

# APS March Meeting 2016

Baltimore, Maryland

<http://www.aps.org/meetings/march/index.cfm>

**Monday, March 14, 2016 8:00AM - 11:00AM –**

**Session A1 DCMP: Charge Order and the Pseudogap in the Underdoped Cuprates** Ballroom I - Tom Devereaux, Stanford University

**8:00AM A1.00001 Towards a complete Fermi surface in underdoped high  $T_c$  superconductors<sup>1</sup>**

NEIL HARRISON, nharrison@lanl.gov — The discovery of magnetic quantum oscillations in underdoped high  $T_c$  superconductors raised many questions, and initiated a quest to understand the origin of the Fermi surface the like of which had not been seen since the very first discovery of quantum oscillations in elemental bismuth. While studies of the Fermi surface of materials are today mostly assisted by computer codes for calculating the electronic band structure, this was not the case in the underdoped high  $T_c$  materials. The Fermi surface was shown to be reconstructed into small pockets, yet there was no hint of a viable order parameter. Crucial clues to understanding the origin of the Fermi surface were provided by the small value of the observed Fermi surface cross-section, the negative Hall coefficient and the small electronic heat capacity at high magnetic fields. We also know that the magnetic fields were likely to be too weak to destroy the pseudogap and that vortex pinning effects could be seen to persist to high magnetic fields at low temperatures. I will show that the Fermi surface that appears to fit best with the experimental observations is a small electron pocket formed by connecting the nodal 'Fermi arcs' seen in photoemission experiments, corresponding to a density-wave state with two different orthogonal ordering vectors. The existence of such order has subsequently been detected by x-ray scattering experiments, thereby strengthening the case for charge ordering being responsible for reconstructing the Fermi surface. I will discuss new efforts to understand the relationship between the charge ordering and the pseudogap state, discussing the fate of the quasiparticles in the antinodal region and the dimensionality of the Fermi surface. The author acknowledges contributions from Suchitra Sebastian, Brad Ramshaw, Mun Chan, Yu-Te Hsu, Mate Hartstein, Gil Lonzarich, Beng Tan, Arkady Shekhter, Fedor Balakirev, Ross McDonald, Jon Betts, Moaz Altarawneh, Zengwei Zhu, Chuck Mielke, James Day, Doug Bonn, Ruixing Liang, Walter Hardy.

<sup>1</sup>supported by BES "Science of 100 tesla" program.

**8:36AM A1.00002 Three-dimensional charge density wave order in YBCO at high magnetic field**

WEI-SHENG LEE, Stanford Institute of Materials and Energy Sciences, SLAC National Accelerator Lab. and Stanford University — Charge density wave (CDW) correlations have been shown to universally exist in cuprate superconductors. However, their nature at high magnetic fields, *e.g.* inferred from nuclear magnetic resonance, Hall coefficient, and sound velocity measurements, is distinct from that measured by x-ray scattering at zero and low fields. In this talk, I will discuss our recent experiment which combines a pulsed magnet with an x-ray free electron laser to characterize the CDW in  $\text{YBa}_2\text{Cu}_3\text{O}_{6.67}$  via x-ray scattering in fields up to 28 Tesla. While the zero-field CDW order, which develops below  $\sim 150$  K, is essentially two dimensional, a three-dimensionally ordered CDW emerges at magnetic fields beyond 15 Tesla and at temperatures below the zero-field superconducting transition temperature. While the two CDW arrange differently along the c-axis, they share the same incommensurate periodicity in the  $\text{CuO}_2$  plane. Our observations imply that the two forms of CDW and high-temperature superconductivity are intimately linked.

**9:12AM A1.00003 Fractionalized Fermi liquids and the pseudogap<sup>1</sup>**

SUBIR SACHDEV, Harvard Univ — Fractionalized Fermi liquids (FL\*) are metals with Fermi surfaces of electron-like quasiparticles; however the volume enclosed by the Fermi surface is not equal to the Luttinger value determined by the density of all electrons. There are general non-perturbative arguments that any such state with a non-Luttinger volume must also have emergent gauge excitations which have vanishing energy on manifolds of non-trivial topology. In doped antiferromagnets with hole density  $p$ , the Luttinger volume of a closed Fermi surface of holes is  $1 + p$  in the state without antiferromagnetic order. Simple FL\* models of doped antiferromagnets will be described with ground states which preserve all symmetries, and have hole pockets of total volume  $p$ . Such models provide natural explanations for a number of recent observations on the pseudogap phase of the hole-doped cuprate superconductors. Confinement transitions of such FL\* phases to conventional phases will also be described.

<sup>1</sup>Supported by NSF Grant DMR-1360789

**9:48AM A1.00004 Charge order in cuprates: from hole to electron doping.**

ANDREA DAMASCELLI, University of British Columbia, Quantum Matter institute — Charge ordering has resurged as a prominent phenomenon in the physics of high- $T_c$  cuprates. In this talk I will review our recent results from  $\text{Bi2201}$  [1,2] and YBCO hole-doped cuprates [3,4], as well as electron doped NCCO [5]. With the early discovery of stripe-like order in La-based cuprates, this establishes charge ordering instabilities to be omnipresent in all cuprate families. I will discuss the connection between charge ordering and pseudogap phenomenology [2,5], similarities and asymmetries between hole and electron doping [2,5], and the native local symmetry of charge modulations [3,4].

1) J.A. Rosen et al., Nature Communications 4, 1977 (2013). 2) R. Comin et al., Science 343, 390 (2014). 3) R. Comin et al., Science 347, 1335 (2015). 4) R. Comin et al., Nature Materials, 14, 796-800 (2015). 5) E.H. da Silva Neto et al., Science 347, 282 (2015).

**10:24AM A1.00005 Short ranged orders in numerical data and STM data, their mechanism and roles.**

EUN-AH KIM, Cornell Univ — With the recent experimental break through establishing the short-ranged spin and charge order as universal phenomena in under-doped cuprates, both the origin and the role of these local ordering tendencies take the center stage of cuprates research. In this talk, I will present analysis of short-ranged charge order observed in both our numerical data on multi-band spin-Fermi on model and scanning tunneling spectroscopy data. I will discuss the implications of the results in the context of the origin and the role of charge order.

**Monday, March 14, 2016 8:00AM - 11:00AM –**

**Session A2 DCMP DAMOP: Frontiers in the Theory of Non-Equilibrium Physics: From Nanosystems to Cold Atoms** Ballroom II - Marcos Rigol, Pennsylvania State University

**8:00AM A2.00001 Out-of-equilibrium phenomena and Transport in Cold Atoms<sup>1</sup>**, THIERRY GIAMARCHI, DQMP, University of Geneva — Transport of particle or charge current between two reservoirs is one of the most studied phenomenon in the context of condensed matter. Despite its apparent simplicity this phenomenon is in fact a case of an out of equilibrium situation requiring in principle new theoretical tools and concepts for its solution. One way to sweep the difficulty under the rug has been usually to tackle this problem in the linear response, where one can come back to the comfortable case of equilibrium. There are however many cases when the linear response is not enough and when a full solution of the non-equilibrium problem is needed. This is in particular the case for quantum point contacts or junctions where the full current-voltage characteristics gives direct information on the physics of the problem. In the recent years, in complement to condensed matter experimental realizations, due to the full control on the parameters of the problem and the fact that they realize isolated quantum systems cold atoms have proven a fantastic laboratory to produce out of equilibrium situations. This ranges from the case of quenches, to more recently via experiments of the ETHZ group to the case of real transport between reservoirs. This experimental activity has in turn thus stimulated strongly theoretical developments in this field. I will discuss in this talk some of the recent advances and realizations both at the experimental and of course the theoretical level. I will in particular focus on a recent study [1] which was able to realize a tunable, ballistic quantum point contact between two fermi reservoirs with a tunable interaction allowing to reach unitarity and to provide a theoretical description of the out-of equilibrium corresponding problem. In such a system the current has been shown to originate from multiple Andreev reflections which leads to a very non-linear current-chemical potential characteristics. The geometry of the contact can be changed showing a competition between superfluidity and thermally activated transport which leads to a conductance minimum and poses several theoretical questions for its theoretical description. [1] "Connecting strongly correlated superfluids by a quantum point contact", D. Husemann, S. Uchino, S. Krinner, M. Lebrat, T. Giamarchi, T. Esslinger and J.-P. Brantut, arXiv:1508.00578 (2015).

<sup>1</sup>Work supported in part by Swiss NSF under division II and the ARO-MURI Non-equilibrium Many-body Dynamics grant (W911NF-14-1-0003)

**8:36AM A2.00002 'Consistent bosonization-debosonization': A resolution of the non-equilibrium transport puzzle blazes a new path forward**, NAYANA SHAH, University of Cincinnati — In this talk, we will critically reexamine the bosonization-debosonization procedure for systems including certain types of localized features (although more general scenarios are possible). By focusing on the case of a tunneling junction out of equilibrium, I will show that the conventional approach gives results that are not consistent with the exact solution of the problem even at the qualitative level and highlight the inconsistencies that can adversely affect the results of all types of calculations. I will subsequently report on a 'Consistent bosonization-debosonization procedure that we have developed to resolve the aforementioned non-equilibrium transport puzzle and argue that this framework should be widely applicable [1]. I will touch upon its application for the two-lead Kondo problem [2] that besides being a key theoretical prototype of a strongly correlated system is also of immediate experimental relevance in many ways (see also related talk by Bolech). [1] Nayana Shah, C. J. Bolech, arXiv:1508.03078, [2] C. J. Bolech, Nayana Shah, arXiv:1508.03079

**9:12AM A2.00003 Non-equilibrium Aspects of Quantum Integrable Systems<sup>1</sup>**, NATAN ANDREI, Rutgers University — The study of non-equilibrium dynamics of interacting many body systems is currently one of the main challenges of modern condensed matter physics, driven by the spectacular progress in the ability to create experimental systems - trapped cold atomic gases are a prime example - that can be isolated from their environment and be highly controlled. Many old and new questions can be addressed: thermalization of isolated systems, nonequilibrium steady states, the interplay between non equilibrium currents and strong correlations, quantum phase transitions in time, universality among others. In this talk I will describe nonequilibrium quench dynamics in integrable quantum systems. I'll discuss the time evolution of the Lieb-Liniger system, a gas of interacting bosons moving on the continuous infinite line and interacting via a short range potential. Considering a finite number of bosons on the line we find that for any value of repulsive coupling the system asymptotes towards a strongly repulsive gas for any initial state, while for an attractive coupling, the system forms a maximal bound state that dominates at longer times. In the thermodynamic limit -with the number of bosons and the system size sent to infinity at a constant density and the long time limit taken subsequently- I'll show that the density and density-density correlation functions for strong but finite positive coupling are described by GGE for translationally invariant initial states with short range correlations. As examples I'll discuss quenches from a Mott insulator initial state or a Newton's Cradle. Then I will show that if the initial state is strongly non translational invariant, e.g. a domain wall configuration, the system does not equilibrate but evolves into a nonequilibrium steady state (NESS). A related NESS arises when the quench consists of coupling a quantum dot to two leads held at different chemical potential, leading in the long time limit to a steady state current. Time permitting I will also discuss the quench dynamics of the XXZ Heisenberg chain.

<sup>1</sup>Research supported by NSF Grant DMR 1410583

**9:48AM A2.00004 Universal behavior after a quantum quench in interacting field theories<sup>1</sup>**, ADITI MITRA, New York University — The dynamics of an isolated quantum system represented by a field theory with  $O(N)$  symmetry, and in  $d \geq 2$  spatial dimensions, is investigated after a quantum quench from a disordered initial state to the critical point. A perturbative renormalization-group approach involving an expansion around  $d=4$  is employed to study the time-evolution, and is supplemented by an exact solution of the Hartree-Fock equations in the large- $N$  limit. The results show that the dynamics is characterized by a prethermal regime controlled by elastic dephasing where excitations propagate ballistically, and a light cone emerges in correlation functions in real space. The memory of the initial state, together with the absence of time-scales at the critical point, gives rise to universal power-law aging which is characterized by a new non-equilibrium short-time exponent. The dynamics of the entanglement following a quench is also explored, and reveals that while the time evolution of the entanglement entropy itself is not much different between a free bosonic theory and an interacting bosonic theory, the low-energy entanglement spectrum on the other hand shows clear signature of the non-equilibrium short-time exponent related to aging. This work was done in collaboration with Y. Lemonik (NYU), M. Tavora (NYU), A. Chiocchetta (SISSA), A. Maraga (SISSA), and A. Gambassi (SISSA).

<sup>1</sup>Supported by NSF-DMR 1303177

**10:24AM A2.00005 Exploring the nonequilibrium dynamics of ultracold quantum gases by using numerical tools<sup>1</sup>**, FABIAN HEIDRICH-MEISNER, LMU Munich, Germany — Numerical tools such as exact diagonalization or the density matrix renormalization group method have been vital for the study of the nonequilibrium dynamics of strongly correlated many-body systems. Moreover, they provided unique insight for the interpretation of quantum gas experiments, whenever a direct comparison with theory is possible. By considering the example of the experiment by Ronzheimer et al. [1], in which both an interaction quench and the release of bosons from a trap into an empty optical lattice (sudden expansion) was realized, I discuss several nonequilibrium effects of strongly interacting quantum gases. These include the thermalization of a closed quantum system and its connection to the eigenstate thermalization hypothesis [2], nonequilibrium mass transport [1], dynamical fermionization [3], and transient phenomena such as quantum distillation or dynamical quasicondensation [4]. I highlight the role of integrability in giving rise to ballistic transport in strongly interacting 1D systems [1] and in determining the asymptotic state after a quantum quench [5]. The talk concludes with a perspective on open questions concerning 2D systems and the numerical simulation of their nonequilibrium dynamics [6].

[1] Ronzheimer et al., Phys. Rev. Lett. 110, 205301 (2013)

[2] Sorg et al., Phys. Rev. A 90, 033606 (2014)

[3] Vidmar et al., Phys. Rev. B 88, 235117 (2013)

[4] Vidmar et al., Phys. Rev. Lett. 115, 175301 (2015)

[5] Mei et al., arXiv:1509.00828

[6] Hauschild, Pollmann, FHM, arXiv:1509.00696

<sup>1</sup>Supported by Deutsche Forschungsgemeinschaft (DFG) via FOR 801.

## Monday, March 14, 2016 8:00AM - 11:00AM –

Session A3 DCMP GMAG: Recent Progress on 'Order by Disorder' Phenomena Ballroom III - Israel Klich, University of Virginia

### 8:00AM A3.00001 Order From disorder in Frustrated Spin Systems<sup>1</sup>

PIERS COLEMAN, Rutgers Univ — This talk will review the phenomenon of "Order from disorder": the mechanism by which fluctuations remove a degeneracy within a frustrated spin system. An important consequence of order-from-disorder, is the ability of frustrated Heisenberg spin systems to overcome the Mermin-Wagner theorem, developing new forms of discrete order, even when the spins themselves remain disordered with a finite correlation length. The most well-known example, is the two-dimensional frustrated  $J_1 - J_2$  Heisenberg model, which undergoes a finite temperature Ising phase transition into a stripy or "nematic" state, even though the spins do not order until absolute zero[1,2]. Nematic ordering of this kind is believed to occur in the iron-based superconductors, such as  $BaFe_2As_2$ . More recently, it has been possible to theoretically study the triangular-honeycomb versions of the  $J_1 - J_2$  model, called a windmill model[3-4], in which order-from disorder drives the development of six-state clock order. Remarkably, in this case, order-from-disorder leads to an intermediate power-law spin phase, despite the underlying Heisenberg spins.

[1]C. L. Henley, Phys. Rev. Lett. 62, 2056 (1989).

[2]P. Chandra, P. Coleman, and A. I. Larkin, Phys. Rev. Lett. 64, 88 (1990).

[3]P. P. Orth, P. Chandra, P. Coleman, and J. Schmalian, Phys. Rev. Lett. 109, 237205 (2012).

[4]P. P. Orth, P. Chandra, P. Coleman, and J. Schmalian, Phys. Rev. B 89, 094417 (2014).

[4]B. Jeevanesan, P. Chandra, P. Coleman, P. P. Orth, Phys. Rev. Lett. 115, 177201 (2015).

<sup>1</sup>This research was supported by DOE Basic Energy Sciences grant DE-FG02-99ER45790

### 8:36AM A3.00002 Love triangles, quantum fluctuations and spin jam

SEUNG-HUN LEE, University of Virginia — When magnetic moments are interacting with each other in a situation resembling that of complex love triangles, called frustration, a large set of states that are energetically equivalent emerge. This leads to exotic spin states such as spin liquid and spin ice. Recently, we presented evidence for the existence of a topological glassy state, that we call spin jam, induced by quantum fluctuations.[1,2] The case in point is  $SrCr_9pGa_{12-9p}O_{19}$  (SCGO(p)), a highly frustrated magnet, in which the magnetic Cr ions form a quasi-two-dimensional triangular system of bi-pyramids. This system has been an archetype in search for exotic spin states. Understanding the nature of the state has been a great intellectual challenge. Our new experimental data and theoretical spin jam model provide for the first time a coherent understanding of the phenomenon. Furthermore, the findings strongly support the possible existence of purely topological glassy states. Reference: [1] *Spin jam induced by quantum fluctuations in a frustrated magnet*, J. Yang et al., Proc. Natl. Acad. Sci. of U.S.A. Vol. 127, 11519-11523 (2015). [2] *Glassiness and exotic entropy scaling induced by quantum fluctuations in a disorder-free frustrated magnet*, I. Klich, S.-H. Lee, K. Iida, Nature Communications 5, 3497 (2014).

### 9:12AM A3.00003 The many faces of order-by-disorder in rare-earth pyrochlore magnets

MICHEL J P GINGRAS, University of Waterloo — Order-by-disorder (ObD) is a concept of central importance in the field of frustrated magnetism. Saddled with large accidental degeneracies, a subset of states, those that support the largest quantum and/or thermal fluctuations, may be selected to form true long-range order. More formally, one often begins describing a system in terms of some order parameter  $m$  with the low-energy description framed in terms of an effective action  $\Gamma_0(m)$ . In each ObD scenario, one starts from an artificial limit where there is an accidental degeneracy; that is the effective action at this point,  $\Gamma_0(m)$ , has an accidental symmetry. One may then view ObD phenomena as cases where the corrections to  $\Gamma_0(m)$  arise through some form of fluctuation corrections, may they be thermal, quantum or virtual, towards an enlarged higher energy Hilbert space. In the rare-earth pyrochlore oxides, of formula  $R_2M_2O_7$ , the trivalent magnetic rare-earth ions  $R^{3+}$  (e.g  $R = Gd, Er, Yb$ ;  $M = Ti, Sn$  is non-magnetic) reside on a three-dimensional pyrochlore lattice of corner-sharing tetrahedra. This architecture is prone to a high degree of magnetic frustration, with the  $R_2M_2O_7$  pyrochlore materials having been found over the past twenty years to display a gamut of exotic phenomena. In this talk, I will discuss three such phenomena: (i) the intermediate partially-ordered multiple- $k$  state between 0.7K and 1K in the  $Gd_2Ti_2O_7$  Heisenberg antiferromagnet <sup>1</sup>, (ii) the ordered  $\psi_2$  state selection in the  $XY$   $Er_2Ti_2O_7$  antiferromagnet <sup>2</sup> and (iii) the puzzling high sample sensitivity of the  $Yb_2Ti_2O_7$  "quantum spin ice" candidate <sup>3</sup>. I will argue that in all three cases, some form of fluctuation corrections to their simplest  $\Gamma_0(m)$  description play a significant role in the state selection and experimentally observed behaviors.

<sup>1</sup> PRL 114, 130601 (2015)

<sup>2</sup> arXiv:1510.04292

<sup>3</sup> arXiv:1505.05499

### 9:48AM A3.00004 Order by Disorder in the XY Pyrochlore Antiferromagnet $\text{Er}_2\text{Ti}_2\text{O}_7$ <sup>1</sup>, BRUCE D.

GAULIN, McMaster University — Crystal field effects associated with  $\text{Er}^{3+}$  magnetic moments in  $\text{Er}_2\text{Ti}_2\text{O}_7$  give rise to local XY anisotropy and effective quantum  $S=1/2$  spins which are antiferromagnetically coupled on this materials cubic pyrochlore lattice [1].  $\text{Er}_2\text{Ti}_2\text{O}_7$  orders into a non-collinear antiferromagnetic  $\Psi_2$  state below  $\sim 1.2$  K, in zero magnetic field, but the mechanism for its ground state selection has been a puzzle for more than a decade. We have carried out inelastic neutron scattering measurements on single crystal samples of  $\text{Er}_2\text{Ti}_2\text{O}_7$  at low temperatures and in the presence of a strong [110] magnetic field, allowing us to determine the underlying spin Hamiltonian for this quantum antiferromagnet [2, 3]. These results point to ground state selection via an order-by-quantum-disorder mechanism [3], and a concomitant order-by-disorder gap of  $\sim 0.05$  meV has also been observed [4], associated with the pseudo-Goldstone modes in the low field ordered state. In addition, we have explored the sensitivity of the ground state selection to magnetic dilution by preparing and studying single crystals of  $\text{Er}_{2-x}\text{Y}_x\text{Ti}_2\text{O}_7$  [5]. These studies are particularly topical in light of two theoretical predictions [6,7] that the  $\Psi_2$  ordered state may be unstable to formation of the related  $\Psi_3$  phase at low temperatures, in the presence of quenched disorder. [1] J.D.M. Champion et al., Phys. Rev. B 68, 020401 (2003). [2] J.P.C. Ruff et al., Phys. Rev. Lett., 101, 147205 (2005). [3] L. Savary et al. Phys. Rev. Lett., 109, 167201 (2012). [4] K.A. Ross et al. Phys. Rev. Lett. 112, 057201 (2014). [5] J.F. Niven, Proc. R. Soc. A, 470: 20140387 (2014). [6] V. S. Maryasin and M. E. Zhitomirsky, Phys. Rev. B 90, 094412 (2014). [7] A. Andreanov and P. A. McClarty, Phys. Rev. B 91, 064401 (2015).

<sup>1</sup>Research supported by NSERC of Canada and the Canadian Institute for Advanced Research

### 10:24AM A3.00005 Quantum order-by-disorder and excitations in anisotropic kagome-lattice antiferromagnets<sup>1</sup>, ALEXANDER CHERNYSHEV, University of California, Irvine — Our recent works have advanced theoretical understanding of

the quantum effects in kagome-lattice antiferromagnets and have provided insights into the quantum order-by-disorder mechanism, important for a broad class of frustrated spin systems. In particular, we have challenged a general expectation that the quantum and thermal order-by-disorder mechanisms always select the same ground state. We have shown that the non-linear terms in the quantum hamiltonian of the anisotropic kagome-lattice antiferromagnets can yield a rare example of the ground state that is different from the one favored by thermal fluctuations. We have also demonstrated that the order selection is generated by topologically non-trivial tunneling processes, yielding a new energy scale in the system.

Related to the ground-state selection mechanism are the non-linear effects in the spectra of the kagome-lattice systems. Further progress has been made in understanding spectral properties of realistic kagome-lattice antiferromagnets such as Fe-jarosite, for which we have demonstrated a remarkable wipe-out effect for a significant portion of the spectrum. This phenomenon is related to an existence of the so-called "flat mode," a ubiquitous feature of the kagome-lattice and other highly-frustrated antiferromagnets, and is due to a resonant-like decay processes involving two of such modes.

References: [1] A. L. Chernyshev and M. E. Zhitomirsky, "Quantum Selection of Order in an XXZ Antiferromagnet on a Kagom'e Lattice", Phys. Rev. Lett. 113, 237202 (2014). [2] A. L. Chernyshev, "Strong quantum effects in an almost classical antiferromagnet on a kagome lattice", Phys. Rev. B 92, 094409 (2015). [3] A. L. Chernyshev and M. E. Zhitomirsky, "Order and excitations in large-S kagome-lattice antiferromagnets", Phys. Rev. B 92, 144415 (2015). (Editors' Suggestion).

<sup>1</sup>Supported by the DoE

## Monday, March 14, 2016 8:00AM - 11:00AM –

### Session A4 DPOLY GSOFIT GSNP: Polymer Dynamics: An Honor Session for Sir Sam Edwards

Ballroom IV - Gary Grest, Sandia National Laboratories

### 8:00AM A4.00001 : Polymer Dynamics from Edwards to Today , MASAO DOI, Nagoya University —

### 8:36AM A4.00002 Polymer dynamics, the Edwards tube model and neutron scattering. , JULIA

HIGGINS, Department of Chemical Engineering, Imperial College, London — Sam Edwards' papers with Masao Doi describing polymer dynamics and rheology based on the tube model were published just as high resolution quasi-elastic neutron scattering experiments achieved the resolution capable of observing directly some of the effects of the tube. The talk will summarize these experiments as well as later work on polymer inter-diffusion across interfaces observed by neutron reflection, where again the tube model is used to interpret the data.

### 9:12AM A4.00003 Recent advances with generalized entropy theory of glass-formation in polymers<sup>1</sup>, KARL FREED, University of Chicago — The generalized entropy theory (GET) of glass-formation in polymers is a combination of the

lattice cluster theory (LCT) for the configurational entropy density with the Adam-Gibbs (AG) theory for the structural relaxation time. A greatly simplified form of the GET (whose expression for the free energy is roughly double that of Flory-Huggins theory) accurately reproduces the four characteristic temperatures of glass-formation (the onset, crossover, glass transition, and Kauzmann temperatures) of the full GET to within 4K for a series of models of polymers composed of semi-flexible chains having the structure of poly(n-alpha olefins). The theory is now simple enough to be used in courses in polymer physics. Although the successes of the GET provide a strong validation of the final form of the AG theory provided the configurational entropy is used, the physical basis of the AG theory has remained an enigma. Hence, we have developed a new, more general, statistical mechanical derivation of AG theory that explains the previously perplexing observations that the string-like elementary excitations have the mass and temperature dependence of systems undergoing equilibrium self-assembly.

<sup>1</sup>This work is supported by the (U.S.) Department of Energy (DOE), Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE- SC0008631.

### 9:48AM A4.00004 The Ordinary-Extraordinary Transition in Dynamics of Solutions of Charged Macromolecules , MURUGAPPAN MUTHUKUMAR, University of Massachusetts — Dynamic light scattering measurements on

dilute salt-free polyelectrolyte solutions have shown over the past three decades that there are two distinctive diffusive modes: fast and slow. The diffusion coefficient deduced from the fast mode has been found to be essentially independent of molar mass and polymer concentration and it is merely a factor of four smaller than that of small electrolyte ion such as sodium or potassium ion. The diffusion coefficient deduced from the slow mode is much smaller suggestive of clumps of many chains although these chains are similarly charged. Upon addition of sufficient amount of small molecular salts, the fast and slow modes merge together and the deduced diffusion coefficient is within the expected value for uncharged polymers. We will present a theory for these observed behaviors based on the coupling between the polyelectrolyte chains and their counterions.

**10:24AM A4.00005 Nanotribology of charged polymer brushes<sup>1</sup>**, JACOB KLEIN, Weizmann Institute of Science — Polymers at surfaces, whose modern understanding may be traced back to early work by Sam Edwards<sup>1</sup>, have become a paradigm for modification of surface properties, both as steric stabilizers and as remarkable boundary lubricants<sup>2</sup>. Charged polymer brushes are of particular interest, with both technological implications and especially biological relevance where most macromolecules are charged. In the context of biolubrication, relevant in areas from dry eye syndrome to osteoarthritis, charged polymer surface phases and their complexes with other macromolecules may play a central role. The hydration lubrication paradigm, where tenaciously-held yet fluid hydration shells surrounding ions or zwitterions serve as highly-efficient friction-reducing elements, has been invoked to understand the excellent lubrication provided both by ionized<sup>3</sup> and by zwitterionic<sup>4</sup> brushes. In this talk we describe recent advances in our understanding of the nanotribology of such charged brush systems. We consider interactions between charged end-grafted polymers, and how one may disentangle the steric from the electrostatic surface forces<sup>5</sup>. We examine the limits of lubrication by ionized brushes, both synthetic and of biological origins, and how highly-hydrated zwitterionic chains may provide extremely effective boundary lubrication<sup>6</sup>. Finally we describe how the lubrication of articular cartilage in the major joints, a tribosystem presenting some of the greatest challenges and opportunities, may be understood in terms of a supramolecular synergy between charged surface-attached polymers and zwitterionic groups<sup>7</sup>. 1. Dolan & Edwards, *Proc. Roy. Soc. A*, **337**, 509 (1974). 2. Klein et al. *Nature*, **370**, 634 (1994). 3. Raviv et al., *Nature*, **425**, 163 (2003). 4. Chen et al., *Science*, **323** 1698 (2009). 5. Peretz et al., to be published. 6. Tairy et al., *Macromolecules*, **48**, 140 (2015). 7. Seror et al., *Nature Communications*, 6:6497 (2015); Jahn et al., *Annual Reviews of Biomedical Engineering* (2016)

<sup>1</sup>Work supported by European Research Council (HydrationLube), Israel Science Foundation (ISF), Petroleum Research Fund of the American Chemical Society, ISF-NSF China Joint Program

**Monday, March 14, 2016 8:00AM - 11:00AM —**  
**Session A5 GMAG DCMP FIAP: Magnetic Resonance and Spin-Dependent Optical Phenomena in Semiconductors** 301 - Masashi Shiraishi, U. Kyoto

**8:00AM A5.00001 Optimizing Frequency-Modulated CW EDMR in silicon**, LIHUANG ZHU, KIPP VAN SCHOOTEN, CHANDRASEKHAR RAMANATHAN, Dartmouth College — Electrically detected magnetic resonance (EDMR) is a powerful method of probing dopant and defect spin states in semiconductor devices. Moreover, at the single dopant level, these spin states are heavily investigated as potential qubit systems, though facile electronic access to single dopants is exceedingly difficult. We therefore characterize detection sensitivities of frequency-modulated CW-EDMR of phosphorus donors in silicon Si:P using a home-built 2.5 GHz system (~80 mT) at 5 K. An arbitrary waveform generator controls the frequency modulation, allowing us to optimize the signal to noise ratio (SNR) of both the dangling bond and phosphorus donor signals against multiple experimental parameters, such as modulation amplitude and modulation frequency. The optimal range of frequency modulation parameters is constrained by the relaxation time of the phosphorous electron at 5 K, resulting in the same sensitivity limit as field modulated CW-EDMR, but offers some technical advantages; e.g. reducing the relative contribution of magnetic field induced currents and eliminating the need for field modulation coils. We further characterize the EDMR SNR in Si:P as a function of optical excitation energy by using a narrow line laser, tunable across donor exciton and band gap states.

**8:12AM A5.00002 Electron Spin Resonance in a 2D Fermi Liquid with Spin-Orbit Coupling**, SAURABH MAITI, MUHAMMAD IMRAN, DMITRII MASLOV, University of Florida — Electron spin resonance (ESR) is usually interpreted as a single-particle phenomenon protected from the effect of many-body correlations. We show that this is not the case in a two-dimensional Fermi liquid (FL) with spin-orbit coupling (SOC). Depending on whether the magnetic field is below or above some critical value, ESR in such a system probes up to three collective chiral-spin modes, augmented by the presence of the field, or the Larmor mode, augmented both by SOC and FL renormalizations. We argue that ESR can be used as a probe not only for SOC but also for many-body physics.

**8:24AM A5.00003 Electric dipolar spin resonance in systems with a valley dependent  $g$ -factor**, MARKO RANCIC, GUIDO BURKARD, Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — We theoretically investigate the electric dipole spin resonance (EDSR) in a single Si/SiGe quantum dot in the presence of a magnetic field gradient, e.g., produced by a micromagnet. The control of electron spin states can be achieved by applying an oscillatory electric field, which induces periodic oscillations in real space of the electron spin inside the quantum dot. This motion inside a magnetic field gradient produces an effective periodic in-plane magnetic field, and allows for driven spin rotations near resonance. The magnetic field gradient induces a valley dependent  $g$ -factor and a valley dependent Rabi frequency. Our first goal is to quantitatively and qualitatively describe valley dependent  $g$ -factors and a valley dependent Rabi frequencies using a microscopic model. A valley dependent  $g$ -factor combined with inter-valley scattering gives rise to a novel electron spin decoherence mechanism. The second goal of our study is to describe the drop of coherence in the presence of inter-valley scattering, and furthermore, to discuss the interplay between valley and spin relaxation. All relevant decoherence mechanisms are quantitatively evaluated by solving a Lindblad master equation.

**8:36AM A5.00004 Electrically and optically detected spin echo of hopping carriers in organic semiconductors<sup>1</sup>**, VAGHARSH MKHITARYAN, VIATCHESLAV DOBROVITSKI, Ames Laboratory, Iowa State University, Ames, Iowa 50011 — We develop a theory for electrically and optically detected primary (2-pulse) and stimulated (3-pulse) spin echo produced by the polaron pairs coupled to the nuclear spins in organic semiconductors. The theory employs fully quantum description of the nuclear and polaron spins, and explains how the structure of the echo signal (electron spin echo envelope modulation, ESEEM) depends on the statistics and rate of the polaron hopping. For the primary spin echo the envelope modulation is strong for slow hopping; both modulation amplitude and dephasing time  $T_2$  decrease with increasing hopping rate. As the hopping rate increases further,  $T_2$  starts to increase again due to motional narrowing, while the primary echo signal becomes exponential without modulation. The stimulated spin echo signal also shows strong envelope modulation for slow polaron hopping. For faster hopping the stimulated echo (unlike the primary echo) shows a modulation which does not disappear for fast hopping, and has the frequency of the nuclear Larmor precession. Besides describing the recent spin echo measurements in  $\pi$ -conjugated polymers [1], our work provides a way to directly determine the polaron hopping dynamics from the spin echo experiments. [1] H. Malissa et al, *Science* 345, 1487 (2014).

<sup>1</sup>This work was supported by the Department of Energy-Basic Energy Sciences under Contract No. DE-AC02-07CH11358

**8:48AM A5.00005 Tuning magnetic exchange interactions in crystalline thin films of substituted Cobalt Phthalocyanine<sup>1</sup>**, NAVEEN RAWAT, LANE MANNING, KIM-NGAN HUA, RANDALL HEADRICK, Univ of Vermont, MICHAEL BISHOP, STEPHEN MCGILL, National High Magnetic Field Lab, florida, RORY WATERMAN, MADALINA FURIS, Univ of Vermont — Magnetic exchange interactions in diluted organometallic crystalline thin film alloys of Phthalocyanines (Pcs) made of a organo-soluble derivatives of Cobalt Pc and metal-free (H<sub>2</sub>Pc) molecule and is investigated. To this end, we synthesized a organosoluble CoPc and successfully employed a novel solution-based pen-writing deposition technique to fabricate long range ordered thin films of mixtures of different ratios ranging from 1:1 to 10:1 H<sub>2</sub>Pc:CoPc. Our previous magnetic circular dichroism (MCD) results on the parent CoPc crystalline thin films identified different electronic states mediating exchange interactions and indirect exchange interaction competing with superexchange interaction. This understanding of spin-dependent exchange interaction between delocalized  $\pi$ -electrons with unpaired d spins along with the excitonic delocalization character enabled the further tuning of these interactions by essentially varying the spatial distance between the spins. Furthermore, high magnetic field ( $B < 25$  T) MCD and magneto-photoluminescence show evidence of spin-polarized band-edge excitons in the same materials.

<sup>1</sup>This work was possible due to support by the National Science Foundation, Division of Materials Research MRI, CAREER and EPM program awards: DMR- 0722451, DMR- 0821268, DMR-1307017 and DMR-1056589, DMR-1229217

**9:00AM A5.00006 Measurement of hyperfine fields and the  $\Delta g$ -effect in  $\pi$ -conjugated polymer-based OLEDs using multi-frequency electrically detected magnetic resonance**, GAJADHAR JOSHI, HANS MALISSA, RICHARD MILLER, LILLIE OGDEN, DOUGLAS BAIRD, SHIRIN JAMALI, MARZIEH KAVAND, KAPIL AMBAL, Univ of Utah, JOHAN VAN TOL, NHMFL FSU, JOHN LUPTON, Universitaet Regensburg, CHRISTOPH BOEHME, Univ of Utah — Magneto-opto-electronic properties of organic semiconductors, such as organic magnetoresistance or magneto-electroluminescence, are strongly influenced by the interplay of proton induced hyperfine fields to which charge carrier spins are coupled [Nguyen et al., Nat. Mater. 9, 345-352 (2010), Mcamey et al. Phys. Rev. Lett. 104, 017601 (2010)]. In addition, the weak but non-negligible and highly inhomogeneously distributed spin-orbit effects caused by the material's structural disorder can affect spin-dependent processes. In order to quantitatively access and discriminate between these mechanisms, we investigate the inhomogeneous broadening of polaron spin-resonances using electrically detected magnetic resonance (EDMR) spectroscopy at various magnetic fields between 3mT and 12T. While random local hyperfine fields cause an external magnetic field-independent line broadening, spin-orbit contributions give rise to a distribution of the charge carrier g-factors. This  $\Delta g$  effect leads to a resonance line-width contribution that is proportional to the external magnetic field. We observe an EDMR line that is largely field-independent in the low-magnetic field, but shows substantial broadening of line shape at higher fields.

**9:12AM A5.00007 Magnetoresistance detected spin collectivity in organic light emitting diodes**, HANS MALISSA, DAVID P WATERS, GAJADHAR JOSHI, MARZIEH KAVAND, MARK E LINES, Department of Physics and Astronomy, University of Utah, PAUL L BURN, Centre for Organic Photonics & Electronics, School of Chemistry & Molecular Biosciences, The University of Queensland, JOHN M LUPTON, Department of Physics and Astronomy, University of Utah and Institut fuer Experimentelle und Angewandte Physik, Universitaet Regensburg, CHRISTOPH BOEHME, Department of Physics and Astronomy, University of Utah — Organic magnetoresistance (OMAR) typically refers to the significant change in the conductivity of thin layers of organic semiconductors at low static magnetic fields ( $< 10$  mT). When radio frequency (rf) radiation is applied to an organic semiconductor under bipolar injection, and in the presence of small magnetic fields  $B$ , magnetic resonance can occur, which is observed as a change of the OMAR effect [Baker et al., Nat. Commun. 3, 898 (2012)]. When  $B$  and the resonant driving field are stronger than local hyperfine fields, an ultrastrong coupling regime emerges, which is marked by collective spin effects analogous to the optical Dicke effect [Roundy and Raikh, Phys. Rev. B 88, 125206 (2013)]. Experimentally, this collective behavior of spins can be probed in the steady state OMAR of organic light-emitting diodes (OLEDs) at room temperature by observation of a sign reversal of the OMAR change under rf irradiation. Furthermore, in the presence of strong driving fields, an ac Zeeman effect can be observed through OMAR [Waters et al., Nat. Phys. 11, 910 (2015)], a unique window to observe room temperature macroscopic spin quantum coherence.

**9:24AM A5.00008 Microwave frequency modulation for improving polarization transfer in DNP experiments<sup>1</sup>**, MALLORY GUY, CHANDRASEKHAR RAMANATHAN, Department of Physics and Astronomy, Dartmouth College — Dynamic nuclear polarization (DNP) is a driven process that transfers the inherently high electron polarization to surrounding nuclear spins via microwave irradiation at or near the electron Larmor frequency. In a typical DNP experiment, the amplitude and frequency of the applied microwaves are constant. However, by adding time dependence in the form of frequency modulation, the electron excitation bandwidth is increased, thereby increasing the number of electron spins active in the polarization transfer process and improving overall efficiency. Both triangular and sinusoidal modulation show a 3 fold improvement over monochromatic irradiation. In the present study, we compare the nuclear spin polarization after DNP experiments with no modulation of the applied microwaves, triangular and sinusoidal modulation, and modulation schemes derived from the sample's ESR spectrum. We characterize the polarization as a function of the modulation amplitude and frequency and compare the optimal results from each modulation scheme. Working at a field of 3.34 T and at a temperature of 4 K, we show that by using a modulation scheme tailored to the electronic environment of the sample, polarization transfer is improved over other modulation schemes. Small-scale simulations of the spin system are developed to gain further insight into the dynamics of this driven open system. This understanding could enable the design of modulation schemes to achieve even higher polarization transfer efficiencies.

<sup>1</sup>With support from NSF (CHE-1410504) and by NIH (U19-A1091173).

**9:36AM A5.00009 Resonant and Time-Resolved Spin Noise Spectroscopy**, XINLIN SONG, BRENNAN PURSLEY, VANESSA SIH, University of Michigan — Spin noise spectroscopy is a technique which can probe the system while it remains in equilibrium. It was first demonstrated in atomic gases and then in solid state systems. Most existing spin noise measurement setups digitize the spin fluctuation signal and then analyze the power spectrum. Recently, pulsed lasers have been used to expand the bandwidth of accessible dynamics and allow direct time-domain correlation measurements. Here we develop and test a model for ultrafast pulsed laser spin noise measurements as well as a scheme to measure spin lifetimes longer than the laser repetition period. For the resonant spin noise technique, analog electronics are used to capture correlations from the extended pulse train, and the signal at a fixed time delay is measured as a function of applied magnetic field. [1]

[1] B. C. Pursley, X. Song, and V. Sih, arXiv: 1508.07383

**9:48AM A5.00010 Modification of electron spin properties in a GaAs epilayer by an in-plane electric field<sup>1</sup>**, MICHAEL MACMAHON, VANESSA SIH, Department of Physics, University of Michigan, Ann Arbor, MI 48109 — The interaction of electron spins with accelerating electric fields in bulk gallium arsenide results in many effects that are relevant to proposed spin-based devices. For example, in-plane electric fields have been shown to change the g-factor<sup>2</sup>, generate spin polarization<sup>3</sup>, and decrease the spin lifetime<sup>4</sup>. Most such studies have used only very low electric fields, typically less than 100 V/cm. We investigate the dependence of spin lifetime on electric field at high electric fields and separate the contribution due to heating.

<sup>1</sup>This work was supported in part by ONR and the Rackham Graduate School.

<sup>2</sup>M. Luengo-Kovacs et al., *Phys. Rev. B* **91**, 201110 (2015)

<sup>3</sup>B. M. Norman et al., *Phys. Rev. Lett.* **112**, 056601 (2014)

<sup>4</sup>M. Furis et al., *Appl. Phys. Lett.* **89**, 102102 (2006)

**10:00AM A5.00011 3T and nonlocal 4T Hanle measurements of spin accumulation in the persistent photoconductor  $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As:Si}^1$** , JOON-IL KIM, K. KOUNTOURIOTIS, T. LIU, S. VON MOLNAR, P. XIONG, Florida State University, J. LU, X.Z. YU, J.H. ZHAO, Institute of Semiconductors, Chinese Academy of Sciences — 3-terminal (3T) and nonlocal 4-terminal (4T) Hanle measurements have been performed on a spin injection/detection device with patterned Fe electrodes and  $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As:Si}$ , a persistent photoconductor, as the channel. The persistent photoconductivity facilitates *in situ* incremental photo-doping of the AlGaAs channel, which enables direct comparisons of the 3T and 4T Hanle results on the same device over a broad range of carrier densities across the insulator-metal transition. Although their magnitudes differ by about an order of magnitude, the 3T and 4T Hanle signals exhibit broad similarities in their dependencies on the injection current and carrier density, as well as the resulting spin lifetimes. Specifically, at each bias current, the magnitudes of both the 3T and 4T Hanle signals are observed to decrease exponentially with increasing carrier density of the AlGaAs deep into the metallic state. The spin lifetimes extracted from the 3T and 4T Hanle curves, both via the FWHM of the Lorentzian fit and the 1D spin drift-diffusion model analysis, show similar values and evolution with the carrier density.

<sup>1</sup>Work supported by NSF grant DMR-1308613.

**10:12AM A5.00012 Wurtzite Spin-Lasers**, GAOFENG XU, SUNY Buffalo, PAULO E. FARIA JUNIOR, GUILHERME M. SIPAHI, University of Sao Paulo, Brazil, IGOR ZUTIC, SUNY Buffalo — Lasers in which spin-polarized carriers are injected provide paths to different practical room temperature spintronic devices, not limited to magnetoresistive effects [1]. While theoretical studies of such spin-lasers have focused on zinc-blende semiconductors as their active regions, the first electrically injected carriers at room temperature were recently demonstrated in GaN-based wurtzite semiconductors [2], recognized also for the key role as highly-efficient light emitting diodes [3]. By focusing on a wurtzite quantum well-based spin-laser, we use accurate electronic structure calculations to develop a microscopic description for its lasing properties. We discuss important differences between wurtzite and zinc-blende spin-lasers. [1] P. E. Faria Junior, G. Xu, J. Lee, N. C. Gerhardt, G. M. Sipahi, and I. Zutic, Phys. Rev. B 92, 075311 (2015). [2] J.-Y. Cheng, T.-M. Wond, C.-W. Chang, C.-Y. Dong, and Y.-F. Chen, Nat. Nanotech. 9, 845 (2014); I. Zutic and P. E. Faria Junior, Nat. Nanotech. 9, 750 (2014). [3] S. Nakamura, Rev. Mod. Phys. 87, 1139 (2015).

**10:24AM A5.00013 Manipulation of spin transfer torque using light<sup>1</sup>**, MASSIMO RONTANI, KARSTEN VENDELBJERG, CNR-NANO Research Center S3, Modena, Italy, LU SHAM, Dept of Physics, University of California San Diego — We show that the spin transfer torque induced by a spin-polarized current on a nanomagnet as the current flows through a semiconductor-nanomagnet-semiconductor junction is externally controlled by shining the junction off-resonantly with a strong laser beam. The excitonic coherence driven by the laser dresses the virtual electron-hole pairs coupling conduction and valence bands and inducing an evanescent state in the proximity of the nanomagnet. The Fano-like quantum interference between this localized state and the continuum spectrum is different in the two spin channels and hence it dramatically alters the spin transport, leading to the coherent control of the spin transfer torque.

<sup>1</sup>This work is supported by EU-FP7 Marie Curie Initial Training Network INDEX.

**10:36AM A5.00014 Microscopic description of a spin laser<sup>1</sup>**, PAULO E. FARIA JUNIOR, University of Sao Paulo, GAOFENG XU, SUNY Buffalo, JEONGSU LEE, University of Regensburg, NILS C. GERHARDT, Ruhr-University Bochum, GUILHERME M. SIPAHI, University of Sao Paulo / SUNY Buffalo, IGOR ZUTIC, SUNY Buffalo — Spin lasers provide interesting possibilities for spintronic applications at room temperature[1]. They have the same elements of a conventional laser, but the injected carriers are spin polarized which allows the output light polarization to have either positive or negative helicity. These devices are commonly implemented as VCSELs, which have the advantage of tuning the photon energy by the cavity design. We investigate a spin VCSEL with a AlGaAs/GaAs quantum well active region using band structure calculations and spin-dependent optical gain. In addition to the desirable properties for steady-state operation and cavity designs, we also show that by applying a uniaxial strain, large values of birefringence  $> 200$  GHz can be achieved[2]. Combined with spin injected carriers, the birefringence in the device allows polarization dynamics much faster than photon intensity dynamics[3]. Our theoretical prediction for high-frequency birefringence was experimentally demonstrated in similar spin VCSELs[4]. [1] I. Zutic and P. E. Faria Junior, Nat. Nanotech. 9, 750 (2014). [2] P. E. Faria Junior et al., PRB 92, 075311 (2015). [3] N. C. Gerhardt et al., APL 99, 151107 (2011). [4] T. Pusch et al., Electron. Lett. 51, 1600 (2015).

<sup>1</sup>FAPESP (2011/19333-4, 2012/05618-0 and 2013/23393-8), CNPq (246549/2012-2), DFG (GE 1231/2-1), NSF-ECCS, DOE-BES and US ONR.

**10:48AM A5.00015 Modulating Spin Relaxation with Light and a Novel Spintronic Room Temperature Infrared Photodetector<sup>1</sup>**, MD IFTEKHAR HOSSAIN, Dept of ECE,VCU, Richmond, VA,23284, SAUMIL BANDYOPADHYAY, EECE Dept., MIT, Cambridge, MA 02139, JAYASIMHA ATULASIMHA, Dept of MNE,VCU, Richmond, VA,23228, SUPRIYO BANDYOPADHYAY, Dept of ECE,VCU, Richmond, VA,23284 — We report modulating the spin relaxation rate in an InSb nanowire with infrared (IR) light. The nanowire is fashioned into a spin valve with cobalt and nickel contacts using electrochemical self-assembly. The spin relaxation length is long in the dark since ~96% of the electrons occupy the lowest conduction subband at room temperature, which results in near elimination of the D'yakonov-Perel' (DP) spin relaxation. Under IR illumination, electrons are excited to higher subbands by IR photons, resulting in the revival of the DP relaxation and a threefold shortening of the spin relaxation length [1]. This changes the resistance of the spin valve and therefore has applications in a novel spintronic IR photodetector that can ideally work at room temperature with infinite light-to-dark contrast ratio, infinite detectivity and zero dark current if all other spin relaxation mechanisms are eliminated and spins can be injected into the nanowire and detected with 100% efficiency. This work is supported by the NSF under grant CMMI-1301013. [1] M. I. Hossain, et al., Nanotechnology, 26, 281001(2015)

<sup>1</sup>This work is supported by the NSF under grant CMMI-1301013.

**Monday, March 14, 2016 8:00AM - 10:48AM –**  
**Session A6 GMAG DMP: Metal Oxide Nanoparticles** 302 - Erik Brok, NIST

### 8:00AM A6.00001 Magnetic ordering in lanthanide-molybdenum oxide nanostructure arrays ,

JOSEPH HAGMANN, SON LE, National Institute of Standards and Technology, LYNN SCHNEEMEYER, PATTI OLSEN, Montclair State University, TIGLET BESARA, THEO SIEGRIST, Florida State University, DAVID SEILER, CURT RICHTER, National Institute of Standards and Technology — Reduced ternary molybdenum oxides, or bronzes, offer an attractive materials platform to study a wide variety of remarkable physical phenomena in a system with highly varied structural chemistry. Interesting electronic behaviors, such as superconductivity, charge density waves, and magnetism, in these materials arise from the strong hybridization of the 4d states of high-valent Mo with O p orbitals. We investigate a series of molybdenum bronze materials with Lanthanide-Mo<sub>16</sub>O<sub>44</sub> composition that can be described as a three-dimensional array of metallic Mo<sub>8</sub>O<sub>32</sub> nanostructures computationally predicted to contain a single charge with spin separated by insulating MoO<sub>4</sub> tetrahedra. This study reveals novel magnetic ordering in Lanthanide-Mo<sub>16</sub>O<sub>44</sub> systems arising, not from the inclusion of magnetic elements, but rather from an exchange interaction between cubic Mo<sub>8</sub>O<sub>32</sub> units. Here, we report the magnetometry and transport behaviors of a series of Lanthanide-Mo<sub>16</sub>O<sub>44</sub> materials, emphasizing an observed low-temperature phase transition signifying the onset of antiferromagnetic ordering between the arrayed nanostructures, and relate these behaviors to their experimentally-characterized structures to reveal the intriguing physics of these correlated electronic systems.

### 8:12AM A6.00002 Thermogravimetric and Magnetic Studies of the Oxidation and Reduction

Reaction of SmCoO<sub>3</sub> to Nanostructured Sm<sub>2</sub>O<sub>3</sub> and Co , BRIAN KELLY, Department of Physics and Astronomy, University of Delaware, RONALD CICHOCKI, Department of Chemistry and Biochemistry, University of Delaware, GERALD POIRIER, Advanced Materials Characterization Laboratory, University of Delaware, KARL UNRUH, Department of Physics and Astronomy, University of Delaware — The SmCoO<sub>3</sub> to nanostructured Sm<sub>2</sub>O<sub>3</sub> and Co oxidation and reduction reaction has been studied by thermogravimetric analysis (TGA) measurements in forming gas (FG) and inert N<sub>2</sub> atmospheres, x-ray diffraction (XRD) and vibrating sample magnetometry (VSM). The TGA measurements showed two clearly resolvable reduction processes when heating in FG, from the initial SmCoO<sub>3</sub> phase through an intermediate nanostructured mixture of Sm<sub>2</sub>O<sub>3</sub> and CoO when heated to 330C for several minutes, and then the conversion of CoO to metallic Co when heated above 500C. These phases were confirmed by XRD and VSM. Similar measurements in N<sub>2</sub> yielded little mass change below 900C and coupled reduction processes at higher temperatures. Isoconversional measurements of the CoO to Co reduction reaction in FG yielded activation energies above 2eV/atom in the nanostructured system. This value is several times larger than those reported in the literature or obtained by similar measurements of bulk mixtures of Sm<sub>2</sub>O<sub>3</sub> and CoO, suggesting the nanostructuring was the source of the large increase in activation energy.

### 8:24AM A6.00003 Roles of Surface and Interface Spins in Exchange Coupled Nanostructures<sup>1</sup>

, MANH-HUONG PHAN, Department of Physics, University of South Florida, Tampa, FL 33620, USA — Exchange bias (EB) in magnetic nanostructures has remained a topic of global interest because of its potential use in spin valves, MRAM circuits, magnetic tunnel junctions, and spintronic devices. The exploration of EB on the nanoscale provides a novel approach to overcoming the superparamagnetic limit and increasing the thermoremanence of magnetic nanoparticles, a critical bottleneck for magnetic data storage applications. Recent advances in chemical synthesis have given us a unique opportunity to explore the EB in a variety of nanoparticle systems ranging from core/shell nanoparticles of Fe/ $\gamma$ -Fe<sub>2</sub>O<sub>3</sub>, Co/CoO, and FeO/Fe<sub>3</sub>O<sub>4</sub> to hollow nanoparticles of  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub> and hybrid composite nanoparticles of Au/Fe<sub>3</sub>O<sub>4</sub>. Our studies have addressed the following fundamental and important questions: (i) Can one decouple collective contributions of the interface and surface spins to the EB in a core/shell nanoparticle system? (ii) Can the dynamic and static response of the core and shell be identified separately? (iii) Can one tune “minor loop” to “exchange bias” effects in magnetic hollow nanoparticles by varying the number of surface spins? (iv) Can one decouple collective contributions of the inner and outer surface spins to the EB in a hollow nanoparticle system? (v) Can EB be induced in a magnetic nanoparticle by forming its interface with a non-magnetic metal? Such knowledge is essential to tailor EB in magnetic nanostructures for spintronics applications. In this talk, we will discuss the aforementioned findings in terms of our experimental and atomistic Monte Carlo studies.

<sup>1</sup>The work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-FG0207ER46438.

### 9:00AM A6.00004 Synthesis and magnetic properties of highly crystalline Fe<sub>3</sub>O<sub>4</sub> nanorods , R

DAS, K STOJAK REPA, V KALAPPATTIL, Univ. of South Florida, J ALONSO, Univ. of South Florida, BCMaterials, MH PHAN, H SRIKANTH, Univ. of South Florida — Anisotropic one-dimensional magnetic nanostructures have drawn considerable attention due to their high surface to volume ratio, which drastically influences physical and chemical properties. In the past decade, most attention has been paid to the synthesis of Fe<sub>3</sub>O<sub>4</sub> nanoparticles (NPs), mainly focusing on a spherical morphology. In this work, we report the first systematic study of the magnetic properties of highly crystalline Fe<sub>3</sub>O<sub>4</sub> nanorods (NRs), which were synthesized by the hydrothermal method. XRD and TEM confirm the formation of highly crystalline Fe<sub>3</sub>O<sub>4</sub> NRs with narrow size distribution. For high aspect ratio NRs (656nm), room temperature saturation magnetization is close to that of bulk Fe<sub>3</sub>O<sub>4</sub> (~90emu/g) and much larger than that of spherical NPs of the same volume (60-70emu/g). DC magnetization vs. temperature data display a sharp change in the magnetization at 120K, which is attributed to the Verwey transition, whose presence affirms the excellent crystallinity of Fe<sub>3</sub>O<sub>4</sub> NRs. Owing to their high effective anisotropy and saturation magnetization, the Fe<sub>3</sub>O<sub>4</sub> NRs show enhanced heating efficiency relative to their spherical NP counterparts when tested in a standard hyperthermia set-up.

### 9:12AM A6.00005 Ferroic ordering and charge-spin-lattice order coupling in Gd doped Fe<sub>3</sub>O<sub>4</sub> nanoparticles ,

SUVRA LAHA, EHAB ABDELHAMID, MAHESHIKA PALIHAWADANA ARACHCHIGE, Wayne State University, AMBESH DIXIT, Indian Institute of Technology Jodhpur, GAVIN LAWES, Wayne State University, VAMAN NAIK, University of Michigan Dearborn, RATNA NAIK, Wayne State University — Rare earth doped spinels have been extensively studied for their potential applications in magneto-optical recording and as MRI contrast agents. In the present study, we have investigated the effect of gadolinium doping (1-5 at.%) on the magnetic and dielectric properties of Fe<sub>3</sub>O<sub>4</sub> nanoparticles synthesized by the chemical co-precipitation method. The structure and morphology of the as-synthesized gadolinium doped Fe<sub>3</sub>O<sub>4</sub> (Gd-Fe<sub>3</sub>O<sub>4</sub>) nanoparticles were characterized by XRD, SEM and TEM, and the magnetic properties were measured by a Quantum Design physical property measurement system. We find that the penetration of excess Gd<sup>3+</sup> ions into Fe<sub>3</sub>O<sub>4</sub> spinel matrix significantly influences the average crystallite size and saturation magnetization in Gd-Fe<sub>3</sub>O<sub>4</sub>. The average crystallite size, estimated from XRD using Scherrer equation, increases with increasing Gd doping percentage and the saturation magnetization drops monotonically with excess Gd<sup>3+</sup> ions. Interestingly, Gd-Fe<sub>3</sub>O<sub>4</sub> develops enhanced ferroelectric ordering at low temperatures. The details of the temperature dependent dielectric, ferroelectric and magnetocapacitance measurements to understand the onset of charge-spin-lattice coupling in Gd-Fe<sub>3</sub>O<sub>4</sub> system will be presented.

### 9:24AM A6.00006 A comparison of methods for the determination of the magnetocrystalline anisotropy constant in an Fe<sub>3</sub>O<sub>4</sub>-based ferrofluid ,

RONALD TACKETT, MEGAN ALLYN, Kettering University, VIJAYENDRA GARG, ADERBAL DE OLIVEIRA, University of Brasilia, PREM VAISHNAVA, Kettering University — The dynamics of the relaxation behavior of superparamagnetic nanoparticles is governed by many factors such as the anisotropy constant, composition, size and nature of coating of the nanoparticles particles. We report values of the anisotropy constant (K) for magnetite nanoparticle (size ~12 nm) coated with dextran and suspended in water by dc and ac magnetization measurements, Mossbauer spectroscopy and the temperature dependent specific absorption rate (SAR) measurement. The magnetite nanoparticles were synthesized by co-precipitation and characterized by X-ray diffraction (XRD) and Transmission electron microscopy (TEM). The K values from dc magnetic susceptibility, Mossbauer spectroscopy, ac magnetic susceptibility, and that obtained by temperature dependent SAR measurements are all within the range of the accepted values in the literature. Merits and demerits of the four methods of determining K values will be discussed. We will also report on the temperature dependence of the anisotropy constant and the NEel relaxation constant.

**9:36AM A6.00007 Effect of magnetic anisotropy and particle size distribution on temperature dependent magnetic hyperthermia in  $\text{Fe}_3\text{O}_4$  ferrofluids**, MAHESHIKA PALIHAWADANA ARACHCHIGE, Wayne State University, HUMESHKAR NEMALA, Illinois Wesleyan University, VAMAN NAIK, University of Michigan Dearborn, RATNA NAIK, Wayne State University — Magnetic hyperthermia (MHT) has a great potential as a non-invasive cancer therapy technique. Specific absorption rate (SAR) which measures the efficiency of heat generation, mainly depends on magnetic properties of nanoparticles such as saturation magnetization ( $M_s$ ) and magnetic anisotropy (K) which depend on the size and shape. Therefore, MHT applications of magnetic nanoparticles often require a controllable synthesis to achieve desirable magnetic properties. We have synthesized  $\text{Fe}_3\text{O}_4$  nanoparticles using two different methods, co-precipitation (CP) and hydrothermal (HT) techniques to produce similar XRD crystallite size of 12 nm, and subsequently coated with dextran to prepare ferrofluids for MHT. However, TEM measurements show average particle sizes of 13.8 3.6 nm and 14.6 3.6 nm for HT and CP samples, implying the existence of an amorphous surface layer for both. The MHT data show the two samples have very different SAR values of 110 W/g (CP) and 40W/g (HT) at room temperature, although they have similar  $M_s$  of 70 4 emu/g regardless of their different TEM sizes. We fitted the temperature dependent SAR using linear response theory to explain the observed results. CP sample shows a larger magnetic core with a narrow size distribution and a higher K value compared to that of HT sample.

**9:48AM A6.00008 The investigation of smart magnetic nanoparticles for use in the hyperthermia treatment of cancer**, MEGAN ALLYN, Kettering University, PARASHU KHAREL, South Dakota State University, PREM VAISHNAVA, RONALD TACKETT, Kettering University — The magnetic fluid hyperthermia (MFH) treatment of cancer has emerged as a possible low-side-effect alternative to traditional chemotherapy- and radiation-based therapy. As the nanoparticles absorb energy from a low amplitude RF magnetic field they heat up; however, currently used hyperthermia systems require external temperature monitoring as the nanoparticles can easily heat to temperature greater than the desired window between 42C and 46C. To combat this, we are investigating smart magnetic nanoparticles whose Curie temperatures fall within the desired range. In order to do this, we have doped non-magnetic cations onto the structure of the AFM  $\text{LaMnO}_3$ . We report synthesis of  $\text{La}_{1-x}\text{M}_x\text{MnO}_3$  (M = Ba, Ca, Sr; x = 0.10 0.25) nanoparticles via sol-gel method for use in temperature-controlled MFH. These nanoparticles were characterized via powder x-ray diffraction and found to have the expected R-3c perovskite structure. For elemental analysis, energy dispersive spectroscopy was performed using scanning electron microscopy. The temperature dependence of the magnetization was investigated using vibrating sample magnetometry (VSM) to determine the Curie temperature of the ensembles. The results of the change in temperature vs time and SAR values will be presented.

**10:00AM A6.00009 Magnetically Stimulated Release of a Model Drug From a Magnetic Drug Carrier**, TOM RILEY, BEN EVANS, None — The use of particles in the micro and nanometer ranges has become increasingly important as therapeutic tools in medicine. In particular, magnetically-active particles may allow for magnetically-controlled release of drugs at targeted locations. The drugs can be delivered directly to cancerous tumors at desired concentrations. While hydrogel-based microspheres have been commonly proposed for such purposes, there is also a need for a lipophilic magnetic microsphere for delivery of poorly-soluble pharmaceuticals. We have created a well-dispersed suspension of iron oxide nanoparticles in a silicone matrix, and have used the material to manufacture microspheres in sizes ranging from 100nm to 50 microns. Our spheres are stable in aqueous suspensions, yet their silicone matrix is uniquely suited for the transport and delivery of hydrophobic pharmaceuticals. A high concentration of magnetic nanoparticles (50% wt.) enables magnetic localization, magnetic heating (hyperthermia), and magnetic stimulation to trigger drug release. Using fluorescein as a model drug, we use UV-visible spectroscopy to show a slow native release rate of the hydrophobic fluorescein from the spheres. We use these measurements to quantify the loading capacity of the microspheres, and we show results of magnetically-stimulated drug release using a DM100 field applicator (nanoScale Biomagnetics).

**10:12AM A6.00010 Electric field control of the magnetic order parameter of magnetic pillars embedded in a ferroelectric matrix**, MICHAEL FITZSIMMONS, Oak Ridge National Lab, Q WANG, Argonne National Lab, A CHEN, T LOOKMAN, Q.X. JIA, Los Alamos National Lab, D.A. GILBERT, J.A. BORCHERS, NIST, B HOLLADAY, S SINHA, UCSD — Using polarized beam small angle neutron scattering (SANS) we quantitatively measured the influence of an electric field on correlation of magnetism in a ferroelectric/ferrimagnetic nanocomposite. The nanocomposite consists of ~12 nm wide pillars of  $\text{CoFe}_2\text{O}_4$  (dark regions, inset figure left), a room temperature ferrimagnet, embedded in a ferroelectric,  $\text{BaTiO}_3$ , matrix (light regions, inset figure right). We used a model-free method to extract the correlations of the magnetic structure from the SANS data (figure below). We found a 700 kV/cm electric field induced a change of magnetization of ~2% (scattering geometry, inset figure left). We explain our results using a simple representation for free energy that attributes coupling between electric polarization and magnetic order parameters to strain.

**10:24AM A6.00011 Characterization and Magnetic Properties of Nano-ferrite  $\text{ZnFe}_2\text{-xLa}_x\text{O}_4$  prepared by Co-precipitation method**, ALY ABOU-ALY, Physics department, Faculty of Science, Alexandria University, Alexandria, Egypt, DOAA BAKEER, Physics department, Faculty of Science, Damanhur University, Damanhur, Egypt, NAYERA MOHAMMED, RAMADAN AWAD, MARWA HASEBBO, Physics department, Faculty of Science, Alexandria University, Alexandria, Egypt — Nano size spinel ferrite with nominal compositions  $\text{ZnFe}_{2-x}\text{La}_x\text{O}_4$ ,  $0.0 \leq x \leq 0.3$  were prepared using stoichiometric amounts of  $\text{ZnCl}_2$ ,  $\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$  and  $\text{LaCl}_3 \cdot 7\text{H}_2\text{O}$  by Co-precipitation method. The structures, optical and magnetic properties of the prepared samples were investigated, and compared with similar compositions prepared by different methods. The X-ray powder diffraction analysis shows single-phase cubic spinel structure up to  $x = 0.2$ . The lattice parameter "a" significantly increases with increasing x, which confirms the substitution of La at Fe sites. The crystallite size, estimated by different methods, has been found in the range of 7-14 nm. This crystallite size is found to be less than that prepared by sol gel combustion method. The FTIR spectra indicate the presence of absorption bands in the range of 390- 561 $\text{cm}^{-1}$ . The magnetic hysteresis was studied using vibrating sample magnetometer (VSM). The saturation magnetization, coercivity and remnents magnetization have nonsystematic change as the La-substitution increases. This is because the magnetic properties of Nano- ferrites are strongly dependent on the cation distribution among tetrahedral and octahedral sites in the cubic spinel structure.

**10:36AM A6.00012 Magnetite nano-islands on Graphene<sup>1</sup>**, NATHANIEL ANDERSON, QIANG ZHANG, Ames Laboratory and Iowa State University, RICHARD ROSENBERG, Advance Photon Source, Argonne National Laboratory, DAVID VAKNIN, Ames Laboratory and Iowa State University — X-ray magnetic circular dichroism (XMCD) of ex-situ iron nano-islands grown on graphene reveals that iron oxidation spontaneously leads to the formation of magnetite nano-particles - i.e. the formation of the inverse spinel  $\text{Fe}_3\text{O}_4$ . Fe islands have been grown with two different heights (20 and 75 MLs) on epitaxial graphene and we have determined their magnetic behavior both as function of temperature and applied external field. Our XAS and XMCD at an applied magnetic field of  $B = 5$  T show that the thin film (20 MLs) is totally converted to magnetite whereas the thicker film (75 MLs) exhibits magnetite properties but also those of pure metal iron. For both samples, temperature dependence of the XMCD shows clear transitions at ~120 K consistent with the Verwey transition of bulk magnetite. XMCD at low temperatures shows a weak hysteresis and provide the average spin  $\langle S_z \rangle$  and angular-momentum  $\langle L_z \rangle$  moments, the dipolar  $\langle T_z \rangle$  term, and the total moment  $\langle M_z \rangle$ . In addition, manipulation and comparison of the XMCD data from both samples allows us to extract information about the pure iron nano-islands from the thicker sample.

<sup>1</sup>Ames Laboratory is supported by the U.S. DOE, BES, MSE Contract No. DE-AC02-07CH11358. APS is supported by U.S. DOE contract No. DE-AC02-06CH11357.

**Monday, March 14, 2016 8:00AM - 11:00AM —**

**Session A7 APS SPS: Undergraduate Research/SPS I 303 - Crystal Bailey, American Physical Society**

**8:00AM A7.00001 Identifying the relation between trapping force of Laser Tweezers and Size of Microsphere particles<sup>1</sup>**, ALEXANDRA DIABRE, Seton Hall University — Optical trapping technique is the method in which micron and sub-micron particles can be studied. In this technique the laser pressure radiation creates the essential force to trap particles. This force depends on several parameters including the particles' indices of refraction, the specification of the beads surrounding environment and the characteristics of the implemented laser. On this work we present the outcome of the experiment we designed to analyze the trapping force. In this experiment we used micro sized beads with different indices of refraction, changed the viscosity of the surrounding environment of the beads and adjusted the power of the laser implemented. By analyzing the motion of the beads in several trials, the trapping force was estimated and its dependency to the parameters mentioned above was identified. Finally the outcomes of our experiment were compared with the theoretical reported results.

<sup>1</sup>This work was conducted under the supervision by Dr. Mitra Feizabadi

**8:12AM A7.00002 Scanning Tunneling Microscopy of Charge Density Wave states in TbTe<sub>3</sub>**, AARON KRAFT, LING FU, BISHNU SHARMA, Clark University, IAN FISHER, Stanford University, MICHAEL BOYER, Clark University — Charge density wave (CDW) states are broken symmetry states which involve a periodic lattice distortion and an opening of a band gap. While these states are prevalent in condensed matter systems, often coexisting with other states such as superconductivity, much is still not understood about the microscopic properties of CDWs or their onset through T<sub>CDW</sub>. For these reasons we use scanning tunneling microscopy (STM) to study CDW states in TbTe<sub>3</sub> where T<sub>CDW</sub> ~335 K. We will present temperature dependent STM data through T<sub>CDW</sub> as well as our efforts in modeling the combined effects of crystal lattice structure, CDW states, and wave-vector mixing to understand the periodicities detected in our topographic images.

**8:24AM A7.00003 Thermal Properties of Nd-Doped PrOs<sub>4</sub>Sb<sub>12</sub> Extracted From Measurement of Specific Heat<sup>1</sup>**, TAYLOR MCCULLOUGH-HUNTER, Physics Department, California State University, Fresno, SHOJI HISHIDA, PEI-CHUN HO, Department of Physics, California State University, Fresno, BRIAN MAPLE, Department of Physics, University of California, San Diego, TATSUYA YANAGISAWA, Department of Physics, Hokkaido University, Japan — PrOs<sub>4</sub>Sb<sub>12</sub> has attracted interest due to its unconventional heavy fermion superconductivity, interest that has increased once the Nd-doped compound was shown at certain concentrations of Nd to simultaneously display ferromagnetism and superconducting properties at low temperatures. In order to better understand the more exotic low temperature behavior exhibited by this system, it is necessary to characterize its normal-state properties. Therefore, the molar specific heat of Pr<sub>1-x</sub>Nd<sub>x</sub>Os<sub>4</sub>Sb<sub>12</sub> is measured using finite heat pulse relaxation calorimetry. A curve-fit of the temperature-dependent molar specific heat allows an estimation of the Debye and Einstein temperatures, as well as the electronic specific heat coefficient. These properties are examined across x to determine the behavior of the system with respect to Nd-concentration. The results from the measurements will be discussed during the presentation.

<sup>1</sup>Research at CSU-Fresno is supported by NSF DMR-1506677; at UCSD by NSF DMR-1206553 and US DOE DE FG02-04ER46105; at Hokkaido Univ. by Grant-in-Aid No 2600342

**8:36AM A7.00004 Pressure Dependence of the Magnetic Response of the S = 1 Polymeric Chain [Ni(HF<sub>2</sub>)(3-Clpy)<sub>4</sub>]BF<sub>4</sub>.<sup>1</sup>**, JAYNISE PEREZ, Univ of Puerto Rico - Mayaguez, MARCUS PEPRAH, PEDRO QUINTERO, MARK MEISEL, Dept. of Physics and NHMFL, Univ. of Florida, JAMIE MANSON, Dept. of Chemistry, Eastern Washington Univ. — [Ni(HF<sub>2</sub>)(3-Clpy)<sub>4</sub>]BF<sub>4</sub> (py = pyridine) is an S = 1 antiferromagnetic polymeric chain with a single-ion anisotropy (zero-field splitting) of D/kB = 4.3 K and an intrachain exchange interaction value of J/kB = 4.86 K at ambient pressure [1]. The ratio of these parameters (D/J = 0.88) places this system close to a quantum critical point at D/J ≈ 1, which falls between the Haldane and the Large-D phases. The temperature dependence of the low-field (1 kG) magnetic susceptibility was measured as a function of pressure, up to 1.49 GPa, using a homemade piston-clamp cell [2]. The data indicate the antiferromagnetic component is suppressed with increasing pressure. [1] J.L. Manson et al., Inorg. Chem. 51 (2012) 7520. [2] M.K. Peprah, PhD thesis, University of Florida (2015).

<sup>1</sup>Supported, in part, by the NSF via DMR-1202033 (MWM), DMR- 1306158 (JLM), DMR-1461019 (UF Physics REU support for JMP), and DMR-1157490 (NHMFL), and by the State of Florida.

**8:48AM A7.00005 High pressure differential conductance measurements of (Pb,Sn)Se**, TIFFANY PAUL, DERRICK VANGENNEP, DANIEL JACKSON, AMLAN BISWAS, JAMES HAMLIN, Department of Physics, University of Florida, Gainesville, FL 32608 — Topological transitions have been recognized as a new type of quantum phase transition. Recently, a number of papers have reported scanning tunneling microscope (STM) measurements of the Landau level spectra of topologically non-trivial materials. Such measurements can offer substantial insight into the nature of the transition between topologically distinct phases. Although applied pressure represents an attractive means to drive a topological quantum phase transition, STM measurements can not be performed under high pressure conditions. In this talk, I will discuss our recent attempts to observe Landau level spectra in compressed (Pb,Sn)Se using differential conductance measurements. Acknowledgements: TAP supported by REU NSF DMR-1461019. Pressure cell development and measurements at high magnetic fields supported by the National High Magnetic Field Laboratory User Collaboration Grants Program. Synthesis, characterization, and high pressure measurements supported by NSF DMR-1453752.

**9:00AM A7.00006 Phase Transitions in Nanostructured Mn<sub>0.18</sub>TaS<sub>2</sub><sup>1</sup>**, LUCAS BEVING, MATHEW FLEMING, PAYTON BURKEN, PAUL SHAND, TIMOTHY KIDD, LAURA STRAUSS, University of Northern Iowa — Phase transitions in a sample of Mn-intercalated TaS<sub>2</sub> were investigated. The concentration of manganese relative to tantalum was determined to be 18%. The phase transitions of the sample were explored using a variety of techniques: Curie-Weiss, Critical Scaling, Arrott-Noakes, and Kouvel-Fisher. All but the first method include the use of critical exponents defined using the spontaneous magnetization and susceptibility in zero applied field. The sample was found to undergo a transition from paramagnetism to an ordered state below 100 K. Two of the aforementioned methods were converted to computational methods. These same methods for determining the transition temperature and critical exponents may also indicate the existence of a second transition very close to the first. These results have been extracted using the theory of scaling.

<sup>1</sup>Research supported by National Science Foundation Grant No. DMR 1206530

**9:12AM A7.00007 Lattice thermal conductance of quantum wires with disorder**, ERIK VYHMEISTER, Andrews University, SELMAN HERSHFELD, University of Florida — We model the lattice thermal conductance in long quantum wires connected to two large heat baths at different temperatures in the harmonic approximation. The thermal conductance is computed with the Landauer formula for phonons, where it is related to the sum over all transmission probabilities for phonons through the wire. The net transmission probability is computed using a recursive Green function technique, which allows one to study long wires efficiently. We consider several different kinds of disorder to reduce the lattice thermal conductivity: periodic rectangular holes of varying sizes and shapes, periodic triangular holes, and narrow bands, averaged over randomness to account for variance in manufacturing. Depending on the model, the thermal conductance was reduced by 80 percent or more from the perfectly ordered wire case. Funded by NSF grant DMR-1461019.

**9:24AM A7.00008 3-D matrix template-assisted growth of oriented oxide nanowire arrays using glancing angle pulsed laser deposition**, N WRIGHT, Univ of Connecticut - Storrs, D MATEO-FELICIANO, A OSTOSKI, P MUKHERJEE, S WITANACHCHI, Univ of South Florida — Nanosphere lithography is a combination of different methods to nanofabrication. In this work nanosphere lithography is used to study the growth of Zinc Oxide Nano-columns (ZnO NCs) on different diameter Silica Nanosphere (SNS) self-assembled templates. ZnO NCs are promising building blocks for many existing and emerging optical, electrical, and piezoelectric devices, specifically, the seeded growth of other oxide materials. Recently, reports have shown a ferroelectric phase of zinc stannate ( $\text{ZnSnO}_3$ ) and while lead zirconium titanate oxide (PZT) has been the main material of interest in ferroelectric and piezoelectric applications, the toxicity of lead has been of great concern. The possibility of developing lead free piezoelectric materials is of great interest in the ferroelectric community. Langmuir-Blodgett method was used to construct a self-assembled monolayer of SNSs on silicon substrates. Oriented ZnO NCs were grown on top of the spheres using the glancing angle pulsed laser deposition technique. Columns were formed in a spatially ordered closed-packed hexagonal configuration. Growth of ZnO NCs was studied as function of ambient Oxygen pressure with SNS size ranging from 250-1000 nm. Cross-sectional Scanning Electron Microscopy and X-ray diffraction (XRD) were used to study the template structure. Relative aspect ratios were studied and showed tunability of column dimensions with sphere size. XRD revealed ZnO NC arrays were c-axis oriented with hexagonal wurtzite structure.

**9:36AM A7.00009 Observation of Interlayer Excitons in Monolayer  $\text{MoSe}_2$ - $\text{WSe}_2$  Heterostructure on BN Substrate<sup>1</sup>**, ALICE HUANG, Rutgers University, ESSANCE RAY, KYLE SEYLER, PASQUAL RIVERA, ERIC WONG, PAUL NYUGEN, GENEVIEVE CLARK, XIAODONG XU, University of Washington, GROUP OF XIAODONG XU TEAM — Interlayer excitons have previously been observed in monolayer MX2 heterostructures exhibiting type II band alignment. Specifically, interlayer excitons in  $\text{MoSe}_2$ - $\text{WSe}_2$  heterostructures have been thoroughly characterized with photoluminescence (PL) and photoluminescence excitation spectroscopy (PLE). However, electrical control of the interlayer exciton exhibits PL intensity dependence that is inconsistent with the dipole and electric field model - possibly owing to carrier charge effects - and requires further elucidation. The addition of BN substrate, which has been shown to (1) smooth the surface and (2) reduce carrier charge inhomogeneity of graphene devices, presents itself as a potential solution. In this preliminary study, we fabricated an  $\text{MoSe}_2$ - $\text{WSe}_2$  heterostructure on BN substrate. Photoluminescence (PL) measurements on the device confirm the presence of interlayer excitons at approximately 1.40 eV, consistent with  $\text{MoSe}_2$ - $\text{WSe}_2$  heterostructures. Furthermore, the PL characterization reveals unreported spectral features for both the interlayer and intralayer excitons.

<sup>1</sup>NSF REU, University of Washington Seattle

**9:48AM A7.00010 Magneto-Optical Study of Lithographically Patterned Ferromagnetic Multilayer  $(\text{Co/Pt})_8$  Micro-Channels<sup>1</sup>**, ALEXIS BOWERS, Lock Haven Univ, NITIN SAMARTH, SUSAN KEMPINGER, ROBERT FRALEIGH, Pennsylvania State University — Controlled domain movement in magnetic structures has become promising for applications in magnetic memory systems and data processing. This study examines magnetic domain nucleation and propagation within a series of lithographically patterned Co/Pt micro-channels with perpendicular magnetic anisotropy (PMA). Magnetic domains are nucleated and then manipulated using out-of-plane sweep protocols and studied in situ using magneto-optical Kerr effect (MOKE) imaging. Co/Pt multilayers were fabricated with optical lithography and sputter deposition. Effects of channel width and annealing are presented. Annealing the Co/Pt after fabrication as a function of time and temperature resulted in increasing the coercivity of the unpatterned film, decreasing the coercivity of the micro-channels, and reducing the average domain size in both. Atomic force microscopy (AFM) characterization of the micro-channels showed non-uniform deposition near feature edges. MOKE imaging demonstrated that the feature edges had a much lower coercivity (70G) than the middle of the channel/pad (150G) or the unpatterned film (250G). We found that an oscillating field protocol to re-initialize soft domains near feature edges proved to be more effective than a traditional field sweep to initialize a domain wall in the channel. Once a domain wall was formed, we explored a combination of constant and pulsed field protocols to manipulate the domain wall.

<sup>1</sup>2015 Penn State REU in Interdisciplinary Materials and Physics

**10:00AM A7.00011 Nuclear Magnetic Resonance Study of 3D Dirac Semimetal,  $\text{Na}_3\text{Bi}$ <sup>1</sup>**, AMELIA ESTRY, National High Magnetic Field Laboratory, NICK CURRO, KENT SHIRER, MATTHEW LAWSON, JOHN CROCKER, BLAINE BUSH, PETER KLAVINS, CHING (JIM) LIN, TANAT KISSIKOV, Department of Physics, University of California, Davis, ADAM DIOGUARDI, Los Alamos National Laboratory, ROBERT CAVA, Department of Chemistry, Princeton University — Dirac semimetals (DS) are a hot topic of research in topological materials because their unique properties indicate a potential in electronic applications. The electron band structure of ordinary semimetals differ from insulators and conductors as the top of the valence band and bottom of the conduction band have a small overlap. In DS, this overlap occurs only at discrete points, known as Dirac points. At the Dirac points, the relationship of energy to momentum (dispersion relation) is linear, allowing electrons near the Dirac points to behave as massless particles. Of particular interest are the three-dimensional Dirac semimetals, where this interesting band structure is present along all three dimensions. We attempt to probe the local conditions of a three-dimensional DS,  $\text{Na}_3\text{Bi}$ , using nuclear magnetic resonance (NMR) to perturb the spin states of the nuclei. Studying each of the nuclei sites of  $\text{Na}_3\text{Bi}$  using NMR can provide insight into the interactions among the nuclei and between the nuclei and the surrounding electrons.  $\text{Na}_3\text{Bi}$  has a complex NMR spectrum which requires further study to understand.

<sup>1</sup>Special thanks to the National Science Foundation for funding the UC Davis REU

**10:12AM A7.00012 A MATLAB GUI to study Ising model phase transition**, CURTISLEE THORNTON, TRINANJAN DATTA, Georgia Regents University — We have created a MATLAB based graphical user interface (GUI) that simulates the single spin flip Metropolis Monte Carlo algorithm. The GUI has the capability to study temperature and external magnetic field dependence of magnetization, susceptibility, and equilibration behavior of the nearest-neighbor square lattice Ising model. Since the Ising model is a canonical system to study phase transition, the GUI can be used both for teaching and research purposes. The presence of a Monte Carlo code in a GUI format allows easy visualization of the simulation in real time and provides an attractive way to teach the concept of thermal phase transition and critical phenomena. We will also discuss the GUI implementation to study phase transition in a classical spin ice model on the pyrochlore lattice.

**10:24AM A7.00013 Spin wave Feynman diagram vertex computation package**, ALEXANDER PRICE, Georgia Regents University, PHILIP JAVERNICK, University of North Carolina at Chapel Hill, TRINANJAN DATTA, Georgia Regents University — Spin wave theory is a well-established theoretical technique that can correctly predict the physical behavior of ordered magnetic states. However, computing the effects of an interacting spin wave theory incorporating magnons involve a laborious by hand derivation of Feynman diagram vertices. The process is tedious and time consuming. Hence, to improve productivity and have another means to check the analytical calculations, we have devised a Feynman Diagram Vertex Computation package. In this talk, we will describe our research groups effort to implement a Mathematica based symbolic Feynman diagram vertex computation package that computes spin wave vertices. Utilizing the non-commutative algebra package NCAAlgebra as an add-on to Mathematica, symbolic expressions for the Feynman diagram vertices of a Heisenberg quantum antiferromagnet are obtained. Our existing code reproduces the well-known expressions of a nearest neighbor square lattice Heisenberg model. We also discuss the case of a triangular lattice Heisenberg model where non collinear terms contribute to the vertex interactions.

**10:36AM A7.00014 A critical comparison of electrical methods for measuring spin-orbit torques<sup>1</sup>**, XUANZI ZHANG, YU-MING HUNG, LAURA REHM, ANDREW D. KENT, New York University — Direct (DC) and alternating current (AC) transport measurements of spin-orbit torques (SOTs) in heavy metal-ferromagnet heterostructure with perpendicular magnetic anisotropy have been proposed and demonstrated [1,2]. A DC method measures the change of perpendicular magnetization component while an AC method probes the first and second harmonic magnetization oscillation in responses to an AC current ( $\sim 1$  kHz). Here we conduct both types of measurements on  $\beta$ -Ta/CoFeB/MgO in the form of patterned Hall bars (20  $\mu$ m linewidth) and compare the results. Experiments results are qualitatively in agreement with a macro spin model including Slonzewski-like and a field-like SOTs. However, the effective field from the ac method is larger than that obtained from the DC method. We discuss the possible origins of the discrepancy and its implications for quantitatively determining SOTs. [1] L. Liu, C. Pai, Y. Li, H. Tseng, D. Ralph, and R Buhrman, Science 336, 1126 (2012). [2] J. Kim, J. Sinha, M. Hayashi, M. Yamanouchi, S. Fukami, T.Szuki, S. Mitani, and H. Ohno, Nature Mater. 12, 3522 (2013).

<sup>1</sup>Research supported by the SRC-INDEX program, NSF-DMR-1309202 and NYU-DURF award.

**10:48AM A7.00015 Analysis of Methods to Excite Head-Tail Motion Within the Cornell Electron Storage Ring**, NAOMI GENDLER, Reed College, MIKE BILLING, JIM SHANKS, Cornell University — The main accelerator complex at Cornell consists of two rings around which electrons and positrons move: the synchrotron, where the particles are accelerated to 5 GeV, and the Storage Ring, where the particles circulate at a fixed energy, guided by quadrupole and dipole magnets, with a steady energy due to a sinusoidal voltage source. Keeping the beam stable in the Storage Ring is crucial for its lifetime. A long-lasting, invariable beam means more accurate experiments, as well as brighter, more focused X-rays for use in the Cornell High Energy Synchrotron Source (CHESS). The stability of the electron and positron beams in the Cornell Electron Storage Ring (CESR) is important for the development of accelerators and for usage of the beam in X-ray science and accelerator physics. Bunch oscillations tend to enlarge the beam's cross section, making it less stable. We believe that one such oscillation is "head-tail motion," where the bunch rocks back and forth on a pivot located at the central particle. In this project, we write a simulation of the bunch that induces head-tail motion with a vertical driver. We also excite this motion physically in the storage ring, and observe a definite head-tail signal. In the experiment, we saw a definite persistence of the drive-damp signal within a small band around the head-tail frequency, indicating that the head-tail frequency is a natural vertical mode of the bunch that was being excited. The signal seen in the experiment matched the signal seen in the simulation to within an order of magnitude.

**Monday, March 14, 2016 8:00AM - 11:00AM —**

**Session A11 DMP: Pairing Interaction and Gap Symmetry in Fe-based Superconductors** 307 -

Rafael Fernandes, University of Minnesota

**8:00AM A11.00001 Glide-Plane Symmetry and Superconducting Gap Structure of Iron-Based Superconductors<sup>1</sup>**, THOMAS MAIER, Oak Ridge National Lab — This talk will provide a review [1] of the implications of the glide plane symmetry of a single Fe-pnictide/chalcogen plane on the structure of the superconducting gap. It will be shown that  $\eta$ -pairing with non-zero total momentum occurs inevitably in this system, but that its contribution to the superconducting condensate has the usual even parity symmetry and time reversal symmetry is preserved. I will demonstrate that for a single plane the gap function, which appears in physical quantities, is identical to that found in 1 Fe per unit cell pseudo-crystal momentum calculations and discuss the effects of the symmetry breaking out-of-plane hopping integrals in three dimensions. [1] Y. Wang, T. Berlijn, P. J. Hirschfeld, D. J. Scalapino, T. A. Maier, Phys. Rev. Lett. 114, 107002 (2015).

<sup>1</sup>A portion of this research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

**8:36AM A11.00002 Robust measurement of superconducting gap sign changes via quasiparticle interference: an application to 111 compounds<sup>1</sup>**, ILYA EREMIN, DUSTIN ALTENFELD, Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany, PETER HIRSCHFELD, Department of Physics, University of Florida, Gainesville, Florida 32611, USA, IGOR MAZIN, Code 6393, Naval Research Laboratory, Washington, DC 20375, USA — While quasiparticle interference (QPI) measurements based on scanning tunneling spectroscopy are often proposed as definitive tests of gap structure, the analysis typically relies on details of the model employed. Here using the simplified two-band model system we propose, that the temperature dependence of momentum-integrated QPI data can be used to identify gap sign changes in a qualitative way, and present an illustration for  $s_{\pm}$  and  $s_{++}$  states in a system with typical Fe-pnictide Fermi surface. Using ARPES derived band structures within 10 orbital model Hamiltonian we analyze the QPI spectra in LiFeAs and Co-doped NaFeAs compounds and show that the sign-changing gap can be clearly identified using non-magnetic impurity scattering.

<sup>1</sup>P.J.H. was supported by NSF-DMR-1005625, and I.I.M. by the U.S. Office of Naval Research through the Naval Research Laboratory's Basic Research Program. The work of DA and IE was supported by the Focus Program 1458 Eisen-Pnictide of the DFG

**8:48AM A11.00003 Features of Superconducting Gaps Revealed by STM/STS in Iron Based Superconductors With and Without Hole Pockets<sup>1</sup>**, HAI-HU WEN, Nanjing University, HAI-HU WEN TEAM — The pairing mechanism and gap structure in iron based superconductors (IBS) remains unresolved. We have conducted extensive STM/STS study on the Na(Fe<sub>1-x</sub>T<sub>x</sub>)As (T=Co, Cu, Mn)[1], Ba<sub>1-x</sub>K<sub>x</sub>Fe<sub>2</sub>As<sub>2</sub>[2], KFe<sub>2</sub>As<sub>2</sub>[3], and Li<sub>1-x</sub>Fe<sub>x</sub>OHFeSe[4] single crystals. We found the clear evidence of the in-gap quasi-particle states induced by the non-magnetic Cu impurities in Na(Fe<sub>0.97-x</sub>Co<sub>0.03</sub>Cu<sub>x</sub>)As, giving strong evidence of the  $S^{\pm}$  pairing. Furthermore, we show the presence of the bosonic mode with the energy identical to that of the neutron resonance and a simple linear relation  $\Omega/k_B T_c \approx 4.3$ , being explained a consequence of the Spairing. The STS spectrum in Li<sub>1-x</sub>Fe<sub>x</sub>OHFeSe clearly indicates the presence of double superconducting gaps with  $\Delta_1 \approx 14.3$  meV and  $\Delta_2 \approx 8.6$  meV. Further analysis based on QPI allows us to assign the larger (smaller) gap to the outer (inner) hybridized electron pockets[4]. The huge value  $2\Delta_1/k_B T_c = 8.7$  discovered here undoubtedly proves the strong coupling mechanism. [1] H. Yang et al., Nature Communications 4, 2947 (2013). [2] Z. Y. Wang, et al., Nature Physics 9, 42(2013). [3] D. L. Fang, X. Shi et al., arXiv: Condmat.1412.0945. Phys. Rev. B 2015. [4] Z. Y. Du et al., arXiv: Condmat. 1506.04645.

<sup>1</sup>This work was supported by the Ministry of Science and Technology of China, National Natural Science Foundation of China.

**9:00AM A11.00004 Specific Heat in High Magnetic Fields of  $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$** , CAMILLA M. MOIR, FSU/NHMFL, JOSE A. GALVIS, NHMFL, PHILLIP WALMSLEY, Stanford, JAMES G. ANALYTIS, UC Berkeley, JIUN-HAW CHU, IAN R. FISHER, Stanford, ARKADY SHEKHTER, NHMFL, GREG S. BOEBINGER, FSU/NHMFL, SCOTT C. RIGGS, NHMFL — We measure the magnetic field dependence of the specific heat in  $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$  with  $x$  ranging from  $x=0.31$  to  $x=0.6$  in fields up to 34.5T. We report three important observations:  $\sqrt{H}$  behavior indicating a nodal superconducting gap with a linear energy dispersion, saturation of the heat capacity at the magnetic field that corresponds to the resistive onset [1], and a calculated quasiparticle mass using the increase in the electronic specific heat coefficient when entering the normal state,  $\Delta\gamma = \gamma(34.5\text{T}) - \gamma(0\text{T})$ , as a measure of the normal state specific heat. [1] James G. Analytis, H-H. Kuo, Ross D. McDonald, Mark Wartenbe, P. M. C. Rourke, N. E. Hussey & I. R. Fisher. *Nature Phys.* 10, 194–197 (2014)

**9:12AM A11.00005 Direct evidence for a pressure induced nodal superconducting gap in the  $\text{Ba}_{0.65}\text{Rb}_{0.35}\text{Fe}_2\text{As}_2$  superconductor**, ZURAB GUGUCHIA, Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, Switzerland, ALEX AMATO, PSI, JIAN KANG, University of Minnesota, USA, HUBERTUS LUETKENS, PABITRA K. BISWAS, PSI, GIACOMO PRANDO, IFW Dresden, Germany, FABIAN V. ROHR, Universität Zurich, Switzerland, ZBIGNIEW BUKOWSKI, Institute of Low Temperature and Structure Research, Poland, ALEXANDER SHENGELAYA, Tbilisi State University, Georgia, HUGO KELLER, Universität Zurich, Switzerland, ELVEZIO MORENZONI, PSI, RAFAEL M. FERNANDES, University of Minnesota, USA, RUSTEM KHASANOV, PSI — In contrast to other unconventional superconductors, in the Fe-based superconductors (Fe-HTSs) both  $d$ -wave and extended  $s$ -wave pairing symmetries are close in energy. Probing the proximity between these different superconducting (SC) states and identifying experimental parameters that can tune them is of central interest. We report high-pressure muon spin rotation experiments on the temperature-dependent magnetic penetration depth in the optimally doped nodeless  $s$ -wave Fe-HTS  $\text{Ba}_{0.65}\text{Rb}_{0.35}\text{Fe}_2\text{As}_2$ . Upon pressure, a strong decrease of the penetration depth is observed, while the SC transition temperature remains nearly constant. More importantly, the low-temperature behavior of the inverse squared magnetic penetration depth, which is a direct measure of the superfluid density, changes qualitatively from an exponential saturation at zero pressure to a linear-in- $T$  behavior at higher pressures, indicating that hydrostatic pressure promotes the appearance of nodes in the SC gap.

**9:24AM A11.00006 Thermoelectric signatures of time-reversal symmetry breaking states in multiband superconductors**, MIKHAIL SILAEV, JULIEN GARAUD, EGOR BABAIEV, KTH, The Royal Institute of Technology — We demonstrate that superconductors which break time-reversal symmetry can exhibit thermoelectric properties, which are entirely different from the Ginzburg mechanism. As an example, we show that in the  $s+i$  superconducting state there is a reversible contribution to thermally induced supercurrent, whose direction is not invariant under time-reversal operation. Moreover in contrast to Ginzburg mechanism it has a singular behavior near the time-reversal symmetry breaking phase transition. A local hot spot in such superconductors is surrounded by a multipolar magnetic field, sensitive to the presence of domain walls and crystalline anisotropy of superconducting states. A non-stationary heating process produces an electric field and a charge imbalance in different bands. These effect can be measured and used to distinguish  $s+i$  and  $s+id$  superconducting states in the candidate materials such as  $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ .

**9:36AM A11.00007 Raman resonance due to magnetic fluctuations in iron-based superconductors**, JIASHEN CAI, ALBERTO HINOJOSA, ANDREY CHUBUKOV, University of Minnesota — We perform theoretical analysis of polarization-sensitive Raman spectroscopy on  $\text{NaFe}_{1-x}\text{Co}_x\text{As}$  and  $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ , focusing on two features seen in the  $B_{1g}$  symmetry channel (in one Fe unit cell notation): the strong temperature dependence of the static, uniform Raman response in the normal state and the existence of a collective mode in the superconducting state. We show that both features can be explained by the coupling of fermions to pairs of magnetic fluctuations via the Aslamazov-Larkin process. We argue that the singular temperature dependence in the normal state comes from the Aslamazov-Larkin vertex, while the resonance is due to the interaction between two propagating spin fluctuations in an  $s^{+-}$  superconductor.

**9:48AM A11.00008 Electron pairing in the presence of incipient bands in iron-based superconductors<sup>1</sup>**, ANDY LINSCHIED, XIAO CHEN, SAURABH MAITI, PETER HIRSCHFELD, University of Florida — Recent experiments on certain Fe-based superconductors (SC) have hinted at a role for paired electrons in incipient bands that are close to, but do not cross the Fermi level. Within a simple multiband weak-coupling BCS approximation, we categorize the problem into two cases: case(I) where SC arises from the incipient band pairing alone, and case(II) where it is induced on an incipient band by pairing due to Fermi-surface based interactions. Negative conclusions regarding the importance of incipient bands are largely based on case(I). However, we show explicitly that models under case(II) can explain the mild suppression of  $T_c$ , as well as robust large gaps on an incipient band. We also model the interplay between phonon and spin fluctuation (SF) driven SC and describe the bootstrap of electron-phonon SC by SF coupling the incipient and the regular bands. We argue that pairing on incipient bands may be important in several Fe-based materials, including  $\text{LiFeAs}$ ,  $\text{FeSe}$  intercalates and  $\text{FeSe}$  monolayers on  $\text{SrTiO}_3$ , and indeed may contribute to high  $T_c$  in some cases. In addition, we address the question whether this conclusion holds if the SF interaction is derived explicitly in the incipient band scenario and retardation effects are included on the level of the Eliashberg equations.

<sup>1</sup>SM was supported by NHMFL through NSF-DMR-1157490, AL and PJH were supported in part by DOE DE-FG02-05ER46236

**10:00AM A11.00009 Smearing of the Lifshitz transition by superconductivity<sup>1</sup>**, ALEXEI KOSHELEV, KONSTANTIN MATVEEV, Materials Science Division, Argonne National Laboratory — We consider a multiband metal with deep primary bands and a shallow secondary one [1]. In the normal state the system undergoes Lifshitz transition when the bottom of the shallow band crosses the Fermi level. In the superconducting state Cooper pairing in the shallow band is induced by the deep ones. As a result, the density of electrons in the shallow band remains finite even when the bottom of the band is above the Fermi level. We study the density of states in the system and find qualitatively different behaviors on the two sides of the Lifshitz transition. On one side of the transition the density of states diverges at the energy equal to the induced gap, whereas on the other side it vanishes. We argue that this physical picture describes the recently measured gap structure in shallow bands of iron pnictides and selenides. [1] A. E. Koshelev and K. A. Matveev *Phys. Rev. B* **90**, 140505(R) (2014)

<sup>1</sup>This work was supported by the U.S. Department of Energy, Office of Science, Materials Sciences and Engineering Division.

**10:12AM A11.00010 Microscopic theory of superconductivity near a Lifshitz transition<sup>1</sup>**, VIVEK MISHRA, THOMAS MAIER, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN-37831, USA., DOUG SCALAPINO, Department of Physics, University of California, Santa Barbara, CA-93106, USA. — Observation of robust superconductivity in some of the iron based superconductors in the vicinity of a Lifshitz point has attracted many theoretical and experimental studies. The majority of these studies have been phenomenological. Here we discuss a microscopic treatment of the pairing mechanism for a bilayer Hubbard model, which goes through a Lifshitz transition. We study pairing driven by spin-fluctuations by solving the strong coupling Eliashberg equations and make a systematic comparison of the results with non-perturbative dynamical cluster quantum Monte Carlo calculations. Our findings are quite general and we will discuss their application to some of the iron based superconductors.

<sup>1</sup>Research sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U. S. Department of Energy.

**10:24AM A11.00011 Topological Phase Transitions in Line-nodal Superconductors<sup>1</sup>**, GIL YOUNG CHO, SANGEUN HAN, EUN-GOOK MOON, KAIST — Fathoming interplay between symmetry and topology of many-electron wave-functions deepens our understanding in quantum nature of many particle systems. Topology often protects zero-energy excitation, and in a certain class, symmetry is intrinsically tied to the topological protection. Namely, unless symmetry is broken, topological nature is intact. We study one specific case of such class, symmetry-protected line-nodal superconductors in three spatial dimensions (3d). Mismatch between phase spaces of order parameter fluctuation and line-nodal fermion excitation induces an exotic universality class in a drastic contrast to one of the conventional  $\phi^4$  theory in 3d. *Hyper-scaling violation* and *relativistic dynamic scaling* with unusually large quantum critical region are main characteristics, and their implication in experiments is discussed. For example, continuous phase transition out of line-nodal superconductors has a *linear* phase boundary in a temperature-tuning parameter phase-diagram.

<sup>1</sup>This work was supported by the Brain Korea 21 PLUS Project of Korea Government and KAIST start-up funding.

**10:36AM A11.00012 Orbital-selective pairing: a  $\tau 3$  B<sub>1g</sub> pairing candidate state for the alkaline iron selenides.**, RONG YU, Renmin University of China, EMILIAN M NICA, QIMIAO SI, Rice University — The iron-based unconventional superconductors are inherently multi-orbital systems and show remarkable variation in the Fermi-surfaces and pairing symmetries. In the alkaline iron selenides cases, ARPES experiments indicate fully gapped superconducting states, which suggests s-wave pairing, while neutron-scattering studies show resonances in the spin-spectrum with wave vectors across the electron Fermi pockets, suggesting d-wave pairing. We propose a novel superconducting state composed of a direct product of an s-wave form factor and a rotational symmetry-breaking orbital matrix in the  $d_{xz}/yz$  sectors [1]. It belongs to the B<sub>1g</sub> representation of the D<sub>4h</sub> point group, allowing for the overall change in sign between the pairing field at the electron pockets close to the 1-Fe BZ edge. While it supports a spin resonance, it also produces a fully gapped quasiparticle spectrum, making it a candidate pairing state for the alkaline iron selenide compounds. Our results also show how such a state can become energetically competitive in the regime of quasi-degeneracy between the s and d-wave pairing states. In a broader context, this pairing provides an alternative to the *s+id* to reconstruct the degenerate pairing states, while preserving the time-reversal symmetry. We discuss possible analogs in other multi-band strong-coupling superconductors such as the heavy fermions. [1] "Emergent superconducting state from quasi-degenerate s- and d-wave pairing channels in iron-based superconductors," E. M. Nica, R. Yu, and Q. Si, arXiv:1505.04170v1 (2015).

**10:48AM A11.00013 Searching for the Genes of Unconventional High Temperature Superconductors**, JIANGPING HU, Purdue University & Institute of Physics, CAS — In the past, both cuprates and iron-based superconductors were discovered accidentally. Lacking of successful predictions on new high T<sub>c</sub> materials is one of major obstacles to reach a consensus on the high T<sub>c</sub> mechanism. In this talk, we discuss two emergent principles, which are called as the correspondence principle and the selective magnetic pairing rule, to unify the understanding of both cuprates and iron-based superconductors. These two principles provide a unified explanation why the d-wave pairing symmetry and the s-wave pairing symmetry are robust respectively in cuprates and iron-based superconductors. In the meanwhile, the above two principles explain the rareness of unconventional high T<sub>c</sub> superconductivity, identify necessary electronic environments required for high T<sub>c</sub> superconductivity and finally serve as direct guiding rules to search new high T<sub>c</sub> materials. We predict that the third family of unconventional high T<sub>c</sub> superconductors exist in the compounds which carry two dimensional hexagonal lattices formed by cation-anion trigonal bipyramidal complexes with a *d<sub>xy</sub> filling configuration on the cation ions. Their superconducting states are expected to be dominated by the d<sub>xy</sub> + id pairing symmetry and their maximum T<sub>c</sub> should be higher than those of iron-based superconductors. Verifying the prediction can convincingly establish the high T<sub>c</sub>*

**Monday, March 14, 2016 8:00AM - 11:00AM –**

**Session A12 DLS: Advances in Real-Time Measurement of Structural Transformations** 308 - Roseanne Sension, University of Michigan

**8:00AM A12.00001 Tabletop Extreme Ultraviolet Spectroscopy of Element-Specific Organometallic Photophysics**, JOSH VURA-WEIS, University of Illinois at Urbana-Champaign — High-harmonic extreme ultraviolet (XUV) spectroscopy has the potential to provide the elemental, oxidation-state, and spin-state specificity of core-level spectroscopy with the convenience and ultrafast time resolution of tabletop laser sources. We will show that M-edge spectroscopy of first-row transition metal complexes (3p→3d excitation) is a sensitive probe of the electronic structure of organometallic complexes in solution. Furthermore, this technique can be used to determine the relaxation dynamics of these molecules in the first few femtoseconds to nanoseconds after photoexcitation.

**8:36AM A12.00002 Advancing the molecular movie: Femtosecond X-ray scattering of an electrocyclic chemical reaction<sup>1</sup>**, MICHAEL MINITTI, SLAC National Accelerator Laboratory — Since it began operation in 2009, SLAC's Linac Coherent Light Source (LCLS) has allowed scientists to make new types of X-ray measurements that were once thought unattainable by delivering one trillion X-ray photons in incredibly short bursts of less than a few femtoseconds. It was promised that this astonishing quantity of photons, delivered in such a small slice of time, could capture the motions of atoms in chemical reactions. Now we have used this capability to make a "molecular movie" of a molecule undergoing a chemical reaction from start to finish, with frames just a few femtoseconds long. We assembled the movie by taking individual X-ray snapshots of the molecules that show the positions of their atoms at each moment in time. Comparing these results to computer simulations of the reaction, we determined the routes the individual molecules followed as it's structure rearranged. This is the first step in developing robust methods for visualizing molecular motions in chemistry, biology, and materials science at the atomic scale. Please enjoy the movie!

<sup>1</sup>SLAC National Accelerator Laboratory U.S. DOE, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-76SF00515

**9:12AM A12.00003 Structure and Dynamics with Ultrafast Electron Microscopes**, BRADLEY SIWICK, McGill University, Department of Physics, Center for the Physics of Materials — In this talk I will describe how combining ultrafast lasers and electron microscopes in novel ways makes it possible to directly 'watch' the time-evolving structure of condensed matter, both at the level of atomic-scale structural rearrangements in the unit cell and at the level of a material's nano- microstructure. First, I will briefly describe my group's efforts to develop ultrafast electron diffraction using radio- frequency compressed electron pulses in the 100keV range, a system that rivals the capabilities of xray free electron lasers for diffraction experiments. I will give several examples of the new kinds of information that can be gleaned from such experiments. In vanadium dioxide we have mapped the detailed reorganization of the unit cell during the much debated insulator-metal transition. In particular, we have been able to identify and separate lattice structural changes from valence charge density redistribution in the material on the ultrafast timescale. In doing so we uncovered a previously unreported optically accessible phase/state of vanadium dioxide that has monoclinic crystallography like the insulator, but electronic structure and properties that are more like the rutile metal. We have also combined these dynamic structural measurements with broadband ultrafast spectroscopy to make detailed connections between structure and properties for the photoinduced insulator to metal transition. Second, I will show how dynamic transmission electron microscopy (DTEM) can be used to make direct, real space images of nano-microstructural evolution during laser-induced crystallization of amorphous semiconductors at unprecedented spatio-temporal resolution. This is a remarkably complex process that involves several distinct modes of crystal growth and the development of intricate microstructural patterns on the nanosecond to ten microsecond timescales all of which can be imaged directly with DTEM.

**9:48AM A12.00004 Understanding subcellular function on the nanometer scale in real time: Single-molecule imaging in living bacteria** , JULIE BITEEN, Univ of Michigan - Ann Arbor — It has long been recognized that microorganisms play a central role in our lives. By beating the diffraction limit that restricts traditional light microscopy, single-molecule fluorescence imaging is a precise, noninvasive way to sensitively probe position and dynamics, even in living cells. We are pioneering this super-resolution imaging method for unraveling important biological processes in live bacteria, and I will discuss how we infer function from subcellular dynamics (Tuson and Biteen, *Analytical Chemistry* 2015). In particular, we have understood the mechanism of membrane-bound transcription regulation in the pathogenic *Vibrio cholerae*, revealed an intimate and dynamic coupling between DNA mismatch recognition and DNA replication, and measured starch utilization in an important member of the human gut microbiome.

**10:24AM A12.00005 Orbital-specific mapping of chemical dynamics with ultrafast x-rays** , PHILIPPE WERNET, Helmholtz-Zentrum Berlin — Charge and spin density changes at the metal sites of transition-metal complexes and in metalloproteins determine reactivity and selectivity. To understand their function and to optimize complexes for photocatalytic applications the changes of charge and spin densities need to be mapped and ultimately controlled. I will discuss how time-resolved soft x-ray spectroscopy enables a fundamental understanding of local atomic and intermolecular interactions and their dynamics on atomic length and time scales of Ångströms and femtoseconds. The approach consists in using time-resolved, atom- and orbital-specific x-ray spectroscopy and quantum chemical theory to map the frontier-orbital interactions and their evolution in real time of ultrafast chemical transformations. We recently used femtosecond resonant inelastic x-ray scattering (RIXS, the x-ray analog of resonant Raman scattering) at the x-ray free-electron laser LINAC Coherent Light Source (LCLS, Stanford, USA) to probe the reaction dynamics of a transition-metal complex in solution on the femtosecond time scale. Spin crossover and ligation are found to define the excited-state dynamics. It is demonstrated how correlating orbital symmetry and orbital interactions with spin multiplicity allows for determining the reactivity of short-lived reaction intermediates. I will discuss how this complementary approaches that probe structural dynamics and how it can be extended to map the local chemical interactions and their dynamical evolution in metalloproteins.

**Monday, March 14, 2016 8:00AM - 11:00AM –**  
**Session A13 GQI: Quantum Characterization, Verification and Validation** 309 - Charles Tahan, Laboratory for Physical Sciences

**8:00AM A13.00001 Estimating the coherence of noise** , JOEL WALLMAN, Univ of Waterloo — To harness the advantages of quantum information processing, quantum systems have to be controlled to within some maximum threshold error. Certifying whether the error is below the threshold is possible by performing full quantum process tomography, however, quantum process tomography is inefficient in the number of qubits and is sensitive to state-preparation and measurement errors (SPAM). Randomized benchmarking has been developed as an efficient method for estimating the average infidelity of noise to the identity. However, the worst-case error, as quantified by the diamond distance from the identity, can be more relevant to determining whether an experimental implementation is at the threshold for fault-tolerant quantum computation. The best possible bound on the worst-case error (without further assumptions on the noise) scales as the square root of the infidelity and can be orders of magnitude greater than the reported average error. We define a new quantification of the coherence of a general noise channel, the unitarity, and show that it can be estimated using an efficient protocol that is robust to SPAM. Furthermore, we also show how the unitarity can be used with the infidelity obtained from randomized benchmarking to obtain improved estimates of the diamond distance and to efficiently determine whether experimental noise is close to stochastic Pauli noise.

**8:36AM A13.00002 Gate-set tomography and beyond** , ROBIN BLUME-KOHOUT, Sandia National Laboratories — Four years ago, there was no reliable way to characterize and debug quantum gates. Process tomography required perfectly pre-calibrated gates, while randomized benchmarking only yielded an overall error rate. Gate-set tomography (GST) emerged around 2012-13 in several variants (most notably at IBM; see PRA 87, 062119) to address this need, providing complete and calibration-free characterization of gates. At Sandia, we have pushed the capabilities of GST well beyond these initial goals. In this talk, I'll demonstrate our open web interface, show how we characterize gates with accuracy at the Heisenberg limit, discuss how we put error bars on the results, and present experimental GST estimates with  $1e-5$  error bars. I'll also present preliminary results of GST on 2-qubit gates, including a brief survey of the tricks we use to make it possible. I'll conclude with an analysis of GST's limitations (e.g., it scales poorly), and the techniques under development for characterizing and debugging larger (3+ qubit) systems.

**9:12AM A13.00003 Toward a new culture in verified quantum operations** , STEVE FLAMMIA, University of Sydney — Measuring error rates of quantum operations has become an indispensable component in any aspiring platform for quantum computation. As the quality of controlled quantum operations increases, the demands on the accuracy and precision with which we measure these error rates also grows. However, well-meaning scientists that report these error measures are faced with a sea of non-standardized methodologies and are often asked during publication for only coarse information about how their estimates were obtained. Moreover, there are serious incentives to use methodologies and measures that will continually produce numbers that improve with time to show progress. These problems will only get exacerbated as our typical error rates go from 1 in 100 to 1 in 1000 or less. This talk will survey existing challenges presented by the current paradigm and offer some suggestions for solutions that can help us move toward fair and standardized methods for error metrology in quantum computing experiments, and towards a culture that values full disclosure of methodologies and higher standards for data analysis.

**9:48AM A13.00004 Applying QCVV protocols to real physical systems.**<sup>1</sup> , EASWAR MAGESAN, IBM TJ Watson Research Center — As experimental systems move closer to realizing small-scale quantum computers with high fidelity operations, errors become harder to detect and diagnose. Verification and validation protocols are becoming increasingly important for detecting and understanding the precise nature of these errors. I will outline various methods and protocols currently used to deal with errors in experimental systems. I will also discuss recent advances in implementing high fidelity operations which will help to understand some of the tools that are still needed on the road to realizing larger scale quantum systems.

<sup>1</sup>Work partially supported by ARO under contract W911NF-14-1-0124

**10:24AM A13.00005 Applying benchmarking protocols to encoded qubits with non-Markovian errors** , SETH MERKEL, HRL Laboratories, LLC. — An essential goal for any quantum information processing platform is to develop the tools necessary to validate high-fidelity quantum gates. This effort has produced a suite of benchmarking and tomographic protocols that have been applied to a wide variety of physical implementations. All these protocols, however, were designed with strict error assumptions that can and will be violated by physical errors, especially as we push to lower and lower error rates. In this talk we look at randomized benchmarking with encoded states (from which leakage errors may occur) in the presence of non-Markovian noise and under the influence of sequence-length dependent filtering errors. These circumstances may apply to a variety of physical systems, but are particularly pertinent for  $1/f$  charge noise and hyperfine leakage noise in electrically controlled quantum dot qubits. We demonstrate how these errors affect the outcome of randomized benchmarking, including the signatures of said errors and the confidence with which we can report an average gate fidelity.

**Monday, March 14, 2016 8:00AM - 10:24AM –**

**Session A14 FHP: Peer Review: History and Issues** 310 - Robert Crease, Stony Brook University

**8:00AM A14.00001 Plagiarism and Trust in Peer Review** , MARIO BIAGIOLI, University of California, Davis — No abstract available.

**8:36AM A14.00002 The Curious Origins of the Scientific Referee** , ALEX CSISZAR, Department of the History of Science, Harvard University — Where did the figure of the scientific referee come from, and why? Beginning in the 1820s, in the midst of reform movements in English science and in English politics, a number of British scientific societies established formal systems for reading and reporting on manuscripts by special readers, who soon became known as referees. In this personage came to be juxtaposed elements of the legal expert, the trustworthy gentleman, the state bureaucrat, and even the anonymous literary reviewer. But when the scientific referee appeared on the scene of British science, it was not certain who he was, or what he was supposed to be for. The initial impetus for the Royal Society of London's referee system had been as much about generating publicity as making anonymous judgments. But gradually the referee report became shrouded in secrecy, and the referee was increasingly viewed as an agent for conferring rewards on authors in exchange for contributions to knowledge. The conception of the referee as primarily a gatekeeper of knowledge became dominant only later in the century, as scientific practitioners came to perceive the existence of a special set of texts called the scientific literature that could be marked off from other periodicals and which required protecting. The notion that some form of peer review – as it came to be known during the Cold War – was a *sine qua non* of legitimate scientific journals was an even later development.

**9:12AM A14.00003 In Referees We Trust? Controversies over Grant Peer Review in the Late Twentieth Century** , MELINDA BALDWIN, Harvard University — While many accounts of external refereeing assume that it has been a consistent part of science since the seventeenth century, the practice developed far more slowly and haphazardly than many observers realize, and it was not until after the Second World War that "peer review" became considered an essential part of scientific publishing or grant-making. This talk will explore refereeing procedures at American grant-giving organizations in the twentieth century, focusing especially on the National Science Foundation and the National Institutes of Health. The creators of the NSF and the NIH put refereeing systems in place at their foundation. However, the form and function of these systems differed from modern "peer review" in several important ways. At the NSF the initial purpose of the referee process was to advise the NSF program directors, not to dictate funding decisions. At the NIH, small "study sections" devoted to particular subjects made recommendations to the NIH leadership, which rendered final judgments. However, beginning in the 1960s a series of controversies about NIH and NSF grants placed refereeing procedures at these organizations under more intense scrutiny. These debates culminated in six days of Special Oversight Hearings into the NSF's peer review process in the summer of 1975. Following the hearings, both the NSF and NIH reformed their review processes to place more emphasis on referees' opinions about grant proposals, making peer review increasingly responsible for decision-making. These controversies illustrate that refereeing continued to undergo significant changes in form and purpose throughout the twentieth century, and further suggest that both the scientific community and the public placed increased emphasis on the role of the referee during the late twentieth century.

**9:48AM A14.00004 Where is the trust in the peer review dynamic?** , DANIEL UCKO<sup>1</sup>, Stony Brook University/American Physical Society APS — The motto of the Royal Society is "nullius in verba", which translates roughly as "take nobody's word for it", and this motto is furthermore emblematic of the conduct of science. We want facts and not opinions, verified results and not conjecture. From the time that we first started communicating scientific results, it has been recognized that scientific claims must be verified by someone who is not the maker of those claims, and who furthermore has no stake in the matter, in other words, a claim needs to be evaluated objectively. Peer review as a method of evaluation can be thought of as akin to an experiment, where the review process tests the hypothesis of a submitted paper. Peer review is however also a social process with human actors: authors, referees, and editors. As a process, peer review depends on trust, but in what way does that manifest? There are many agents in peer review: in addition to the human actors, there is also the institution that is the journal, as well as the publisher (e.g. APS) that stands behind the journal. People can also have trust in the very concept of peer review. If we accept as a proposition that publications are witnesses to science in the same way that people who attend scientific demonstrations are witnesses of an experiment, then how much do we trust this witness? A few further questions arise:

- If referees (and sometimes authors) are anonymous, what does this do to the mechanisms of trust?
- Is trust only possible between human agents, or can you trust a process or a journal in a similar way to trusting a certain car brand?
- Is an absence of trust the same as distrust?
- Is trust rational, or cognitive, or is it a practice?

In this paper I will attempt to locate the trust and ask how trust is earned, and, conversely, how it can be lost, using peer review as example.

<sup>1</sup>I have a joint affiliation with Stony Brook University and APS and would like both listed, in that order, in the abstract

**Monday, March 14, 2016 8:00AM - 11:00AM –**

**Session A15 DCMP DMP: Graphene: Quantum Hall Effect** 314 - Paul Campbell, Naval Research Laboratory

**8:00AM A15.00001 Valley Hall Effect in the presence of strain fluctuation in graphene systems<sup>1</sup>** , WENYU SHAN, DI XIAO, Carnegie Mellon University — We develop a theory of valley Hall transport in graphene on hexagonal boron nitride substrate, where the strain-induced random gauge potential becomes the dominant source of disorder. We find a large value (if not quantized) of valley Hall conductivity in the band transport regime, for a wide class of strain-fluctuation modes. Such exotic property is a consequence of a generic enhanced coordinate shift under vector disorder scattering for Dirac systems. When applied to monolayer or bilayer graphene, our theory reproduces the large valley Hall angle and finite-temperature behaviors of valley Hall conductivity observed in experiments. Our theory provides an alternative interpretation of experimental results for nonlocal transport in graphene, instead of previous understanding based on the equilibrium current in ground state.

<sup>1</sup>This work is supported by DOE Basic Energy Sciences Grant No. DE-SC0012509 (D. X. and W. S.).

**8:12AM A15.00002 Observation of fractional Bloch band quantum Hall states in graphene/h-BN superlattices**, LEI WANG, Physics, Cornell University, YUANDA GAO, Mechanical Engineering, Columbia University, BO WEN, Physics, Columbia University, JAMES HONE, Mechanical Engineering, Columbia University, CORY DEAN, Physics, Columbia University — The Hofstadter energy spectrum provides a uniquely tunable system to study emergent topological order in the regime of strong interactions. Previous experiments, however, have been limited to low Bloch band fillings where only the Landau level index plays a role. Here we report measurements of high mobility graphene superlattices where the complete unit cell of the Hofstadter spectrum is accessible. We observe coexistence of conventional fractional quantum Hall effect (QHE) states together with the integer QHE states associated with the fractal Hofstadter spectrum. At large magnetic field, we observe signatures of another series of states, which appears at fractional Bloch filling index. These fractional Bloch band QHE states are not anticipated by existing theoretical pictures and point towards a distinct type of many-body state.

**8:24AM A15.00003 Spin and valley resolved Landau level crossing in tri-layer ABA stacked graphene.**, BISWAJIT DATTA, Tata Institute of Fundamental Research, Mumbai, India, VISHAKHA GUPTA, Birla Institute of Technology & Science, Pilani, Goa campus, Tata Institute of Fundamental Research, Mumbai, India, ABHINANDAN BORAH, Tata Institute of Fundamental Research, Mumbai, India, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Japan, MANDAR DESHMUKH, Tata Institute of Fundamental Research, Mumbai, India — We present quantum Hall measurements on a high quality encapsulated tri-layer graphene device. Low temperature field effect mobility of this device is around  $500,000 \text{ cm}^2/\text{Vs}$  and we see SdH oscillations at a magnetic field as low as 0.3 T. Quantum Hall measurements confirm that the chosen tri layer graphene is Bernal (ABA) stacked. Due to the presence of both mass-less monolayer like Dirac fermions and massive bi-layer like Dirac fermions in Bernal stacked tri-layer graphene, there are Landau level crossings between monolayer and bi-layer bands in quantum Hall regime. Although most of the Landau Level crossings are predominantly present on the electron sides, we also observe signatures of the crossings on the hole side. This behaviour is consistent with the asymmetry of electron and hole in ABA tri-layer graphene. We observe a series of crossings of the spin and valley resolved Landau Levels.

**8:36AM A15.00004 Landau Level Crossings in Dual-Gated Bilayer Graphene at Large Displacement Fields**, CHENG PAN, YONG WU, BIN CHENG, SHI CHE, CHUN NING LAU, MARC BOCKRATH, University of California, Riverside — Previous work shows that Landau levels in bilayer graphene with the same orbital index  $N$  but different spin and valley degrees of freedom can form superpositions at a finite electric field[1-2]. Using the technique of one dimensional edge contacts[3] we fabricate dual-gated boron-nitride-encapsulated bilayer graphene device with a graphite local gate, which enables us to apply large electric fields and observe Landau level crossings between levels with neighboring orbital indices. We will discuss our latest results. [1] R. T. Weitz et al., Science 330, 812-816 (2010). [2] K. Lee et al., Science 345, 58-61 (2014). [3] L. Wang et al., Science 342, 614-617 (2013)

**8:48AM A15.00005 Quantum Hall Effect in Bernal-stacked tetralayer graphene**, YANMENG SHI, SHI CHE, TIMOTHY ESPIRITU, ZIQI PI, Department of Physics and Astronomy, University of California Riverside, Riverside, CA 91765, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, 1-1 Namiki, Tsukuba, Japan, CHUN NING LAU, Department of Physics and Astronomy, University of California Riverside, Riverside, CA 91765 — Bernal-stacked few layer graphene is of particular interest due to its unique tunable band structure. Here we study the electric transport of Bernal-stack tetralayer graphene that are encapsulated by boron nitride sheets. The device shows a clear Landau fan with multiple Landau level crossing features. We will present the dependence of its quantum Hall properties on electric and magnetic fields, and compare with theoretical calculations.

**9:00AM A15.00006 Quantum Hall resistance standard in graphene devices under relaxed experimental conditions**, F. SCHOPFER, R. RIBEIRO-PALAU, F. LAFONT, J. BRUN-PICARD, LNE, D. KAZAZIS, Laboratoire de Photonique et de Nanostructures, CNRS, A. MICHON, Centre de Recherche sur l'Hétéroépitaxie et ses Applications, CNRS, F. CHEYNIS, Aix Marseille Université, CNRS, CINAM, O. COUTURAUD, C. CONSEJO, B. JOUAULT, Laboratoire Charles Coulomb, CNRS, Montpellier Université, W. POIRIER, LNE — Large-area and high-quality graphene devices synthesized by CVD on SiC are used to develop reliable electrical resistance standards, based on the quantum Hall effect (QHE), with state-of-the-art accuracy of  $1 \times 10^{-9}$  and under an extended range of experimental conditions of magnetic field (down to 3.5 T), temperature (up to 10 K) or current (up to 0.5 mA). These conditions are much relaxed as compared to what is required by GaAs/AlGaAs standards and will enable to broaden the use of the primary quantum electrical standards to the benefit of Science and Industry for electrical measurements. Furthermore, by comparison of these graphene devices with GaAs/AlGaAs standards, we demonstrate the universality of the QHE within an ultimate uncertainty of  $8.2 \times 10^{-11}$ . This suggests the exact relation of the quantized Hall resistance with the Planck constant and the electron charge, which is crucial for the new SI to be based on fixing such fundamental constants. These results show that graphene realizes its promises and demonstrates its superiority over other materials for a demanding application. Nature Nanotech. 10, 965-971, 2015, Nature Commun. 6, 6806, 2015

**9:12AM A15.00007 Scaling behavior of the quantum Hall plateau-plateau transition in graphene p-n-p junctions**, WEI-HUA WANG, IAMS, Academia Sinica, CHENG-HUA LIU, National Taiwan University, PO-HSIANG WANG, Academia Sinica, TAK-PONG WOO, CHUN-WEI CHEN, CHI-TE LIANG, National Taiwan University — We present the observation of scaling behavior in graphene p-n-p junctions achieved by controlled metallic diffusion. Generally, metal deposition on graphene surface introduces substantial carrier scattering, which undermines the high mobility of intrinsic graphene. However, we discover a weakly functionalized regime of the deposited contact with small carrier scattering, while p-type doping of graphene is realized due to the metal oxide formation. Consequently, the resulted graphene channel are composed of p-type doped and an intrinsic regions. The high-quality graphene p-n-p junctions is evidenced by a pronounced quantum Hall effect and Shubnikov-de Haas oscillations. Remarkably, we observed a well-defined QH plateau-plateau transition of zeroth Landau level, yielding a scaling exponent of  $\kappa = 0.21 \pm 0.01$ . Moreover, the graphene p-n-p junctions exhibit weak localization behavior, and the coherence length was found to be correlated to carrier scattering in the graphene devices.

**9:24AM A15.00008 Landau Level Mixing in the  $\nu = 0$  Quantum Hall State of Graphene<sup>1</sup>**, BRADEN FESHAMI, HERBERT FERTIG, Department of Physics, Indiana University — The  $\nu = 0$  quantum Hall state in graphene has been the focus of many studies over the last several years. Recent experimental developments have allowed for the possibility of tuning the strength of the Zeeman interaction by tilting a graphene sample in the presence of an external magnetic field. Many of the theoretical frameworks for these systems involve projecting into the zeroth Landau level (LL) and specifying effective interaction parameters to simplify the calculation. We explore the effects of keeping a larger number of LLs, allowing for the possibility of Landau level mixing, within a self-consistent Hartree-Fock theory of the system. We include a SU(4) symmetric, Coulombic-like, interaction, and introduce microscopic on-site and nearest-neighbor interactions. Phase diagrams are constructed over a range of these two microscopic interaction strengths for different magnetic field strengths and Zeeman couplings.

<sup>1</sup>Supported by US-Israel BSF and the NSF

**9:36AM A15.00009 Unconventional Quantum Hall Edge-Bulk Correlation in Gated Graphene Devices**, YONG-TAO CUI, Stanford University, BO WEN, Columbia University, ERIC MA, GEORGI DIANKOV, Stanford University, ZHENG HAN, Columbia University, FRANCOIS AMET, Stanford University, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, Japan, DAVID GOLDBABER-GORDON, Stanford University, CORY DEAN, Columbia University, ZHI-XUN SHEN, Stanford University — The quantum Hall effect in a two dimensional electron system (2DES) has been understood as chiral edge states circulating a highly insulating bulk when the bulk Landau levels are completely filled. We combine edge-sensitive charge transport with scanning Microwave Impedance Microscopy that probes the bulk transition through Landau levels, to directly examine such edge-state picture in gated graphene devices. Surprisingly, comparison of these measurements reveals that quantized transport typically occurs below complete filling of bulk Landau levels, different from the conventional picture in semiconductor-based 2DESs. We suggest that gate-induced charge accumulation near edges leads to a complex edge state configuration in which counter-propagating edge states could exist at the same edge. The backscattering between these states, together with an incompressible strip separating the bulk and the edge region, can explain the observed deviations.

**9:48AM A15.00010 Collective Bulk and Edge Modes through the Quantum Phase Transition in Graphene at  $\nu = 0$** <sup>1</sup>, GANPATHY MURTHY, University of Kentucky, EFRAT SHIMSHONI, Bar-Ilan University, Israel, HERBERT FERTIG, Indiana University, Bloomington — Undoped graphene in a strong, tilted magnetic field exhibits a radical change in conduction upon changing the tilt-angle, which can be attributed to a quantum phase transition[1] from a canted antiferromagnetic (CAF) to a ferromagnetic (FM) bulk state at filling factor  $\nu = 0$ . This behavior signifies a change in the nature of the collective ground state and excitations across the transition. Using the time-dependent Hartree-Fock approximation, we study the collective neutral (particle-hole) excitations in the two phases, both in the bulk and on the edge of the system[2]. The CAF has gapless neutral modes in the bulk, whereas the FM state supports only gapped modes in its bulk. At the edge, however, only the FM state supports gapless charge-carrying states. Linear response functions are computed to elucidate their sensitivity to the various modes. The response functions demonstrate that the two phases can be distinguished by the evolution of a local charge pulse at the edge[3]. 1. M. Kharitonov, Phys. Rev. B **85**, 155439 (2012). 2. G. Murthy, E. Shimshoni, and H. A. Fertig, Phys. Rev. B **90**, 241410(R) (2014). 3. G. Murthy, E. Shimshoni, and H. A. Fertig, arxiv:1510.04255 (2015).

<sup>1</sup>NSF 1066293 (Aspen), US-Israel BSF 2012120 (GM, EF,HAF), ISF 231/14 (ES), NSF-DMR 1306897 (GM), NSF-DMR 1506460 (HAF).

**10:00AM A15.00011 Observation of helical edge states and fractional quantum Hall effect in a graphene electron-hole bilayer**, JASON YUANHONG LUO, JAVIER SANCHEZ-YAMAGISHI, Massachusetts Institute of Technology, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute of Materials Science, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology — 1D electronic systems are common theoretical building blocks for constructing quantum circuits, motivating a search for new experimental systems where 1D edge states of different quantum numbers can be coupled to each other by design. Twisted bilayer graphene allows for the stacking of two separate 1D quantum hall edge states, thus providing a natural sandbox for studying different types of edge state interactions. Via doping to form an electron-hole bilayer at moderate magnetic fields, we can induce edge modes of opposite chiralities and spin polarizations on different layers, thereby creating helical edge states reminiscent of a two-dimensional quantum spin Hall system. We report magnetotransport measurements of high-quality twisted bilayer graphene, showing how non-local measurements allow us to elucidate the nature and robustness of the helical edge states, as well as hints of fractional edge state interactions that are observable at higher magnetic fields.

**10:12AM A15.00012 Emergence of Helical Edge Conduction in Graphene in the  $\nu = 0$  Quantum Hall State**<sup>1</sup>, HERBERT FERTIG, Indiana University, PAVEL TIKHONOV, EFRAT SHIMSHONI, Bar-Ilan University, GANPATHY MURTHY, University of Kentucky — The conductance of graphene subject to a strong, tilted magnetic field exhibits a dramatic change with tilt-angle, interpreted as an evidence for the transition from a canted antiferromagnetic (CAF) to a ferromagnetic (FM)  $\nu = 0$  quantum Hall state. We develop a theory for the electric transport in this system based on the spin-charge connection, whereby the evolution in the nature of collective spin excitations throughout this quantum phase transition is reflected in the charge-carrying modes. To this end we study quantum fluctuations of the spin-valley configuration in a system with an edge, and derive an effective theory describing collective charge edge excitations coupled to neutral bulk excitations. Focusing particularly on the FM phase, naively expected to exhibit perfect conductance due to the emergence helical edge modes, we analyze the mechanism whereby the coupling to bulk excitations assists in generating back-scattering. Finally, we calculate the conductance as a function of temperature and the Zeeman energy the parameter that tunes the transition between the two phases.

<sup>1</sup>Support provided by the US-Israel BSF, ISF, and NSF.

**10:24AM A15.00013 Edge State Structure of the  $\nu = 0$  quantum Hall State in monolayer Graphene**, ANGELIKA KNOTHE, Universite Paris-Sud 11 and University of Freiburg, THIERRY JOLICOEUR, Universite Paris-Sud 11 — Single-layer graphene at neutrality under a magnetic field is a many-body insulator whose phase structure is under intense scrutiny. When tilting the applied magnetic field, there is a phase transition towards a conducting state. A plausible description is to start from a SU(4) spin-valley symmetric quantum Hall ferromagnet and add some lattice-scale anisotropies in valley space. In the manifold of ground states captured by this approach, it has been proposed that graphene undergoes a transition between a canted antiferromagnetic state and a ferromagnetic state. While this picture is clear in the bulk of the system, it remains to understand the effect of this phase change on the current-carrying edge states that are formed at the physical boundaries of a real sample. We use an extended Hartree-Fock approach to describe a finite-size system with a simple model for the edge and extract the one-body spectrum. We then describe the current-carrying edge textures.

**10:36AM A15.00014 Andreev reflection in edge states of time reversal invariant Landau levels**, K. G. S. H. GUNAWARDANA, Ames Laboratory, Iowa State University, BRUNO UCHOA, University of Oklahoma — We describe the conductance of a normal-superconducting junction in systems with Landau levels that preserve time-reversal symmetry. Those Landau levels have been observed in strained honeycomb lattices. The current is carried along the edges in both the normal and superconducting regions. When the Landau levels in the normal region are half filled, the Andreev reflection is maximal and the conductance plateaus have a peak as a function of the filling factor. The height of those peaks is quantized at  $4e^2/h$ . The interface of the junction has Andreev edge states, which form a coherent superposition of electrons and holes that can carry a net valley current. We identify unique experimental signatures for superconductivity in time-reversal-invariant Landau levels.

**10:48AM A15.00015 Andreev conversion of quantum Hall edge state in graphene**, GIL-HO LEE, SEAN HART, DI WEI, KATIE HUANG, Harvard University, DMITRI EFETOV, MIT, TAKASHI TANIGUCHI, KENJI WATANABE, NIMS, AMIR YACOBY, PHILIP KIM, Harvard University — Understanding the interplay between superconductivity (SC) and quantum Hall effect (QHE) has been a long-sought theoretical and experimental problem. SC contacts to QHE systems enable us to study interesting physics, such as Cooper pair injection into ballistic 2D channels, Andreev edge states, and emergent excitations of non-Abelian anyons. We developed an in-situ etching technique for highly transparent superconducting contact (NbN) to hBN encapsulated graphene channels. The high critical field of NbN electrodes ( $H_{c2} > 30$  T) and the high quality of our graphene devices allows us to experimentally access a wide range of magnetic field where SC and QHE coexist. In order to probe the Andreev conversion of QH edge states, we measure the chemical potential of normal electrodes located on the upstream and the downstream QH edge states relative to a narrow grounded superconducting electrode. We observed that the chemical potential in downstream has sign opposite to the one measured in upstream suggesting Andreev conversion of incident electrons to outgoing holes across the narrow superconducting contact. We systematically investigated this phenomena as a function of temperature, magnetic field, bias voltage and the width and length of the superconducting electrode.

**Monday, March 14, 2016 8:00AM - 11:00AM —**

**Session A16 DMP: 2D Devices: Sensors and Detectors 315 - Ke Zou, Yale University**

**8:00AM A16.00001 On-Chip High-Responsivity Graphene–Boron Nitride Photodetector Integrated with Si Waveguide**, YUANDA GAO, Columbia University, REN-JYE SHUIE, DIRK ENGLUND, Massachusetts Institute of Technology, JAMES HONE, Columbia University — Graphene and other two-dimensional (2D) materials have emerged as promising materials for broadband and high-speed photodetection [1] and optical modulation [2]. These optoelectronic capabilities can augment complementary metal–oxide– semiconductor (CMOS) devices for high-speed and low-power optical interconnects. Here, we demonstrate an on-chip ultrafast photodetector based on a two-dimensional heterostructure consisting of high-quality graphene encapsulated in hexagonal boron nitride. Coupled to the optical mode of a silicon waveguide, this 2D heterostructure-based photodetector exhibits a maximum responsivity of 0.36 A/W and high-speed operation with a 3 dB cutoff at 42 GHz [3]. From photocurrent measurements as a function of the top-gate and source-drain voltages, we conclude that the photoresponse is consistent with hot electron mediated effects. 1. Gan, X. et al. Chip-integrated ultrafast graphene photodetector with high responsivity. *Nat. Photonics* 7, 883–887 (2013). 2. Gao, Y. et al. High-Speed Electro-Optic Modulator Integrated with Graphene-Boron Nitride Heterostructure and Photonic Crystal Nanocavity. *Nano Lett.* 15(3), 2001-2005 (2015) 3. Shiue, R.-J. et al. High-Responsivity Graphene–Boron Nitride Photodetector and Autocorrelator in a Silicon Photonic Integrated Circuit. *Nano Lett.* Article ASPA

**8:12AM A16.00002 Buckled Graphene-like Materials in Ultrafast and Superstrong Optical Fields**, HAMED KOOCHAKI KELARDEH, VADYM APALKOV, MARK STOCKMAN, Georgia State University — We discuss the theoretical investigation of buckled Dirac materials (silicene and germanene) interacting with ultrashort and ultrastrong optical pulses. Highly intensive few-cycle fields strongly modify the electronic and optical properties of these two dimensional materials. The strong nonlinearity of the system for the fields applied ( $V/\text{\AA}$ ), will cause the violation of the charge (C) and parity (P) and time reversal symmetries. Such symmetry violations are related to the electron transfer between the sublattices produced by the normal field component and result in nonreciprocity, optical rectification and the appearance of a cross current. We also note a direct resemblance between silicene and field-effect transistors (FET). In FETs, the (perpendicular) gate field changes the carrier concentration and thereby, controls its conductance. Analogously, in silicene, the normal field component of the pulse, transfers carriers between two sublattices, and consequently modulates the response function of silicene to the in-plane field. **Reference:** H. K. Kelardeh, V. Apalkov, and M. I. Stockman, *Ultrafast field control of symmetry, reciprocity, and reversibility in buckled graphene-like materials*, *Phys. Rev. B* **92** (4), 045413 (2015).

**8:24AM A16.00003 Optical Detection of Local Electric Field Dynamics in Solutions by Waveguide-integrated Graphene Device**, JASON HORNG, HALLEH BALCH, UC Berkeley, FENG WANG TEAM — The spatio-temporal dynamics of local electric fields in ionic solutions plays a central role in various chemical and biological processes ranging from batteries technologies to neuron signaling. A non-invasive, precise detection scheme for measuring local electric fields dynamics has long been sought for. Here, we report a sensitive, high-speed, high spatial resolution optical imaging method for local electric fields based on the unique optoelectronic properties of graphene. With enhancement from a waveguide involving critical coupling concept, we show that our graphene optical sensor provides an ideal platform for studying dynamics of local electric field fluctuations in different nonequilibrium solutions.

**8:36AM A16.00004 Passive optical switches based on endohedral fullerenes**, YONGCHANG DONG, Clemson Univ, DEEPIKA SAINI COLLABORATION, LUIS A. ECHEGOYEN COLLABORATION, RAMAKRISHNA PODILA COLLABORATION — Although there have been many attempts to find better nanomaterial-based optical limiters & switches in recent years, currently there are only a few effective options for high-energy lasers. Reverse saturable absorption in fullerenes has been widely used to realize excellent passive optical limiters for the visible region up to 650 nm. The electronic structure of fullerenes can be modified by the encapsulation of endohedral clusters to achieve exotic quantum states of matter such as superconductivity. Building on this concept, in this talk, we show that three tri-metallic nitride endohedral fullerenes could alter the HOMO-LUMO gap and allow passive optical switching with a low limiting threshold ( $0.3 \text{ J/cm}^2$ ) and a wider operation window up to 1064 nm (average pulse energy  $>0.5 \text{ mJ}$  in ns regime).

**8:48AM A16.00005 Kirigami Graphene Transistors for Biological Sensing**, MICHAEL REYNOLDS, Cornell University, MORGAN BROWN, Oregon State University, KATHRYN MCGILL, PATRICIA DAVIDSON, JAN LAMMERDING, Cornell University, ETHAN MINOT, Oregon State University, JESSE GOLDBERG, PAUL MCEUEN, Cornell University — As flexible, locally amplifying probes, graphene transistors have potential applications in biological sensing, particularly for read-out of extracellular potentials. We present here electrolyte-gating measurements of stretchable graphene transistors aimed at exploring this application. The graphene is etched into patterns inspired by the Japanese paper art of kirigami to permit in-plane stretching<sup>1</sup>. Using a technique developed in our group for manipulating these devices in solution, we can maneuver and stretch devices in an electrolyte solution while monitoring their electrical response. These devices show proximity-dependent gating to voltages on an additional small metal probe near the device, and we quantify the nature and sensitivity of this response. The flexibility of these devices makes them promising as wearable electronics for cells, and we present early results on interactions between graphene devices and cardiomyocyte cells.

<sup>1</sup>Blees, M. K. et al. Graphene kirigami. *Nature* (2015).

**9:00AM A16.00006 Nanopores in suspended WS<sub>2</sub> membranes for DNA sequencing**, GOPINATH DANDA, Department of Electrical and Systems Engineering, University of Pennsylvania, PAUL MASIH DAS, YUNG-CHIEN CHOU, JEROME MLACK, CARL NAYLOR, Department of Physics and Astronomy, University of Pennsylvania, NESTOR PEREA-LOPEZ, ZHONG LIN, Department of Physics, The Pennsylvania State University, LAURA BETH FULTON, Department of Mechanical Engineering, University of Pittsburgh, MAURICIO TERRONES, Department of Physics, The Pennsylvania State University, A. T. CHARLIE JOHNSON, MARIJA DRNDIC, Department of Physics and Astronomy, University of Pennsylvania — Recent advances in solid-state nanopore sensor systems for DNA detection and analysis have been supported by using increasingly thinner materials to the point of utilizing atomically thin two-dimensional materials such as graphene and MoS<sub>2</sub>. However, these materials still have issues with pore wettability and signal-to-noise ratios displayed in DNA translocation measurements. Recently, the fabrication and operation of nanopores in MoS<sub>2</sub> have been demonstrated, but the wetting properties and signal-to-noise ratios of transition metal dichalcogenides are yet to be understood and further improved. Here we fabricate suspended WS<sub>2</sub> nanopore devices with sub-10 nm pore diameters using a novel nanomaterial transfer method and TEM nanosculpting to study and better understand nanopore wetting properties and performance in DNA translocation measurements.

**9:12AM A16.00007 Electronic nanobiosensors based on two-dimensional materials<sup>1</sup>**, JINGLEI PING, Univ of Pennsylvania — Atomically-thick two-dimensional (2D) nanomaterials have tremendous potential to be applied as transduction elements in biosensors and bioelectronics. We developed scalable methods for synthesis and large-area transfer of two-dimensional nanomaterials, particularly graphene and metal dichalcogenides (so called “MX<sub>2</sub>” materials). We also developed versatile fabrication methods for large arrays of field-effect transistors (FETs) and micro-electrodes with these nanomaterials based on either conventional photolithography or innovative approaches that minimize contamination of the 2D layer. By functionalizing the FETs with a computationally redesigned water-soluble mu-opioid receptor, we created selective and sensitive biosensors suitable for detection of the drug target naltrexone and the neuropeptide enkephalin at pg/mL concentrations. We also constructed DNA-functionalized biosensors and nano-particle decorated biosensors by applying related bio-nano integration techniques. Our methodology paves the way for multiplexed nanosensor arrays with all-electronic readout suitable for inexpensive point-of-care diagnostics, drug-development and biomedical research. With graphene field-effect transistors, we investigated the graphene/solution interface and developed a quantitative model for the effect of ionic screening on the graphene carrier density based on theories of the electric double layer. Finally, we have developed a technique for measuring low-level Faradaic charge-transfer current (fA) across the graphene/solution interface via real-time charge monitoring of graphene microelectrodes in ionic solution. This technique enables the development of flexible and transparent pH sensors that are promising for *in vivo* applications.

<sup>1</sup>The author acknowledges the support from the Defense Advanced Research Projects Agency (DARPA) and the U. S. Army Research Office under grant number W911NF1010093.

**9:48AM A16.00008 Enhancing the performance of Graphene NEMS<sup>1</sup>**, MARSHA PARMAR, Indian Inst of Science — In recent past Nanoelectromechanical systems (NEMS) have got several sensing based applications such as force, spin, charge and mass sensors. These devices due to their smaller size, operate in very high frequency regime (MHz - GHz) and have very high quality factors (10<sup>2</sup> -10<sup>5</sup>). Nevertheless these devices are limited by their comparatively smaller linear operational range. Electromechanical devices based on 2D materials are extremely sensitive to strain. We studied the effect of strain on the performance of single layer Graphene NEMS. Our results reveal that the strain in Graphene NEMS can be tuned to increase the linear operational range. We report a 25 dB increase in dynamic range by tuning the strain from 10<sup>-3</sup> at room temperature to 10<sup>-2</sup> at 200K. This increase in dynamic range is also accompanied by partial cancellation of elastic and electrostatic nonlinearities. The resulting mass resolution estimated from the experimental data is 100 yg.....<sup>1</sup> which is one order of magnitude better than previously reported values. Reference: 1. Parmar, M. M., Gangavarapu, P. R. Y. & Naik, A. K. Dynamic range tuning of graphene nanoresonators. *Applied Physics Letters* **107**, 113108 (2015).

<sup>1</sup>1.Department of Science and technology, India. 2.CSIR, India.

**10:00AM A16.00009 Biosensors based on DNA-Functionalized Graphene**, RAMYA VISHNUBHOTLA, JINGLEI PING, AMEY VRUDHULA, A.T. CHARLIE JOHNSON, Univ of Pennsylvania — Since its discovery, graphene has been used for sensing applications due to its outstanding electrical properties and biocompatibility. Here, we demonstrate the capabilities of field effect transistors (FETs) based on CVD-grown graphene functionalized with commercially obtained DNA oligomers and aptamers for detection of various biomolecular targets (e.g., complementary DNA and small molecule drug targets). Graphene FETs were created with a scalable photolithography process that produces arrays consisting of 50-100 FETs with a layout suitable for multiplexed detection of four molecular targets. FETs were characterized via AFM to confirm the presence of the aptamer. From the measured electrical characteristics, it was determined that binding of molecular targets by the DNA chemical recognition element led to a reproducible, concentration-dependent shift in the Dirac voltage. This biosensor class is potentially suitable for applications in drug detection. This work is funded by NIH through the Center for AIDS Research at the University of Pennsylvania.

**10:12AM A16.00010 Direct observation of PMMA removal from graphene surface**, XIAOHAN WANG, HARRY CHOU, LI TAO, ANDREW DICK, ANDREI DOLOCAN, DEJI AKINWANDE, C. GRANT WILLSON, Univ of Texas, Austin — PMMA is often used as a carrier layer for transfer of CVD graphene from copper to other substrates. After transfer, the PMMA is removed by chemical or thermal treatment. However, regardless of the method used, polymer residues are left on the graphene surface, which degrade the performance of graphene-based devices. Here, we present a systematic study of PMMA removal after graphene transfer. Raman and FET measurements were applied to monitor the polymer dissolution in an acetone bath. Isotope labeling and in-situ TOF-SIMS, XPS, Raman and AFM all show chemical changes in surface residues upon vacuum annealing. These data along with strategies to clean the graphene surface will be presented.

**10:24AM A16.00011 Carbon nanotube as a local drag sensor**, AUSTIN CHENG, Harvard University, JEAN-DAMIEN PILLET, Columbia University, PHILIP KIM, Harvard University — We report a Columb drag measurement in a carbon nanotube (CNT) and graphene hybrid device. In this device, the CNT and graphene serve as a 1D and 2D electronic system respectively and are separated by a thin hexagonal boron nitride (h-BN). By flowing a drive current in one conductor, due to electron-electron interactions, a drag voltage is developed in the other conductor. In the case where a current is applied to graphene, the CNT can act as a local drag sensor that probes the microscopic effects of electronic interactions hidden in graphene. We demonstrate this drag sensor capability by applying a magnetic field in graphene and show the transition from compressible states to incompressible states.

**10:36AM A16.00012 Amino Acids Interaction with Boron Nitride Nanomaterials**, KEVIN WATERS, RAVINDRA PANDEY, Michigan Technological University, SHASHI KARNA, US Army Research Laboratory — Stability and electronic properties of bioconjugated BN nanostructures are investigated. The biomolecules considered are amino acids ranging from monomers to peptides, and the low- dimensional BN nanostructures are monolayer and tubular configurations. Specifically, we examine the role of an aqueous background in stabilizing such bioconjugated nanostructures by employing the continuum solvent model. It is expected that the calculated results will provide guidance for selective sensing of biomolecules by the next generation nanomaterials.

**10:48AM A16.00013 Biomolecular interactions of emerging two-dimensional materials with aromatic amino acids**, SAI SUNIL KUMAR MALLINENI<sup>1</sup>, MEHMET KARAKAYA<sup>2</sup>, RAMAKRISHNA PODILA<sup>3</sup>, APPARAO RAO<sup>4</sup>, None — The present work experimentally investigates the interaction of aromatic amino acids, viz., tyrosine, tryptophan, and phenylalanine with novel two-dimensional (2D) materials including graphene (G), graphene oxide (GO), and boron nitride (BN). Photoluminescence, micro-Raman spectroscopy and cyclic voltammetry were employed to investigate the nature of interactions and possible charge transfer between 2D materials and amino acids. Consistent with previous theoretical studies<sup>[1,2]</sup>, graphene and BN were observed to interact with amino acids through  $\pi$ - $\pi$  interactions. Furthermore, we found that GO exhibits strong interactions with tryptophan and tyrosine as compared to graphene and BN, which we attribute to the formation of H-bonds between tryptophan and GO as shown theoretically in Ref. 2. On the other hand, phenylalanine did not exhibit much difference in interactions with G, GO, and BN.(1) The Journal of Chemical Physics 130, 124911 (2009) (2) J. Phys. Chem. Lett. 2013, 4, 3710–3718

<sup>1</sup>Clemson Nanomaterials Center,Clemson University, Clemson,SC,USA.

<sup>2</sup>Clemson Nanomaterials Center,Clemson University, Clemson,SC,USA.

<sup>3</sup>Laboratory of Nano-biophysics and COMSET, Clemson University, Clemson,SC,USA

<sup>4</sup>Clemson Nanomaterials Center,Clemson University, Clemson,SC,USA.

**Monday, March 14, 2016 8:00AM - 10:48AM –**

**Session A17 DMP: Graphene: Growth and Synthesis** 316 - Joshua Robinson, Pennsylvania State University

**8:00AM A17.00001 Materials Science and Engineering with Two-dimensional Atomic Layers**

, PULICKEL M. AJAYAN, Rice University — There has been tremendous interest in recent years to study two-dimensional atomic layers which form building blocks of many bulk layered materials and devices. This talk will focus on the materials science aspects of 2D atomic layer, in particular the emerging structures based on transition metal chalcogenides. Several aspects that include synthesis, characterization and device fabrication will be explored with the objective of achieving all 2D functional structures for future technologies. The concept of nanoscale engineering and the goal of creating new artificially stacked van der Waals solids will be discussed through a number of examples. The challenges involved in scalable synthesis, doping, defect engineering, surface modifications of monolayers and the controlled creation of stacked structures and in-plane junctions from multiple compositions will be discussed. Some of anticipated applications of these materials will also be discussed.

**8:36AM A17.00002 Large area single crystalline graphene growth on copper foil**, JAEHYUCK JUNG,

HOANG DANH PHAN, LEE CHANGGU, Sungkyunkwan Univ, GRAPHENE ENGINEERING LAB TEAM — Graphene synthesis methods using chemical vapor deposition (CVD) have been developed dramatically in these years but still it is challenging to make large size single crystal grains which have similar properties with pristine graphene. Here we report a pita-pocket method of growing large area single crystalline graphene on copper foil. We made holes on top of the closed copper pocket to provide stable gas flow inside of pocket, and copper domains with (111) crystal orientation, which gives an advantage for hexagonal graphene crystal growth, were formed continuously during synthesis. Liquid crystal analysis and electron backscatter diffraction (EBSD) were used to observe the copper crystallographic orientation. Also we compared with a traditional pocket method and an opened flat copper foil method. Graphene from the other methods had poly-crystallinity with different orientation in contrast to graphene from the hole-pocket method.

**8:48AM A17.00003 Strain-Engineering the Gauge Potential of Dirac fermions in PECVD-grown Graphene**, CHEN-CHIH HSU, MARCUS TEAGUE, JAIQING WANG, NAI-CHANG YEH, Dept. of Physics, Caltech — Non-trivial strain can induce pseudo-magnetic fields in graphene so that the electronic properties of Dirac fermions can be tuned by controlling the strain on graphene. Here we employ nearly strain-free single-domain PECVD-graphene<sup>1</sup> to induce controlled strain by placing graphene on nanostructured substrates. Strain-induced gauge potentials and pseudo-magnetic fields can be manifested by the local tunneling conductance peaks at quantized energies.<sup>2,3</sup> Additionally, pseudo-magnetic field-induced local spontaneous time-reversal symmetry breaking can be revealed by spatially alternating presence and absence of the zero mode in the tunneling conductance spectra.<sup>2,3</sup> We also employ molecular dynamics simulations to determine the spatial distribution of the pseudo-magnetic field for a given nanostructure. We find that a tetrahedron-like nanostructure can be an effective valley splitter to separate the trajectories of Dirac fermions of opposite pseudo-spins. Proper design and arrangement of several valley filters can function as a valley propagator to guide valley-polarized currents. We plan to verify the valley Hall effect associated with a valley splitter and to assess the feasibility of realistic valleytronic applications. 1. D.A. Boyd et al. Nat. Comm. 6, 6620 (2015). 2. N.-C. Yeh et al. Surface Science 605, 1649-1656 (2011). 3. N.-C. Yeh et al. Acta Mechanica Sinica (in press).

**9:00AM A17.00004 ABSTRACT WITHDRAWN –**

**9:12AM A17.00005 SPALEED Studies of the Growth of Zero to Mono-layer Graphene on SiC(0001)<sup>1</sup>**, M. HUPALO, Ames Laboratory, M. T. HERSHBERGER, Iowa State University and Ames Laboratory, H. HATTAB, Ames Laboratory, D. C. MCDUGALL, Iowa State University and Ames Laboratory, M. HORN VON HOEGEN, University of Duisburg-Essen, M. C. TRINGIDES, Iowa State University and Ames Laboratory — The growth of graphene on SiC was studied in detail with SPA LEED to understand the transition from zero to monolayer graphene with increasing temperature starting at 1200C. Both the changing diffraction spots with annealing and their line shapes are studied in detail until a fully completed monolayer is obtained with only 6x6 spots remaining. In particular we focus on two strong features not investigated previously: (i) superstructures spots at  $\pi/13$  locations present between the specular and the graphene spots. These spots are possibly related to different coincidence lattices before graphene locks into its final 6x6 orientation. (ii) The presence of a very broad background intensity covering ~60% of the BZ both around the specular and graphene spots whose origin is still unknown. Detailed studies of the dependence of this background component on energy and comparison between the graphene and specular spots suggest that the origin is not due to the standard variation with electron energy, i.e. a  $g(s)$  curve caused by the topography. Throughout the literature this broad background has been seen in graphene grown in different types of substrates. We comment on possible reasons for the origin of the background.

<sup>1</sup>Ames Laboratory is operated by the US-DOE under Contract No. DE-AC02-07CH11358.

**9:24AM A17.00006 Growth of Graphene on Cu Single Crystal Substrates**, TYLER MOWLL, ENG

WEN ONG, University at Albany-SUNY, PARUL TYAGI, Global Foundries, ZACHARY ROBINSON, College at Brockport-SUNY, CARL VENTRICE, SUNY Polytechnic Institute — A common technique for synthesizing single-layer graphene films is CVD on Cu foil substrates. However, the presence of crystalline defects in the CVD graphene films results in a reduction in the transport properties. In order to achieve a better understanding of the influence of the surface termination of the Cu substrate on the crystallization of graphene during the CVD process, a systematic study of graphene growth on Cu(100), Cu(110), and Cu(111) crystals has been performed. The graphene synthesis is done in a UHV chamber that has been modified to perform graphene growth at pressures as high as 100 mTorr. The precursor gas used is ethylene. This growth procedure allows for the preparation of the clean Cu surfaces in UHV, growth under typical CVD conditions, and characterization of the graphene in UHV, without exposing the sample to atmospheric contaminants. Our results indicate that the surface termination of the Cu substrate has a strong influence on the decomposition rate of the ethylene and the rotational alignment of the graphene grains as they nucleate on each surface. For Cu(111), single-domain graphene growth can be achieved for ethylene pressures of 5 mTorr or less. For both Cu(100) and Cu(110), a minimum of two graphene domains is always observed.

**9:36AM A17.00007 Strain sensing through the optical properties of graphene: Comparing indentation of epitaxial- and CVD-grown graphene**, ERIN L. WOOD, YANFEI YANG, NIST, Gaithersburg, MD, USA, WILL GANNETT, NIST, Boulder, CO, USA, GORDON A. SHAW, RANDOLPH E. ELMQUIST, NIST, Gaithersburg, MD, USA, MARK W. KELLER, NIST, Boulder, CO, USA, ANGELA R. HIGHT WALKER, NIST, Gaithersburg, MD, USA — The unprecedented mechanical and electrical properties of graphene have garnered great interest, yet critical understanding of deformation processes is needed before robust devices are realized. Raman spectroscopy is an information rich, non-destructive probe of mechanical, structural, and electrical properties of graphene through analysis of the prominent bands; D, G, and G'. Previous reports on strained graphene have been largely limited to graphene transferred to flexible substrates and have produced divergent results regarding shifting and splitting in the G band. To systematically evaluate strain, we compare as-grown graphene on either Cu or SiC to the blank substrates which are well understood. Strain was applied by micro- or nano-indentation and Raman mapping was collected of the deformed area providing validation of the applied strain. Confocal Raman microscopy is diffraction limited, however, and localized strain cannot be spatially resolved at the nanoscale. To overcome this, an AFM probe was co-located within the Raman laser focus to obtain sub-diffraction spatial resolution. This also increases the sensitivity to the surface, allowing for observation of the D peak within a micron of nano-indents, which was unseen in confocal Raman spectroscopy.

**9:48AM A17.00008 Oxygen-Activated Growth and Bandgap Tunability of Large Single-Crystal Bilayer Graphene** , YUFENG HAO, JAMES HONE, columbia univerisity, RODNEY RUOFF, UNIST, LUIGI COLOMBO, Texas Instruments, THE HONE GROUP TEAM — Distinct from zero-bandgap single-layer graphene, Bernal-stacked bilayer graphene (BLG) is a semiconductor whose bandgap can be tuned by a transverse electric field, making it a unique material for a number of electronic and photonic devices. In this presentation, we will focus on the most recent progress in the identification of new growth mechanisms towards large-area single-layer BLG on Copper: multiple control experiments and first-principles calculations are used to support the proposed mechanisms. We emphasize that trace amount of impurities on metal surface are critical to initiate graphene growth and affect the growth kinetics. Furthermore, contrary to the traditional viewpoint that graphene growth is always surface-limited process, our new observations strongly suggest that metal bulk plays a role to feed carbon species for graphene growth. State-of-the-art structural characterizations and electrical transport measurements of the CVD graphene layers will be presented as well.

**10:00AM A17.00009 In-Situ Measurements of Graphene Mechanics During Annealing** , AARON HUI, ROBERTO DE ALBA, ABHILASH SEBASTIAN, JEEVAK PARPIA, Cornell University — Graphene shows great potential as a material for a new generation of mechanical nanodevices. However, current methodologies used for fabricating graphene structures involve polymer resists for transfer and patterning, which degrades mechanical performance. To improve surface quality, high current or high temperature annealing of graphene is commonly employed. Previous studies of graphene mechanics have focused on performance after annealing or temperature-dependent behavior from 4K-300K. Here we present real-time, in-situ measurements of graphene mechanical resonance during high temperature annealing from 300K-600K. Upon heating, reversible changes in mechanical frequency are indicative of graphene thermal contraction. Discontinuous and irreversible changes are also seen, corresponding to graphene slipping and mass desorption. Both reversible and irreversible changes in quality factor are also observed. Characterizing the effects of annealing on the structural properties of graphene will enable more precise engineering for particular applications, such as mass sensing.

**10:12AM A17.00010 Effective structural properties in polycrystalline graphene** , ZUBAER HOSSAIN, University of Delaware — This talk will discuss effective structural properties in polycrystalline graphene under the presence of atomic scale heterogeneity. Polycrystallinity is ubiquitous in solids, but theories describing their effective behavior remain limited, particularly when heterogeneity is present in the form of nonuniform deformation or composition. Over the decades, exploration of the effective transport and strength properties of heterogeneous systems has been carried out mostly with random distribution of grains or regular periodic structures under various approximations, in translating the underlying physics into a single representative volume element. Although heterogeneity can play a critical role in modulating the basic behavior of low-dimensional materials, it is difficult to capture the local characteristics accurately by these approximations. Taking polycrystalline graphene as an example material, we study the effective structural properties (such as Young's Modulus, Poisson's ratio and Toughness) by using a combination of density functional theory and molecular dynamic simulations. We identify the key mechanisms that govern their effective behavior and exploit the understanding to engineer the behavior by doping with a carefully selected choice of chemical elements.

**10:24AM A17.00011 Pump-induced far-infrared reflection in quasi-intrinsic graphene** , MARTIN MITTENDORFF, RYAN J. SUESS, THOMAS E. MURPHY, University of Maryland, College Park, MD 20742, USA, HARALD SCHNEIDER, MANFRED HELM, STEPHAN WINNERL, Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden, Germany — We present an experimental far-infrared pump-probe study on multilayer epitaxial graphene that is complemented by a straightforward theoretical model. To gain deeper insights into the pump-induced change in the complex conductivity in the far-infrared, pump-probe measurements recording both transmission and reflection were performed. These measurements reveal a pump-induced increase of the transmission at low pump fluence, and a decreased transmission at high pump fluence due to a strong pump-induced reflection. Modelling the temperature dependent conductivity for interband and intraband processes in combination with an energy balance equation reproduces the observed results.

**10:36AM A17.00012 Atomic intercalation – a practical method to determine the nanoscale adhesion energy of graphene on HOPG<sup>1</sup>** , JUN WANG, Oak Ridge National Lab, DAN SORESCU, National Energy Technology Laboratory (NETL), U.S. Department of Energy, SEOKMIN JEON, ALEXEI BELIANINOV, SERGEI KALININ, ARTHUR BADDORF, PETRO MAKSYMOVYCH, Oak Ridge National Lab — A detailed analysis of atomic intercalates in graphite provides a direct estimate of the nanoscale elastic adhesion of a graphene sheet atop highly ordered pyrolytic graphite (HOPG). Atomic intercalation is carried out using conventional ion sputtering, creating “blisters” in the top-most layer of the HOPG surface. Scanning tunneling microscopy coupled with image analysis and density functional theory is used to reconstruct the atomic positions and the strain map within the deformed graphene sheet. To estimate the adhesion energy we invoke an analytical model originally devised for macroscopic deformations of graphene. This model yields a value of  $0.221 \pm 0.011 J/m^2$  for the adhesion energy of graphite, which is in surprisingly good agreement with reported experimental and theoretical values. This implies that mechanical properties of graphene scale at least to lengths of a few nanometers. The simplicity of our method enables analysis of elastic mechanical properties in many two-dimensional layered materials and provides a unique opportunity to investigate the local variability of mechanical properties on the nanoscale.

<sup>1</sup>Acknowledgements: Experiments were conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

## Monday, March 14, 2016 8:00AM - 11:00AM – Session A18 GMAG DMP FIAP: Spin-Hall I 317 - Arne Brataas, Norwegian University

**8:00AM A18.00001 In-plane current induced spin orbit effects in nanometer scale Hall bar of  $\beta$ -W/Ta/CoFeB/MgO/Ta multilayers<sup>1</sup>** , AVYAYA J. NARASIMHAM, State University of New York, Albany, YU-MING HUNG, Department of Physics, New York University, MENG ZHU, SUNY Polytechnic Institute, Albany , ANDREW D. KENT, Department of Physics, New York University, VINCENT P.LABELLA, SUNY Polytechnic Institute, Albany — The giant spin Hall effect (GSHE) is caused by spin orbit interactions in a semiconductor or metal that result in a spin current that is transverse to the charge current. Recent spin Hall effect studies in the beta phase metals Ta and W show that transverse spin currents are strong enough to switch an adjacent magnetic layer. Films with perpendicular magnetic anisotropy (PMA) can exhibit uniform magnetizations and higher thermal stability. Inserting a 1 nm Ta insert-layer between the CoFeB and W induces PMA which is confirmed by vibrating sample magnetometer and anomalous Hall voltage measurements.  $\beta$ -W(5)/Ta(1) channel and the adjacent CoFeB/MgO/Ta layers are patterned into a 100 nm wide Hall bar structures. Effect of in-plane current induced change in coercivity while sweeping in-plane magnetic field are studied. An empirical model to quantitatively understand the switching will be presented.

<sup>1</sup>SRC-NRI-INDEX -Spin Logic

**8:12AM A18.00002 Spin Orbit Torque in TbCo Films with Bulk Perpendicular Magnetic Anisotropy**, KOHEI UEDA, MAXWELL MANN, AIK-JUN TAN, GEOFFREY. S. D. BEACH, MIT — Spin-orbit torque (SOT) has generated considerable interest for manipulating magnetization in spintronic devices with ultra-low dissipation. Recent research has demonstrated that highly efficient magnetization control can be driven by current-induced SOT in ferromagnet/heavy metals bilayers with strong spin orbit coupling. However, most work on SOT has focused on ultra-thin magnetic films with interfacial perpendicular magnetic anisotropy (PMA), whereas future devices will require bulk PMA for sufficient thermal stability. Recently, Zhao et al reported SOT induced magnetization switching in a bulk PMA material; however, the films examined were still rather thin. Here we examine spin orbit torques in TbCo alloy films with bulk PMA, sandwiched between top and bottom Ta layers. By performing conventional harmonic and current-induced switching measurements, we quantified the current-induced effective fields generated by damping-like (DL) and field-like (FL) torques. The DL torque is much larger than FL torque, and corresponds to an effective spin Hall angle consistent with that of Ta. Owing to the relatively small saturation magnetized of these ferrimagnetic materials, the current-induced effective field is comparable to that observed in nm-thick Co films, despite the much larger film thicknesses used here. These results demonstrate ferromagnetic alloys with bulk PMA can be engineered to simultaneously provide thermal stability and efficient SOT switching.

**8:24AM A18.00003 Spin-orbit torque induced reversible coercivity change in Co/Pd multilayer thin films.**, SANDEEP KUMAR, Univ of California - Riverside — In this work we report reversible reduction in coercivity of Co/Pd multilayer thin films under high-density direct current biasing. We carried out in-situ focused magneto optic Kerr effect based hysteresis measurement while the specimen was under DC bias. The experiments show a reversible reduction in coercivity during the application of direct current. We propose this reduction occurs due to the spin-orbit torques (Rashba) generated at high current densities. Using an in-situ transmission electron microscope biasing experiment, we also showed the presence of dissymmetric lattice structure of Co/Pd multilayers. Our results suggest that the Rashba torque is the dominant spin-orbit torque since coercivity change is a bulk phenomenon as compared to spin Hall effect.

**8:36AM A18.00004 Novel current driven domain wall dynamics in synthetic antiferromagnets<sup>1</sup>**, SEE-HUN YANG, IBM Almaden Research Center — It was reported [1,2] that the domain walls in nanowires can be moved efficiently by electrical currents by a new type of torque, chiral spin torque (CST), the combination of spin Hall effect and Dzyaloshinskii-Moriya interaction. Recently we demonstrated that ns-long current pulses can move domain walls at extraordinarily high speeds (up to  $\sim 750$  m s<sup>-1</sup>) in synthetic antiferromagnetic (SAF) nanowires that have almost zero net magnetization [3], which is much more efficient compared with similar nanowires in which the sub-layers are coupled ferromagnetically (SF). This high speed is found to be due to a new type of powerful torque, exchange coupling torque (ECT) that is directly proportional to the strength of the antiferromagnetic exchange coupling between the two sub-layers, showing that the ECT is effective only in SAF not in SF. Moreover, it is found that the dependence of the wall velocity on the magnetic field applied along the nanowire is non-monotonic. Most recently we predict a Walker-breakdown-like domain wall precession in SAF nanowires in the presence of in-plane field based on the model we develop, and this extraordinary precession has been observed [4]. In this talk I will discuss this in details by showing a unique characteristics of SAF sublayers' DW boost-and-drag mechanism along with CST and ECT. [1] Kwang-Su Ryu, Luc Thomas, See-Hun Yang, and Stuart Parkin, "Chiral Spin Torque at Magnetic Domain Walls", Nature Nanotechnology 8, 527-533 (2013). [2] Satoru Emori, Uwe Bauer, Sung-Min Ahn, Eduardo Martinez, and Geoffrey S. D. Beach, "Current-driven dynamics of chiral ferromagnetic domain walls", Nature Materials 12, 611-616 (2013). [3] See-Hun Yang, Kwang-Su Ryu, and Stuart Parkin, "Domain-wall velocities of up to 750 m s<sup>-1</sup> driven by exchange-coupling torque in synthetic antiferromagnets", Nature Nanotechnology 10, 221-226 (2015). [4] See-Hun Yang, Chirag Garg, Paul Amari, Charles Rettner, and Stuart Parkin, in preparation. [5] Stuart Parkin and See-Hun Yang, "Memory on the Racetrack", Nature Nanotechnology 10, 195-198 (2015).

<sup>1</sup> Novel current driven domain wall dynamics in synthetic antiferromagnets

**9:12AM A18.00005 Spin-Hall Switching of In-plane Exchange Biased Heterostructures**, MAXWELL MANN, GEOFFREY BEACH, Massachusetts Inst of Tech-MIT — The spin Hall effect (SHE) in heavy-metal/ferromagnet bilayers generates a pure transverse spin current from in-plane charge current, allowing for efficient switching of spintronic devices with perpendicular magnetic anisotropy [1,2,3,4]. Here, we demonstrate that an AFM deposited adjacent to the FM establishes a large in-plane exchange bias field, allowing operation at zero HIP. We sputtered Pt(3nm)/Co(0.9nm)/Ni80Co20O(tAF) stacks at room-temperature in an in-plane magnetic field of 3 kOe. The current-induced effective field was estimated in Hall cross devices by measuring the variation of the out-of-plane switching field as a function of JIP and HIP. The spin torque efficiency, dHSL/dJIP, is measured versus HIP for a sample with tAF=30 nm, and for a control in which NiCoO is replaced by TaOx. In the latter, dHSL/dJIP varied linearly with HIP. In the former, dHSL/dJIP varied nonlinearly with HIP and exhibited an offset indicating nonzero spin torque efficiency with zero HIP. The magnitude of HEB was 600 Oe in-plane. [1] D'yakonov and Perel JETP Lett., 1971. [2] Hirsch, PRL 1999. [3] Kato et al. Science, 2004. [4] Liu et al. PRL 2012.

**9:24AM A18.00006 Few-nanosecond pulse switching with low write error for in-plane nanomagnets using the spin-Hall effect**, SRIHARSHA ARADHYA, GRAHAM ROWLANDS, SHENGJIE SHI, JUNSEOK OH, D. C. RALPH, ROBERT BUHRMAN, Cornell University — Magnetic random access memory (MRAM) using spin transfer torques (STT) holds great promise for replacing existing best-in-class memory technologies in several application domains. Research on conventional two-terminal STT-MRAM thus far has revealed the existence of limitations that constrain switching reliability and speed for both in-plane and perpendicularly magnetized devices. Recently, spin torque arising from the giant spin-Hall effect in Ta, W and Pt has been shown to be an efficient mechanism to switch magnetic bits in a three-terminal geometry [1-3]. Here we report highly reliable, nanosecond timescale pulse switching of three-terminal devices with in-plane magnetized magnetic tunnel junctions. We obtain write error rates (WER) down to  $\sim 10^{-5}$  using pulses as short as 2 ns, in contrast to conventional in-plane STT-MRAM devices where write speeds were limited to a few tens of nanoseconds for comparable WER. Utilizing micro-magnetic simulations, we discuss the differences from conventional MRAM that allow for this unanticipated and significant performance improvement. Finally, we highlight the path towards practical application enabled by the ability to separately optimize the read and write pathways in three-terminal devices. [1] L. Liu et al., Science, 336, 2012; [2] C-F. Pai et al., APL, 101, 2012; [3] M-H. Nguyen et al., APL, 106, 2015.

**9:36AM A18.00007 Magnetization dynamics in LSMO/Pt nanowires in the presence of spin orbit torques**, HANKYU LEE, IGOR BARSUKOV, CHRISTOPHER SAFRANSKI, ALEJANDRO JARA, YU-JIN CHEN, University of California, Irvine, ADRIAN SWARTZ, BONGJU KIM, GLAM, Stanford Univ., HAROLD HWANG, GLAM, Stanford Univ., SLAC Nat. Accel. Lab., ILYA KRIVOROTOV, University of California, Irvine — La<sub>0.7</sub>Sr<sub>0.3</sub>MnO<sub>3</sub> (LSMO) possesses attractive magnetic properties for nanowire spin torque oscillators (STOs) driven by spin orbit torques: low magnetic damping, low saturation magnetization and high spin polarization. In this context, good understanding of magnetization dynamics in LSMO/Pt bilayer nanowires is important. Here, we report measurements of the spectral properties of spin-wave modes in LSMO/Pt nanowires magnetized along the two principal in-plane axes. In electrically-detected ferromagnetic resonance (FMR) we observe excitation of multiple spin wave modes, including non-aligned modes when the nanowire is magnetized perpendicular to its axis. Spectral linewidth of the FMR resonances gives quantitative information on the Gilbert damping parameter of the nanowire. In comparison to extended LSMO/Pt films, the magnetic damping in the nanowire is reduced due to the suppression of two-magnon scattering. We will present data on the effect of high bias current density applied to the wire on the frequency and linewidth of the observed spin wave resonances.

**9:48AM A18.00008 Study of spin orbit torque switching in ferrimagnetic  $Gd_x(Fe_{90}Co_{10})_{100-x}$  alloy<sup>1</sup>**, NIKLAS ROSCHEWSKY, Department of Physics, University of California, Berkeley, TOMOYA MATSUMURA, TAKESHI KATO, Department of Electrical Engineering and Computer Science, Nagoya University Furo-cho, Chikusa-ku, SATOSHI IWATA, Advanced Measurement Technology Center, Nagoya University Furo-cho, Chikusa-ku, SURAJ CHEEMA, JAMES CLARKSON, Department of Materials Science and Engineering, University of California, Berkeley, SAYEED SALAHUDDIN, Department of Electrical Engineering and Computer Sciences, University of California, Berkeley — Magnetization switching in ferromagnetic metals (FM) with spin-orbit torques (SOT) is a well established technique. The SOT originates from spin accumulation at the interface of the FM generated by the spin Hall effect in an adjacent heavy metal. Here we report measurements of SOT in the alloy  $Gd_x(Fe_{90}Co_{10})_{100-x}$ , where the transition metal sub-lattice and the rare earth sub-lattice couple antiferromagnetically. By varying the composition  $x$  of the alloy we can tune the total magnetization. Anomalous Hall effect measurements are conducted to study the effect of SOT on the  $Gd_x(Fe_{90}Co_{10})_{100-x}$  magnetization.

<sup>1</sup>This work was supported by Department of Energy Basic Energy Sciences Award no DE -SC0012371

**10:00AM A18.00009 Nanowire spin Hall oscillators: width dependence**, ANDREW SMITH, Univ of California - Irvine, TOBIAS SCHNEIDER, Helmholtz-Zentrum Dresden - Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstrae 400, 01328 Dresden, German, LIU YANG, ILYA KRIVOROTOV, Univ of California - Irvine — We present experimental studies of auto-oscillatory magnetization dynamics in nanowire spin Hall oscillators (SHOs) as a function of the wire width ranging from 0.17  $\mu$ m to 2  $\mu$ m. These SHOs consist of long Pt(7 nm)/Py(5 nm)/AlOx(2 nm) wires on a sapphire substrate. Direct current generating anti-damping spin torque is applied to a section of the wire between two leads separated by a 2  $\mu$ m gap, which defines the SHO active region.<sup>1</sup> All devices show onset of auto-oscillations at similar critical current densities. For the 0.17  $\mu$ m and 0.34  $\mu$ m wide nanowire SHOs, auto-oscillatory modes arising from the bulk and edge eigenmodes of the nanowire are clearly seen in the emission spectra. For SHO devices based on wider wires, the bulk auto-oscillatory modes dominate the emission spectrum due to the larger wire volume occupied by the bulk modes. Our work demonstrates robust operation of nanowire-based SHOs over a wide range of nanowire widths and presents an example of a spin torque oscillator with the active area extended into the  $m^2$  domain. [1] Zheng Duan et al, Nature Communications 5, 5616 (2014)

**10:12AM A18.00010 Non-adiabatic spin-transfer torque independent of the spin relaxation rate**, KYOUNG-WHAN KIM, NIST - Natl Inst of Stds & Tech, KYUNG-JIN LEE, Korea University, HYUN-WOO LEE, POSTECH, MARK STILES, NIST - Natl Inst of Stds & Tech — Non-adiabatic spin-transfer torques play an important role in magnetization dynamics. For example, they determine current-induced magnetic domain wall velocity. A well-known mechanism for non-adiabatic spin-transfer torques arises from spin relaxation and is directly proportional to the spin relaxation rate. Here we report mechanism that is independent of the spin relaxation rate. This mechanism is related to the recently reported intrinsic damping-like spin-orbit torque, which is proportional to an electric field but is independent of the conductivity, and hence the scattering rate. Likewise, the mechanism we report is independent of the scattering rate. It originates from the effective spin-orbit coupling that arises in systems with magnetic textures as we previously reported for related processes. In this work, we demonstrate the existence of such a spin-transfer torque, which is a contribution to the non-adiabatic spin-transfer torque and is independent of scattering rates. We also demonstrate that the magnitude of this torque can be much larger than other mechanisms for non-adiabatic spin-transfer torques, and may be the dominant contribution in some systems.

**10:24AM A18.00011 Optical detection of spin Hall effect in metals**, OLAF VAN T ERVE, AUBREY HANBICKI, CONNIE LI, BEREND JONKER, Naval Research Lab — Spin Hall effects in metals have been successfully measured using electrical methods such as nonlocal spin valve transport, ferromagnetic resonance or spin torque transfer experiments. These methods require complex processing techniques and measuring setups. Here we present room temperature measurements of the spin Hall effect in non-magnetic metals such as Pt and  $\beta$ -W using a standard bench top magneto-optic Kerr effect (MOKE) system. With this system, one can readily determine the angular dependence of the induced polarization on the bias current direction. When a bias current is applied, the spin Hall effect causes electrons of opposite spin to be scattered in opposite directions, resulting in a spin accumulation at the surface of the film. The MOKE signal tracks the applied square wave bias current with an amplitude and phase directly related to the spin Hall angle. Using this technique, we show that the spin-Hall angle of  $\beta$ -W is opposite in sign and significantly larger than that of Pt. In addition, we use this technique to detect spin diffusion from  $\beta$ -W into Al thin films, as well as spin diffusion from the topological surface states of  $Bi_2Se_3$  into Al. We will also show direct modulation of the reflected light up to 100 kHz, using Bi doped Cu samples. This work was supported by internal programs at NRL.

**10:36AM A18.00012 Spin Hall magnetoresistance in ultra thin Pt/LSMO.**, NA LEI, Beihang University, YU BAI, ZHAO DING, JIAN SHAO, WENGANG WEI, LIFENG YIN, YIZHENG WU, JIAN SHEN, Fudan University — Spin Hall magnetoresistance (SMR) in a non-/ferro-magnetic (NM/FM) bilayer is an angular dependence of resistance of the NM layer on the magnetization of FM layer [1]. It provides an easy approach to the spin Hall effect in a simple bilayer system, however similar effects mixed in the system and might complicated the data analysis and interpretation. Here we present a case of ultra thin Pt/LSMO, in which LSMO (below 7 unit cells) layer is an insulating magnetic oxide with Curie temperature of 120K. Below 120K, our results clearly show the coexistence of the anisotropic magnetoresistance (AMR) and SMR effects. However, far away above Curie temperature, where the LSMO is paramagnetic, the magnetoresistance doesn't disappear but even increase, which is distinct from the case of Pt/YIG [2]. Here it is neither SMR nor AMR, and an additional mechanism is required. Anomalous Hall effect was also performed, which is consistent with SMR measurement. We propose some physical pictures which could attribute to this magnetoresistance in paramagnetic state. Reference: [1] H. Nakayama, M. Althammer, Y.-T. Chen, K. Uchida, et al., Phys. Rev. Lett. 110(20), 206601 (2013). [2] K. Uchida, Z. Qiu, T. Kikkawa, R. Iguchi, E. Saitoh, Appl. Phys. Lett. 106, 052405 (2015).

**10:48AM A18.00013 Spin Transport in Ferromagnetic and Antiferromagnetic Insulators<sup>1</sup>**, SHAN-SHAN SU, GEN YIN, YIZHOU LIU, Department of Electrical and Computer Engineering, University of California, Riverside, JIADONG ZANG, Department of Physics, University of New Hampshire, YAFIS BARLAS, Department of Physics and Astronomy, University of California, Riverside, ROGER LAKE, Department of Electrical and Computer Engineering, University of California, Riverside — Recently, experiments of spin pumping have been done for system with antiferromagnetic oxides (AFMOs) as a spacer between YIG and Pt [1-3]. Observation of spin transport through the AFMO and the enhancement of spin pumping signal in the system due to the insertion of AFMO have been reported [1,2]. In this research, we model the spin transport in Pt/YIG/Pt and Pt/YIG/AFMO/Pt heterostructures using the Landau-Lifshitz-Gilbert equations coupled with the non-equilibrium Green's function equations. We show that a pure spin current generated at the first Rashba SOC electrode is carried by magnon through YIG, which can be converted back to spin pumping signal at the second electrode. The spin dynamical details at the heterostructure can determine the transport efficiency. The effect of different magnetization orientations and finite temperatures will be addressed. [1]C. Hahn et al., EPL 108, 57005 (2014) [2]H. Wang et al., Phys. Rev. Lett. 113, 097202 (2014) [3]H. Wang et al., Phys. Rev. B 91, 220419 (2015)

<sup>1</sup>This work was supported by the SHINES under Award SC0012670.

**Monday, March 14, 2016 8:00AM - 11:00AM —**

**Session A19 GMAG DMP: Manganites and Cobaltites** 318 - Junjie Zhang, Argonne National Laboratory

**8:00AM A19.00001 Investigating short-range magnetism in strongly correlated materials via magnetic pair distribution function analysis and *ab initio* theory**, BENJAMIN FRANDSEN, Columbia University, KATHARINE PAGE, Oak Ridge National Laboratory, MICHELA BRUNELLI, European Synchrotron Radiation Facility, JULIE STAUNTON, University of Warwick, SIMON BILLINGE, Columbia University — Short-range magnetic correlations are known to exist in a variety of strongly correlated electron systems, but our understanding of the role they play is challenged by the difficulty of experimentally probing such correlations. Magnetic pair distribution function (mPDF) analysis is a newly developed neutron total scattering method that can reveal short-range magnetic correlations directly in real space, and may therefore help ameliorate this difficulty. We present temperature-dependent mPDF measurements of the short-range magnetic correlations in the paramagnetic phase of antiferromagnetic MnO, an archetypal strongly correlated transition-metal oxide. We observe significant correlations on a  $\sim 1$  nm length scale that differ substantially from the low-temperature long-range-ordered spin arrangement. With no free parameters, *ab initio* calculations using the self-interaction-corrected local spin density approximation of density functional theory quantitatively reproduce the magnetic correlations to a high degree of accuracy. These results yield valuable insight into the magnetic exchange in MnO and showcase the utility of the mPDF technique for studying magnetic properties of strongly correlated electron systems.

**8:12AM A19.00002 Magnetic Order in the Mixed-Spin Triangular Lattice Antiferromagnet  $\text{Na}_x\text{MnO}_2$** , ROBIN CHISNELL, DAN PARSHALL, NIST Center for Neutron Research, XIN LI, Harvard, AMBER LARSON, University of Maryland, TAKEHITO SUZUKI, JOSEPH CHECKELSKY, MIT, EFRAIN RODRIGUEZ, University of Maryland, JEFFREY LYNN, NIST Center for Neutron Research —  $\text{Na}_x\text{TMO}_2$  (TM = transition metal) materials consist of alternating layers of Na and TM ions with the TM ions arranged on a geometrically frustrated triangular lattice. Na can be easily and reversibly removed from these materials, making them of interest for application in rechargeable batteries and allowing for exploration of their rich phase diagrams as a function of Na concentration. Na ordering is an important factor in ground state selection, and is driven by electrostatic interactions in many  $\text{Na}_x\text{TMO}_2$  systems. The TM = Mn series differs in that Na ordering is driven by a cooperative Jahn-Teller effect, due to the coexistence of Jahn-Teller active  $\text{Mn}^{3+}$  and inactive  $\text{Mn}^{4+}$  ions. This effect also results in an ordered arrangement of the  $\text{Mn}^{3+}$  and  $\text{Mn}^{4+}$  ions, and thus of spin-2 and spin-3/2 moments. For  $x = 5/8$ , we have recently shown the coexistence of charge and magnetic stripe orderings [1]. Here, we present the results of neutron diffraction measurements performed on single crystal samples of  $\text{Na}_x\text{MnO}_2$  and discuss the details of the magnetic structure in the magnetically ordered phase.

[1] X. Li *et al.* Nature Mater. **13**, 586 (2014).

**8:24AM A19.00003 Spin polarized scanning tunneling microscopy of bilayer manganite  $\text{La}_{2-2x}\text{Sr}_{1+2x}\text{Mn}_2\text{O}_7$  single crystals.**<sup>1</sup>, XINZHOU TAN, ALEX DE LOZANNE, JIANSI ZHOU, JOHN GOODENOUGH, Univ of Texas, Austin — We employ spin-polarized scanning tunneling microscopy to investigate the (001) surface of bilayer manganite  $\text{La}_{2-2x}\text{Sr}_{1+2x}\text{Mn}_2\text{O}_7$  single crystals with  $x = 0.32$  at various temperature and different magnetic fields. A spin reorientation transition (SRT) at this doping level starts around 70K, when the ferromagnetic spins change from out of plane to in plane configuration. Tracing the SRT while applying magnetic field along the c axis we are going to investigate the corresponding magnetic domain wall structure and motion in detail by spin polarized tunneling. Moreover, we are also going to search for the emergence of skyrmions near the same doping level.

<sup>1</sup>This work is supported by NSF DMR-1507874

**8:36AM A19.00004 ABSTRACT WITHDRAWN —**

**8:48AM A19.00005 Electronic, structural and magnetic properties of  $\text{LaMnO}_3$  phase transition at high temperature**, PABLO RIVERO, Louisiana State University, VINCENT MEUNIER, Rensselaer Polytechnic Institute, WILLIAM SHELTON, Louisiana State University — We have developed a theoretical approach for investigating systems that contain a range of correlation that varies with experimentally controlled parameters. We applied this method to the  $\text{LaMnO}_3$  compound [1,2,3] to accurately describe the antiferromagnetic (AFM) insulating ground-state, the metal-to-insulator transition and the high temperature ferromagnetic (FM) state, where we observe a half-metallic behavior. [1]: T. Saitoh, A. E. Bocquet, T. Mizokawa, H. Namatame, A. Fujimori, M. Abbate, Y. Takeda, and M. Takano, *Phys. Rev. B*, **13942** (1995). [2]: J. S. Zhou, and J. B. Goodenough, *Phys. Rev. B*, **R15002** (1999). [3]: J. Rodríguez-Carvajal, M. Hennion, F. Moussa, A. H. Mouden, L. Pinsard, and A. Revcolevschi, *Phys. Rev. B*, **R3189** (1998).

**9:00AM A19.00006 Spin wave damping in colossal magnetoresistive  $\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$** , JOEL HELTON, SUSUMU JONES, US Naval Academy, MATTHEW STONE, Oak Ridge National Laboratory, DMITRY SHULYATEV, National University of Science and Technology "MISIS", DANIEL PARSHALL, JEFFREY LYNN, NIST Center for Neutron Research — The hole-doped perovskite  $\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$  is best known for the colossal magnetoresistance displayed at a combined ferromagnetic and metal-insulator phase transition ( $T_C = 257$  K). Previous studies have reported that the spin wave excitations in the ferromagnetic phase become anomalously damped near the Brillouin zone boundary, though a later work suggested that this was a measurement artifact due to an optical phonon branch. We have used the ARCS time-of-flight neutron spectrometer to investigate the spin wave excitations of  $\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3$  at  $T = 100$  K and find a damping for spin waves at energies exceeding 20 meV that cannot be explained solely by proximity to the phonon branch. With additional measurements using the BT7 triple-axis neutron spectrometer, the spin wave damping is explored as a function of reduced wavevector, excitation energy, and temperature.

**9:12AM A19.00007 Biquadratic and ring exchange interactions in orthorhombic perovskite manganites**, NATALYA FEDOROVA, CLAUDE EDERER, NICOLA SPALDIN, Materials Theory, ETH Zurich, ANDREA SCARAMUCCI, Laboratory for Developments and Methods, Paul Scherrer Institut — We use *ab initio* electronic structure calculations within the GGA+U approximation to density functional theory (DFT) to determine the microscopic exchange interactions in the series of orthorhombic rare-earth manganites ( $\text{o-RMnO}_3$ ). Our motivation is to construct a model Hamiltonian (excluding effects due to spin-orbit coupling), which can provide an accurate description of the magnetism in these materials. First we map the exchange couplings for several representatives of  $\text{o-RMnO}_3$  series onto a Heisenberg Hamiltonian and find a clear deviation from the Heisenberg-like behavior. We demonstrate that this deviation can be explained only by the presence of relatively strong higher order exchange interactions (biquadratic and four-spin ring couplings) and show that they have the strongest effect in compounds, where nearest-neighbor exchange interactions are weakened due to the presence of large  $\text{GdFeO}_3$ -type distortion. Finally we discuss how these higher order terms determine magnetic ground states, influence magnetic excitations and define the multiferroic properties of  $\text{o-RMnO}_3$ .

**9:24AM A19.00008 Role of Entropy and Structural Parameters in the Spin State Transition of  $\text{LaCoO}_3$** , BISMAYAN CHAKRABARTI, TURAN BIROL, KRISTJAN HAULE, Rutgers, The State University of New Jersey — The spin state transition in  $\text{LaCoO}_3$  has eluded description for decades despite concerted theoretical and experimental effort. In this study, we approach this problem using fully charge consistent Density Functional Theory + Dynamical Mean Field Theory (DFT+DMFT). We show, from first principles, that  $\text{LaCoO}_3$  cannot be described by a single, pure spin state at any temperature, but instead shows a gradual change in the population of higher spin multiples as temperature is increased. We explicitly elucidate the critical role of the lattice expansion and oxygen octahedral rotations in the spin state transition. We also show that the spin state transition and the metal-insulator transition in the compound occur at different temperatures. In addition, our results shed light on the importance of electronic entropy, which has so far been ignored in all first principles studies of this material.

### 9:36AM A19.00009 LaCoO<sub>3</sub> (LCO) - Dramatic changes in Magnetic Moment in fields to 500T<sup>1</sup>

, Y. LEE, B. N. HARMON, Ames Laboratory, U.S. DOE and Dept. of Physics and Astronomy, Iowa State University — LCO has attracted great attention over the years (>2000 publications) because of its unusual magnetic properties; although in its ground state at low temperatures it is non-magnetic. A recent experiment<sup>[1]</sup> in pulsed fields to 500T showed a moment of  $\sim 1.3\mu_B$  above 140T, and above  $\sim 270T$  the magnetization rises, reaching  $\sim 3.8\mu_B$  by 500T. We have performed first principles DFT calculations for LCO in high fields. Our earlier calculations<sup>[2]</sup> explained the importance of a small rhombohedral distortion in the ground state that leads to a suppression of the  $1.3\mu_B$  moment for fields below  $\sim 140T$ . By allowing fairly large atomic displacements in high fields, moments of  $\sim 4\mu_B$  are predicted. [1] V. V. Platonov *et al.* Phys. Solid State **54**, 279 (2012) [2] Y. Lee and B. N. Harmon *et al.* J. Appl. Phys. **113**, 17E145 (2013)

<sup>1</sup>This work was supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences, Materials Science and Engineering Division under contract No. DE-AC02-07CH11358.

### 9:48AM A19.00010 ABSTRACT WITHDRAWN —

10:00AM A19.00011 Interplay between frustration, magnetism and sodium vacancy ordering in Na<sub>0.84</sub>CoO<sub>2</sub>, STANISLAW GALESKI, KURT MATTENBERGER, BERTRAM BATLOGG, Laboratory for Solid State Physics, ETH Zurich, Switzerland — We have performed an extensive survey of low temperature specific heat of Na<sub>0.84</sub>CoO<sub>2</sub>. Heat capacity measurements were performed with an AC steady state method using a membrane nanocalorimeter. Thanks to the 10-30 nanogram sample mass we were able to perform well controlled ultra-fast cooling (500K/s) from high temperatures to temperatures where the sodium ions become immobile. This allowed us to take snapshots of different high temperature sodium configurations, relate them to particular structural transitions and at the same time establish their influence on the low temperature magnetic order. Through correlation with XRD data we demonstrate that the least ordered sodium configuration increases the T<sub>c</sub> of the 22K transition by 2K.

10:12AM A19.00012 Angle-resolved photoemission on the delafossite oxide metal PtCoO<sub>2</sub>, VERONIKA SUNKO, University of St Andrews, PALLAVI KUSHWAHA, Max Planck Institute for Chemical Physics of Solids, P.J.W. MOLL, Laboratory for Solid State Physics, ETH Zurich, Switzerland, L. BAWDEN, J.M. RILEY, University of St Andrews, NABHANILA NANDI, HELGE ROSNER, M.P. SCHMIDT, F. ARNOLD, E. HASSINGER, Max Planck Institute for Chemical Physics of Solids, T.K. KIM, M. HOESCH, Diamond Light Source, A.P. MACKENZIE, Max Planck Institute for Chemical Physics of Solids, P.D.C. KING, University of St Andrews — The delafossite structural series of oxides has recently attracted considerable attention because of the remarkable and varied properties of the compounds in the series. Here we consider the Pt-based 5d delafossite oxide PtCoO<sub>2</sub>, the most conductive oxide known [1]. From angle-resolved photoemission and density-functional theory, we show that the underlying Fermi surface is a single cylinder of nearly hexagonal cross-section, with very weak dispersion along k<sub>z</sub>. Despite being predominantly composed of d-orbital character, the conduction band is remarkably steep, with an average effective mass of only 1.14m<sub>e</sub>. Moreover, the sharp spectral features observed in photoemission remain well-defined with little additional broadening for over 500 meV below E<sub>F</sub>, pointing to suppressed electron-electron scattering. Together, our findings establish PtCoO<sub>2</sub> as a model nearly-free electron system and an ideal testbed for elucidating the ultrahigh conductivity in delafossite oxides. [1] Kushwaha P. *et al.*, Sci. Adv. **1**, 9 (2015)

10:24AM A19.00013 Theory for the Spin State and Spectroscopic Modes of Multiferroic CaBaCo<sub>4</sub>O<sub>7</sub><sup>1</sup>, RANDY FISHMAN, Oak Ridge National Laboratory, SANDOR BORDACS, ISTVAN KEZMARKI, VILMOS KOCIS, Budapest University of Technology and Economics, URMAS NAGEL, TOOMAS ROOM, National Institute of Chemical Physics Department, Y. TOKUNAGA, Y. TAKAHASHI, Y. TAGUCHI, Y. TOKURA, RIKEN Center for Emergent Matter Science — With alternating Kagome and triangular lattices, the type I multiferroic CaBaCo<sub>4</sub>O<sub>7</sub> is highly frustrated. Magnetic frustration produces a non-collinear, ferrimagnetic spin state with a net magnetic moment of about 1 m<sub>B</sub> along the b axis below 60 K. Based on the field dependence of the three observed spectroscopic modes between 0.8 and 2.7 THz and on the field dependence of the magnetization up to 14 T, we construct a microscopic model for this compound. Using the symmetry of the crystal, the model is constructed in terms of eight independent nearest-neighbor exchange interactions as well as both in-plane and easy-axis anisotropies. With three observed Co species (spins 1.45, 1.0, and 1.2), the magnetic unit cell contains 16 spins. Our results indicate that the easy-plane and hexagonal anisotropy in the triangular layers is far larger than the anisotropy in the kagome layers. The observed spin-induced polarization along the c axis is produced by magnetostriction. We also predict other spin-wave modes outside the window of the spectroscopic measurements.

<sup>1</sup>Research Sponsored by the Department of Energy, Office of Sciences, Basic Energy Sciences, Materials Sciences and Engineering Division

10:36AM A19.00014 Investigation of the magnetic properties in double perovskite R<sub>2</sub>CoMnO<sub>6</sub> single crystals (R=rare earth: La to Lu)<sup>1</sup>, M. K. KIM, J. Y. MOON, H. Y. CHOI, S. H. OH, N. LEE, Y. J. CHOI, Yonsei Univ, LABORATORY FOR INNOVATIVE FUNCTIONAL MATERIALS TEAM — We have successfully synthesized the series of the double-perovskite R<sub>2</sub>CoMnO<sub>6</sub> (R=rare earth: La to Lu) single crystals and have investigated their magnetic properties. The ferromagnetic order of Co<sup>2+</sup>/Mn<sup>4+</sup> spins emerges mainly along the c axis. Upon decreasing the size of rare earth ion, the magnetic transition temperature decreases linearly from 204 K for La<sub>2</sub>CoMnO<sub>6</sub> to 48 K for Lu<sub>2</sub>CoMnO<sub>6</sub>, along with the enhancement of monoclinic distortion. The temperature and magnetic-field dependences of magnetization reveal the various magnetic characteristics such as the metamagnetic transition in R=Eu, the isotropic nature of rare earth moment in R=Gd, and the reversal of magnetic anisotropy in R=Tb and Dy. Our results offer comprehensive information for understanding the roles of mixed-valent magnetic ions and rare earth magnetic moments on the magnetic properties.

<sup>1</sup>R2CoMnO6 single crystals, double-perovskite, magnetic anisotropy, rare earth

10:48AM A19.00015 Enhanced magnetic coercivity and maximum energy product in double-perovskite Y<sub>2</sub>CoMnO<sub>6</sub> single crystals, HWAN YOUNG CHOI, S.H. OH, J.Y. MOON, M.K. KIM, D.G. OH, N. LEE, Y.J. CHOI, Yonsei university — We have investigated the influence of different annealing conditions on the magnetic properties on the single crystals of double-perovskite Y<sub>2</sub>CoMnO<sub>6</sub>. The ferromagnetic moment along the c-axis with the large magnetic coercivity and high squareness ratio was observed. Particularly, in the quenched specimen, the magnetic functionality has been greatly improved compared to that of the as-grown crystal. The magnetic coercivity and maximum energy product have been increased by  $\sim 120\%$  and  $\sim 50\%$ , respectively, by comprising substantial disorders and defects. Our result renders an efficient route to improve the magnetic functionality in mixed-valent magnets.

## Monday, March 14, 2016 8:00AM - 10:36AM —

### Session A20 GMAG DMP FIAP: Spin Superfluidity and Dzyaloshinskii-Moriya Interaction 319

- Dario Arena, University of Southern Florida

## 8:00AM A20.00001 Spin superfluidity and long-range transport in thin-film ferromagnets ,

HANS SKARSVÅG, CECILIA HOLMQVIST, ARNE BRATAAS, Norwegian University of Science and Technology (NTNU) — In ferromagnets, magnons may condense into a single quantum state. Analogous to superconductors, this quantum state may support transport without dissipation. Recent works suggest that longitudinal spin transport through a thin-film ferromagnet is an example of spin superfluidity. Although intriguing, this tantalizing concept ignores long-range dipole interactions; here, we demonstrate that such interactions dramatically affect spin transport.<sup>1</sup> In single-film ferromagnets, "spin superfluidity" only exists at length scales (a few hundred nanometers in yttrium iron garnet) somewhat larger than the exchange length. Over longer distances, dipolar interactions destroy spin superfluidity. Nevertheless, we predict the re-emergence of spin superfluidity in tri-layer ferromagnet–normal metal–ferromagnet films that are  $\sim 1\ \mu\text{m}$  in size. Such systems also exhibit other types of long-range spin transport in samples that are several micrometers in size.

<sup>1</sup>H. Skarsvåg, C. Holmqvist and A. Brataas, arXiv:1506.06029

## 8:12AM A20.00002 Magnetization dynamics in exchange coupled antiferromagnet spin superfluids<sup>1</sup> ,

YIZHOU LIU, Department of Electrical and Computer Engineering, Univ of California - Riverside, YAFIS BARLAS, Department of Physics and Astronomy, Univ of California - Riverside, GEN YIN, Department of Electrical and Computer Engineering, Univ of California - Riverside, JIADONG ZANG, Department of Physics and Material Science Program, University of New Hampshire, ROGER LAKE, Department of Electrical and Computer Engineering, Univ of California - Riverside — Antiferromagnets (AFMs) are commonly used as the exchange bias layer in magnetic recording and spintronic devices. Recently, several studies on the spin transfer torque and spin pumping in AFMs reveal much more interesting physics in AFMs. Properties of AFMs such as the ultrafast switching within picoseconds and spin superfluidity demonstrate the potential to build AFM based spintronic devices. Here, we study the magnetization dynamics in an exchange coupled AFM systems. Beginning from the Landau-Lifshitz-Gilbert equation, we derive a Josephson-like equation for the exchange coupled system. We investigate the detailed magnetization dynamics by employing spin injection and spin pumping theory. We also propose a geometry that could be used to measure this magnetization dynamics.

<sup>1</sup>This work was supported as part of the Spins and Heat in Nanoscale Electronic Systems (SHINES) an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award SC0012670.

## 8:24AM A20.00003 Superfluidity of magnons in ferromagnetic films ,

CHEN SUN, Texas A&M University, THOMAS NATTERMANN, University of Cologne, VALÉRY POKROVSKY, Texas A&M University, Landau Institute for Theoretical Physics — The magnon Bose-Einstein condensation in Yttrium Iron Garnet films at room temperature was discovered by the Münster experimental group (S.O. Demokritov) in 2006. Since the magnon condensate is coherent the natural question is whether the condensate is superfluid. Though the normal magnon density exceeds the condensate density in about 100 times, the velocity of the superfluid part is by 5-7 decimal orders larger than that of the normal part at the same field gradients. Thus, the spin current is dominated by the condensate, i.e. superfluid. A deeper obstacle is that the phase trapping is inconsistent with the free motion whose phase linearly depends on coordinate. The superfluidity can start only after submission of a finite (threshold) energy to the condensate by an external source. At energy close to threshold, the phase on long intervals of length remains close to the trapped values and changes by  $2\pi$  on a comparatively short intervals (phase solitons). The superfluid velocity remains almost zero between solitons and acquires finite value inside solitons. At large energy the superfluidity of magnons becomes close to a uniform flow.

## 8:36AM A20.00004 Two-Fluid Theory for Spin Superfluidity in Magnetic Insulators ,

BENEDETTA FLEBUS, Univ of Utrecht, SCOTT BENDER, YAROSLAV TSERKOVNÝAK, UCLA, REMBERT DUINE, Univ of Utrecht, UU TEAM, UCLA TEAM — We investigate coupled spin and heat transport in easy-plane magnetic insulators. These materials display a continuous phase transition between normal and condensate states that is controlled by an external magnetic field. Using hydrodynamic equations supplemented by Gross-Pitaevski phenomenology and magnetoelectric circuit theory, we derive a two-fluid model to describe the dynamics of thermal and condensed magnons, and the appropriate boundary conditions in a hybrid normal-metal–magnetic-insulator–normal-metal heterostructure. We discuss how the emergent spin superfluidity can be experimentally probed via a spin Seebeck effect measurement.

## 8:48AM A20.00005 Magneto-optical Phase Transition in a Nanostructured Co/Pd Thin Film<sup>1</sup> ,

CHIDUBEM NWOKOYE, LAWRENCE BENNETT, EDWARD DELLA TORRE, ABID SIDDIQUE, MING ZHANG, MICHAEL WAGNER, Institute for Magnetic Research, Department of Electrical and Computer Engineering, The George Washington University, Washington, DC 20052, USA, FRANK NARDUCCI, Naval Air Systems Command, Avionics, Sensors and E\*Warfare Department, Patuxent River, MD 20670, USA — Interest in the study of magnetism in nanostructures at low temperatures is growing. We report work that extends the magnetics experiments in [1] that studied Bose-Einstein Condensation (BEC) of magnons in confined nanostructures. We report experimental investigation of the magneto-optical properties, influenced by photon-magnon interactions, of a Co/Pd thin film below and above the magnon BEC temperature. Comparison of results from SQUID and MOKE experiments revealed a phase transition temperature in both magnetic and magneto-optical properties of the material that is attributed to the magnon BEC. Recent research in magnonics has provided a realization scheme for developing magnon BEC qubit gates for a quantum computing processor [2]. Future research work will explore this technology and find ways to apply quantum computing to address some computational challenges in communication systems. [1] Bennett L. H. and Della Torre, E. (2014) J. Mod. Phys. 5, 693. [2] Andrianov S. N. and Moiseev, S. A. (2014) Phys. Rev. A 90,042303.

<sup>1</sup>We recognize financial support from the Naval Air Systems Command Section 219 grant.

## 9:00AM A20.00006 Bose-Einstein condensation of confined magnons in nanostructures: the first 30 years and some recent experiments ,

LAWRENCE BENNETT, EDWARD DELLA TORRE, CHIDUBEM NWOKOYE, ABID SIDDIQUE, MOHAMMADREZA GHAREMANI, Institute for Magnetic Research, Department of Electrical and Computer Engineering, The George Washington University, Washington, DC 20052, USA — The Bose-Einstein condensation (BEC) theory was proposed in 1924 by Bose and Einstein. They showed that a non-interacting gas of bosons condenses into a coherent BEC in which a macroscopic number of bosons occupy the lowest-energy single particle state below a critical temperature [1]. An extension of this phenomenon to magnons, spin-wave quanta that behave as bosonic quasiparticles, in magnetic nanoparticles has been observed [2,3]. The BEC of magnons has unique characteristics differentiating it from atomic BEC, creating the potential for a whole new variety of interesting behaviors and applications that include high temperature Bose-Einstein condensation and novel nanomagnetic devices. We report the review of the theoretical and experimental work done in the first 30 years and present recent experimental research related to the topic. [1] Bose, S. N. (1924) Zeitschrift für Physik, 26, 178; Einstein, A. and Sitzungsber. K. (1925) Preuss. Akad. Wiss., Phys. Math. Kl. 3. [2] Swartzendruber, L. J., Rugkwamsook, P., Bennett, L. H., and Della Torre, E. (2000) J. Appl. Phys., 87, 5684. [3] Bennett L. H., and Della Torre E. (2014) J. Mod. Phys., 5, 693.

**9:12AM A20.00007 Extinction of phase transition and spin transport on site diluted quantum two-dimensional antiferromagnet in Bose-Einstein condensation<sup>1</sup>**, LEONARDO DOS SANTOS LIMA, Departamento de Física e Matemática, Centro Federal de Educação Tecnológica de Minas Gerais — We study the two-dimensional Heisenberg antiferromagnetic model with ion single anisotropy in the square lattice in the presence of nonmagnetic impurities at  $T = 0$  using the SU(3) Schwinger boson theory. In particular, we discuss the influence of site disorder on the quantum phase transition of this model at  $D_c$  that separates the Néel phase,  $D < D_c$ , which is gapless, from the disordered phase, gapped phase,  $D > D_c$ . We find that the long-range order in  $D < D_c$  for the model without impurities is destroyed for a concentration of nonmagnetic impurities  $x_c \approx 0.15$ . We have studied also the spin transport of this model. In particular we discuss the influence of site disorder on the spin conductivity of the model and the influence of quantum phase transition on it. We find a large influence of the site dilution at the ac conductivity or continuum conductivity, and on the spin stiffness  $D_S$  that generates information about the dc conductivity. The point of extinction of  $D_c$  *withxdoesnotgenerateaninfluenceonthespinconductivity*.

<sup>1</sup>CNPq, FAPEMIG, CAPES

**9:24AM A20.00008 Resonant x-ray magnetic diffraction of  $q = 0$  antiferromagnetic order in  $\text{Cd}_2\text{Os}_2\text{O}_7$  under high pressure**, YEJUN FENG, Argonne National Lab, YISHU WANG, California Institute of Technology, A. PALMER, The University of Chicago, J.-Q. YAN, D. MANDRUS, Univ. Tennessee and Oak Ridge National Lab, J.W. KIM, Argonne National Lab, T. F. ROSENBAUM, California Institute of Technology — The pyrochlore structured  $\text{Cd}_2\text{Os}_2\text{O}_7$  manifests a continuous metal-insulator transition at ambient pressure. Associated with the rise of the insulating phase is the formation of an all-in/all-out type of spin arrangement for Os ions on each tetrahedron unit, resulting in antiferromagnetic order with a  $q=0$  wave vector. The nature of the insulating phase is not understood due to the interplay of different degrees of freedom with almost degenerate energy scales characteristic of 5d transition metal compounds. Here we probe directly the pressure evolution of the antiferromagnetism using resonant x-ray magnetic diffraction techniques. We track the antiferromagnetic state to 18 GPa at 4 K, gradually suppressing the strength of the magnetic order and locating the boundary of an apparent continuous quantum phase transition.

**9:36AM A20.00009 Very large Rashba coupling by a staggered crystal field in the inversion-symmetric  $\text{BaNiS}_2$  semi-metal<sup>1</sup>**, ANDREA GAUZZI, DAVID SANTOS-COTTON, MICHELE CASULA, IMPMC-Sorbonne Universités, GABRIEL LANTZ, LPS-Université Paris Sud, YANNICK KLEIN, IMPMC-Sorbonne Universités, EVANGELOS PAPALAZAROU, MARINO MARSI, LPS-Université Paris Sud — By means of a single-crystal angular resolved photoemission spectroscopy study combined with first principles calculations, we give evidence of a giant Rashba coupling  $\alpha_R \approx 0.25$  eV Å leading to an energy splitting as large as  $\Delta\epsilon \approx 150$  meV in a novel situation of an inversion-symmetric system - the  $\text{BaNiS}_2$  semi-metal - composed of comparatively light elements. This finding is explained by a huge staggered crystal field  $\approx 1.4$  V/Å associated with a peculiar non-symorphic square-pyramidal structure, which produces a local inversion asymmetry at the Ni site. We show that this very effective mechanism of Rashba coupling enables large changes of the electronic structure of solids without using either heavy elements or external fields.

<sup>1</sup>Partially funded by the Emergence program of the UPMC-Sorbonne Universities.

**9:48AM A20.00010 Low-temperature magneto-thermal conductivity of the helimagnet  $\text{Cu}_2\text{OSeO}_3$ <sup>1</sup>**, NARAYAN PRASAI, SUNXIANG HUANG, JOSHUA L. COHN, University of Miami, BENJAMIN TRUMP, GUY G. MARCUS, TYREL M. MCQUEEN, CHIA LING CHEN, Johns Hopkins University — We report measurements of thermal conductivity ( $\kappa$ ) in the range  $0.6 \text{ K} \leq T \leq 200 \text{ K}$  for single crystals of the helimagnetic insulator  $\text{Cu}_2\text{OSeO}_3$ . A maximum in  $\kappa$  near  $T = 8 \text{ K}$  with  $\kappa_{max} \sim 300 \text{ W/mK}$  implies a very high lattice quality for an oxide. The magneto-thermal conductivity at  $T \leq 10 \text{ K}$  and influence of spin-reorientation transitions associated with low- $T$  magnetic phases will be discussed for different orientations of the magnetic field relative to the crystallographic and heat flow directions.

<sup>1</sup>This material is based upon work supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Material Sciences and Engineering, under grants No. DEFG02-12ER46888 (Univ. Miami) and No. DEFG02-08ER46544 (Johns Hopkins Univ.)

**10:00AM A20.00011 Anisotropic RKKY and Dzyaloshinsky-Moriya interactions in a two-dimensional spin-polarized electron gas with Rashba and Dresselhaus spin-orbit coupling**, MOHAMMAD MAHDI VALIZADEH, SASHI SATPATHY, University of Missouri - Columbia — Chiral order in magnetic structures is currently an area of considerable interest and leads to such structures as the skyrmion lattice. The chiral structures originate from the Dzyaloshinsky-Moriya (DM) interactions caused by broken symmetry and the presence of the spin-orbit interaction. We study the indirect exchange interaction between two localized magnetic moments mediated by a spin-polarized 2DEG in the presence of both Rashba and Dresselhaus spin-orbit coupling. We find anisotropic RKKY and DM interactions, e. g., of the form  $J_1(S_{1x}S_{2x} + S_{1y}S_{2y}) + J_2S_{1z}S_{2z}$  in the former case, in the presence of a non-zero spin polarization. The magnitude of the vector and tensor DM interactions are estimated and compared to recent experiments on magnetic thin films.

**10:12AM A20.00012 Minimal Ingredients for Orbital Texture Switches at Dirac Points in Strong Spin-Orbit Coupled Materials**, JUSTIN WAUGH, University of Colorado at Boulder, THOMAS NUMMY, University of Colorado at Boulder, STEPHEN PARHAM, DANIEL DESSAU, University of Colorado at Boulder — Recent angle resolved photoemission spectroscopy measurements on strong spin-orbit coupled materials have shown an in-plane orbital texture switch at their respective Dirac points. This feature has also been demonstrated in a few materials ( $\text{Bi}_2\text{Se}_3$ ,  $\text{Bi}_2\text{Te}_3$ , and BiTeI) through DFT calculations. Here we present a minimal orbital-derived tight binding model to calculate the electron wave-function in a two-dimensional crystal lattice. We show that the orbital components of the wave-function demonstrate an orbital-texture switch in addition to the usual spin switch seen in spin polarized bands. This orbital texture switch is determined by the existence of three main properties: local or global inversion symmetry breaking, strong spin-orbit coupling, and non-local physics (the electrons are on a lattice). Using our model we demonstrate that the orbital texture switch is ubiquitous and to be expected in many real systems. The orbital hybridization of the bands is the key aspect for understanding the unique wave function properties of these materials, and this minimal model helps to establish the quantum perturbations that drive these hybridizations.

**10:24AM A20.00013 A mechanism for orbital angular momentum and giant spin-splitting in solids and nanostructures**, SEHOON OH, HYOUNG JOON CHOI, Department of Physics, IPAP, and Center for Computational Studies of Advanced Electronic Material Properties, Yonsei University, Seoul 03722, Korea — Giant spin-splitting (GSS) of electronic bands, which is several orders of magnitude greater than Rashba model, has been observed in various systems including noble-metal surfaces, thin film of transition-metal dichalcogenides, often accompanied by the orbital angular momentum (OAM). Here, we study structural and orbital conditions for emergence of a GSS by using tight-binding and first-principles calculations. We find that broken mirror symmetry of local atomic structure around an atom can produce non-zero OAM at the atom. This OAM results in a GSS if the atom is a high-atomic number element. We demonstrate these structural and orbital conditions in the cases of simple atomic chains,  $\text{WSe}_2$  monolayer, Au(111) surface, and bulk HgTe. Based on this mechanism of the spin-splitting, we suggest methods to control the GSS, which can be used in applications such as spintronic devices. This work was supported by NRF of KOREA (Grant No. 2011-0018306) and KISTI supercomputing center (Project No. KSC-2015-C3-039).

**Monday, March 14, 2016 8:00AM - 11:00AM —**

**Session A21 GMAG DMP: Magnetic Layers** 320 - Mark Meisel, University of Florida

**8:00AM A21.00001 Specific Heat Studies of a 2D  $S = \text{Heisenberg Antiferromagnet}$** , CHRISTOPHER LANDEE, FAN XIAO, Department of Physics, Clark University, SIMON GERBER, MICHEL KENZELMANN, Paul Scherrer Institute, NU XU, ANDERS SANDVIK, Department of Physics, Boston University — We report on the field-dependent specific heat of a highly two-dimensional Heisenberg,  $S = 1/2$  antiferromagnet (2D QHAF),  $[\text{Cu}(\text{pz})_2(2\text{-OHpy})_2](\text{ClO}_4)_2$ , where pz = pyrazine and 2-OHpy = 2-pyridone. The copper atoms and pyrazine molecules form distorted rectangular layers of pyrazine-bridged copper(II) ions with the pyridone molecules normal to the layers, providing exceptional spacing between layers [1]. The zero-field specific heat of this compound (1.8 – 35 K) is compared to the recent QMC simulations of the specific heat for the 2D QHAF. Under applied field, the temperature dependence of the specific heat varies smoothly, but no field-induced ordering is observed. This behavior differs from the field-induced ordering in the 2D QHAF  $\text{Cu}(\text{pz})_2(\text{ClO}_4)_2$  reported previously [2]. [1] V. Selmani, C. P. Landee, M. M. Turnbull, J. L. Wikaira, and F. Xiao. Inorg. Chem. Comm. 13, 1399-1401 (2010), doi: 10.1016/j.inoche.2010.07.045 [2] N. Tsyrlin, F. Xiao, A. P. Schneidewind, H. M. Rönnow, J. Gavilano, C. P. Landee, M. M. Turnbull, M. Kenzelmann. Phys. Rev. B, 81, 134409 (2010), doi: 10.1103/PhysRevB.81.134409.

**8:12AM A21.00002 Thickness- and magnetic-field-driven suppression of antiferromagnetism in  $\text{V}_5\text{S}_8$  single crystals**, WILL HARDY, Applied Physics Graduate Program, Smalley-Curl Institute, Rice University, JIANGTAN YUAN, Department of Materials Science and NanoEngineering, Rice University, PANPAN ZHOU, Department of Physics and Astronomy, Rice University, JUN LOU, Department of Materials Science and NanoEngineering, Rice University, DOUGLAS NATELSON, Department of Physics and Astronomy, Rice University — The search for novel materials approaching the  $2d$  limit can be expanded beyond the transition metal dichalcogenides (TMDs) to related compounds, widening the range of available physical phenomena and tuning parameters.  $\text{V}_5\text{S}_8$ , a metal with an antiferromagnetic (AFM) ground state below  $\sim 32$  K, displays a prominent spin-flop transition at  $\sim 4.2$  T. Here we study the AFM state in thin CVD-grown single crystals of  $\text{V}_5\text{S}_8$ , focusing on temperatures close to  $T_{\text{Néel}}$ , where the exact transition temperature depends on the crystal thickness. Magnetoresistance (MR) measurements performed just below  $T_{\text{Néel}}$  reveal magnetic hysteresis, likely a result of a first-order magnetic field-driven breakdown of the AFM state. In thin crystals, on the order of 10 nm thick, monotonic MR measurements suggest that antiferromagnetism is suppressed as the thickness nears the  $2d$  limit. This work demonstrates the possibility of growing single crystals of a relatively complicated magnetic system with thicknesses approaching one unit cell, thereby allowing the tuning of magnetic properties by a field-driven phase transition.

**8:24AM A21.00003 Field induced phase transition in layered honeycomb spin system  $\alpha\text{-RuCl}_3$  studied by thermal conductivity**<sup>1</sup>, IAN LEAHY, ALEX BORNSTEIN, University of Colorado, Boulder, CO 80309, KWANG-YONG CHOI, Chung-Ang University, Seoul, South Korea, MINHYEA LEE, University of Colorado, Boulder, CO 80309 —  $\alpha\text{-RuCl}_3$ , a quasi two-dimensional honeycomb lattice is known to be a candidate material to realize the Heisenberg-Kitaev spin model of a highly anisotropic bond-dependent exchange interaction. We investigate in-plane thermal conductivity ( $\kappa$ ) as a function of temperature ( $T$ ) and in-plane applied field ( $H$ ). At  $H = 0$ , the onset of a strong increase in  $\kappa$  marks the spontaneous long range ordering temperature,  $T_c = 6.5\text{K}$ , corresponding to zigzag antiferromagnetic ordering. A broad peak appearing below  $T_c$  in  $\kappa$  was found to be suppressed significantly as  $H$  increases up to  $\approx 7\text{T}$ , implying the system undergoes a field-induced transition from ordered to a new spin-disordered state analogous to the transverse-field Ising model. Further increasing  $H$  above  $7.1\text{T}$ , the large field seems to begin polarizing spins thus increasing the phonon mean free path, resulting in a significant rise in  $\kappa$ . This tendency is clearly shown in the field dependence of  $\kappa$  below  $T_c$ , which has a pronounced minimum at  $H_{\text{min}} = 7.1\text{T}$ . We will discuss our scaling analysis to characterize this field-induced phase transition and compare to the transverse-field Ising spin system.

<sup>1</sup>Work at the University of Colorado was supported by the US DOE Basic Energy Sciences under Award No. DE-SC0006888

**8:36AM A21.00004 Fingerprints of the field-induced Berezinskii-Kosterlitz-Thouless transition in quasi-two-dimensional quantum magnets**<sup>1</sup>, ALŽBETA ORENDÁČOVÁ, P.J. Šafárik University, Košice — The two-dimensional (2d) easy-plane (XY) model provides a prototypical description of 2d systems exhibiting topological excitations, which drive the Berezinskii-Kosterlitz-Thouless (BKT) transition that occurs in 2d superfluids, electron plasmas, Josephson junction arrays, ultracold atomic 2d Bose gases, etc. The excitations in the 2d XY model are spin waves and vortices. In the BKT scenario, at low temperatures, all vortices (V) and antivortices (AV) are bound to V-AV pairs, and spin waves dominate in this quasi-long-range-ordered phase with an infinite correlation length,  $\xi$ , and an algebraic decay of correlations. At a critical temperature,  $T_{\text{BKT}}$ , the V-AV pairs start to unbind, driving the transition to a free vortex phase above  $T_{\text{BKT}}$ , characterized by an exponential divergence of  $\xi$  [1]. Vortices remain stable also in quantum 2d anisotropic Heisenberg systems with a very weak XY anisotropy [2]. The BKT scenario appears even in 2d isotropic Heisenberg magnets due to frustration [3] or an external magnetic field [4]. I will focus on quasi-2d spin  $1/2$  Heisenberg antiferromagnets with extremely weak spin anisotropy [5]. These highly anisotropic layered Cu(II) organo-metallic insulators with relatively low saturation fields, about 6 T, enabled a comprehensive study in a wide range of magnetic fields and temperatures. A response of all compounds to the application of a magnetic field mimics 2d behavior with fingerprints of a field-induced Berezinskii-Kosterlitz-Thouless phase transition. [1] J. V. José (Ed.), 40 Years of Berezinskii-Kosterlitz-Thouless Theory, World Scientific, 2013. [2] A. Cuccoli et al., Phys. Rev. Lett. 90 (2003) 167205. [3] B. Jeevanesan et al., Phys. Rev. Lett. 115 (2015) 177201. [4] A. Cuccoli et al., Phys. Rev. B 68 (2003) 060402(R). [5] R. Tarasenko et al., Phys. Rev. B 87 (2013) 174401.

<sup>1</sup>ITMS 26220120005, VEGA 1/0143/13 and APVV-14-0073 are acknowledged for a financial support.

**9:12AM A21.00005 Magnetic Property Determination of Nickel Niobate ( $\text{NiNb}_2\text{O}_6$ )**, TIMOTHY MUNSIE, MURRAY WILSON, ALANNAH HALLAS, YIPENG CAI, Department of Physics and Astronomy, McMaster University, TRAVIS WILLIAMS, ADAM ACZEL, Oak Ridge National Laboratory, HANNA DABKOWSKA, Brockhouse Institute for Materials Research, JOHN GREEDAN, Department of Chemistry, McMaster University, GRAEME LUKE, Department of Physics and Astronomy, McMaster University — We have synthesized a novel polymorph of the material nickel niobate,  $\text{NiNb}_2\text{O}_6$ , in a previously undetermined space group. We have examined the material using SQUID magnetometry and have observed a magnetic transition at approximately 14 K, and a second magnetic feature below 2 K. We have determined these materials using muon spin rotation and relaxation at TRIUMF National Lab in Vancouver, Canada and using neutron scattering on the HB-3A beamline of the High Flux Isotope Reactor at Oak Ridge National Labs, TN. Using these techniques we were able to determine that the magnetic structure is highly two-dimensional. This talk will discuss the nature of the phase transition and its evolution through low temperatures.

**9:24AM A21.00006 Direct Visualization of Surface Phase of Oxygen Molecules Physisorbed on the Ag(111) Surface: A Two-dimensional Quantum Spin System**, SHUNJI YAMAMOTO, YASUO YOSHIDA, ISSP, The Univ. of Tokyo, HIROSHI IMADA, YOUSOO KIM, SISL, RIKEN, YUKIO HASEGAWA, ISSP, The Univ. of Tokyo — Oxygen molecule ( $O_2$ ) is one of the smallest molecular magnets with an  $S=1$  quantum spin. This makes  $O_2$  attractive as a building block of low-dimensional (LD) quantum spin systems. Recently, the existence of a spin in physisorbed  $O_2$  on Ag(111) was confirmed by the ortho-para conversion of molecular hydrogen. Therefore, there is a strong need for STM-based techniques with single-molecule resolution in order to verify the potential of the  $O_2$ /Ag(111) for LD quantum spin systems. Here we report the real-space observation of oxygen molecules physisorbed on an Ag(111) surface by using low-temperature scanning tunneling microscopy and spectroscopy. A well-ordered  $O_2$  structure was observed, and the lattice was distorted from an isosceles triangular lattice. The distortion can be explained by the competition between the magnetic and elastic instabilities of the  $O_2$  lattice. In differential tunneling conductance spectra, we found no feature of the Kondo resonance at 4.7 K; in contrast, the physisorbed  $O_2$  on Ag(110) showed a clear Kondo resonance at 18 K. Based on these observations, we discuss the realization of an  $S=1$  two-dimensional antiferromagnetic quantum spin system.

**9:36AM A21.00007 Extent of the Z2 topological phase in the quantum dimer model**, MARC SCHULZ, FIONA J BURNELL, Univ of Minn - Minneapolis — The possibility that topological order is realized in the anti-ferromagnetic Heisenberg model on the Kagome lattice has been supported by increasing numerical evidence over the last years. In particular, effective low-energy descriptions in terms of quantum dimers models provide valuable insights. It has been shown that the phase diagram of the quantum dimer model contains a point at which the Hamiltonian is exactly solvable and realizes a Z2 topological phase. We study the extent of this phase around the exactly solvable point. Therefore we consider the low-energy spectrum which we determine by means of high-order perturbation theory.

**9:48AM A21.00008 Effect of hydrogenation on magnetic properties of heavy transition-metal dichalcogenides<sup>1</sup>**, PRIYANKA MANCHANDA, S. -H. LIOU, AXEL ENDERS, D. J. SELLMYER, RALPH SKOMSKI, University of Nebraska, Lincoln — Two-dimensional transition-metal dichalcogenides (2D TMDs) are emerging as a unique class of materials because of their underlying fundamental physics and technological applications in electronics, sensors, energy storage, photonics, and spintronics. The outstanding electronic properties of 2D TMDs can be further tuned by various external means, such as control of external electric field, chemical functionalization, alloying, and strain. The electronic and magnetic properties of chemical functionalized 2D TMDs is of special interest. Experimentally, adsorbed fluorine has been shown very recently to create a small magnetic moment of 0.06 emu/g in  $MoS_2$  nanosheets. Although several studies as well as review articles on the properties of TMDs have been published in the past few years, Mo and W chalcogenides are most widely studied among the “beyond-graphene” 2D TMDs. However, studies of chemical functionalization on TMDs containing heavy TMDs such as Ta and Pt are still infancy. In the present work, we investigate the effect of hydrogenation on the magnetism of  $PtSe_2$  monolayers using density-functional theory. We find that the hydrogen induces a magnetic moment of 0.7  $\mu_B$  per unitcell. This work has been supported by ARO, and DOE-BES.

<sup>1</sup>This work has been supported by ARO, and DOE-BES.

**10:00AM A21.00009 Calculating small interchain exchange parameters in Copper Pyrazine Dinitrate<sup>1</sup>**, IORWERTH THOMAS, STEWART CLARK, TOM LANCASTER, Durham University — The coordination polymer copper pyrazine dinitrate ( $Cu(pyz)(NO_3)_2$ ) is a one-dimensional antiferromagnet that undergoes a magnetic phase transition to a state of long-range three dimensional magnetic order (LRO) below a temperature of 110 mK. The precise nature of the LRO is dependent on the strength of interchain interactions, which are very weak compared to the dominant superexchange interaction along the chain. It is therefore possible that different approaches to ab initio calculations of exchange interaction parameters may be subject to small systematic effects that would lead to erroneous results. In order to investigate whether such a problem arises in this case, we use the GGA+U approach to Density Functional Theory to compare the results obtained by two methods of calculating these parameters: the dimer fragment approach and the periodic method, and relate them to both experiment and previous calculations performed using the hybrid approach.

<sup>1</sup>Supported by the Templeton Foundation as part of the Durham Emergence Project

**10:12AM A21.00010 Time-Dependent Behavior in Arrays of Coupled Heisenberg Spin Chains**, ROBERT KONIK, Brookhaven Natl Lab, ANDREW JAMES, London Centre for Nanoscience, J-S CAUX, Universiteit van Amsterdam — We employ matrix product state methods combined with data from exact solvability to study infinite arrays of coupled XXZ Heisenberg spin chains of finite length under a time dependent perturbation. We present results for both sudden changes (quantum quenches) as well more gradual changes in the interchain coupling. We benchmark our results and methods against perturbation theory as well as available equilibrium results on two dimensional Heisenberg models. We discuss these results in light of recent pump-probe resonant inelastic x-ray scattering experiments on the iridate compound  $Sr_2IrO_4$ .

**10:24AM A21.00011 Excitations in the quantum paramagnetic phase of the quasi-one-dimensional Ising magnet  $CoNb_2O_6$  in a transverse field: Geometric frustration and quantum renormalization effects<sup>1</sup>**, IVELISSE CABRERA, Clarendon Laboratory, University of Oxford/NIST Center for Neutron Research, J. D. THOMPSON, R. COLDEA, D. PRABHAKARAN, Clarendon Laboratory, University of Oxford, R. I. BEWLEY, T. GUIDI, ISIS Facility, Rutherford Appleton Laboratory, J. A. RODRIGUEZ-RIVERA, NIST Center for Neutron Research, C. STOCK, NIST Center for Neutron Research/The University of Edinburgh — We report extensive single-crystal inelastic neutron scattering measurements of the magnetic excitations in the quasi 1D Ising ferromagnet  $CoNb_2O_6$  in the quantum paramagnetic phase to characterize the effects of the finite interchain couplings. In this phase, we observe that excitations have a sharp, resolution-limited line shape at low energies and over most of the dispersion bandwidth, as expected for spin-flip quasiparticles. We map the full bandwidth along the strongly dispersive chain direction and resolve clear modulations of the dispersions in the plane normal to the chains, characteristic of frustrated interchain couplings in an antiferromagnetic isosceles triangular lattice. The dispersions can be well parametrized using a linear spin-wave model that includes interchain couplings and further neighbor exchanges. The observed dispersion bandwidth along the chain direction is smaller than that predicted by a linear spin-wave model using exchange values determined at zero field. We attribute this effect to quantum renormalization of the dispersion beyond the spin-wave approximation in fields slightly above the critical field, where quantum fluctuations are still significant.

<sup>1</sup>We acknowledge support from EPSRC Grant No. EP/H014934/1, the Oxford Clarendon Fund Scholarship and NSERC of Canada.

**10:36AM A21.00012 Quantum Acoustic Magnetic Resonance Imaging and Spectroscopy:** VIOLETA ZAMORANO, V CELLI, B SHIVARAM, University of Virginia — We present a new modality to characterize single molecule and molecular magnets and propose that it can be used as a powerful spectroscopy and imaging tool. Heisenberg type Hamiltonians representing realistic molecules with appropriate crystal field terms are solved and the magnetic field dependence of the resulting quantum spin energy levels enumerated. The results through thermodynamic identities yield the bulk modulus which is shown to be sensitive to the crystal field parameters at low temperatures. Thus high field low temperature measurements of the sound velocity in molecular and single molecule magnets open the road to a completely new method of understanding such systems.

**10:48AM A21.00013 Molecular quantum magnetism with strong spin-orbit coupling in inorganic solid  $\text{Ba}_3\text{Yb}_2\text{Zn}_5\text{O}_{11}$** , SANG-YOUN PARK, SUNGDAE JI, JAE-HOON PARK, MPPC-CPM, Pohang Univ of Sci & Tech, SEUNGHWAN DO, KWANG-YONG CHOI, Dept. of Physics, Chung-Ang University, DONGJIN JANG, BURKHARD SCHMIDT, MANUEL BRANDO, Max Planck Institute for Chemical Physics of Solids, NICHOLAS BUTCH, NIST Center for Neutron Research — The molecular magnet, assembly of finite number of spins which are isolated from environment, is a model system to study the quantum information process such as the qubit or spintronic devices. In past decades, the molecular magnet has been mostly realized in organic material, however, it has difficulty synthesizing materials or controlling their properties, meanwhile tremendous endeavors to search inorganic molecular magnet are continuing. Here, we propose  $\text{Ba}_3\text{Yb}_2\text{Zn}_5\text{O}_{11}$  as a candidate of inorganic molecular magnet. This material consists of an alternating 3D-array of small and large tetrahedron containing antiferromagnetically coupled four pseudospin-1/2 Yb ions, and magnetic properties are described by an isolated tetrahedron without long-range magnetic ordering. Inelastic neutron scattering measurement with external magnetic field reveals that extraordinarily huge Dzyaloshinsky-Moriya (DM) interaction originating from strong spin-orbit coupling in Yb isospin is the key to explain energy level of tetrahedron in addition to Heisenberg exchange interaction and Zeeman effect. Magnetization measurement shows the Landau-Zener transition between avoided crossing levels caused by DM interaction.

**Monday, March 14, 2016 8:00AM - 10:48AM —**

**Session A22 DCOMP: Electrons, Phonons, and Electron-Phonon Scattering I** 321 - David Singh, University of Missouri

**8:00AM A22.00001 Ab initio phonon limited transport**, MATTHIEU VERSTRAETE, Univ de Liege — We revisit the thermoelectric (TE) transport properties of two champion materials, PbTe and SnSe, using fully first principles methods. In both cases the performance of the material is due to subtle combinations of structural effects, scattering, and phase space reduction. In PbTe anharmonic effects are completely opposite to the predicted quasi-harmonic evolution of phonon frequencies and to frequently (and incorrectly) cited extrapolations of experiments. This stabilizes the material at high T, but also tends to enhance its thermal conductivity, in a non linear manner, above 600 Kelvin. This explains why PbTe is in practice limited to room temperature applications. SnSe has recently been shown to be the most efficient TE material in bulk form. This is mainly due to a strongly enhanced carrier concentration and electrical conductivity, after going through a phase transition from 600 to 800 K. We calculate the transport coefficients as well as the defect concentrations *ab initio*, showing excellent agreement with experiment, and elucidating the origin of the double phase transition as well as the new charge carriers. AH Romero, ECU Gross, MJ Verstraete, and O Hellman PRB 91, 214310 (2015) O. Hellman, IA Abrikosov, and SI Simak, PRB 84 180301 (2011)

**8:36AM A22.00002 High throughput solution of Boltzmann transport equation: phonons, thermal conductivity and beyond**, JOSE PLATA, PINKU NATH, DEMET USANMAZ, Duke University, CORMAC TOHER, Duke Univ, MARCO FORNARI, Central Michigan University, MARCO BUONGIORNO NARDELLI, University of North Texas, STEFANO CURTAROLO, Duke University — Quantitatively accurate predictions of the lattice thermal conductivity have important implications for key technologies ranging from thermoelectrics to thermal barrier coatings. Of the many approaches with varying computational costs and accuracy, which have been developed in the last years, the solution of the Boltzmann transport equation (BTE) is the only approach that guarantees accurate predictions of this property. We have implemented this methodology in the AFLOW [1] high throughput materials science framework, which enables us to compute these anharmonic force constants and solve BTE to obtain the lattice thermal conductivity and related properties automatically in a single step. This technique can be combined with less expensive methodologies previously implemented in AFLOW [2] to create an efficient and fast framework to accelerate the discovery of materials with interesting thermal properties. [1] S. Curtarolo et al., Comp. Mat. Sci. 58, 218 (2012). [2] C. Toher, et. al, Phys. Rev. B 90, 174107, 2014

**8:48AM A22.00003 Parallel calculations of vibrational properties in complex materials: negative thermal expansion and elastic inhomogeneity.**<sup>1</sup>, F.D. VILA, J.J. REHR, U. of Washington — Effects of thermal vibrations are essential to obtain a more complete understanding of the properties of complex materials. For example, they are important in the analysis and simulation of x-ray absorption spectra (XAS). In previous work<sup>2</sup> we introduced an *ab initio* approach for a variety of vibrational effects, such as crystallographic and XAS Debye-Waller factors, Debye and Einstein temperatures, and thermal expansion coefficients. This approach uses theoretical dynamical matrices from which the locally-projected vibrational densities of states are obtained using a Lanczos recursion algorithm. In this talk I present recent improvements to our implementation, which permit simulations of more complex materials with up to two orders of magnitude larger simulation cells. The method takes advantage of parallelization in calculations of the dynamical matrix with VASP. To illustrate these capabilities we discuss two problems of considerable interest: negative thermal expansion in  $\text{ZrW}_2\text{O}_8$ ; and local inhomogeneities in the elastic properties of supported metal nanoparticles. Both cases highlight the importance of a local treatment of vibrational properties.

<sup>1</sup>Supported by DOE grant DE-FG02-03ER15476, with computer support from DOE-NERSC.

<sup>2</sup>F. D. Vila *et al.* Phys. Rev. B **76**, 014301 (2007).

**9:00AM A22.00004 Lattice dynamics and electron-phonon coupling calculations using non-diagonal supercells**<sup>1</sup>, JONATHAN LLOYD-WILLIAMS, University of Cambridge, BARTOMEU MONSERRAT, Rutgers University — Quantities derived from electron-phonon coupling matrix elements require a fine sampling of the vibrational Brillouin zone. Converged results are typically not obtainable using the direct method, in which a perturbation is frozen into the system and the total energy derivatives are calculated using a finite difference approach, because the size of simulation cell needed is prohibitively large. We show that it is possible to determine the response of a periodic system to a perturbation characterized by a wave vector with reduced fractional coordinates  $(m_1/n_1, m_2/n_2, m_3/n_3)$  using a supercell containing a number of primitive cells equal to the least common multiple of  $n_1$ ,  $n_2$ , and  $n_3$ . This is accomplished by utilizing supercell matrices containing nonzero off-diagonal elements. We present the results of electron-phonon coupling calculations using the direct method to sample the vibrational Brillouin zone with grids of unprecedented size for a range of systems, including the canonical example of diamond. We also demonstrate that the use of nondiagonal supercells reduces by over an order of magnitude the computational cost of obtaining converged vibrational densities of states and phonon dispersion curves.

<sup>1</sup>J.L.-W. is supported by the Engineering and Physical Sciences Research Council (EPSRC). B.M. is supported by Robinson College, Cambridge, and the Cambridge Philosophical Society. This work was supported by EPSRC grants EP/J017639/1 and EP/K013564/1.

## 9:12AM A22.00005 Ab Initio Electronic Relaxation Times and Transport in Noble Metals<sup>1</sup>

JAMAL I. MUSTAFA, University of California at Berkeley and Lawrence Berkeley National Lab, MARCO BERNARDI, California Institute of Technology, JEFFREY B. NEATON, STEVEN G. LOUIE, University of California at Berkeley and Lawrence Berkeley National Lab — Relaxation times employed to study electron transport in metals are typically assumed to be constants and obtained empirically using the Drude model. Here, we employ ab initio calculations to compute the electron-phonon relaxation times of Cu, Ag, and Au, and find that they vary significantly on the Fermi surface, spanning  $\sim 15$ – $45$  fs. We compute room temperature resistivities in excellent agreement with experiment by combining *GW* bandstructures, Wannier-interpolated band velocities, and ab initio relaxation times. Our calculations are compared to other approximations used for the relaxation times. Additionally, an importance sampling scheme is introduced to speed up the convergence of resistivity and transport calculations by sampling directly points on the Fermi surface.

<sup>1</sup>This work was supported by NSF Grant No. DMR15-1508412 and U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at LBNL's NERSC facility.

## 9:24AM A22.00006 First-principles calculation of LO phonon scattering in BaSnO<sub>3</sub><sup>1</sup>

KARTHIK KRISHNASWAMY, BURAK HIMMETOGLU, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — BaSnO<sub>3</sub> (BSO) has drawn interest owing to the recent discovery of high electron mobility, highest among the perovskite materials. In our theoretical work, we calculate the electron scattering rate due to LO phonon scattering from first-principles density functional calculations. The calculated mobility is much higher than the experimentally observed value, suggesting defect scattering as the primary limiting factor in currently grown BSO samples, and that reducing the defect density can enhance BSOs mobility significantly.

<sup>1</sup>This work was supported by the LEAST Center and by ONR.

## 9:36AM A22.00007 Consequences of ionic and covalent bonding in Ge-Sb-Te phase change materials

SAIKAT MUKHOPADHYAY, Materials Science and Technology Division, Oak Ridge National Laboratory, JIFENG SUN, Department of Physics and Astronomy, University of Missouri, ALASKA SUBEDI, Max Planck Institute for the Structure and Dynamics of Matter, THEO SIEGRIST, Department of Chemical and Biomedical Engineering, FAMU-FSU College of Engineering, Tallahassee, DAVID SINGH, Department of Physics and Astronomy, University of Missouri — Structural transformation of Ge<sub>2</sub>Sb<sub>2</sub>Te<sub>5</sub> has attracted a great deal of research as it involves two states (crystalline and amorphous) that are stable at ambient temperature but with remarkably different physical properties, in particular, very different optical constants. The differences in physical properties in these states have been explained in terms of resonant bonding that has been generalized to the description of covalent systems with high symmetry structures such as benzene and graphite. However, given the local lattice distortions noted from both experimental and theoretical investigations, it is clear that the meaning of “resonant bonding” in GST is very different from that in graphite or benzene and the precise nature of bonding in this phase has not been fully established. In this talk, based on our first-principles calculations, we show that there is a strong competition between ionic and covalent bonding in the cubic phase, and establish a link between the origins of phase change memory properties and giant responses of piezoelectric materials.

## 9:48AM A22.00008 ABSTRACT WITHDRAWN —

## 10:00AM A22.00009 Novel, discontinuous polaron transition in a two-band model<sup>1</sup>

MIRKO M. MOELLER, GEORGE A. SAWATZKY, MONA BERCIU, Univ British Columbia — The coupling of charge carriers (electrons or holes) to phonons leads to the formation of a polaron, a coherent quasi-particle consisting of the charge carrier and the cloud of phonons surrounding it and moving coherently with it. Here we present exact diagonalization and momentum average approximation results for the single polaron properties of a two-band model with phonon modulated hopping, inspired by the perovskite BaBiO<sub>3</sub>. For large coupling we find that the ground state momentum changes *discontinuously* from  $k = \pi$  to  $k = 0$ . Such sharp transitions of the polaron's ground state properties cannot occur in the well-studied models of the Holstein or Fröhlich type in which the carrier-phonon coupling modulates the on-site energies. However, they can occur in models where the carrier-phonon coupling modulates the hopping integrals such as the SSH model for which a similar yet smooth transition of the ground state momentum was recently shown to exist. We compare our findings to the SSH model and point out qualitative differences which we believe to be due to the two band nature of our model versus the single band SSH model.

<sup>1</sup>This work was supported by NSERC, QMI and the UBC 4YF.

## 10:12AM A22.00010 Quasiparticle properties of the nonlinear Holstein model at finite doping and temperature.

SHAOZHI LI, Univ of Tennessee, Knoxville, BETH NOWADNICK, Cornell University, STEVEN JOHNSTON, Univ of Tennessee, Knoxville — Models with linear electron-phonon (e-ph) interactions often predict the formation of small polarons with large lattice displacements. This directly violates the approximations made in deriving the linear model, which implies that one should consider higher order terms in the interaction. Previously we have shown that even small positive nonlinear e-ph interactions dramatically suppress charge-density-wave formation and s-wave superconductivity relative to the linear model [EPL. 109, 27007 (2015)]. In this talk, we present a determinant quantum Monte Carlo study of the single-particle properties of quasiparticles and phonons in a two-dimensional Holstein model that includes an additional nonlinear e-ph interaction. We show that a small positive nonlinear e-ph interaction reduces the effective coupling between electrons and phonons and hardens the effective phonon frequency. Conversely, a small negative nonlinear interaction can enhance e-ph coupling resulting in heavier quasiparticles. In addition, we find that an effective linear model fails to simultaneously capture the quantitative effects of the nonlinearity of both the electronic and phononic degrees of freedom, even though it can qualitatively reproduce properties.

## 10:24AM A22.00011 Entanglement of nuclear spins and phonons in ideal solids.

VADIM OGANESYAN, CUNY-CSI, STEVEN MORGAN, GREGORY BOUTIS, CUNY-Brooklyn College — We investigate quantum many-body dynamics of nuclei in solids, in particular as they are affected by dynamical excitations of the underlying matrix, i.e. phonon modulation of dipolar couplings. Our recent work documented consequences of this coupling in calcium fluoride, where small changes in the spectrum of the free induction decay (FID) were measured, roughly consistent with theoretical estimates based on a simplified elastic model. Such theory also predicts temperature dependent enhancement of the diffusion constant of dipolar order, essentially due to growth in the phonon mean-free path.

## 10:36AM A22.00012 Chiral Phonons and Electrical Resistivity of Ferromagnetic Metals at Low Temperatures<sup>1</sup>

EDGARDO SOLANO CARRILLO, ANDREW J. MILLIS, Columbia University — In the presence of a magnetic field (produced for example by the exchange field of a ferromagnet) phonons become chiral, with left and right circularly polarized modes in addition to the longitudinal or zero-helicity mode. The scattering of spin-split electrons by chiral phonons is investigated, with particular attention to the question of whether the scattering can account for the linear resistivity observed in metallic ferromagnets at low temperature. The theory is shown to explain the observed spin relaxation time of Ni.

<sup>1</sup>ESC was supported by the Fulbright-Colciencias fellowship and AJM by NSF-DMR-1308236.

**Monday, March 14, 2016 8:00AM - 11:00AM –**

**Session A23 DMP: Novel Plasmonic Effects and Devices** 322 - Natalia Litchinitser, State University of New York, Buffalo

**8:00AM A23.00001 Plasmonic Nanomaterials for Optical-to-Electrical Energy Conversion**

MATTHEW SHELDON, Texas AM University — High-quality semiconductor solids have been the dominant photovoltaic materials platform for decades. Although several alternative approaches have been proposed, e.g. dye-sensitized cells or polymeric solids, none compete in terms of cost and conversion efficiency, the crucial benchmarks for industrial scale implementation. However, semiconductors suffer from several fundamental limitations relating to the microscopic mechanism of power conversion that preclude them, even theoretically, from achieving conversion efficiency at the Carnot limit of 95%. Indeed, the fundamentally different tasks of semiconductors in photovoltaic devices, both as optical absorbers, and separately, for electron-hole pair separation and collection, often demand opposing trade-offs in materials optimization. Alternatively, recent advances in subwavelength metal optics, e.g. nanophotonics, metamaterials, and plasmonics, provide several new examples where nanostructured metals perform the separate tasks of absorption and charge separation necessary for photovoltaic power conversion. Nanostructured metals are extremely efficient broadband absorbers of radiation, with tailorable optical properties throughout the visible and infrared spectrum. It is traditionally assumed that the lack of a band gap and consequent fast electronic relaxation (fs) and short mean free path (100 nm) hinders efficient carrier collection. However, new phenomena resulting from the remarkable energy concentration and nanoscale collection geometry afforded by plasmonic systems suggest new strategies may be possible that use all metal structures. In this talk, I will describe two ongoing studies in our laboratory that exemplify opportunities for metal-based optical energy conversion: (1) Excitation with circularly polarized illumination can induce strong, persistent electrical drift currents in resonant metal nanostructures via the inverse faraday effect. (2) Plasmonic absorption in metal nanostructures provides an entirely new mechanism for generating electrochemical potential from photons. This behavior is termed a 'plasmoelectric effect' (*Science*, 2014).

**8:36AM A23.00002 Hot carrier metamaterial detectors and energy converters**

LISA KRAYER, JEREMY N MUNDAY, Univ of Maryland-College Park — Metamaterials can be used to manipulate the flow of light in ways not typically available with traditional materials. Beyond their optical properties, metamaterials can be used as the basis for optoelectronic devices through the incorporation of a metal-semiconductor interface. The absorbed radiation in the metal can excite surface plasmons, which nonradiatively decay into hot electrons or holes that can be injected into the base semiconductor and contribute to photocurrent generation. In this talk, we will present our latest work on metamaterial photo-detectors and solar energy converters.

**8:48AM A23.00003 Non-equilibrium hot carrier dynamics in plasmonic nanostructures**

PRINEHA NARANG, RAVISHANKAR SUNDARAMAN, ADAM JERMYN, Caltech, EMILIANO CORTES, STEFAN A. MAIER, Imperial College, London, WILLIAM A. GODDARD, III, Caltech — Decay of surface plasmons to hot carriers is a new direction that has attracted considerable fundamental and application interest, yet a fundamental understanding of ultrafast plasmon decay processes and the underlying microscopic mechanisms remain incomplete. Ultrafast experiments provide insights into the relaxation of non-equilibrium carriers at the tens and hundreds of femtoseconds time scales, but do not yet directly probe shorter times with nanometer spatial resolution. Here we report the first ab initio calculations of non equilibrium transport of plasmonic hot carriers in metals and experimental observation of the injection of these carriers into molecules tethered to the metal surface. Specifically, metallic nanoantennas functionalized with a molecular monolayer allow for the direct probing of electron injection via surface enhanced Raman spectroscopy of the original and reduced molecular species. We combine first principles calculations of electron-electron and electron-phonon scattering rates with Boltzmann transport simulations to predict the ultrafast dynamics and transport of carriers in real materials. We also predict and compare the evolution of electron distributions in ultrafast experiments on noble metal nanoparticles.

**9:00AM A23.00004 Plasmon drag in esheric percolation series of metallic arrays**

XUEYUAN WU, JIANTAO KONG, KRYSZTOF KEMPA, MICHAEL J. BURNS, MICHAEL J. NAUGHTON, Boston College — Perforated thin metallic films, which evolve from hole to island arrays, form an Escheric percolation series. The plasmonic response of such a series has been investigated [1], with critical phenomena observed near the percolation threshold. In this work, we investigate the plasmon drag effect in such structures, and propose a microscopic explanation for the recently discovered plasmoelectric effect [2]. [1] E. M. Akinoglu, T. Sun, J. Gao, M. Giersig, Z.F. Ren, and K. Kempa, "Evidence for critical scaling of plasmonic modes at the percolation threshold in metallic nanostructures", *Appl. Phys. Lett.* **103**, 171106 (2013). doi: 10.1063/1.4826535 [2] M.T. Sheldon, J. v.Groep, A.M. Brown, A. Polman, H.A. Atwater, "Plasmoelectric potentials in metal nanostructures", *Science* **346**, 828-831 (2014). doi: 10.1126/science.1258405

**9:12AM A23.00005 Collective plasmonic oscillations in nanostrips arrays and sine wave gratings. Comparative study**

NATALIA NOGINOVA, Norfolk State Univ, SOHEILA MASHHADI, SARAH WILSON, FRANCES WILLIAMS, Norfolk State University, JARRETT VELLA, AUGUSTINE URBAS, AFRL, Wright-Patterson AFB, MATTHEW LEPAIN, MAXIM DURACH, Georgia Southern University — Excitation of collective plasmonic modes and their effects on optical behavior were experimentally and theoretically studied in 1 D arrays of gold nanostrips in comparison with those in continuous gold films with a sine wave profile and similar periodicity. Two kinds of collective resonance modes are efficiently excited in gold strips, with participation of gold-air and gold-glass interfaces. These modes correspond to maxima in the angular dependence of reflection, as opposed to minima observed at surface plasmon polariton conditions in a continuous sine wave grating. Spectral and polarization dependences are obtained. A theoretical approach based on the novel combined transfer-matrix coupled-wave analysis and coordinate transformation method is shown to well describe experiments.

**9:24AM A23.00006 Semiconductor-free hot carrier devices for energy harvesting and photodetection.**

TAO GONG, JEREMY MUNDAY, University of Maryland, College Park — The maximum efficiency for a single-junction solar cell is around 30% by the Shockley-Queisser (SQ) limit. The energy loss is typically through a thermalization process between the excited high-energy carriers, e.g. hot carriers, and the lattice. Therefore, the collection of the hot carriers before thermalization would allow for reduced power loss. Recently, photodetectors based on metal-semiconductor Schottky junctions have been exploiting hot electron effects to allow sub-bandgap absorption and hence show promise as near IR wavelength detectors. Here we present a simple, semiconductor-free hot carrier device based on transparent conducting oxides (TCO) electrodes. We experimentally demonstrate the hot carrier generation and extraction under monochromatic and broadband light illumination of normal and oblique incidence. Under optimized conditions, a power conversion efficiency >10% is predicted for high-energy photon excitation. The performance of the device shows further improvement by employing nanostructures, which couple the incident light into surface plasmons, leading to absorption enhancement. This semiconductor-free device provides an alternative way of energy harvesting and photodetection.

### **9:36AM A23.00007 High-contrast and fast electrochromic switching enabled by plasmonics**

ALBERT TALIN, Sandia National Labs, TING XU, ERICH WALTER, AMIT AGRAWAL, CHRISTOPHER BOHN, JEYAVEL VELMURUGAN, WENQI ZHU, HENRI LEZEC, NIST — With vibrant colors and simple, room-temperature processing methods, electrochromic polymers have long attracted attention as active materials for flexible, low-power consuming devices such as smart windows and displays. However, despite their many advantages, slow switching speed and complexity of combining several separate polymers to achieve full-color gamut has limited electrochromic materials to niche applications. Here we exploit the enhanced light-matter interaction associated with the deep-subwavelength mode confinement of surface plasmon polaritons propagating in metallic nanoslit arrays coated with ultra-thin electrochromic polymers to build a novel configuration for achieving high-contrast and fast electrochromic switching. The switchable configuration retains the short temporal charge-diffusion characteristics of thin electrochromic films while maintaining the high optical-contrast associated with thicker electrochromic coatings. We further demonstrate that by controlling the pitch of the nanoslit arrays, it is possible to achieve a full-color response with high-contrast and fast switching-speeds while relying on just one electrochromic polymer.

### **9:48AM A23.00008 Alloyed Noble Metal Nanoparticles with Tunable Optical Properties**

GARRETT C. WESSLER, CHEN GONG, Institute for Research in Electronics and Applied Physics, Dept. of Materials Science & Engr., Univ. of Maryland College Park, MARIAIA REBELLO DE SOUSA DIAS, Institute for Research in Electronics and Applied Physics, Univ. of Maryland College Park, JOSHUA A. TAILON, LOURDES G. SALAMANCA-RIBA, Dept. of Materials Science & Engr., Univ. of Maryland College Park, MARINA S. LEITE, Institute for Research in Electronics and Applied Physics, Dept. of Materials Science & Engr., Univ. of Maryland College Park — Noble metal nanoparticles (NPs) have been widely used in sensing, optics, and catalysis applications by taking advantage of surface plasmon resonance (SPR). This response is slightly tuned by varying the size and shape of the NPs; however, a method to obtain truly on-demand plasmonic responses is still lacking due to the intrinsic nature of a metal's dielectric function. Here, we fabricate size and composition controlled metal alloy NP arrays by deposit-and-anneal methods and through-template depositions. We control the composition of the metal NPs by co-sputtering and by alternating electron-beam evaporation of the Ag and Au targets. To characterize the NPs, macroscopic transmission measurements are combined with spectrally dependent near-field scanning optical microscopy to show the local optical properties around the NPs. By varying the atomic fraction of Ag and Au in the alloys, we modulate the optical properties of the NPs for different applications. For example, hot carrier plasmonic devices necessitate high absorption in the visible range, while photovoltaic applications require low absorption by the NPs.

### **10:00AM A23.00009 Plasmonic thickness variation study of gold nanostructures in ultraviolet-visible light regime**

PIJUSH GHOSH, DESALEGN TADESSE DEBU, DAVID FRENCH, STEPHEN BAUMAN, JOSEPH B. HERZOG, Univ of Arkansas-Fayetteville — Noble metal nanostructures exhibit strong surface plasmon resonances in the ultraviolet-visible light range that are not present in bulk metal. In this study, we have observed the plasmonic properties of different sized gold nanodisks and nanorods with varying thickness. The samples were fabricated by electron beam lithography on silicon dioxide substrates. Depending on the thickness of the nanostructures, strong and well-defined surface plasmon resonances were found (wavelength 400nm - 1000nm). For experimental and theoretical results, we have used Dark field spectroscopy and finite element method, respectively. We found that resonance peak was shifted with nanostructure thickness. By using Dark field spectroscopy, the scattered light from individual structures can be analyzed with less background noise and the incident light was at an angle to the substrate.

### **10:12AM A23.00010 Complex Near-Field Plasmonic Response of Au Nanospirals<sup>1</sup>**

JORDAN HACHTEL, RODERICK DAVIDSON, Vanderbilt University, ANDREW LUPINI, BENJAMIN LAWRIE, Oak Ridge National Laboratory, RICHARD HAGLUND, SOKRATES PANTELIDES, Vanderbilt University — Complex metallic nanostructures that support unique near-field surface plasmon modes have shown applications across the fields of photovoltaics, bio-sensing, and even quantum computing. Chiral Au nanospirals not only possess a non-symmetric morphology that results in second-harmonic generation, but possess multiple distinct near-field plasmonic modes that cover a wide range of plasmon frequencies. We use cathodoluminescence (CL) and electron energy loss spectroscopy (EELS) within a scanning transmission electron microscopy (STEM) to study the surface plasmons and map them with nanoscale precision. The two techniques are complementary as EELS measures excitations in the sample, while CL measures the subsequent radiative decays. We STEM-EELS/CL to map and analyze the spatial profile, intensity and polarization response of the intricate near-field plasmon modes in these versatile nanostructures.

<sup>1</sup>This work was funded by the Department of Energy grant DE-FG02-09ER46554 and the Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division

### **10:24AM A23.00011 Infrared Resonances in Plasmonic Nanorod and Nanoarc Antennas**

ANDREW LAWSON, University of Maryland, College Park, MD USA, CHASE ELLIS, JOSEPH TISCHLER, U.S. Naval Research Laboratory, Washington, DC USA, ODED RABIN, University of Maryland, College Park, MD USA — Tunability of the frequency and polarization of localized surface plasmon resonances (LSPR) of nanostructures is crucial for their implementation in nanophotonics applications such as photovoltaics, chiroptical spectroscopy, and infrared detection. We report spectroscopic data of plasmonic nanorods and nanoarcs collected by polarized Fourier transform infrared reflectance spectroscopy (FTIR). The effects of the nanostructure material, geometry and substrate material are investigated by patterning gold and aluminum structures with varying length on silicon and glass substrates, as well as on anodic aluminum oxide, a cost effective alternative to standard transparent substrates. By varying such parameters for straight rods and arcs, we find that the measured LSPR frequencies of our nanostructures span the mid-infrared spectral range ( $\lambda=2-12$  microns). However, we find that bending the nanostructures (i.e., forming arcs rather than straight rods) results in additional resonances with unique polarizations not observed in straight nanorods. We find that the nanorods exhibit half-wave antenna behavior which can be modeled using antenna theory with a linearly scaled effective wavelength which accounts for structure dimensions and material.

### **10:36AM A23.00012 Localized and Propagating Surface Plasmons in Aluminum Nanostructures: The Effect of Metal Deposition Method on Resonance Quality and Depolarization<sup>1</sup>**

VLADIMIR LIBERMAN, KENNETH DIEST, COREY STULL, MATTHEW COOK, DONNA LENNON, MORDECHAI ROTHCHILD, MIT Lincoln Laboratory, STEFAN SCHOECH, J. A. Woollam Co., Inc. — The field of plasmonics has provided revolutionary concepts in sensing, nano-optics and energy harvesting. Al plasmonics has recently emerged as an alternative, CMOS-compatible nanofabrication platform for applications in the UV-visible ranges. Previously, we found that high-temperature sputtered Al films showed significantly better plasmonic response than conventional evaporated films. Here, we extend this thin film work to patterned aluminum nanostructures that support both localized and propagating plasmon modes. The nanostructures from sputtered and evaporated aluminum are fabricated side-by-side in a CMOS compatible state-of-the-art facility. The quality of plasmonic resonances is analyzed with Mueller Matrix spectroscopic ellipsometry over a wide range of incidence angles and wavelengths. Full band structure is experimentally obtained and verified with full-field simulations. We find a strong enhancement in the ellipsometric depolarization parameter near the wavelengths of plasmonic resonance. The depolarization parameter is interpreted as a powerful connection between the near and the far field, providing a diagnostic of the quality of plasmonic resonances.

<sup>1</sup>The Lincoln Laboratory portion of this work was sponsored by the Assistant Secretary of Defense for Research & Engineering under Air Force Contract FA8721-05-C-0002.

**10:48AM A23.00013 Optical forces in a cluster of cylinders.**<sup>1</sup> , JINYING XU, Fuzhou University — We present a rigorous multiple-scattering method to calculate the optical force exerted on a cylinder placed near a cluster of parallel cylinders. Various kinds of cluster structure with both dielectric and left-hand materials are considered. It is shown that optical forces are sensitive to the position of the test cylinder, the material of the cylinders in the cluster or the structure of the system. The optical force is strong within frequency bands corresponding to surface-plasmon excitations of the cylinders.

<sup>1</sup>This work was supported by the National Natural Science Foundation of China (Grant No. 11304258).

**Monday, March 14, 2016 8:00AM - 11:00AM –**  
**Session A24 DMP: Electronic Transport through Individual Nanostructures** 323 - Pierre Darancet, Argonne National Laboratory

**8:00AM A24.00001 Quantum Transport and Emergence of Superradiant States** , AMIN TAYEBI, VLADIMIR ZELEVINSKY, Michigan State University — Quantum transport is investigated in the framework of the Feshbach projection formalism. This approach provides an alternative to popular methods such as the Feynman diagrammatic techniques and the master equation. The suggested method, being practically simpler, is quite general, not perturbative and reveals new physics, including the sharp redistribution of decay widths and the emergence of short-lived “superradiant” states and long-lived “trapped” states for sufficiently strong coupling to the leads. The superradiant states significantly enhance the transport phenomenon. An additional advantage of the formalism is its flexibility, which allows for a straightforward incorporation of disorder and additional degrees of freedom, such as phonons. Numerical results of transport through specific structures is presented. The interplay of superradiance and polaronic self-localization effects is discussed.

**8:12AM A24.00002 Validity criteria for scattering rates obtained with Fermi’s golden rule in semi-classical transport** , KRISTOF MOORS, KU Leuven, imec, BART SORE, imec, KU Leuven, U Antwerpen, WIM MAGNUS, imec, U Antwerpen — Fermi’s golden rule is often invoked to obtain scattering rates due to imperfections for semi-classical transport in different condensed matter systems. As it is an estimate for relatively small perturbations, its validity depends on the system and imperfection properties under consideration. We present a formal way to obtain easy to handle validity criteria, based on general system parameters, e.g. system size and momentum of the electron states, and the statistical properties of the imperfections. The criteria can also be obtained with a simple set of Feynman rules and corresponding diagrams. We show concrete examples of validity criteria for electron transport in metallic nanowires with several elastic scattering mechanisms, e.g. point defect or grain boundary scattering. We observe realistic nanowire examples where the scattering rate appears to be valid but also cases where the criteria are clearly violated. The latter indicates that higher order effects come into play, such as electrons being trapped between grain boundaries or at a rough surface, which cannot be described using Fermi’s golden rule. The presented validity criteria are therefore very useful to check whether or not the transport properties predicted by a semi-classical transport simulation can be trusted.

**8:24AM A24.00003 Parallel Quantum Circuit in a Tunnel Junction**<sup>1</sup> , OMID FAIZY NAMARVAR, GHASEN DRIDI, CHRISTIAN JOACHIM, PicoLab, CEMES-CNRS, GNS THEORY GROUP TEAM — In between 2 metallic nanopads, adding identical and independent electron transfer paths in parallel increases the electronic effective coupling between the 2 nanopads through the quantum circuit defined by those paths. Measuring this increase of effective coupling using the tunnelling current intensity can lead for example for 2 paths in parallel to the now standard  $G = G_1 + G_2 + 2\sqrt{G_1 G_2}$  conductance superposition law (1). This is only valid for the tunnelling regime (2). For large electronic coupling to the nanopads (or at resonance),  $G$  can saturate and even decay as a function of the number of parallel paths added in the quantum circuit (3). We provide here the explanation of this phenomenon: the measurement of the effective Rabi oscillation frequency using the current intensity is constrained by the normalization principle of quantum mechanics. This limits the quantum conductance  $G$  for example to go when there is only one channel per metallic nanopads. This effect has important consequences for the design of Boolean logic gates at the atomic scale using atomic scale or intramolecular circuits.

**References:**

- (1) Joachim et al, Phys. Rev. B, 59, 16011 (1999).
- (2) C. Joachim, Nature Nano., 7, 620 (2012).
- (3) Sadeghi et al; PNAS 2015, 112, 9, 26

<sup>1</sup>This has the financial support by European PAMS project

**8:36AM A24.00004 Multi-channel quantum dragons from rectangular nanotubes with even-odd structure**<sup>1</sup> , GODFRED INKOOOM, MARK NOVOTNY, Mississippi State University — Recently, a large class of nanostructures called quantum dragons have been discovered theoretically [1]. Quantum dragons are nanostructures with correlated disorder but have an electron transmission probability  $T(E)=1$  for all energies  $E$  when connected to idealized leads. Hence for a single channel, the electrical conductance for a two-probe measurement should give the quantum of conductance  $G_o = \frac{2e^2}{h}$ . The time independent Schrödinger equation for the single band tight binding model is solved exactly to obtain  $T(E)$ . We have generalized the matrix method and the mapping methods of [1] in order to study multi-channel quantum dragons for rectangular nanotubes with even-odd structure. The studies may be relevant for experimental rectangular nanotubes, such as MgO, copper phthalocyanine or some types of graphyne. [1] M.A. Novotny, Phys. Rev. B 90 165103 [14 pages] (2014).

<sup>1</sup>Supported in part by NSF grant DMR-1206233.

**8:48AM A24.00005 Effect of broadening in the weak coupling limit of vibrationally coupled electron transport through molecular junctions and the analogy to quantum dot circuit QED systems** , RAINER HARTLE, Institut für theoretische Physik, Georg-August-Universität Göttingen, MANAS KULKARNI, Department of Physics, New York City College of Technology, City University of New York — We [1] investigate the nonequilibrium population of a vibrational mode in the steady state of a biased molecular junction, using a rate equation approach. We focus on the limit of weak electronic-vibrational coupling and show that, in the resonant transport regime and for sufficiently high bias voltages, the level of vibrational excitation increases with decreasing coupling strength, assuming a finite and non-zero value. An analytic behavior with respect to the electronic-vibrational coupling strength is only observed if the influence of environmental degrees of freedom is explicitly taken into account. We consider the influence of three different types of broadening: hybridization with the electrodes, thermal fluctuations and the coupling to a thermal heat bath. Our results apply to vibrationally coupled electron transport through molecular junctions but also to quantum dots coupled to a microwave cavity, where the photon number can be expected to exhibit a similar behavior. [1] Rainer Hartle, Manas Kulkarni, Phys. Rev. B 91, 245429 (2015)

**9:00AM A24.00006 Landauer's formula with finite-time relaxation: Kramers' crossover in electronic transport**<sup>1</sup>, DANIEL GRUSS, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, KIRILL VELIZHANIN, Theoretical Division, Los Alamos National Laboratory, MICHAEL ZWOLAK, Center for Nanoscale Science and Technology, National Institute of Standards and Technology — Landauer's formula relates the conductance of a region of interest to its transmission probability. It is the standard theoretical tool to examine ballistic transport in nano- and meso-scale junctions and devices. This view of transport as transmission necessitates a simplified view of transmission, one occurring through an essentially fixed structure. Starting from a description of transport that includes relaxation of electrons in the reservoirs, we derive a Landauer-like formula for the steady-state current. We demonstrate that the finite relaxation time gives rise to three regimes of behavior. Weak relaxation within a small region nearby to the junction gives a contact limited current. Strong relaxation also influences the current by localizing electrons, distorting their natural dynamics and reducing the current. In an intermediate regime, the standard Landauer view is recovered. This behavior is analogous to Kramers' turnover in chemical reactions.

<sup>1</sup>Supported by UMD/CNST Cooperative Research Agreement, Award 70NANB10H193

**9:12AM A24.00007 ABSTRACT WITHDRAWN —**

**9:24AM A24.00008 Kondo-correlated transport in single molecule ferromagnetic break junction devices with controllable electrode magnetization alignment**, GAVIN SCOTT, TING-CHEN HU, Bell Labs - Murray Hill — A quantum dot attached to electrodes with magnetizations that can be switched between parallel and anti-parallel alignment has been proposed as a platform for investigating quantum criticality associated with the destruction of Kondo entanglement. We have fabricated single molecule break junction devices with elliptical ferromagnetic electrodes designed to suit this purpose. Low temperature transport measurements, supported by micromagnetic simulations, were used to investigate the magnetoresistance response on control samples during the magnetization reversal process. We show results of Kondo-correlated transport as the source and drain contacts are switched between parallel and anti-parallel magnetization configurations.

**9:36AM A24.00009 Tuning Charge and Correlation Effects for a Single Molecule on a Graphene Device**, HSIN-ZON TSAI, UCB Physics, SEBASTIAN WICKENBURG, UCB Physics and LBNL MSD, JIONG LU, UCB Physics, NUS Chemistry, NUS GRC, JOHANNES LISCHNER, UCB Physics, LBNL MSD, ARASH A. OMRANI, ALEXANDER RISS, CHRISTOPH KARRASCH, HAN SAE JUNG, RAMIN KHAJEH, DILLON WONG, UCB Physics, KENJI WATANABE, TAKASHI TANIGUCHI, NIMS Japan, ALEX ZETTL, UCB Physics, LBNL MSD, and Kavli ENSI, STEVEN G. LOUIE, UCB Physics and LBNL MSD, MICHAEL F. CROMMIE, UCB Physics, LBNL MSD, and Kavli ENSI — Controlling electronic devices down to the single molecule level is a grand challenge of nanotechnology. Single-molecules have been integrated into devices capable of tuning electronic response, but a drawback for these systems is that their microscopic structure remains unknown due to inability to image molecules in the junction region. Here we present a combined STM and nc-AFM study demonstrating gate-tunable control of the charge state of individual F4TCNQ molecules at the surface of a graphene field effect transistor. This is different from previous studies in that the Fermi level of the substrate was continuously tuned across the molecular orbital energy level. Using STS we have determined the resulting energy level evolution of the LUMO, its associated vibronic modes, and the graphene Dirac point (ED). We show that the energy difference between ED and the LUMO increases as EF is moved away from ED due to electron-electron interactions that renormalize the molecular quasiparticle energy. This is attributed to gate-tunable image-charge screening in graphene and corroborated by ab initio calculations.

**9:48AM A24.00010 Probing voltage induced bond rupture in a molecular junction**<sup>1</sup>, HAIXING LI, Department of Applied Physics and Applied Mathematics, Columbia University, TIMOTHY SU, NATHANIEL KIM, Department of Chemistry, Columbia University, PIERRE DARANCET, Argonne National Laboratory Center for Nanoscale Materials, JAMES LEIGHTON, MICHAEL STEIGERWALD, COLIN NUCKOLLS, Department of Chemistry, Columbia University, LATHA VENKATARAMAN, Department of Applied Physics and Applied Mathematics, Columbia University — We use scanning tunneling microscope break junction to study electric field breakdown at the single molecule level. We investigate breakdown phenomena in atomic chains composed of Si—Si, Si—O, Si—C, Ge—Ge and C—C bonds that are commonly found in the low- $\kappa$  dielectric material. We see different bond rupture behaviors in a range of molecular backbones, and use the results from a statistically large number of measurements to determine which bond breaks. We find that Si—Si and Ge—Ge bonds rupture above a 1V bias. We also find that the Si—C bond is more robust than Si—O or Si—Si bond at above 1V. Finally, we illustrate how an additional conductance pathway in parallel to the Si—Si bond changes bond rupture behavior under an electric field. We carry out ab initio calculations on these systems and demonstrate that the mechanism for bond rupture under electric field involves "heating" of the molecule through electron-vibrational mode coupling.

<sup>1</sup>Haixing Li is supported by Semiconductor Research Corporation and New York CAIST program. We thank the NSF for the support of these studies under grant no. CHE-1404922.

**10:00AM A24.00011 ABSTRACT WITHDRAWN —**

**10:12AM A24.00012 Bias-dependent enhancement of the Fano factor in atomic-scale Au junctions**, LOAH STEVENS, PAVLO ZOLOTAVIN, RUOYU CHEN, DOUGLAS NATELSON, Rice University — We report measurements of current noise in STM-style Au break junctions at 77K, focusing on the dependence of the Fano factor on applied bias. In room temperature investigations of similar systems, measured noise at low bias (<150 mV) was observed to agree well with Landauer-Büttiker theory for shot noise at a fixed electronic temperature. At higher biases, however, measured noise exhibited a superlinear dependence on scaled bias above the low bias expectations. In the present experiment at cryogenic temperatures, we also observe this nonlinear increase of noise. We will discuss this behavior in terms of an enhancement of the Fano factor above the predicted model for minimum open transmission channels, and how the data constrain possible explanations of this excess noise. Furthermore, we will examine channel mixing in transport through the junction from measured Fano factor and conductance.

**10:24AM A24.00013 Electron Transport in Short Peptide Single Molecules**<sup>1</sup>, JING CUI, Department of Physics, Columbia University, JOSEPH BRISENDINE, Department of Physics, The City College of New York, FAY NG, COLIN NUCKOLLS, Department of Chemistry, Columbia University, RONALD KODER, Department of Physics, The City College of New York, LATHA VENKATARAMAN, Department of Applied Physics and Applied Mathematics — We present a study of the electron transport through a series of short peptides using scanning tunneling microscope-based break junction method. Our work is motivated by the need to gain a better understanding of how various levels of protein structure contribute to the remarkable capacity of proteins to transport charge in biophysical processes such as respiration and photosynthesis. We focus here on short mono, di and tri-peptides, and probe their conductance when bound to gold electrodes in a native buffer environment. We first show that these peptides can bind to gold through amine, carboxyl, thiol and methyl-sulfide termini. We then focus on two systems (glycine and alanine) and show that their conductance decays faster than alkanes terminated by the same linkers. Importantly, our results show that the peptide bond is less conductive than a sigma carbon-carbon bond.

<sup>1</sup>This work was supported in part by NSF-DMR 1507440

**10:36AM A24.00014 Controlled fabrication of DNA molecular templates for the deposition and electrical measurement of 1D metal nanowires**, JORGE BARREDA, LONGQIAN HU, LIUQI YU, ZHIBIN WANG, JUNFEI XIA, JINGJIAO GUAN, PENG XIONG, Florida State University, GUAN'S GROUP TEAM, XIONG'S GROUP TEAM — Stretched DNA nanowires (NWs) offer a convenient substrate for the fabrication and measurement of 1D metal NWs of width down to nm [1]. So far the fabrication of the DNA templates has relied on somewhat random self-assembly processes. Here we demonstrate a process with high degree of control over the length, spacing, diameter, and orientation of the metal NWs: A one-step dewetting of a DNA solution on a PDMS stamp with an array of micropillars with well-defined pitch yields DNA NWs suspended across the micropillars along a chosen direction [2]. The DNA NWs are then transferred via micro-contact printing onto a Si/SiO<sub>2</sub>/SiN<sub>x</sub> substrate with a lithographically fabricated trench defined by an opening in the SiN<sub>x</sub> layer and undercut in the SiO<sub>2</sub> layer. The template with DNA NWs stretched across the trench is placed in a high-vacuum evaporator for metal deposition, resulting in a metal NW of width defined by the diameter of the DNA template (<10 nm) and length determined by the width of the trench. Quasi-four terminal I-V measurements are performed in situ with incremental metal deposition. Concomitant with a transition from strongly nonlinear IV to Ohmic behavior with increasing thickness, the NW resistance is observed to decrease exponentially. [1] Hopkins, David S., et al. Science 308.5729 (2005): 1762-1765. [2] Guan, Jingjiao, et al. Soft Matter 3.11 (2007): 1369-1371.

**10:48AM A24.00015 Electron field emission from Ge nanoclusters on Si.**, VERONIKA BUROBINA, University of California - San Diego — We analyzed the electron field emission from Ge nanoclusters grown on Si substrate by the method of molecular beam epitaxy. The emission properties were studied with the use of scanning tunneling microscopy. The phenomenological model of the field emission mechanism was applied to estimate current density from the surface of the pointed Ge/Si nanostructures.

**Monday, March 14, 2016 8:00AM - 10:48AM —**

**Session A25 DCMP: Superconductivity: Odd Parity** 324 - Daniel Agterberg, University of Wisconsin, Milwaukee

**8:00AM A25.00001 Identifying detrimental effects for multi-band superconductivity - Application to Sr<sub>2</sub>RuO<sub>4</sub>**<sup>1</sup>, ALINE RAMIRES, Institute for Theoretical Sciences - ETH Zurich, MANFRED SIGRIST, Institute for Theoretical Physics - ETH Zurich — Spin polarization and anti-symmetric spin-orbit coupling are detrimental to Cooper pairing in the spin singlet and spin triplet channel, respectively. These are the well-known features of paramagnetic limiting and selection rules in non-centrosymmetric superconductors. We propose a general scheme to probe the compatibility of arbitrary pairing states with given normal state properties in model systems. This yields a universal criterion which we validate with results based on weak coupling analysis of the stability of different superconducting gaps under time-reversal and inversion symmetry breaking fields. Our criterion does, however, not address directly any aspects concerned with the pairing mechanism. A merit of the criterion is that it can be easily applied to the stability analysis of superconducting states in multi-band systems, to establish gap structures favourable within a given complex band structure. As such it can serve as a tool to identify non-trivial mechanisms to suppress superconductivity under various external influences, in particular, magnetic fields or distortions. We apply our criterion to the multi-band superconductor Sr<sub>2</sub>RuO<sub>4</sub> with the aim to explore possible explanations for the limiting feature observed in the in-plane upper critical field.

<sup>1</sup>\*This work was supported by Dr. Max Rössler, the Walter Haefner Foundation and the ETH Zurich Foundation (AR) and by the Swiss National Science Foundation (MS).

**8:12AM A25.00002 Experimentally observable signatures of odd-frequency pairing in multi-band superconductors**, LUCIA KOMENDOVA, Uppsala University, Sweden, ALEXANDER V. BALATSKY, Nordita, Stockholm, Sweden and Los Alamos National Laboratory, US, ANNICA M. BLACK-SCHAFFER, Uppsala University, Sweden — We report on how hybridization (single-quasiparticle scattering) between two superconducting bands induces odd-frequency superconductivity in a multiband superconductor. Using the Green's functions formalism we derived the odd-frequency pairing correlation and its full frequency dependence. We found that the density of states is modified, at higher energies, from the sum of the two BCS spectra to also include additional hybridization gaps with strong coherence peaks when odd-frequency pairing is present. These gaps constitute clear experimentally measurable signatures of odd-frequency pairing in multiband superconductors. [1] L. Komendova, A. V. Balatsky, and A. M. Black-Schaffer, Phys. Rev. B 92, 094517 (2015).

**8:24AM A25.00003 Odd-parity superconductivity in the vicinity of inversion symmetry breaking in spin-orbit-coupled systems**<sup>1</sup>, VLADYSLAV KOZII, LIANG FU, Massachusetts Institute of Technology, MASSACHUSETTS INSTITUTE OF TECHNOLOGY TEAM — We study superconductivity in spin-orbit-coupled systems in the vicinity of inversion symmetry breaking. We find that due to the presence of spin-orbit coupling, fluctuations of the incipient parity-breaking order generate an attractive pairing interaction in an odd-parity pairing channel, which competes with the *s*-wave pairing. We show that Coulomb repulsion or an external Zeeman field suppresses the *s*-wave pairing and promotes the odd-parity superconducting state. Our work provides a new mechanism for odd-parity pairing and opens a route to novel topological superconductivity.

<sup>1</sup>This work is supported by the David and Lucile Packard foundation.

**8:36AM A25.00004 Triplet p<sub>z</sub>-wave pairing in quasi-one-dimensional A<sub>2</sub>Cr<sub>3</sub>As<sub>3</sub> superconductors (A = K,Rb,Cs)**<sup>1</sup>, FAN YANG, School of Physics, Beijing Institute of Technology, XIANXIN WU, JIANGPING HU, CONGCONG LE, HENG FAN, Institute of Physics, Chinese Academy of Sciences — We construct minimum effective models to investigate the pairing symmetry in the newly discovered quasi-one-dimensional superconductor K<sub>2</sub>Cr<sub>3</sub>As<sub>3</sub>. We show that a minimum three-band model based on the d<sub>z<sup>2</sup></sub>, d<sub>xy</sub>, and d<sub>x<sup>2</sup>-y<sup>2</sup></sub> orbitals of one Cr sublattice can capture the band structures near Fermi surfaces. In both weak and strong coupling limits, the standard random phase approximation and mean-field solutions consistently yield the triplet p<sub>z</sub>-wave pairing as the leading pairing symmetry for physically realistic parameters. The triplet pairing is driven by the ferromagnetic fluctuations within the sublattice. The gap function of the pairing state possesses line gap nodes on the k<sub>z</sub> = 0 plane on the Fermi surfaces. Experimental consequences of the triplet p<sub>z</sub>-wave pairing are also discussed, including the NMR, superfluid density and phase-sensitive dc SQUID experiments.

<sup>1</sup>This work is supported in part by MOST of China (Grants No. 2012CB821400, No. 2011CBA00100, and No. 2015CB921300), NSFC (Grants No. 11190020, No.91221303, No.11334012, and No. 11274041) and the NCET program under Grant No. NCET-12-0038.

**8:48AM A25.00005 Leggett modes in the multi-band superconductor  $\text{Sr}_2\text{RuO}_4$ <sup>1</sup>**, WEN HUANG, McMaster University, MANFRED SIGRIST, Institute for Theoretical Physics, ETH Zurich, CATHERINE KALLIN, McMaster University —  $\text{Sr}_2\text{RuO}_4$  is a prototypical multi-band superconductor, with three bands crossing the Fermi level. These bands exhibit distinct dimensional characteristics, with one quasi-2D  $\gamma$ -band and two quasi-1D  $\alpha$ - and  $\beta$ - bands. As a consequence, the superconducting order parameter on the  $\gamma$ - and  $\alpha/\beta$ -bands may only be weakly Josephson-coupled, in contrast to the stronger coupling between the quasi-1D bands. In this work, we study the Leggett modes associated with the relative phase fluctuations between the bands. We show that a soft Leggett mode exists in the case of comparatively weaker inter-band Josephson coupling between the  $\gamma$ - and  $\alpha/\beta$ -bands. We further analyze the dependence of the inter-band Josephson coupling on spin-orbit coupling, and discuss the possibility of an exotic time-reversal symmetry breaking phase when the Josephson coupling is comparable between all pairs of bands.

<sup>1</sup>Work supported by NSERC and CIFAR in Canada, Pauli Center for Theoretical Studies of ETH Zurich and the Swiss National Science Foundation.

**9:00AM A25.00006 Microscopic model of the Knight shift in anisotropic and correlated metals<sup>1</sup>**, RICHARD KLEMM, BIANCA HALL, University of Central Florida — We present a microscopic model of nuclear magnetic resonance in metals. The spins of the spin-1/2 local nucleus and its surrounding orbital electrons interact with the arbitrary constant  $B_0$  and perpendicular time-oscillatory magnetic inductions  $B_1(t)$  and with each other via an anisotropic hyperfine interaction. An Anderson-like Hamiltonian describes the excitations of the relevant occupied local orbital electrons into the conduction bands, each band described by an anisotropic effective mass with corresponding Landau orbits and an anisotropic spin  $g$  tensor. Local orbital electron correlation effects are included using the mean-field decoupling procedure of Lacroix. The Knight resonance frequency and corresponding linewidth shifts are evaluated to leading orders in the hyperfine and Anderson excitation interactions. While respectively proportional to  $(B_1/B_0)^2$  and a constant for weak  $B_0 \gg B_1$ , both highly anisotropic shifts depend strongly upon  $B_0$  when a Landau level is near the Fermi energy. Electron correlations affect the anisotropy of the linewidth shift.

<sup>1</sup>The authors acknowledge support from an anonymous donor

**9:12AM A25.00007 Odd-frequency Superconductivity in Driven Systems**, CHRISTOPHER TRIOLA, Nordita, ALEXANDER BALATSKY, IMS, Los Alamos National Lab and Center for Quantum Materials, Nordita — We show that Berezinskiis classification of the symmetries of Cooper pair amplitudes in terms of parity under transformations that invert spin, space, time, and orbital degrees of freedom holds for driven systems even in the absence of translation invariance. We then discuss the conditions under which pair amplitudes which are odd in frequency can emerge in driven systems. Considering a model Hamiltonian for a superconductor coupled to an external driving potential, we investigate the influence of the drive on the anomalous Greens function, density of states, and spectral function. We find that the anomalous Greens function develops odd in frequency component in the presence of an external drive. Furthermore we investigate how these odd-frequency terms are related to satellite features in the density of states and spectral function. Supported by US DOE BES E 304.

**9:24AM A25.00008 Majorana zero modes in  $p + ip$  superconducting rings with half quantum flux in the presence of a  $d$ -soliton<sup>1</sup>**, ALI BEYRAMZADEH MOGHADAM, KIRILL SHTENGEL, University of California - Riverside — Half-integer flux quantization has been observed in mesoscopic rings of superconducting  $\text{Sr}_2\text{RuO}_4$ <sup>2</sup>. This finding suggests a chiral  $p + ip$  nature of the superconducting order parameter. Under the assumption that the  $d$ -vector (which parametrizes the triplet pairing) lies in the plane of a 2D superconductor, such rings are expected to support Majorana zero modes at their inner and outer edges. However, such modes have not been directly observed in experiments. More recently, H.-Y. Kee and M. Sigrist argued that the spin-orbit coupling in such systems can stabilize a different spin texture, also consistent with half-quantum vortices<sup>3</sup>. That spin texture is characterized by the presence of a so-called  $d$ -soliton — a radial domain wall between the regions where the  $d$ -vector is oriented in the positive and negative  $z$ -directions. Our theoretical investigation of superconducting rings with  $d$ -solitons confirms the existence of two Majorana zero modes, one at each boundary. Furthermore, the presence of a  $d$ -soliton enhances the hybridization between the localized Majorana modes at the inner and outer boundaries.

<sup>1</sup>This work is supported by NSF Grant No. DMR-1411359.

<sup>2</sup>J. Jang et al. Science **331**, 186 (2011)

<sup>3</sup>H.-Y. Kee, M. Sigrist, arXiv:1307.5859

**9:36AM A25.00009 Scanning SQUID Microscopy of  $\text{Sr}_2\text{RuO}_4$  Under Anisotropic Strain**, CHRISTOPHER A. WATSON, HILARY NOAD, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, Menlo Park, CA, USA, ALEXANDRA GIBBS, ANDREW P. MACKENZIE, CLIFFORD W. HICKS, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, KATHRYN A. MOLER, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, Menlo Park, CA, USA — The proposed  $p_x \pm ip_y$  topological superconducting state of  $\text{Sr}_2\text{RuO}_4$  has motivated a great deal of experimental effort. While some experimental results are consistent with this order parameter, others are not, and the question of the order parameter remains unsettled. Furthermore, it is possible that multiple order parameters are nearly degenerate, such that perturbing the sample may induce a change in order parameter. It was recently demonstrated that  $T_c$  is strongly enhanced under anisotropic strain with  $\langle 100 \rangle$  principle axes; the dependence on strain was essentially quadratic, but with an anomaly at low strains. In this work, we will use a scanning SQUID susceptometer to study the local diamagnetic response of the superconducting state as a function of temperature and applied strain. We will investigate the homogeneity of the superconductivity and the precise dependence of  $T_c$  on strain without inhomogeneity-related broadening.

**9:48AM A25.00010 Realization of a mixed-symmetry superconducting gap in correlated organic metals<sup>1</sup>**, MICHAELA ALTMAYER, DANIEL GUTERDING, HARALD O. JESCHKE, Institute for Theoretical Physics, Goethe-University Frankfurt, Germany, SANDRA DIEHL, TORSTEN METHFESSEL, Institute for Physics, Johannes Gutenberg-University Mainz, Germany, ULRICH TUTSCH, HARALD SCHUBERT, MICHAEL LANG, JENS MÜLLER, MICHAEL HUTH, Department of the Physical Institute, Goethe-University Frankfurt, Germany, MARTIN JOURDAN, HANS-JOACHIM ELMERS, Institute for Physics, Johannes Gutenberg-University Mainz, Germany, ROSER VALENTI, Institute for Theoretical Physics, Goethe-University Frankfurt, Germany — Recent scanning tunneling spectroscopy measurements on the organic charge transfer salt  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu[N(CN)<sub>2</sub>]Br show clear evidence of a highly anisotropic gap structure. Based on an *ab initio* derived model Hamiltonian we employ random phase approximation spin fluctuation theory yielding a composite order parameter of (extended)  $s + d_{x^2-y^2}$  symmetry. Taking explicitly also the shape of the Fermi surface into account we calculate STS spectra that are in excellent agreement to the experimental observations [1]. Moreover we determine the minimal tight binding model to describe the general lattice structure of these compounds accurately and generate a phase diagram for the gap symmetry by varying the hopping parameters. Based on *ab initio* derived parameter sets we predict the gap symmetry of other superconducting  $\kappa$  charge transfer salts.

<sup>1</sup>This work was supported by Deutsche Forschungsgemeinschaft under Grant No. SFB/TR 49.

**10:00AM A25.00011 Quasiparticles near domain walls in hexagonal superconductors<sup>1</sup>**, SOUMYA MUKHERJEE, KIRILL SAMOKHIN, Brock University, Department of Physics — We calculate the energy spectrum of quasiparticles trapped by a domain wall separating different time reversal symmetry-breaking ground states in a hexagonal superconductor, such as UPt<sub>3</sub>. The bound state energy is found to be strongly dependent on the gap symmetry, the domain wall orientation, the quasiparticle's direction of semiclassical propagation, and the phase difference between the domains. We calculate the corresponding density of states and show how one can use its prominent features, in particular, the zero-energy singularity, to distinguish between different pairing symmetries.

<sup>1</sup>Discovery Grant from the Natural Sciences and Engineering Research Council of Canada

**10:12AM A25.00012 Dynamic Quantum Phase Transitions in Holographic Superconductors**, MOON JIP PARK, MATTHEW GILBERT, Univ of Illinois - Urbana — A non-equilibrium quench that crosses a quantum critical point is known to exhibit distinct behavior from trivial quench. This is readily apparent via examination of the Loschmidt echo that contains the Yang-Lee (YL) zeros in the non-equilibrium quench within the vanishing returning rate of ground state when the quantum critical point is crossed. While previous studies on the dynamical quenches are restricted within non-interacting systems, we use of the Loschmidt echo to understand quenches within strongly interacting conformal field theories using holographic mapping. We show that the free energy of the gravitational dual possesses YL zeros at the superconducting critical temperature. We argue that, on the gravitational side, the presence of YL zeros implies that the free energy is invariant under a set of discrete deformations of the metric characterized by the time at which the returning rate vanishes. We illustrate these ideas using a holographic superconductor constructed via the coupling of AdS gravity with a Maxwell field and charged scalar.

**10:24AM A25.00013 Knight shift and spin relaxation in the single band 2D Hubbard model.**, JAMES LEBLANC, XI CHEN, EMANUEL GULL, Univ of Michigan - Ann Arbor — We study in detail the roles of spin and charge fluctuations in the single band 2D Hubbard model. Using dynamical mean field theory and cluster extensions such as the dynamical cluster approximation (DCA), we compute the full two particle susceptibilities in the spin and charge representations. By performing analytic continuations we obtain the temperature and doping dependence of the spin-lattice relaxation ( $T_1^{-1}$ ) and knight shift in the 2D Hubbard model relevant to NMR results on doped cuprates and connect these to RPA results in weak coupling limits.

**10:36AM A25.00014 Magnetism and experimental consequences of  $p_z$ -wave spin triplet state in quasi-one-dimensional  $A_2Cr_3As_3$  superconductors**, XIANXIN WU, Institute of Physics, Chinese Academy of Sciences, FAN YANG, 2School of Physics, Beijing Institute of Technology, CONGCONG LE, JING YUAN, SHENGSHAN QIN, HENG FAN, JIANGPING HU, Institute of Physics, Chinese Academy of Sciences — The recently discovered quasi-one dimensional superconductors  $A_2Cr_3As_3$  ( $A=K,Rb,Cs$ ), are found to possess strong frustrated magnetic fluctuations and are nearby a novel in-out co-planar magnetic ground state. Then, we find that the triplet  $p_z$ -wave pairing is strongly favored. Finally, with  $p_z$  wave pairing state, we obtain the specific heat, superfluid density, Knight shift and spin relaxation rate and find that all these properties at low temperature ( $T \ll T_c$ ) show powerlaw behaviors and are consistent available experiments. Particularly, the superfluid density determined by the  $p_z$ -wave pairing state in this quasi-one dimensional system is anisotropic: the in-plane superfluid density varies as  $\Delta\rho_{\parallel} \sim T$  but the out-plane one varies as  $\Delta\rho_{\perp} \sim T^3$  at low temperature. The anisotropic upper critical field reported in experiment is consistent with the  $S_z = 0$  (i.e.,  $(\uparrow\downarrow + \downarrow\uparrow)$ )  $p_z$ -wave pairing state. We also suggest the phase-sensitive dc-SQUID measurements to pin down the triplet  $p_z$ -wave pairing state. References: [1] X. Wu et al., Chin. Phys. Lett. 32, 057401 (2015). [2] X. Wu et al., Phys. Rev. B 92,104511 (2015). [3] X. Wu et al., arXiv: 1507.07451 (2015)

**Monday, March 14, 2016 8:00AM - 10:48AM –**

**Session A26 DMP: Experimental Advances in Strongly Spin-orbit Coupled Oxides** 325 - Kyle Shen, Cornell

**8:00AM A26.00001 Ultrafast Optical Reflectivity Study of Photo-Carrier Relaxation Dynamics in Perovskite Iridates**, HAO CHU, LIUYAN ZHAO, Caltech, TOM HOGAN, STEPHEN WILSON, University of California, Santa Barbara, DAVID HSIEH, Caltech, CALTECH COLLABORATION, UNIVERSITY OF CALIFORNIA, SANTA BARBARA COLLABORATION — The Ruddlesden-Popper series of perovskite iridates  $Sr_{n+1}Ir_nO_{3n+1}$  lie close to a localization-delocalization boundary, evolving from a Mott-like magnetic insulator in the single layer ( $n=1$ ) compound to a paramagnetic semi-metal in the infinite layer ( $n=\infty$ ) compound. We will discuss the insulator-to-metal transition in perovskite iridates from the point of view of time-resolved optical reflectivity measurements. This technique probes the relaxation dynamics of photo-generated carriers, which are strongly affected by the presence of a charge gap.

**8:12AM A26.00002 Ionic liquid gating  $Sr_2IrO_4$  single crystal<sup>1</sup>**, BOYI YANG, ALLEN GOLDMAN, Univ of Minnesota - Twin Cities — The 5d iridates have attracted much interest due to the prediction of novel electronic phases driven by the interplay of spin-orbit coupling with onsite Coulomb interaction. The compound  $Sr_2IrO_4$ , with a crystal structure similar to that of  $La_2CuO_4$ , was identified as a spin-orbital Mott insulator. It has been doped in various ways in search of a possible superconducting state considering its similarities to the cuprates. Unlike the common ionic liquid gated thin film field effect transistor (FET), here we have fabricated an ionic liquid (DEME-TFSI) gated FET based on the cleaved ab plane surface of a  $Sr_2IrO_4$  single crystal. Due to the insulating behavior of the bulk, the sensitive surface gating effect can be characterized with transport property measurements. We find an insulator to metal transition around 75K upon hole doping, while a minimal gating effect is observed on electron accumulation at the cleaved single crystal surface. The low temperature metallic behavior will be further studied in detail and the latest experimental results will be reported.

<sup>1</sup>This work was primarily supported by the National Science Foundation through the University of Minnesota MRSEC under Award No. DMR-1420013, and partially supported by the National Science Foundation under Award No. DMR-1209578.

**8:24AM A26.00003 Decoupling of the Antiferromagnetic and Insulating States in Tb doped  $\text{Sr}_2\text{IrO}_4$** <sup>1</sup>, H. ZHENG, Center for Advanced Materials and Department of Physics and Astronomy University of Kentucky, Lexington, KY 40506, USA, J.C. WANG, F. YE, Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, S. ASWARTHAM, J. TERZIC, S.J. YUAN, Center for Advanced Materials and Department of Physics and Astronomy University of Kentucky, Lexington, KY 40506, USA, D. HASKEL, Y. CHOI, Advanced Photon Source, Argonne National Laboratory, Argonne IL 60439, USA, S. CHIKARA, National High Magnetic Field Laboratory, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, P. SCHLOTTMANN, Department of Physics, Florida State University, Tallahassee, FL 32306, USA, R. CUSTELCEAN, Chemical Science Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, G. CAO, Center for Advanced Materials and Department of Physics and Astronomy University of Kentucky, Lexington, KY 40506, USA — We report results of a comprehensive study of single-crystal  $\text{Sr}_2\text{Ir}_{1-x}\text{Tb}_x\text{O}_4$  ( $0 \leq x \leq 0.03$ ). This study found that mere 3% ( $x=0.03$ ) tetravalent  $\text{Tb}^{4+}$  substituting for  $\text{Ir}^{4+}$  (rather than  $\text{Sr}^{2+}$ ) completely suppresses the long-range collinear AFM transition but retains the insulating state. Tb doping effectively changes the relative strength of the SOI and the tetragonal CEF and enhances the Hund's rule coupling that competes with the SOI, and destabilizes the AFM state. We observe unconventional correlation between the AFM and insulating states in which the magnetic transition plays no critical role in the formation of the charge gap in the iridate.

<sup>1</sup>This work was supported by NSF through grant DMR-1265162.

**8:36AM A26.00004 Switching the d-wave gap in layered perovskite iridates via spin reorientation**, BUMJOON KIM, Max Planck Institute for Solid State Research — We demonstrate switching of the *d*-wave charge gap in electron-doped  $\text{Sr}_3\text{Ir}_2\text{O}_7$  through changing the spin easy axis. The pristine, undoped  $\text{Sr}_3\text{Ir}_2\text{O}_7$  has *c*-axis collinear antiferromagnetic structure with strong Ising anisotropy, which gaps out magnons with an unprecedentedly large energy scale of 90 meV. However, a metastable phase with *ab* easy-plane anisotropy is found in some surfaces of  $\text{Sr}_3\text{Ir}_2\text{O}_7$ , for which low-energy magnons are expected. Doping electrons to the latter leads to opening of a *d*-wave charge gap below ~30 K, which is not found in the former. Our results indicate the magnetic origin of the *d*-wave gap in electron-doped layered perovskite iridates, and suggest a mechanism to control the charge gap via the spin degrees of freedom.

**9:12AM A26.00005 Isotropic and anisotropic regimes of the spin-dynamics in  $\text{Sr}_2\text{IrO}_4$  : Field-dependent Raman scattering study**<sup>1</sup>, Y. GIM, A. SETHI, Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, 104 South Goodwin Avenue, Urbana, Illinois 61801-2902, Q. ZHAO, J.F. MITCHELL, Material Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA, G. CAO, Center for Advanced Materials, University of Kentucky, Lexington, Kentucky 40506, USA, S.L. COOPER, Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, 104 South Goodwin Avenue, Urbana, Illinois 61801-2902 — Experimental studies of the strong spin-orbit coupled material,  $\text{Sr}_2\text{IrO}_4$ , have provided evidence that the spin dynamics of this material can be described by an isotropic two-dimensional effective Heisenberg description. To study how well this description describes the spin-dynamics of  $\text{Sr}_2\text{IrO}_4$  in different magnetic field regimes, in this talk, we present field-dependent Raman scattering studies of the low-energy spin-dynamics in  $\text{Sr}_2\text{IrO}_4$ . We find that for  $H > 1.5$  T, the spin-dynamics of  $\text{Sr}_2\text{IrO}_4$  are well described by an isotropic, 2D description. However, at low fields,  $H < 1.5$  T, the spin dynamics show evidence for the effects of in-plane anisotropy and interlayer coupling. These effects must therefore be considered when modeling the low-field magnetic and dynamical properties of  $\text{Sr}_2\text{IrO}_4$ .

<sup>1</sup>This work was supported by the National Science Foundation under Grant NSF DMR 14-64090.

**9:24AM A26.00006 From  $J_{\text{eff}} = 1/2$  insulator to p-wave superconductor in single-crystal  $\text{Sr}_2\text{Ir}_{1-x}\text{Ru}_x\text{O}_4$  ( $0 \leq x \leq 1$ )**<sup>1</sup>, SHUJUAN YUAN, SAICHARAN ASWARTHAM, JASMINKA TERZIC, HAO ZHENG, HENGDI ZHAO, Center for Advanced Materials, Department of Physics and Astronomy, University of Kentucky, Lexington, Kentucky 40506, USA, PEDRO SCHLOTTMANN, Physics Department, Florida State University, Tallahassee, FL 32306, USA, GANG CAO, Center for Advanced Materials, Department of Physics and Astronomy, University of Kentucky, Lexington, Kentucky 40506, USA —  $\text{Sr}_2\text{IrO}_4$  is a magnetic insulator assisted by strong spin-orbit coupling (SOC) whereas the  $\text{Sr}_2\text{RuO}_4$  is a p-wave superconductor. Our investigation of structural, transport, and magnetic properties reveals that substituting 4d  $\text{Ru}^{4+}$  ( $4d^4$ ) ions for 5d  $\text{Ir}^{4+}$  ( $5d^5$ ) ions in  $\text{Sr}_2\text{IrO}_4$  directly adds holes to the  $t_{2g}$  bands, reduces the SOC and thus rebalances the competing energies in single-crystal  $\text{Sr}_2\text{Ir}_{1-x}\text{Ru}_x\text{O}_4$ . A profound effect of Ru doping driving a rich phase diagram is a structural phase transition from a distorted  $I4_1/acd$  to a more ideal  $I4/mmm$  tetragonal structure near  $x=0.50$  that accompanies a phase transition from an antiferromagnetic-insulating state to a paramagnetic-metal state. We also make a comparison drawn with Rh doped  $\text{Sr}_2\text{IrO}_4$ , highlighting important similarities and differences.

<sup>1</sup>This work was supported by the National Science Foundation via Grant No. DMR-1265162 and by Department of Energy (BES) through grant No. DE-FG02-98ER45707 (PS).

**9:36AM A26.00007 Probing Novel States of Iridates and Ruthenates under Extreme Conditions**<sup>1</sup>, JASMINKA TERZIC, HAO ZHENG, Center for Advanced Materials and Department of Physics and Astronomy, University of Kentucky, Lexington, KY 40506, USA, PANPAN KONG, CHANQING JIN, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, DANIEL HASKEL, Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, USA, OLEKSANDR KORNETA, Center for Correlated Electron Systems, Institute for Basic Science (IBS), Seoul National University, Seoul 151-742, Korea, SHUJUAN YUAN, GANG CAO, Center for Advanced Materials and Department of Physics and Astronomy, University of Kentucky, Lexington, KY 40506, USA — The highly delicate balance between competing energies in materials of interest makes high-pressure and high-magnetic-field powerful probes for generating novel states. Our studies have uncovered a number of remarkable properties of iridates and ruthenates under extreme conditions: avoidance of metallization at high pressures, absent conventional correlations between magnetic and insulating states in iridates; coexistence of a bulk insulating state and quantum oscillations period in  $1/B$  or  $B$  (depending on the orientation of  $B$  which is applied magnetic field), and colossal magnetoresistivity without spin polarization in ruthenates. We will present and discuss our results with comparison drawn with relevant systems.

<sup>1</sup>This work was supported by NSF via a grant DMR-1265162

**9:48AM A26.00008 Mott Physics in lightly doped  $(\text{Sr}_{1-x}\text{La}_x)_3\text{Ir}_2\text{O}_7$** , GREGORY AFFELDT, TOM HOGAN, University of California, Berkeley and Lawrence Berkeley National Laboratory, CHRISTOPHER SMALLWOOD, University of California, Berkeley, TANMOY DAS, Los Alamos National Laboratory, JONATHAN DENLINGER, SUNG-KWAN MO, Lawrence Berkeley National Laboratory, STEPHEN WILSON, University of California, Santa Barbara, ALESSANDRA LANZARA, University of California, Berkeley and Lawrence Berkeley National Laboratory — The layered perovskite iridates  $\text{Sr}_2\text{IrO}_4$  and  $\text{Sr}_3\text{Ir}_2\text{O}_7$  exhibit a spin-orbit Mott insulating state that becomes metallic upon sufficient carrier doping. While  $\text{Sr}_2\text{IrO}_4$  presents striking similarities to cuprates upon electron doping,  $\text{Sr}_3\text{Ir}_2\text{O}_7$  appears to be a correlated metal. We show a detailed doping and temperature-dependent ARPES study which reveals important similarities between  $(\text{Sr}_{1-x}\text{La}_x)_3\text{Ir}_2\text{O}_7$  and doped  $\text{Sr}_2\text{IrO}_4$ , as well as other doped Mott insulators.

**10:00AM A26.00009 Shubnikov-de Haas oscillation of  $\text{KTaO}_3$  based electron gases**, LUDI MIAO, RENZHONG DU, QI LI, The Pennsylvania State University, QI LI'S LAB TEAM — Two-dimensional electron gases (2DEGs) at transition metal oxide (TMO) surfaces and interfaces have attracted much attention due to their exotic properties such as superconductivity, and ferromagnetism. Recently, 5d TMOs are hotly investigated due to their strong spin-orbit coupling (SOC), an indispensable element for topological insulating states. Among them,  $\text{KTaO}_3$  not only hosts 2DEGs but also involves strong SOC. We have created  $\text{KTaO}_3$  based electron gases, with low temperature mobility as large as  $8000\text{cm}^2\text{V}^{-1}\text{s}^{-1}$ . Shubnikov de Haas oscillations in magnetoresistance have been observed at 1.8 K for field applied along various directions. Contributions from  $d_{xy}$  and  $d_{xz/yz}$  bands are both seen. These oscillation curves exhibit a field direction dependence with 4-fold symmetry, revealing the cubic symmetry of Fermi surface of  $\text{KTaO}_3$  based electron gases. Moreover, the intercept of oscillation indices is close to 0.5, a typical value for systems that involve strong SOC. Our results provide unique insights into the electronic structures of  $\text{KTaO}_3$  based electron gases via magnetotransport measurements.

**10:12AM A26.00010 Pulsed laser deposition and characterizations of pyrochlore iridate thin films**, MATTHEW STARR, JAIME AVILES-ACOSTA, Indiana University, Bloomington, YUANTAO XIE, Virginia Tech, WENKA ZHU, Indiana University, Bloomington, ZHEN LI, Indiana University, Bloomington; Los Alamos National Laboratory, AIPING CHEN, NAN LI, Los Alamos National Laboratory, CHENGGANG TAO, Virginia Tech, QUANXI JIA, Los Alamos National Laboratory, J. J. HEREMANS, Virginia Tech, S. X. ZHANG, Indiana University, Bloomington — Pyrochlore iridates have attracted growing interest in recent years because of their potential to realize novel topological phases. While most of the previous studies have focused on polycrystalline and single crystalline bulk samples, epitaxial thin films offer a unique platform for controllable tuning of material parameters such as oxygen stoichiometry and elastic strain to achieve new electronic states. In this talk, we will present the growth and characterizations of epitaxial thin films of pyrochlore  $\text{Y}_2\text{Ir}_2\text{O}_7$  and  $\text{Bi}_2\text{Ir}_2\text{O}_7$  that are predicted to host topologically non-trivial states. The iridate thin films were grown by pulsed laser deposition at different conditions, and a narrow window for epitaxial growth was determined. Characterizations of crystalline structures were performed using X-ray diffraction and transmission electron microscopy to establish a growth parameter-structure phase diagram. The compositions of thin films were determined by energy dispersive X-ray spectroscopy, and the surface morphologies were characterized using atomic force microscopy and scanning tunneling microscopy. Magneto-transport studies indicate a strong dependence of transport properties on the oxygen stoichiometry and the film thickness.

**10:24AM A26.00011 Strongly enhanced Rashba splitting in the perovskite tantalate-hafnate heterostructure**, SUK BUM CHUNG, Seoul Natl Univ, MINSUNG KIM, Ames Laboratory / Iowa State University — In addition to superconductivity and magnetism, one notable ingredient of the two-dimensional electron gas (2DEG) emerging at the transition metal oxide surface is the Rashba-Dresselhaus spin-orbit interaction, the momentum-dependent spin splitting due to the broken inversion symmetry and atomic spin-orbit coupling. However, it has not been understood how this splitting can be maximized in a physical system without applying external electric field. Here, we present a promising route to realize significant Rashba-type band splitting using thin film heterostructure. Based on a first-principles method and analytic model analysis, a tantalate layer on  $\text{BaHfO}_3$  is shown to host a two-dimensional bands originating from Ta  $t_{2g}$  orbitals with strongly enhanced Rashba-Dresselhaus spin splittings at both the band minima and saddle points. A significant  $t_{2g}$ - $e_g$  coupling that contributes to this enhanced splitting is likely to be a generic feature for the surface 2DEG of transition metal oxide with maximal inversion symmetry breaking. Our results could be important in realizing topological superconductivity and potentially useful for spintronics application.

**10:36AM A26.00012 Elastic and inelastic scattering in  $\text{SrTiO}_{3-\delta}$** , KAMRAN BEHNIA, XIAO LIN, BENOIT FAUQU, ESPCI — Scattering among electrons generates a distinct contribution to electrical resistivity that follows a quadratic temperature dependence. We show that the prefactor of this  $T^2$  resistivity can be tuned by four orders of magnitude in metallic  $\text{SrTiO}_3$  by tuning the concentration of the carriers and consequently, the Fermi energy. The  $T^2$  behavior persists in the single-band dilute limit despite the absence of two known mechanisms for  $T^2$  behavior, distinct electron reservoirs and Umklapp processes. The ultimate origin of the small residual resistivity is the long Bohr radius, which, in a shallow Fermi sea caused by a random distribution of dopants, sets the zero-temperature mobility.

## Monday, March 14, 2016 8:00AM - 11:00AM —

Session A27 DMP: Carbon Nanotube & Related Materials: Growth, Separation, and Assembly  
326 - Zhihong Chen, Purdue University

**8:00AM A27.00001 Nonequilibrium statistical mechanics of nanotube nucleation**, VASILII I. ARTYUKHOV, BORIS I. YAKOBSON, Rice University — A key problem that advanced carbon nanotube applications face is the difficulty of producing pure single-helicity samples. As the elementary processes of nanotube growth are difficult to observe in situ, theoretical understanding of the process is especially important. Direct molecular dynamics simulations offer limited insight due to computational intractability of space- and time-scales involved. We formulated a theory that explains a class of helicity-selective growth experiments, based on classical nucleation theory and crystal growth kinetics.<sup>1</sup> However, a general theory of nanotube growth must also include fast irreversible growth beyond the classical near-equilibrium assumption. Here we construct a coarse-grained model allowing us to rigorously investigate the statistical mechanics of nanotube nucleation and trace how helicity emerges from the global nucleation trajectory ensemble. Importantly, our model can handle the whole range of conditions from perfect reversibility driven by energetics to perfect irreversibility driven by configurational entropy of nanotube caps and edges. Our theory generalizes earlier models in a large advance towards ultimate understanding of helicity-selective synthesis. <sup>1</sup> V.I. Artyukhov, E.S. Penev, and B.I. Yakobson, Nat. Commun. 5, 4892 (2014)

**8:12AM A27.00002 Adsorption of SDS surfactant inside and around carbon nanotubes with DPD simulation**, MINH VO, The University of Oklahoma, DIMITRIOS PAPAVALASSILOU, National Science Foundation — The inner diameter of a carbon nanotube (CNT) is generally from 1 to 20 nm, while its inner space could be filled by certain compounds. In our study, Dissipative Particle Dynamics (DPD) simulations were utilized to investigate the ability of sodium dodecyl sulfate (SDS) to adsorb inside a single-walled CNT. First of all, the DPD interaction parameters for SDS surfactants were validated by determining the CMC of surfactants from DPD calculation. The SDS micelle shape and size in water were also calculated. Water-CNT interactions were obtained from a prior study [1]. When the SDS aqueous system reached equilibrium, an open-ended, hydrophobic CNT (a hollow cylinder in the simulation) was inserted into the solution. The diameter of the CNT varied from 1 to 5 nm. All simulations were run up to  $2 \times 10^6$  time steps at room temperature. For the system of water and CNT, the radial and axial density profiles of water were computed and compared with published Molecular Dynamics results. In the presence of SDS, the distribution of water and SDS inside the CNT was found to be comparable to that in bulk solution after the system reached equilibrium. In addition, the diffusivity and residence time of water and SDS inside CNTs of different were calculated. This study would give insights into the dynamics and morphology of surfactants in nanoconfined structures. References [1] Vo, M.; Papavassiliou, D. V., Molecular Simulation, 2015, DOI:10.1080/08927022.2015.1089989

**8:24AM A27.00003 Intensity Ratio of Resonant Raman Modes for  $(n, m)$  Enriched Semiconducting Carbon Nanotubes**, YANMEI PIAO, National Institute of Standards and Technology, JEFFREY SIMPSON, Towson University, JASON STREIT, GEYOU AO, JEFFREY FAGAN, ANGELA HIGHT WALKER, National Institute of Standards and Technology — Relative intensities of resonant Raman spectral features, specifically the radial breathing mode (RBM) and G modes, of eleven, chirality-enriched, single-wall carbon nanotube (SWCNT) species were established under second-order optical transition excitation. The results demonstrate a significantly under-recognized complexity in the evaluation of Raman spectra for the assignment of  $(n, m)$  population distributions. Strong chiral angle and mod dependencies affect the intensity ratio of the RBM to G modes and can result in misleading interpretations. Furthermore, we report five additional values for chirality dependent  $G^+$  and  $G^-$  Raman peak positions and intensities, supporting accuracy in literature values, and extending the available data to cover more of the small diameter regime by including the first (5,4) second-order, resonance Raman spectra. Together, the Raman spectral library is demonstrated to be sufficient for decoupling multiple species via a spectral fitting process, and enable fundamental characterization even in mixed chiral population samples.

**8:36AM A27.00004 Structure-Controlled Synthesis of Single-Walled Carbon Nanotubes<sup>1</sup>**, YAN LI, Peking University, Beijing, China — Single-walled carbon nanotubes (SWNTs) present structure-determined outstanding properties and SWNTs with a single  $(n, m)$  type are needed in many advanced applications. However, the chirality-specific growth of SWNTs is always a great challenge. Carbon nanotubes and their caps or catalysts can all act as the structural templates to guide the formation of SWNTs with a specified chirality. SWNT growth via a catalyzed chemical vapor deposition CVD process is normally more efficient and therefore of great interest. We developed a new family of catalyst, tungsten-based intermetallic nanocrystals, to grow SWNTs with specified chiral structures. Such intermetallic nanocrystals present unique structure and atomic arrangements, which are distinctly different from the normal alloy nanoparticles or simple metal nanocrystals, therefore can act as the template to grow SWNTs with designed  $(n, m)$  structures. Using W<sub>6</sub>Co<sub>7</sub> catalysts, we realized the selective growth of (12, 6), (16, 0), (14, 4) and other chiralities. By the cooperation of thermodynamic and kinetic factors, SWNTs with high chirality purity can be obtained. .

<sup>1</sup>Structure-Controlled Synthesis of Single-Walled Carbon Nanotubes

**9:12AM A27.00005 Growth of Single-Walled Carbon Nanotubes by High Melting Point Metal Oxide Catalysts<sup>1</sup>**, YANG QIAN, RONG XIANG, HUA AN, TAIKI INOUE, SHOHEI CHIASHI, Department of Mechanical Engineering, The University of Tokyo, SHIGEO MARUYAMA, Department of Mechanical Engineering, The University of Tokyo; National Institute of Advanced Industrial Science and Technology (AIST) — We report on the growth of single-walled carbon nanotubes (SWNTs) from Co oxide catalysts. The concept is using the relatively lower mobility of metal oxide (than metal) to suppress catalyst aggregation at high temperatures. Compared to the SWNTs grown by pre-reduced catalysts, SWNTs grown from oxidized Co catalysts have shown narrower diameter distribution and smaller average diameter. Different growth parameters are discussed regarding the resulting morphology of SWNTs. Transmission electron microscopy (TEM) investigations reveal the information that Co catalysts are transformed to Co<sub>3</sub>O<sub>4</sub> after reduction-calcination process. X-ray photoelectron spectroscopy (XPS) investigations indicate that Co<sub>3</sub>O<sub>4</sub> has decomposed to CoO before growth at a typical growth temperature (800 C) in Ar atmosphere. We propose that CoO has higher melting point than Co and thus is more stable during the growth. Our results indicate that besides the bimetallic catalysts, monometallic catalytic system could also be useful in stabilizing the catalysts to grow chirality-specific SWNTs by transforming the relatively low melting point metal catalysts to high melting point metal oxide catalysts.

<sup>1</sup>Yang Qian was supported through Global Leader Program for Social Design and Management.

**9:24AM A27.00006 Endohedral Volume Control for Improved Single-Wall Carbon Nanotubes**, JOCHEN CAMPO, JEFFREY FAGAN, Materials Science and Engineering Division, National Institute of Standards and Technology, Gaithersburg, Maryland — Liquid-phase processing of single-wall carbon nanotubes (SWCNTs) generally results in the exposure of their core volumes to the environment (opening) due to energy input necessary for purification and solubilization. For aqueous processing this results in SWCNTs routinely getting filled with water, which is detrimental to several properties. Importantly, water filling leads to significant redshifts to, and inhomogeneous broadening of, the electronic transitions of the SWCNTs, as well as a substantial decrease to their fluorescence quantum efficiency. Selection of (remaining) empty (end-capped) SWCNTs to avoid these adverse effects is possible by means of ultracentrifugation, but is a natively low yield process. In this work, SWCNTs are prefilled with linear alkanes or similar organic compounds, serving as a passive, highly homogeneous spacer, blocking the ingestion of water and hence preventing the detrimental consequences. Moreover, the low dielectric nature of the alkane core only weakly affects the local electronic wavefunction of the SWCNTs, effectively simulating empty core conditions and hence yielding much more resolved optical spectra with blue shifted peak positions compared to water filled SWCNTs. It is demonstrated that a wide variety of linear as well as cyclic alkanes can be applied for this purpose, in combination with various SWCNT materials.

**9:36AM A27.00007 Optical excitation of carbon nanotubes drives stoichiometric reaction with diazonium salts**, LYNDSEY POWELL, University of Maryland, YANMEI PIAO, NIST, YUHUANG WANG, University of Maryland, YUHUANG WANG RESEARCH GROUP TEAM — Covalent chemistry is known to lack the precision required to tailor the physical properties of carbon nanostructures. Here we show that, for the first time, light can be used to drive a typically inefficient reaction with single-walled carbon nanotubes in a more stoichiometric fashion. Specifically, our experimental results suggest that light can enhance the reaction rate of diazonium salt with carbon nanotubes by as much as 35-fold, making possible stoichiometric control of the covalent bonding of a functional group to the sp<sup>2</sup> carbon lattice. This light-controlled reaction paves the way for the possibility of highly selective and precise chemistry on single-walled carbon nanotubes and other graphitic nanostructures.

**9:48AM A27.00008 Chirality-controlled synthesis and macro-electronic applications of carbon nanotubes**, CHONGWU ZHOU, University of Southern California — Carbon nanotubes (CNTs) are promising materials for electronic applications due to their interesting properties. Chirality and electronic property controlled preparation are key challenges which need to be solved for practical use of CNTs in electronics. In this talk, I will first introduce our research on chirality-controlled synthesis of CNTs using metal-free carbon seeds. I will talk about chirality-controlled growth of SWCNTs using chirality-sorted nanotube seeds via a vapour phase epitaxy (VPE) cloning approach. Observations on the chirality-dependent growth rate and active lifetime of the nanotube seeds in the VPE process will be presented. Later, I will talk about selective growth of small diameter semiconducting CNTs using organic chemistry synthesized molecular seeds. In the second part, I will talk about the use of pre-separated, semiconducting-enriched CNTs for macro-electronics, printed electronics, and integrated circuits. Our work on the use of CNTs for thin-film transistors, CNT-IGZO hybrid CMOS circuits, and flexible, bendable, and transparent CNT devices and circuits will be presented. These works demonstrate the great potential of CNTs as advanced electronic materials.

**10:24AM A27.00009 Uniformly spaced arrays of purely semiconducting carbon nanotubes**, ABRAM FALK<sup>1</sup>, BHARAT KUMAR, GEORGE TULEVSKI, DAMON FARMER, JAMES HANNON, SHU-JEN HAN, IBM T. J. Watson Research Center, Yorktown Heights, NY — Patterning uniformly spaced arrays of carbon nanotubes (CNTs) is a key challenge for carbon electronics. Our group adopts a hybrid approach to meeting this goal. We use top-down lithography to pattern trenches on chips. We then use surface-selective chemical monolayers to facilitate the bottom-up assembly of solution-processed CNTs into these trenches. Previously, we showed large-scale integration of CNTs based on this approach [1], but modifications to this process have been needed in order to improve the yield and decrease the fraction of non-switching devices. Our latest results show a high degree of selectivity, alignment and yield of successfully placed CNTs at a 100 nm pitch. Electrical measurements confirm that these chemically placed CNTs are nearly 100% semiconducting and of similar quality to randomly dispersed ones. I will then discuss our strategies for increasing the CNT density and extending these results from chip- to wafer-scale electronics. [1] Park et al., Nature Nanotechnology 7, 787-791 (2012)

<sup>1</sup>email: alfalk@us.ibm.com

**10:36AM A27.00010 Nanoscale Structure and Interaction of Compact Assemblies of Carbon Nano-Materials.**, RAJU TIMSINA, XIANGYUN QIU, George Washington University, Washington DC — Carbon-based nano-materials (CNM) are a diverse family of multi-functional materials under research and development world wide. Our work is further motivated by the predictive power of the physical understanding of the underlying structure-interaction-function relationships. Here we present results from recent studies of the condensed phases of several model CNMs in complexation with biologically derived molecules. Specifically, we employ X-ray diffraction (XRD) to determine nanoscale structures and use the osmotic stress method to quantify their interactions. The systems under investigation are dsDNA-dispersed carbon nanotubes (dsDNA-CNT), bile-salt-dispersed carbon nanotubes, and surfactant-assisted assemblies of graphene oxides. We found that salt and molecular crowding are both effective in condensing CNMs but the resultant structures show disparate phase behaviors. The molecular interactions driving the condensation/assembly sensitively depend on the nature of CNM complex surface chemistry and range from hydrophobic to electrostatic to entropic forces.

**10:48AM A27.00011 Synthesis and Investigation of Millimeter-Scale Vertically Aligned Boron Nitride Nanotube Arrays**, ROLAND TAY, HONGLING LI, SIU HON TSANG, LIN JING, DUNLIN TAN, EDWIN HANG TONG TEO, Nanyang Tech Univ — Boron nitride nanotubes (BNNTs) have shown potential in a wide range of applications due to their superior properties such as exceptionally high mechanical strength, excellent chemical and thermal stabilities. However, previously reported methods to date only produced BNNTs with limited length/density and insufficient yield at high temperatures. Here we present a facile and effective two-step synthesis route involving template-assisted chemical vapor deposition at a relatively low temperature of 900 degree C and subsequent annealing process to fabricate vertically aligned (VA) BN coated carbon nanotube (VA-BN/CNT) and VA-BNNT arrays. By using this method, we achieve the longest VA-BN/CNTs and VA-BNNTs to date with lengths of over millimeters (exceeding two orders of magnitude longer than the previously reported length of VA-BNNTs). In addition, the morphology, chemical composition and microstructure of the resulting products, as well as the mechanism of coating process are systematically investigated. This versatile BN coating technique and the synthesis of millimeter-scale BN/CNT and BNNT arrays pave a way for new applications especially where the aligned geometry of the NTs is essential such as for field-emission, interconnects and thermal management.

**Monday, March 14, 2016 8:00AM - 11:00AM —**  
**Session A28 DMP DCMP: Topological Phases** 327 - Yong Chen, Purdue University

**8:00AM A28.00001 Predicting, Realizing and Exploiting Exotic Topological Phases of Quantum Matter**<sup>1</sup>, ARUN BANSIL, Northeastern University — The revolution started by the discovery of topological insulators a few years ago has turned out to be the proverbial tip of the much larger iceberg of exotic phases harbored by quantum matter. Consideration of electronic states protected by time-reversal, crystalline and particle-hole symmetries has led to the prediction of many novel 3D materials, which can support Weyl, Dirac and Majorana fermions, and to new types of insulators such as topological crystalline insulators and topological Kondo insulators, as well as 2D quantum spin Hall insulators with large band gaps capable of surviving room temperature thermal excitations. [1] In this talk, I will discuss our recent theoretical work aimed at predicting topological materials beyond the standard topological insulators and identify cases where robust experimental evidence has been obtained toward their successful materials realization. [2-10] I will also comment on the potential of topological materials as next generation platforms for manipulating spin and charge transport and other applications. [1] A. Bansil, H. Lin and T. Das, Reviews of Modern Physics (2015). [2] S.-Y. Xu et al., Science 349, 613 (2015). [3] I. Zeljkovic et al., Nature Materials 14, 318 (2015). [4] J. He et al., Nature Materials 14, 577 (2015). [5] S.-M. Huang et al., Nature Communications 6, 7373 (2015). [6] S.-Y. Xu et al., Science Advances (2015). [7] I. Zeljkovic, et al., Nature Communications 6, 6559 (2015). [8] M. Neupane et al., Physical Review Letters 114, 016403 (2015). [9] Su-Yang Xu, et al., Nature Physics 11, 748 (2015). [10] C. P. Crisostomo et al., Nano Letters 15, 6568 (2015).

<sup>1</sup>Work supported by the Materials Science & Engineering Division, Basic Energy Sciences, U. S. D. O. E.

Please order the Electronic structure of Na<sub>3</sub>Bi near the Dirac point:optical measurement talk first and Electronic structure of Na<sub>3</sub>Bi near the Dirac point:Theory talk second in the sequence.

**8:36AM A28.00002 Electronic structure of Na<sub>3</sub>Bi near the Dirac point: Optical measurements**<sup>1</sup>, GREGORY S. JENKINS, A. B. SUSHKOV, R. L. CAREY, H. D. DREW, U. of Md College Park, J. KRIZAN, S. KUSHWAHA, R. CAVA, Princeton U., TAY-RONG CHANG, HORNG-TAY JENG, National Tsing Hua U., H. LIN, NUS, C. LANE, B. BARBIELLINI, A. BANSIL, Northeastern U. — The first optical characterization of Na<sub>3</sub>Bi is reported. Reflection measurements on c-plane oriented single-crystals, over the spectral range from 3 meV to 2.5 eV and temperature ranging from 8 to 250K, show a low frequency response consistent with the low doping level  $n \sim 10^{17} \text{ cm}^{-3}$ . The number of observed phonons in the optical spectra is >5, which eliminates the P6<sub>3</sub>/mmc symmetry since point group analysis indicates only 2 IR active phonons. A striking, strongly temperature dependent plasma edge reverses direction at  $T \sim 100\text{K}$ . The behavior is consistent with thermal population effects in a Dirac cone permitting an estimation of the Fermi level. The Lifshitz gap energy is reported.

<sup>1</sup>UMD supported by NSF (DMR-1104343), Princeton supported by the ARO MURI on topological insulators (Grant No. W911NF-12-1-0461) and ARO (W911NF-11-1-0379) and MRSEC program (NSF-DMR-0819860 and DOE DE-FG-02-05ER46200), NU supported by the U.S.D.O.E.

Please order the Electronic structure of Na<sub>3</sub>Bi near the Dirac point:optical measurement talk first and Electronic structure of Na<sub>3</sub>Bi near the Dirac point:Theory talk second in the sequence.

**8:48AM A28.00003 Electronic structure of  $\text{Na}_3\text{Bi}$  near the Dirac point: Theory<sup>1</sup>**, CHRIS LANE, B. BARBIELLINI, A. BANSIL, Northeastern U., TAY-RONG CHANG, HORNG-TAY JENG, National Tsing Hua U., H. LIN, NUS, J. KRIZAN, S. KUSHWAHA, R. CAVA, Princeton U., G. S. JENKINS, A. B. SUSHKOV, R. L. CAREY, H. D. DREW, U. of Md College Park — Band structure calculations have been performed and compared with recent optical experiments. The ground state of the system is found to be not the highly symmetric  $\text{P6}_3/\text{mmc}$  structure, but instead the  $\text{P}\bar{3}\text{c}1$  that involves buckling of the Na-Bi hexagonal planes. The band structure shows very little change between various symmetry configurations, yet the low-energy optical transition matrix elements are dramatically enhanced in the  $\text{P}\bar{3}\text{c}1$  symmetry compared with  $\text{P6}_3/\text{mmc}$ , which results in an electronic response that agrees much more closely with optical data. A peak in the joint density of states driven by the particle-hole asymmetry of the band structure along the  $\Gamma - A$  momentum direction results in a large peak in the imaginary part of the dielectric function. Systematic changes are observed in the low energy Dirac cone Fermi velocity and Lifshitz gap energy with lattice spacing and spin-orbit coupling. The large anisotropies of the Dirac cone and small energy gaps are discussed.

<sup>1</sup>UMD supported by NSF (DMR-1104343), Princeton supported by the ARO MURI on topological insulators (Grant No. W911NF-12-1-0461) and ARO (W911NF-11-1-0379) and MRSEC program (NSF-DMR-0819860 and DOE DE-FG-02-05ER46200), NU supported by the U.S.D.O.E.

**9:00AM A28.00004 Universal signatures of Fermi arcs in quasiparticle interference on the surface of Weyl semimetals**, STEFANOS KOURTIS, JIAN LI, ZHI JUN WANG, B. ANDREI BERNEVIG, Department of Physics, Princeton University, Princeton, NJ 08544, USA — Weyl semimetals constitute a newly discovered class of three-dimensional topological materials with linear touchings of valence and conduction bands in the bulk. The most striking property of topological origin in these materials, so far only observed in photoemission experiments, is the presence of open constant-energy contours in the boundary density of states — the so-called Fermi arcs. In this work, we establish the universal characteristics of Fermi-arc contributions to surface quasiparticle interference. Using a general phenomenological model, we determine the defining interference patterns stemming from the existence of Fermi arcs in a surface band structure. We then trace these patterns in both simple tight-binding models and realistic ab initio calculations. Our results show that definitive signatures of Fermi arcs can be observed in existing and proposed Weyl semimetals using current scanning tunneling spectroscopy setups.

**9:12AM A28.00005 Probing spin-momentum locking of Weyl nodes with neutron scattering**, MICHAEL BJERNGAARD, Department of Physics and Astronomy, Johns Hopkins University, Baltimore, United States of America, BOGDAN GALILO, Department of Mathematics, Imperial College London, London, United Kingdom, ARI TURNER, Department of Physics and Astronomy, Johns Hopkins University, Baltimore, United States of America — We explain how a Weyl semimetal phase can be uniquely identified in the differential cross-section measured by an unpolarized neutron experiment. This differential cross-section has unique features that reflect the scattering between Weyl nodes of either same or opposite Chern numbers / spin-momentum locking. Hence, an unpolarized neutron experiment can uniquely identify Weyl semimetals of both inversion- and time-reversal symmetric classes. This is very desirable, as no experimental probe has yet directly confirmed such phases. Further, we describe how the neutron spectrum can distinguish proposed Weyl semimetals from Dirac semimetals.

**9:24AM A28.00006 Tuning Weyl nodes with a magnetic field**, JENNIFER CANO, BARRY BRADLYN, Princeton Center for Theoretical Science, ZHIJUN WANG, MAX HIRSCHBERGER, N. PHUAN ONG, B. ANDREI BERNEVIG, Princeton University — For Weyl fermions to exist, either inversion or time reversal symmetry must be broken. Here, we consider materials with a normal and/or inverted band structure that display a four band (Dirac) crossing in the presence of both these symmetries. We show that when a magnetic field is applied, thus breaking time reversal, the four band crossing splits into several Weyl nodes, depending on the direction in which the magnetic field is applied as well as on the symmetry group that protected the Dirac crossing. For a particular material realization, relevant to current experiments performed in Princeton, we use a symmetry analysis to predict the position of the Weyl nodes when the magnetic field is along a high-symmetry axis. While the symmetry is not necessary to protect the Weyl crossings, it is a useful tool to find them. Our results agree with both an ab initio and a  $k \cdot p$  effective Hamiltonian analysis.

**9:36AM A28.00007 Spiraling Fermi arcs in Weyl materials<sup>1</sup>**, SONGCI LI, ANTON ANDREEV, Univ of Washington — In Weyl materials the valence and conduction electron bands touch at an even number of isolated points in the Brillouin zone. In the vicinity of these points the electron dispersion is linear and may be described by the massless Dirac equation. This results in nontrivial topology of Berry connection curvature. One of its consequences is the existence of peculiar surface electron states whose Fermi surfaces form arcs connecting projections of the Weyl points onto the surface plane. Band bending near the boundary of the crystal also produces surface states. We show that in Weyl materials band bending near the crystal surface gives rise to spiral structure of energy surfaces of arc states. The corresponding Fermi surface has the shape of a spiral that winds about the projection of the Weyl point onto the surface plane. The direction of the winding is determined by the helicity of the Weyl point and the sign of the band bending potential. For close valleys arc state morphology may be understood in terms of avoided crossing of oppositely winding spirals.

<sup>1</sup>This work is supported by the U.S. Department of Energy Office of Science, Basic Energy Sciences under award number DE-FG02-07ER46452.

**9:48AM A28.00008 Creating chiral anomalies**, BARRY BRADLYN, JENNIFER CANO, ZHIJUN WANG, MAX HIRSCHBERGER, N. PHUAN ONG, B. ANDREI BERNEVIG, Princeton University — Materials with intrinsic Weyl points should present exotic magneto-transport phenomena due to spectral flow between Weyl nodes of opposite chirality - the so-called “chiral anomaly”. However, to date, the most definitive transport data showing the presence of a chiral anomaly comes from Dirac (not Weyl) materials. These semimetals develop Weyl fermions only in the presence of an externally applied magnetic field, when the four-fold degeneracy is lifted. In this talk we examine Berry phase effects on transport due to the emergence of these field-induced Weyl point and (in some cases) line nodes. We pay particular attention to the differences between intrinsic and field-induced Weyl fermions, from the point of view of kinetic theory. Finally, we apply our analysis to a particular material relevant to current experiments performed at Princeton.

**10:00AM A28.00009 Visualizing Weyl Fermions in  $\text{MoTe}_2$  Using Scanning Tunneling Microscopy**, AYELET NOTIS, ERICK ANDRADE, Columbia University, SANG-WOOK CHEONG, Rutgers University, ABHAY PASUPATHY, Columbia University —  $\text{MoTe}_2$ , a transition metal dichalcogenide, has a metastable orthorhombic phase at temperatures below 250 K. This phase is predicted to be a type II Weyl semimetal, providing us an exciting new opportunity to explore Weyl Fermions, a type of particle long sought after but only recently realized as a quasiparticle excitation in a crystal. A topological consequence of the existence of Weyl points in a crystal is the existence of Fermi arc surface states that connect pairs of Weyl points. Here, we present scanning tunneling microscopy and spectroscopy (STM and STS) studies investigating the topography and electronic structure of this material. We resolve the crystal structure of the orthorhombic phase in STM topography, and probe the electronic structure of the Fermi arc states using quasiparticle interference imaging.

**10:12AM A28.00010 Stable Dirac semi-metal in the allotrope of IV elements**, PEIZHE TANG, Stanford Univ, WENDONG CAO, Tsinghua Univ, SHOU-CHENG ZHANG, Stanford Univ, WENHUI DUAN, Tsinghua Univ, ANGEL RUBIO, Max Planck Institute for the Structure and Dynamics of Matter and Center for Free-Electron Laser Science,, ZHANG'S GROUP COLLABORATION, ANGEL'S GROUP COLLABORATION, DUAN'S GROUP COLLABORATION — Three dimensional (3D) topological Dirac semi-metals (SM) represent a novel state of quantum matter with exotic electronic structures, in which a pair of Dirac points with the linear dispersion along all three momentum directions exist in the bulk and are protected by the rotation symmetry. Regarded as the copies of 3D Weyl SMs, the Dirac SMs possess unique Fermi-arcs with helical spin textures on some specific surface planes. Herein, by using first principles calculations with the hybrid functional, we discover a new metastable allotrope of Ge and Sn with the staggered layered dumbbell structure, named as germancite and stancite, to be 3D Dirac SMs with a pair of Dirac points on the rotation axis of  $C_3$ . On the surface parallel to the rotation axis, a pair of topologically non-trivial Fermi arcs are observed to be coexisting with the trivial surface states; and via tuning the Fermi level, the hybridization between them induces a Lifshitz transition on the Fermi surface. Furthermore, the quantum thin film of the germancite is found to be the quantum spin Hall insulator without applying external electric field. These discoveries explore the metastable allotrope of Ge and Sn as topological Dirac SMs showing novel physical properties and future applications.

**10:24AM A28.00011 Chiral magnetic effect and natural optical activity in (Weyl) metals<sup>1</sup>**, DMYTRO PESIN, JING MA, Univ of Utah — We consider the phenomenon of natural optical activity, and related chiral magnetic effect in metals with low carrier concentration. To reveal the correspondence between the two phenomena, we compute the optical conductivity of a noncentrosymmetric metal to linear order in the wave vector of the light wave, specializing to the low-frequency regime. We show that it is the orbital magnetic moment of quasiparticles that is responsible for the natural optical activity, and thus the chiral magnetic effect. While for purely static magnetic fields the chiral magnetic effect is known to have a topological origin and to be related to the presence of Berry curvature monopoles (Weyl points) in the band structure, we show that the existence of Berry monopoles is not required for the dynamic chiral magnetic effect to appear; the latter is thus not unique to Weyl metals. The magnitude of the dynamic chiral magnetic effect in a material is related to the trace of its gyrotropic tensor. We discuss the conditions under which this trace is non-zero; in noncentrosymmetric Weyl metals it is found to be proportional to the energy-space dipole moment of Berry curvature monopoles. The calculations are done within both the semiclassical kinetic equation, and Kubo linear response formalisms.

<sup>1</sup>.This work was supported by NSF Grant No. DMR-1409089

**10:36AM A28.00012 Symmetry-based Search for Topological Weyl Nodes and Nodal-lines in Realistic Materials**, MOTOAKI HIRAYAMA, SHUICHI MURAKAMI, Dept. of Physics, Tokyo Tech.; TIES, Tokyo Tech., RYO OKUGAWA, Dept. of Physics, Tokyo Tech., SHOJI ISHIBASHI, TAKASHI MIYAKE, CD-FMat, National Institute of Advanced Industrial Science and Technology — Topological semimetals such as Weyl semimetals and nodal-line semimetals have been under intensive investigation recently. In this study, to realize such semimetals, we start from any insulators without inversion symmetry, and assume that the gap closes by changing some parameter. We then show that after the gap-closing there are only two possibilities; one is a Weyl semimetal phase, and the other is a nodal-line semimetal, depending on the symmetry and the position of the gap-closing point. Our analysis tells us which cases lead to Weyl semimetal and to the nodal-line semimetal, and this result can be used to find realistic topological semimetals. As an example, we study tellurium [1] using ab initio calculation based on relativistic density functional theory. The electronic structure is calculated by OpenMX [2] and the structural optimization is executed by QMAS [3]. We find that HfS has the nodal line in the mirror symmetry plane, and the nodal-line vanishes by pressure or atomic substitution. We also propose some materials showing the spinless nodal lines and its topological surface states. [1] M. Hirayama, R. Okugawa, S. Ishibashi, S. Murakami, and T. Miyake, Phys. Rev. Lett. 114, 206401 (2015). [2] <http://www.openmx-square.org/> [3] <http://www.qmas.jp/>

**10:48AM A28.00013 Boundary Conditions and Self-Adjoint Extensions of a Continuum Weyl Semimetal Hamiltonian<sup>1</sup>**, MICHAEL VENNETTILLI, Ursinus College, BABAK SERADJEH, Indiana University - Bloomington, ARIJIT KUNDU, Technion - Israel Institute of Technology & Indiana University - Bloomington, MOSTAFA TANHAYI AHARI, Indiana University - Bloomington — A Weyl semimetal is a Dirac material where the spin degeneracy of the energy-momentum Dirac cones is broken. The surface states of Weyl semimetals are expected to permit Fermi arcs connecting the surface-projections of the two Weyl nodes. The existence and physical properties of these surface states depends crucially on the boundary conditions at the surface. Generally speaking, boundary conditions placed on an unbounded Hermitian operator have an intimate relationship with the possible self-adjoint extensions of the operator. Indeed, determining the self-adjoint extensions of the operator naturally classifies all physical boundary conditions on the wavefunctions. We have studied the self-adjoint extensions of a model continuum Hamiltonian for Weyl semimetals and their corresponding classes of surface states. In this way, all possible physical surface spectra of the Weyl semimetal corresponding to different physical realizations of the surface are contained within our result.

<sup>1</sup>This work was supported by the NSF through Grant Nos. DMR-1350663 and PHY-1460882.

**Monday, March 14, 2016 8:00AM - 11:00AM —**  
**Session A29 DCMP: Dirac Semimetal** 328 - Jeffrey Teo, University of Virginia

**8:00AM A29.00001 Ultrafast reflectance of photoexcited Weyl and Dirac semimetals TaAs and ZrSiS**, CHRISTOPHER WEBER, BRYAN BERGGREN, Santa Clara University, KESHAV DANI, Okinawa Institute of Science and Technology, MAZHAR ALI, STUART PARKIN, IBM-Almaden Research Center, LESLIE SCHOOP, BETTINA LOTSCH, Max Planck Institute for Solid State Research, LINGXIAO ZHAO, GENFU CHEN, Beijing National Laboratory for Condensed Matter Physics, — We report ultrafast pump-probe and transient-grating (TG) measurements of the Weyl semimetal TaAs and the Dirac line-node semimetal ZrSiS, and contrast these results with prior measurements on the Dirac semimetal Cd<sub>3</sub>As<sub>2</sub>. After absorption of photons from the pump pulse, we monitor the samples' recovery to equilibrium by measuring the change in reflectance of a time-delayed probe pulse. For TaAs, the reflectance recovers in just 1.2 ps, significantly faster than the 3.1 ps measured in Cd<sub>3</sub>As<sub>2</sub>. This rapid recovery appears not to change when temperature is varied from 300 K to 8 K, when a magnetic field of order 0.3 T is applied, or when the excitation fluence is increased by a factor of 20. TG measurements allow us to assign the changes in reflectance to changes in either the dispersive (real) or absorptive (imaginary) parts of the index of refraction. Intriguingly, and in contrast to Cd<sub>3</sub>As<sub>2</sub>, the initial change in reflectance is caused by an abrupt reduction in the dispersive part, followed by a slower reduction in the absorptive part. For ZrSiS, the recovery after photoexcitation is even faster, at 0.3 ps. We will discuss the implications of these findings for carrier dynamics in topological semimetals.

**8:12AM A29.00002 Ultrafast Photo-Carrier Dynamics and Coherent Phonon Excitations in Topological Dirac Semimetal  $\text{Cd}_3\text{As}_2$** <sup>1</sup>, FEI SUN, QIONG WU, YANLING WU, YICHAO TIAN, YOUGUO SHI, JIMIN ZHAO, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences — Three dimensional (3D) topological Dirac semimetal has attracted growing research interest owing to its intriguing quantum properties such as high bulk carrier mobility and quantum spin Hall effects. However, so far, the ultrafast dynamics of a typical 3D topological Dirac semimetal,  $\text{Cd}_3\text{As}_2$ , as well as its coherent phonon has not been thoroughly investigated. Here we report the ultrafast dynamics of  $\text{Cd}_3\text{As}_2$  by using femtosecond pump-probe spectroscopy. Two distinct relaxation processes was observed, with the lifetimes (at 5 K) of 2.4 ps and 18.6 ps, respectively. Variable temperature experiment from 5 K to 295 K also reveals signatures of phase transitions. Furthermore, coherent optical (8.1 meV) and acoustic (0.036 THz) phonon modes were generated and detected, respectively, with signatures of hybrid-excitation of the two modes.

<sup>1</sup>the National Basic Research Program of China (2012CB821402), the National Natural Science Foundation of China (11274372), and the External Cooperation Program of the Chinese Academy of Sciences (GJHZ1403)

**8:24AM A29.00003 Gate-tunable quantum oscillations in ambipolar  $\text{Cd}_3\text{As}_2$  thin films**, YANWEN LIU, CHENG ZHANG, XIANG YUAN, TANG LEI, CHAO WANG, Fudan Univ, DOMENICO DI SANTE, SILVIA PICOZZI, CNR-SPIN, LIANG HE, Nanjing University, AWADHESH NARAYAN, STEFANO SANVITO, Trinity College, RENCHAO CHE, FAXIAN XIU, Fudan Univ —  $\text{Cd}_3\text{As}_2$ , a three-dimensional (3D) analog of graphene with extraordinary carrier mobility, was predicted to be a 3D Dirac semimetal, a feature confirmed by recent experiments. Here we report on the first observation of a gate-induced transition from band conduction to hopping conduction in single-crystalline  $\text{Cd}_3\text{As}_2$  thin films via electrostatic doping by solid electrolyte gating. The extreme charge doping enables the unexpected observation of p-type conductivity in a 50-nm-thick  $\text{Cd}_3\text{As}_2$  thin film grown by molecular beam epitaxy. More importantly, the gate-tunable Shubnikov-de Haas oscillations and the temperature-dependent resistance reveal a unique band structure and bandgap opening when the dimensionality of  $\text{Cd}_3\text{As}_2$  is reduced. This is also confirmed by our first-principle calculations. The present results offer new insights toward nanoelectronic and optoelectronic applications of Dirac semimetals and provide new routes in the search for the intriguing quantum spin Hall effect in low-dimension Dirac semimetals. Reference: Y. Liu. et.al. NPG Asia Mater. 7, e221 (2015)

**8:36AM A29.00004 Quantum Oscillations in Weyl and Dirac Semimetal Ultra-Thin Films**, DANIEL BULMASH, XIAO-LIANG QI, Stanford University — We show that a thin film of Weyl or Dirac semimetal with a strong in-plane magnetic field becomes a novel two-dimensional Fermi liquid with interesting properties. The Fermi surface in this system is strongly anisotropic, consisting of a combination of chiral bulk channels and the Fermi arcs. The area enclosed by the Fermi surface is proportional to the magnetic field component parallel to the Weyl/Dirac node splitting, which leads to unusual behavior in quantum oscillations when the magnetic field is tilted out of the plane. We estimate the oscillation frequencies and the regimes where such effects could be seen in  $\text{Cd}_3\text{As}_2$  and TaAs.

**8:48AM A29.00005 Dirac Cone Protected by Non-Symmorphic Symmetry and highly dispersive 3D Dirac crossings in  $\text{ZrSiS}$** , LESLIE SCHOOP, Max Planck Institute for Solid State Research, MAZHAR ALI, IBM-Almaden Research Center, CAROLA STRASSER, VIOLA DUPPEL, Max Planck Institute for Solid State Research, STUART PARKIN, IBM-Almaden Research Center, BETTINA LOTSCH, CHRISTIAN AST, Max Planck Institute for Solid State Research — Materials harboring exotic quasiparticles, such as Dirac and Weyl fermions have garnered much attention from the physics and material science communities. Here, we show with angle resolved photoemission studies supported by ab initio calculations that the highly stable, non-toxic and earth-abundant material,  $\text{ZrSiS}$ , has an electronic band structure that hosts several Dirac cones which form a Fermi surface with a diamond-shaped line of Dirac nodes. We also experimentally show, for the first time, that the square Si lattice in  $\text{ZrSiS}$  is an excellent template for realizing the new types of 2D Dirac cones protected by non-symmorphic symmetry and image an unforeseen surface state that arises close to the 2D Dirac cone. Finally, we find that the energy range of the linearly dispersed bands is as high as 2 eV above and below the Fermi level; much larger than of any known Dirac material so far. We will discuss why these characteristics make  $\text{ZrSiS}$  very promising for future applications.

**9:00AM A29.00006 Helical Spin Order from Topological Dirac and Weyl Semimetals**, XIAO-QI SUN, SHOUCHENG ZHANG, Stanford University, ZHONG WANG, Tsinghua University — We study dynamical mass generation and the resultant helical spin orders in topological Dirac and Weyl semimetals, including the edge states of quantum spin Hall insulators, the surface states of weak topological insulators, and the bulk materials of Weyl semimetals. In particular, the helical spin textures of Weyl semimetals manifest the spin-momentum locking of Weyl fermions in a visible manner. The spin-wave fluctuations of the helical order carry electric charge density; therefore, the spin textures can be electrically controlled in a simple and predictable manner.

**9:12AM A29.00007 Magnetotransport in Dirac semimetals: Chiral magnetic effect and quantum oscillations**, GUSTAVO MONTEIRO, ALEXANDER ABANOV, DMITRI KHARZEEV, Stony Brook University — Dirac semimetals are characterized by the linear dispersion of fermionic quasiparticles, with the Dirac point hidden inside a Fermi surface. We study the magnetotransport in these materials using chiral kinetic theory to describe within the same framework both the negative magnetoresistance caused by the chiral magnetic effect and quantum oscillations in the magnetoresistance due to the existence of the Fermi surface [1]. We also consider the role of Fermi Arcs and their contribution for the SdH modes. We discuss the relevance of obtained results to recent measurements on  $\text{Cd}_3\text{As}_2$ .  
[1] G. Monteiro, A. Abanov and D. Kharzeev, Phys. Rev. B 92, 165109 (2015).

**9:24AM A29.00008 Are the surface Fermi arcs in Dirac semimetals topologically protected?**<sup>1</sup>, YUAN MING LU, Department of Physics, The Ohio State University, Columbus, OH 43210, MEHDI KARGARIAN, Department of Physics, University of Maryland, College Park, MD 20742, MOHIT RANDERIA, Department of Physics, The Ohio State University, Columbus, OH 43210 — Motivated by recent experiments probing double Fermi arcs on the surface of Dirac semimetals (DSMs)  $\text{Na}_3\text{Bi}$  and  $\text{Cd}_3\text{As}_2$ , we raise the question posed in the title. We find that, in marked contrast to Weyl semimetals, the Fermi arcs of DSMs are not topologically protected in general, except at certain time-reversal invariant momenta. For a simple 4-band model with a pair of Dirac nodes at  $\mathbf{k} = (0, 0, Q)$  gapless surface states are protected only at  $k_z = 0$ . We identify symmetry allowed bulk perturbations that destroy Fermi arcs, but show that they are necessarily small, i.e., higher order than terms kept in usual  $\mathbf{k} \cdot \mathbf{p}$  theory. We validate our conclusions about the absence of a topological invariant protecting the surface states in DSMs using a K-theory analysis for the space groups of  $\text{Na}_3\text{Bi}$  and  $\text{Cd}_3\text{As}_2$

<sup>1</sup>The authors acknowledge the support of the CEM, an NSF MRSEC, under grant DMR-1420451.

**9:36AM A29.00009 Angular Magnetoresistance and Hall Measurements in New Dirac Material, ZrSiS**, MAZHAR ALI, IBM-Almaden, MPI-Microstructure Physics, LESLIE SCHOOP, BETTINA LOTSCH, MPI-Solid State Research, STUART PARKIN, IBM-Almaden, MPI-Microstructure Physics — Dirac and Weyl materials have shot to the forefront of condensed matter research in the last few years. Recently, the square-net material, ZrSiS, was theorized and experimentally shown (via ARPES) to host several highly dispersive Dirac cones, including the first Dirac cone demanded by non-symmorphic symmetry in a Si square net. Here we report the magnetoresistance and Hall Effect measurements in this compound. ZrSiS samples with  $RRR = 40$  were found to have MR values up to 6000% at 2 K, be predominantly p-type with a carrier concentration of  $\sim 8 \times 10^{19} \text{ cm}^{-3}$  and mobility  $\sim 8500 \text{ cm}^2/\text{Vs}$ . Angular magnetoresistance measurements reveal a peculiar behavior with multiple local maxima, depending on field strength, indicating of a sensitive and sensitive Fermi surface. SdH oscillations analysis confirms Hall and angular magnetoresistance measurements. These results, in the context of the theoretical and ARPES results, will be discussed.

**9:48AM A29.00010 Observation of quasi-two-dimensional Dirac fermions in ZrTe<sub>5</sub>**, XIANG YUAN, CHENG ZHANG, YANWEN LIU, SHOUDONG SHEN, XING SUI, JIE XU, HAOCHI YU, ZHENG HUA AN, JUN ZHAO, HUGEN YAN, FAXIAN XIU, Fudan University — Since the discovery of graphene, layered materials have attracted extensive interests owing to their unique electronic and optical characteristics. Among them, Dirac semimetal, one of the most appealing categories, has been a long-sought objective in layered systems beyond graphene. Recently, layered pentatelluride ZrTe<sub>5</sub> was found to host signatures of Dirac semimetal. However, the low Fermi level in ZrTe<sub>5</sub> strongly hinders a comprehensive understanding of the whole picture of electronic states through photoemission measurements, especially in the conduction band. Here, we report the observation of Dirac fermions in ZrTe<sub>5</sub> through magneto-optics and magneto-transport. By applying magnetic field, we observe a square-root-B-dependence of inter-Landau-level resonance and Shubnikov-de Haas oscillations with non-trivial Berry phase, both of which are hallmarks of Dirac fermions. The angular-dependent SdH oscillations show a clear quasi-two-dimensional feature with highly anisotropic effective mass and Fermi velocity, in stark contrast to the 3D Dirac semimetal such as CdAs<sub>2</sub>. With the confined interlayer dispersion and reducible dimensionality, our work establishes ZrTe<sub>5</sub> as an ideal platform for exploring exotic physical phenomena of Dirac fermions. Another work about the optics on CdAs<sub>2</sub> thin film will also be discussed.

**10:00AM A29.00011 Angle-resolved photoemission study on potential topological insulator ZrTe<sub>5</sub>**, HONGYU XIONG, Stanford University and SLAC National Accelerator Laboratory, JONATHAN SOBOTA, Stanford University, SLAC National Accelerator Laboratory, and Lawrence Berkeley National Laboratory, SHUOLONG YANG, Stanford University and SLAC National Accelerator Laboratory, DOMINIK LEUENBERGER, HADAS SOIFER, SLAC National Accelerator Laboratory, YAN-FENG CHEN, XU HAN, SI-YUAN YU, MING-HUI LU, Nanjing University, MAKOTO HASHIMOTO, DONGHUI LU, PATRICK KIRCHMANN, SLAC National Accelerator Laboratory, ZHI-XUN SHEN, Stanford University and SLAC National Accelerator Laboratory — ZrTe<sub>5</sub> is a layered-structure material which is predicted to exhibit the quantum spin hall effect in its monolayer limit. Bulk ZrTe<sub>5</sub> material is of scientific interest as well, as it might lie within the transition boundary between weak and strong topological insulator. We are using angle-resolved photoemission spectroscopy (ARPES) to investigate the band structure of bulk ZrTe<sub>5</sub>. Synchrotron data with varied photon energies shows little  $k_z$  dependence, which indicates a quasi-two-dimensional band structure; in addition, we observe circular dichroism, which suggests possible spin polarization. We are also working on time-resolved ARPES measurements, hoping to reveal the band structure above the Fermi level, which might give information about the materials topological properties.

**10:12AM A29.00012 Magneto-infrared spectroscopy of Landau levels and Zeeman splitting of three-dimensional massless Dirac Fermions in ZrTe<sub>5</sub>**, R. Y. CHEN, International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China, Z. G. CHEN, National High Magnetic Field Laboratory, Tallahassee, Florida 32310, USA, X.-Y. SONG, International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China, J. A. SCHNEELOCH, G. D. GU, Brookhaven National Lab, Upton, New York 11973, USA, F. WANG, N. L. WANG, International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China — We present a magneto-infrared spectroscopy study on a newly identified three-dimensional (3D) Dirac semimetal ZrTe<sub>5</sub>. We observe clear transitions between Landau levels and their further splitting under magnetic field. Both the sequence of transitions and their field dependence follow quantitatively the relation expected for 3D massless Dirac fermions. The measurement also reveals an exceptionally low magnetic field needed to drive the compound into its quantum limit, demonstrating that ZrTe<sub>5</sub> is an extremely clean system and ideal platform for studying 3D Dirac fermions. The splitting of the Landau levels provides a direct and bulk spectroscopic evidence that a relatively weak magnetic field can produce a sizeable Zeeman effect on the 3D Dirac fermions, which lifts the spin degeneracy of Landau levels. Our analysis indicates that the compound evolves from a Dirac semimetal into a topological line-node semimetal under current magnetic field configuration. Refs: R. Y. Chen et al., Phys. Rev. B 92, 075107 (2015); R. Y. Chen et al., Phys. Rev. Lett. 115, 176404 (2015).

**10:24AM A29.00013 Detection of chiral anomaly and valley transport in Dirac semimetals**, CHENG ZHANG, ENZE ZHANG, YANWEN LIU, Fudan Univ, ZHIGANG CHEN, The University of Queensland, SIHANG LIANG, JUNZHI CAO, XIANG YUAN, LEI TANG, QIAN LI, TENG GU, YIZHENG WU, Fudan Univ, JIN ZOU, The University of Queensland, FAXIAN XIU, Fudan Univ — Chiral anomaly is a non-conservation of chiral charge pumped by the topological nontrivial gauge field, which has been predicted to exist in the emergent quasiparticle excitations in Dirac and Weyl semimetals. However, so far, such pumping process hasn't been clearly demonstrated and lacks a convincing experimental identification. Here, we report the detection of the charge pumping effect and the related valley transport in Cd<sub>3</sub>As<sub>2</sub> driven by external electric and magnetic fields ( $\mathbf{E} \times \mathbf{B}$ ). We find that the chiral imbalance leads to a non-zero gyrotropic coefficient, which can be confirmed by the  $\mathbf{E} \times \mathbf{B}$ -generated Kerr effect. By applying B along the current direction, we observe a negative magnetoresistance despite the giant positive one at other directions, a clear indication of the chiral anomaly. Remarkably, a robust nonlocal response in valley diffusion originated from the chiral anomaly is persistent up to room temperature when B is parallel to E. The ability to manipulate the valley polarization in Dirac semimetal opens up a brand-new route to understand its fundamental properties through external fields and utilize the chiral fermions in valleytronic applications.

**10:36AM A29.00014 A coupled wire model of topological Weyl and Dirac semimetal I: topological insulating texture and gapping interaction**, SYED RAZA, ALEXANDER SIROTA, JEFFREY TEO, University of Virginia — Weyl and Dirac semimetals in three dimensions have semi-robust massless electronic structures. We mimic these gapless systems using an array of coupled Dirac wires, and analytically study the gapping effect of many-body interactions. The Dirac wires are arranged in a way so that the charge conserving model exhibits an antiferromagnetic time reversal symmetry as well as a p2mg wallpaper group symmetry, which contains twofold rotations, reflections and glide planes. The gapless electrons can acquire a mass upon symmetry breaking dimerizations, or more interestingly, symmetry preserving many-body interactions. This involves the introduction of a topological insulating texture in the bulk supported by layers of gapped symmetric interacting surfaces of topological insulators. The resulting massive system is a three dimensional *geometric topological state*.

**10:48AM A29.00015 A coupled wire model of topological Weyl and Dirac fermion II: three-dimensional geometric topological phase**, ALEXANDER SIROTA, SYED RAZA, JEFFREY TEO, University of Virginia — We mimic Weyl and Dirac semimetals in three dimensions by a coupled Dirac wire model, and introduce many-body gapping interactions that preserve symmetries. The construction relies on additional layers of gapped symmetric interacting surfaces of topological insulators, each carrying fractional charge excitations and containing Ising-like surface topological order. The three dimensional stack supports mutually non-local fractional point charges and flux tubes. Moreover the flux tubes, when directed in an appropriate direction, can carry Majorana zero modes and give rise to non-Abelian "3-loop braiding". Due to the highly anisotropic nature of the coupled wire model, the topological phase also exhibits geometric properties beyond a topological field theory description.

# Monday, March 14, 2016 8:00AM - 11:00AM —

## Session A30 DMP DCMF: Ferroelectric Heterostructures 329 - Marty Gregg

**8:00AM A30.00001 Observation of Polar Vortices in Oxide Superlattices**, R RAMESH, Univ of California - Berkeley — The complex interplay of spin, charge, orbital, and lattice degrees of freedom has provided for a plethora of exotic phase and physical phenomena. Among these, in recent years, topological states of matter and spin textures have emerged as fascinating consequences of the electronic band structure and the interplay between spin and spin-orbit coupling in materials. In this work, we leverage the competition between charge, orbital, and lattice degrees of freedom in superlattices of  $\text{PbTiO}_3/\text{SrTiO}_3$  to produce complex, vortex-antivortex pairs (that exhibit smoothly varying ferroelectric polarization with a 10 nm periodicity) that are reminiscent of topological features such as skyrmions and merons. Using a combination of advanced layer-by-layer growth techniques, atomic-resolution mapping of structure and local polar distortions using scanning-transmission electron microscopy, and phase-field modeling approaches we present a comprehensive picture of the nature of the varying polarization profile in such vortex states. The continuous rotation of the polar state into the vortex structures is thought to occur from an interplay of polar discontinuities at the  $\text{PbTiO}_3/\text{SrTiO}_3$  interface (where), the phase transformation strain and gradient energy in the  $\text{PbTiO}_3$  layer, and the strain imposed by the substrate. Finally, the implications of these observations are discussed as they pertain to producing new states of matter and phenomena in ferroic materials.

**8:36AM A30.00002 The ultrafast response of polar vortices under optical excitation**, STOICA, YAKUN YUAN, Pennsylvania State University, ZIJIAN HONG, Materials Science and Engineering, Pennsylvania State University, ANOOP DAMODARAN, University of California, Berkeley, YI ZHU, HUA ZHOU, DONALD WALKO, JOHN FREELAND, APS, Argonne National Laboratory, LONG-QING CHEN, Pennsylvania State University, RAMAMOORTHY RAMESH, VENKATRAMAN GOPALAN, Pennsylvania State University — Polar vortices were recently discovered in  $\text{PbTiO}_3\text{-SrTiO}_3$  nanoscale in the presence of depolarizing fields and mechanical stresses. We have found that these exotic structures, not only possess rich ultrafast responses to fs laser excitation, which is attractive for high-density information storage and nanoscale excitation above the bandgap of  $\text{PbTiO}_3$  layers and structural and second harmonic generation probes of ferroelectric order, but also irreversible nano-ordering transitions were observed. X-ray diffraction and diffuse scattering on nanodomains aided the phase transition measurements. In this talk, we will discuss the dynamic interplay between collinear and toroidal ferroelectric domains aided by the modelling. [1] A.K. Yadav, R. Ramesh et al., "Observation of Polar Vortices in Oxide Superlattices", accepted, Nature (2016).

since it exceeded the space limit <sup>1</sup>DE-SC0012375, DE-AC02-06CH11357, U.S Department of Energy, Office of Science, Office of Basic Energy Sciences

**8:48AM A30.00003 Ultra-thin single crystal perovskite ferroelectric on Silicon.**, SAIDUR BAKAUL, CLAUDY SERRAO, RAMESH RAMAMOORTHY, SAYEED SALAHUDDIN, University of California Berkeley — Single crystalline ultra-thin films (sub-10 nm) of ferroelectric complex oxides are important for tunnelling memory [1] devices. Commercially viable realization of such devices requires their integration with the peripheral Si-based input-output electronics. Integration of single crystalline films of such oxides using direct synthesis remains challenging due to the fundamental crystal chemistry and mechanical incompatibility of dissimilar interfaces. In this work we report epitaxial transfer of ultra-thin single crystalline, oxide films (down to 1 unit cell) onto Si substrates, at room temperature. The thickness of the transferred films has been confirmed by atomic force microscopy. Piezoelectric force microscopy shows ferroelectric property is retained in the transferred film. Electrical transport studies on these transferred ultra-thin films are ongoing. [1] Z. Wen, C. Li, D. Wu, A. Li and N. Ming, Ferroelectric-field-effect-enhanced electroresistance in metal/ferroelectric/semiconductor tunnel junctions. Nat. Mater. 12, 617 (2013)

**9:00AM A30.00004 First-principles simulation of negative capacitance in a polydomain ferroelectric-paraelectric bilayer capacitor under bias**, SHUSUKE KASAMATSU, The Institute for Solid State Physics, the University of Tokyo, SATOSHI WATANABE, Department of Materials Engineering, the University of Tokyo, CHEOL SEONG HWANG, SEUNGWU HAN, Department of Materials Science and Engineering, Seoul National University — The use of negative capacitance materials is gaining attention in recent years as a path to achieving further scaling of nanoelectronic devices [1]. For example, it has been reported that the ferroelectric thin film in a ferroelectric (FE)-paraelectric (PE) bilayer capacitor exhibits negative capacitance, i.e., the bilayer capacitor has a higher capacitance than the capacitor with a single PE layer [2]. However, the mechanism for this effect, especially with regard to the dynamics of polarization domains under bias voltage, is poorly understood. To tackle this issue, we performed first-principles simulation of a metal/FE/PE/metal capacitor with 180° stripe domains under bias using our recently developed orbital-separation approach [3]. We find an antiferroelectric-like behavior with a polydomain-monodomain transition under 0.3 V. Capacitance boost (i.e., negative capacitance) is observed within the monodomain regime, and the transition itself is also found to be a source of capacitance enhancement. [1] G. Catalan et al., Nature Mater. 14, 137 (2015). [2] D. Appleby et al., Nano Lett. 14, 3864, (2014); A. I. Khan et al., Appl. Phys. Lett. 99, 113501 (2011). [3] S. Kasamatsu et al., Phys. Rev. B 84, 085120 (2011); Phys. Rev. B 92, 115124 (2015).

**9:12AM A30.00005 Negative Capacitance in a Ferroelectric Capacitor**, ASIF KHAN, KOROK CHATTERJEE, BRIAN WANG, STEVEN DRAPCHO, LONG YOU, CLAUDY SERRAO, SAIDUR BAKAUL, RAMAMOORTHY RAMESH, SAYEED SALAHUDDIN, UC Berkeley, UC BERKELEY TEAM — The Boltzmann distribution of electrons poses a fundamental barrier to lowering energy dissipation in conventional electronics, often termed as Boltzmann Tyranny<sup>1</sup>. Negative capacitance in ferroelectric materials, which stems from the stored energy of phase transition, could provide a solution, but a direct measurement of negative capacitance has so far been elusive. Here we demonstrate the negative differential capacitance in an epitaxial ferroelectric film, by constructing a simple R-C network and monitoring the voltage dynamics across the ferroelectric capacitor<sup>2</sup>. When a voltage pulse is applied, the voltage across the ferroelectric capacitor is found to be decreasing with time—in exactly the opposite direction to which voltage for a regular capacitor should change. The results are analyzed on the basis of the Landau-Khalatnikov equation, which shows that as the ferroelectric polarization switches its direction, it passes through the unstable negative capacitance region. Analysis of this behavior from a capacitor presents an unprecedented insight into the intrinsic energy profile of the ferroelectric material.

1. Salahuddin et al. Nano Lett. 8, 405 (2008). 2. Khan et al. Nature Mater. 14, 182 (2015).

**9:24AM A30.00006 The interface between ferroelectric and 2D material for a Ferroelectric Field-Effect Transistor**, NAHEE PARK, Center for Integrated Nanostructure Physics, Institute for Basic Science, DOES, Sungkyunkwan University, HAERYONG KANG, DOES, Sungkyunkwan University, SANG-GOO LEE, IBULE Photonics Co. Ltd., YOUNG HEE LEE, DONGSEOK SUH, Center for Integrated Nanostructure Physics, Institute for Basic Science, DOES, Sungkyunkwan University — We have studied electrical property of ferroelectric field-effect transistor which consists of graphene on hexagonal Boron-Nitride (h-BN) gated by a ferroelectric, PMN-PT (i.e.  $(1-x)\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_{3-x}\text{PbTiO}_3$ ) single-crystal substrate. The PMN-PT was expected to have an effect on polarization field into the graphene channel and to induce a giant amount of surface charge. The hexagonal Boron-Nitride (h-BN) flake was directly exfoliated on the PMN-PT substrate for preventing graphene from directly contacting on the PMN-PT substrate. It can make us to observe the effect of the interface between ferroelectric and 2D material on the device operation. Monolayer graphene as 2D channel material, which was confirmed by Raman spectroscopy, was transferred on top of the hexagonal Boron-Nitride (h-BN) by using the conventional dry-transfer method. Here, we can demonstrate that the structure of graphene/hexagonal-BN/ferroelectric field-effect transistor makes us to clearly understand the device operation as well as the interface between ferroelectric and 2D materials by inserting h-BN between them. The phenomena such as anti-hysteresis, current saturation behavior, and hump-like increase of channel current, will be discussed by in terms of ferroelectric switching, polarization-assisted charge trapping.

**9:36AM A30.00007 Symmetry, strain, defects, and the nonlinear optical response of crystalline BaTiO<sub>3</sub>/silicon.**<sup>1</sup>, KRISTY KORMONDY, The University of Texas at Austin, STEFAN ABEL, YOURI POPOFF, MARILYNE SOUSA, DANIELE CAIMI, HEINZ SIEGWART, CHIARA MARCHIORI, IBM Research – Zurich, Säumerstrasse 4, 8803 Rüschlikon, Switzerland, MARTA ROSSELL, Electron Microscopy Center, Empa, ALEX DEMKOV, The University of Texas at Austin, JEAN FOMPEYRINE, IBM Research – Zurich, Säumerstrasse 4, 8803 Rüschlikon, Switzerland — Recent progress has been made towards exploiting the linear electro-optic or Pockels effect in ferroelectric BaTiO<sub>3</sub> (BTO) for novel integrated silicon photonics devices. In such structures, the crystalline symmetry and domain structure of BTO determine which electro-optic tensor elements are accessible under application of an external electric field. For epitaxial thin films of BTO on Si (001), the role of defects in strain relaxation can lead to very different crystalline symmetry even for films of identical thickness. Indeed, through geometric phase analysis of high-resolution scanning transmission electron microscopy images, we map changes of the in-plane and out-of-plane lattice parameters across two 80-nm-thick BTO films. A corresponding 20% difference in the effective electro-optic response was measured by analyzing induced rotation of the polarization of a laser beam ( $\lambda = 1550$  nm) transmitted through lithographically defined electrodes. Understanding, controlling, and modelling the role of BTO symmetry in nonlinear optics is of fundamental importance for the development of a hybrid BTO/Si photonics platform..

<sup>1</sup>Work supported by the NSF (IRES-1358111), AFOSR (FA9550-12-10494), and European Commission (FP7-ICT-2013-11-619456-SITOGA).

**9:48AM A30.00008 Memristive behavior in BaTiO<sub>3</sub> thin films integrated with semiconductors**, SRINIVASA RAO SINGAMANANI, NORTH CAROLINA STATE UNIVERSITY, JOHN PRATER, Army Research Office, JAY NARAYAN, NORTH CAROLINA STATE UNIVERSITY — BaTiO<sub>3</sub> has been studied for emerging non-volatile memory applications. However, most of the previous work has focused on this material when it was deposited on insulating oxide substrates such as SrTiO<sub>3</sub>. Unfortunately, this substrate is not suitable for CMOS-based microelectronics applications. This motivated us to carry out the present work. We have studied the resistive switching behavior in BaTiO<sub>3</sub>/La<sub>0.7</sub>Sr<sub>0.3</sub>MnO<sub>3</sub> (BTO/LSMO) heterostructures integrated with Si (100) using pulsed laser deposition<sup>1,2</sup>. I-V measurements were conducted on BTO (500nm)/LSMO (25nm) devices at 200K, with the compliance current of 10mA. Here, Pt was used as a top electrode and LSMO served as bottom electrode. A few important observations are noted: (a) broad hysteresis in forward and reverse voltage sweeps –ideal for memory applications, (b) the ratio of high resistance to low resistance state is ~600 –important for switching devices, (c) the device is stable at least up to 50 cycles. However, we found that hysteretic behavior was collapsed after 36 cycles upon oxygen annealing of the device at 1 atmospheric pressure, 200° C for 1 hour, inferring the important role of oxygen vacancies in the resistive switching behavior of BTO/LSMO device. The comprehensive experimental data will be presented and discussed.<sup>1,2</sup>S.R.S., et al., J. Appl. Phys., 116, 094103 (2014); J. Appl. Phys., 116, 224104 (2014).

**10:00AM A30.00009 Non-local domain switching in ferroelectric nanostructures**, SEURI JEONG, KWANG-EUN KIM, CHAN-HO YANG, Korea Adv Inst of Sci & Tech — Nanoscale ferroic materials have attracted considerable interest due to their novel properties including electronic, electromechanical and magnetoelectric properties. Until now, exotic ferroelectric structures have been described theoretically such as flux-closure domains, but experimental studies for ferroelectric multi-domains in nanostructures have been a lack of research due to their large domain wall energy. In this study, we realized the radial-quadrant domain structures using strain relaxation known as flexoelectricity. Moreover, we observed that local electric polarization switching can affect distant domain regions to minimize free energy. Our findings provide basic concepts to demonstrate and understand ferroelectric nano-scale multi-domain structures.

**10:12AM A30.00010 Removing pinhole shorts during large scale ferroelectric switching through ionic liquid interfaces**<sup>1</sup>, ANTHONY WONG, University of Tennessee, ANDREAS HERKLOTZ, NINA WISINGER, Oak Ridge National Laboratory, PHILIP RACK, University of Tennessee, THOMAS WARD, Oak Ridge National Laboratory — Ferroelectrics are a classification of materials that spontaneously polarize, accumulating charge at interfaces, and have non-linear hysteretic polarization curves. Switching fields required for ferroelectric materials are often very high, requiring thin insulating layers and high applied voltages. This commonly leads to electric pinholes and limits the areal sizes that can be polarized at a time. Ionic liquids have recently received heavy interest for the formation of electronic double layers which lead to huge electric fields at interfacial regions with low applied biases, and without the thickness constraint associated with conventional capacitors. We will show recent results which demonstrate that ionic liquid gating may offer the ideal solution to switch large regions of a ferroelectric film without limitations associated with pinhole defects. This has great importance to practical applications and fundamental interface studies that require large sample regions to be uniformly polarized.

<sup>1</sup>Supported by the US DOE Office of Basic Energy Sciences, Materials Sciences and Engineering Division and under US DOE grant DE-SC0002136.

**10:24AM A30.00011 ABSTRACT WITHDRAWN —**

**10:36AM A30.00012 Investigation of properties of lithium niobate crystals in confined geometries**, KEITH VEENHUIZEN, Lehigh University, GREG STONE, Pennsylvania State University, BASTIAN KNABE, Department of Microsystems Engineering (IMTEK), SEAN MCANANY, Lehigh University, KARSTEN BUSE, Fraunhofer Institute for Physical Measurement Techniques, HIMANSHU JAIN, VOLKMAR DIEROLF, Lehigh University — The properties of ferroelectric materials in confined geometries, specifically lithium niobate nanocrystals and crystal lines in glass, were studied. Batches of LiNbO<sub>3</sub> nanocrystals have been synthesized from various initial ratios of lithium to niobium using the sol-gel method. The batches were analyzed via Raman spectroscopy and SEM imaging to gain information about their size, morphology, stoichiometry, and defect content. The nanocrystals are very sensitive to the initial stoichiometric ratio in the synthesis step. Raman spectra reveal the resultant nanocrystal stoichiometry depends on the initial stoichiometry of the batch, the spectra also reveal an extra phase is present besides LiNbO<sub>3</sub> in some batches, and high quality spherical nanocrystals can be synthesized at certain initial stoichiometric ratios. In addition, lines of LiNbO<sub>3</sub> were crystallized in lithium-niobo-silica glass systems with varying amounts of silica to understand and control the nucleation and crystallization of the crystals in glass.

**10:48AM A30.00013 Direct writing of functional ferroelectric waveguides in glass**, CARL LIEBIG, JONATHAN GOLDSTEIN, GARY COOK, Air Force Research Laboratories — Femtosecond lasers modify the refractive index of many transparent materials for writing high quality waveguides due to their ability to confine the optical damage to an intended region [1]. They also can precipitate microcrystalline structures in glass and have demonstrated the production of ferroelectric crystals that can be used for optical waveguiding [2,3]. Ferroelectric crystals such as lithium niobate are some of the most widely used optical materials due to their strong electro-optic, piezoelectric, and photorefractive properties. The structure and alignment of the precipitated ferroelectric crystals can be controlled through the incident beam profile, writing speed and the starting material composition[2]. In this study crystalline waveguide structures were be written in 33LiO<sub>2</sub>-33Nb<sub>2</sub>O<sub>5</sub>-34SiO<sub>2</sub> (mol%) glass, characterized, the structural orientation determined, and their waveguiding performance tested. This procedure was then modified to functionalize the precipitated waveguides for photonic and holographic applications. [1] C. Mauchair et al., Opt. Exp. 16, (2008). [2] A. Stone et al., Sci. Reports 5, 10391 (2015). [3] T. Komatsu et al., J. Sol. State Chem. 184, 411 (2011).

**Monday, March 14, 2016 8:00AM - 11:00AM –**

**Session A31 DCP: Advances in Density Functional Theory I** 331 - Donald Truhlar, University of Minnesot

**8:00AM A31.00001 SCAN: An Efficient Density Functional Yielding Accurate Structures and Energies of Diversely-Bonded Materials<sup>1</sup>**, JIANWEI SUN, Temple Univ — The accuracy and computational efficiency of the widely used Kohn-Sham density functional theory (DFT) are limited by the approximation to its exchange-correlation energy  $E_{xc}$ . The earliest local density approximation (LDA) overestimates the strengths of all bonds near equilibrium (even the vdW bonds). By adding the electron density gradient to model  $E_{xc}$ , generalized gradient approximations (GGAs) generally soften the bonds to give robust and overall more accurate descriptions, except for the vdW interaction which is largely lost. Further improvement for covalent, ionic, and hydrogen bonds can be obtained by the computationally more expensive hybrid GGAs, which mix GGAs with the nonlocal exact exchange. Meta-GGAs are still semilocal in computation and thus efficient. Compared to GGAs, they add the kinetic energy density that enables them to recognize and accordingly treat different bonds, which no LDA or GGA can [1]. We show here that the recently developed non-empirical strongly constrained and appropriately normed (SCAN) meta-GGA [2] improves significantly over LDA and the standard Perdew-Burke-Ernzerhof GGA for geometries and energies of diversely-bonded materials (including covalent, metallic, ionic, hydrogen, and vdW bonds) at comparable efficiency. Often SCAN matches or improves upon the accuracy of a hybrid functional, at almost-GGA cost. [1] J. Sun et al., Phys. Rev. Lett. 111, 106401 (2013). [2] J. Sun, A. Ruzsinszky, and J.P. Perdew, Phys. Rev. Lett. 115, 036402 (2015).

<sup>1</sup>This work has been supported by NSF under DMR-1305135 and CNS-09-58854, and by DOE BES EFRC CCDM under DE-SC0012575.

**8:36AM A31.00002 SCAN+rVV10: A promising van der Waals density functional<sup>1</sup>**, HAOWEI PENG, ZENG-HUI YANG, JIANWEI SUN, JOHN PERDEW, Department of Physics, Temple Univeristy — The newly developed “strongly constrained and appropriately normed” (SCAN) meta-generalized-gradient approximation (meta-GGA) can generally improve over the non-empirical Perdew-Burke-Ernzerhof (PBE) GGA not only for strong chemical bonding, but also for the intermediate-range van der Waals (vdW) interaction. However, the long-range vdW interaction is still missing. To remedy this, we propose here pairing SCAN with the non-local correlation part from the rVV10 vdW density functional, with only two empirical parameters. The resulting SCAN+rVV10 yields excellent geometric and energetic results not only for molecular systems, but also for solids and layered-structure materials, as well as the adsorption of benzene on coinage metal surfaces. Especially, SCAN+rVV10 outperforms all current methods with comparable computational efficiencies, accurately reproducing the three most fundamental parameters—the inter-layer binding energies, inter-, and intra-layer lattice constants—for 28 layered-structure materials. Hence, we have achieved with SCAN+rVV10 a promising vdW density functional for general geometries, with minimal empiricism.

<sup>1</sup>This work was supported as part of the Center for the Computational Design of Functional Layered Materials, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award .DE-SC0012575.

**8:48AM A31.00003 The optimized effective potential of meta-generalized gradient approximations in solids<sup>1</sup>**, ZENGHUI YANG, JOHN PERDEW, Department of Physics, Temple University — Unlike the local density approximation(LDA) and the generalized gradient approximation(GGA), calculations with meta-GGAs are usually done according to the generalized Kohn-Sham(gKS) formalism. The exchange-correlation potential of the gKS equation is non-multiplicative, which prevents systematic comparison of meta-GGA bandstructures to those of the LDA and the GGA. We implement the optimized effective potential(OEP) of the meta-GGA for periodic systems, which allows us to carry out meta-GGA calculations in the same KS manner as for the LDA and the GGA. We apply the OEP to several popular meta-GGAs, including the new SCAN functional[Phys. Rev. Lett. 115, 036402(2015)]. We find that the KS gaps of meta-GGAs are close to those of GGAs, and they are smaller than the gKS gaps of meta-GGAs. The well-known grid sensitivity of meta-GGAs is much more severe in OEP calculations.

<sup>1</sup>The authors are supported by the National Science Foundation(Grant No. DMR-1305135).

**9:00AM A31.00004 Characterization of Thin Film Materials using SCAN MetaGGA, an Accurate Nonempirical Density Functional**, IOANA-GIANINA BUDA, CHRISTOPHER LANE, BERNARDO BARBIELLINI, Northeastern University, ADRIENN RUZSINSZKY, JIANWEI SUN, JOHN P. PERDEW, Temple University, ARUN BANSIL, Northeastern University — The exact ground-state properties of a material can be derived from the single-particle Kohn-Sham equations within the framework of the Density Functional Theory (DFT), provided the exact exchange-correlation potential is known. The simplest approximation is the local density approximation (LDA), but it usually leads to overbinding in molecules and solids. On the other hand, the generalized gradient approximation (GGA) introduces corrections that expand and soften bonds. The newly developed nonempirical SCAN (strongly-constrained and appropriately-normed) MetaGGA [Phys. Rev. Lett. 115, 036402] has been shown to be comparable in efficiency to LDA and GGA, and to significantly improve LDA and the Perdew-Burke-Ernzerhof version of the GGA for ground-state properties such as equilibrium geometry and lattice constants for a number of standard datasets for molecules and solids. Here we discuss the performance of SCAN MetaGGA for thin films and monolayers and demonstrate improvements of predicted ground-state properties. Examples include graphene, phosphorene and MoS<sub>2</sub>.

**9:12AM A31.00005 Comparative first-principles study of clean-surface properties of metals**, ABHIRUP PATRA, JIANWEI SUN, JOHN P. PERDEW, Department of Physics, Temple University — Metal surfaces are widely used in different applications from nano-devices to heterogeneous catalysis. Clean-surface properties such as the surface energy, work function and interlayer spacing importantly determine the behavior of metal surfaces. Prior work has been done to understand these properties using high-level methods including the local density approximation (LDA) and the generalized gradient approximation (PBE). In this work, we study (111) (100) and (110) surfaces of Pt, Pd, Cu, Al, Au, Ag, Rh and Ru by extrapolation from a finite number of layers. These surfaces are studied using SCAN, a new member of the computationally-efficient meta-GGA family of density functionals. We have compared the performance of SCAN and three other standard density functionals - LDA, PBE and PBEsol - to available experimental results. We find that the performance of the general-purpose SCAN is at the level of the more-specialized PBEsol, giving accurate metallic properties. Ref: Jianwei Sun, Adrienn Ruzsinszky, John P Perdew, Strongly Constrained and Appropriately Normed Semilocal Density Functional, *Physical Review Letters*115 (3), 036402 (2015). Supported by NSF under DMR-1305135, CNS-09-5884, and by DOE under DE-SC0012575, DE-AC02-05CH11231.

**9:24AM A31.00006 A Non-Local, Energy-Optimized Kernel: Recovering Second-Order Exchange and Beyond in Extended Systems**, JEFFERSON BATES, SAVIO LARICCHIA<sup>1</sup>, ADRIENN RUZSINSZKY, Temple University — The Random Phase Approximation (RPA) is quickly becoming a standard method beyond semi-local Density Functional Theory that naturally incorporates weak interactions and eliminates self-interaction error. RPA is not perfect, however, and suffers from self-correlation error as well as an incorrect description of short-ranged correlation typically leading to underbinding. To improve upon RPA we introduce a short-ranged, exchange-like kernel that is one-electron self-correlation free for one and two electron systems in the high-density limit. By tuning the one free parameter in our model to recover an exact limit of the homogeneous electron gas correlation energy we obtain a non-local, energy-optimized kernel that reduces the errors of RPA for both homogeneous and inhomogeneous solids. To reduce the computational cost of the standard kernel-corrected RPA, we also implement RPA renormalized perturbation theory for extended systems, and demonstrate its capability to describe the dominant correlation effects with a low-order expansion in both metallic and non-metallic systems. Furthermore we stress that for norm-conserving implementations the accuracy of RPA and beyond RPA structural properties compared to experiment is inherently limited by the choice of pseudopotential.

<sup>1</sup>Current affiliation: King's College London

**9:36AM A31.00007 Semiclassical origins of density functionals<sup>1</sup>**, KIERON BURKE, UC Irvine — By careful numerical analysis of non-relativistic atomic correlation energies, we show that (a) the local density approximation becomes relatively exact for the correlation energy as the atomic number approaches infinity, (b) we find the leading correction, which is about 38.5 milliHartrees per atom, (c) show how this correction dominates for larger atoms and (d) how to construct a generalized gradient approximation that respects this limit (See KB, A. Cancio, T. Gould, S. Pittalis, arXiv:1409.4834). The relevance to density functional calculations will also be explained.

<sup>1</sup>Support provided by NSF CHE-1464795

**10:12AM A31.00008 Semiclassical potential functionals for semiconductor quantum wells**, ATTILA CANGI, Max Planck Institute of Microstructure Physics — Parabolic semiconductor quantum wells are considered promising candidates for constructing devices emitting radiation in the largely unexplored THz regime. However, progress is impeded by the difficulty of fine-tuning intersubband transitions in these quantum wells which is achieved by modifying the quantum-well geometry and mixing different materials. We predict the electronic structure of parabolic semiconductor quantum wells highly efficiently by iterating the Kohn-Sham self-consistent cycle without solving the Kohn-Sham equations[1]. We achieve this by combining potential functionals[2,3] with a recently derived semiclassical approximation[4]. This (1) demonstrates our method's efficiency and accuracy for realistic systems and (2) illustrates its utility as a high-throughput method for predicting the electronic structure of technologically intriguing microstructures. [1] A. Cangi, C.R. Proetto, S. Pittalis, K. Burke, and E.K.U. Gross, submitted (2016). [2] A. Cangi, D. Lee, P. Elliott, K. Burke, and E.K.U. Gross, PRL 106, 236404 (2011). [3] A. Cangi, E. K. U. Gross, and K. Burke, PRA 88, 062505 (2013). [4] R.F. Ribeiro, D. Lee, A. Cangi, P. Elliott, and K. Burke, PRL 114, 050401 (2015).

**10:24AM A31.00009 Thermal Corrections to Density Functional Simulations of Warm Dense Matter**, JUSTIN SMITH, AURORA PRIBRAM-JONES, KIERON BURKE, University of California, Irvine — Present density functional calculations of warm dense matter often use the Mermin-Kohn-Sham (MKS) scheme at finite temperature, but employ ground-state approximations to the exchange-correlation (XC) free energy. In the simplest solvable non-trivial model, an asymmetric Hubbard dimer, we calculate the exact many-body energies, the exact Mermin-Kohn-Sham functionals for this system, and extract the exact XC free energy. For moderate temperatures and weak correlation, we show this approximation is excellent, but fails for stronger correlations. Additionally, we use this system to test various conditions that must be satisfied.

**10:36AM A31.00010 Study of the large reduced density gradient limit for the exchange energy**, JOSE GAZQUEZ, JAVIER CARMONA-ESPINDOLA, Universidad Autonoma Metropolitana-Iztapalapa, ALBERTO VELA, Centro de Investigacin y de Estudios Avanzados, SAM TRICKEY, University of Florida — The generalized gradient approximation (GGA) for the Kohn-Sham exchange-correlation functional has become widely used in electronic structure calculations of small, medium and large systems, because it provides rather reasonable results with moderate computational effort. Usually the GGA for exchange (X) is expressed in terms of an analytical expression of the X enhancement function,  $F_x(s)$ , where  $s$  is the reduced density gradient. When a non-empirical approach based on constraint satisfaction is followed, the analytical expression of  $F_x(s)$  is the result of interpolating between the small- and large- $s$  limits. However, neither of those limits is uniquely defined. In both cases there are several possibilities. The present work is a study of the influence of the several large- $s$  limit possibilities upon the calculation of properties that depend on energy differences, versus those that depend on response functions, and excitation energies.

**10:48AM A31.00011 Study of adiabatic connection in ground-state density functional theory**, MANOJ HARBOLA, RABEET CHAUHAN, Indian Inst of Tech-Kanpur, RABEET S. CHAUHAN COLLABORATION — By employing modified [1] variational form of Le-Sech wavefunctions [2] for two-electron systems, accurate wavefunctions for He-like atoms corresponding to their ground-state density are obtained for varying strength, given by a parameter  $\alpha$  ( $0 \leq \alpha \leq 1$ ), of electron-electron interaction. Using these, it is shown explicitly that (i) the total energy varies almost linearly as a function of  $\alpha$ , and (ii) the ionization potential remains unchanged [3] as  $\alpha$  is varied. Furthermore, kinetic energy contribution to the density-functional exchange-correlation energy is calculated using the adiabatic connection formula [4] and shown to match that calculated on the basis of Kohn-Sham calculation. Finally, the exchange-correlation energy obtained for different values of  $\alpha$  is employed to analyze several hybrid exchange-correlation energy functionals in use. [1] R.S. Chauhan and M.K. Harbola, Chem. Phys. Lett. **639C**, 248(2015) [2] C. Le Sech, J. Phys. B: Atom. Mol. Opt. Phys. **30**, L47(1997) [3] M. Levy, J. P. Perdew and V. Sahni, Phys. Rev. A **30**, 2745(1984) [4] R. Harris and R.O. Jones, J. Phys. F: Met. Phys. **4** 1170 (1974); D.C. Langreth and J.P. Perdew, Phys. Rev. B **15**, 2884 (1977)

**Monday, March 14, 2016 8:00AM - 10:48AM —**

**Session A33 DPOLY GSOFT: Charged & Ion-Containing Polymers** 336 - Lisa Hall, Ohio State University

**8:00AM A33.00001 Ionomer Self-assembly in Dilute Solution: a Coarse-grained Molecular Dynamics Study.** , MAHDI GHELICHI, KOUROSH MALEK, MICHAEL EIKERLING, Simon Fraser University — Self-assembly of semiflexible ionomer chains in dilute solution is studied by classical molecular dynamics (MD). Ionomer molecules consist of hydrophobic backbones, grafted with pendant side chains that are terminated by anionic headgroups. Coarse-grained MD simulations show the self-assembly of the semiflexible ionomer chains into cylindrical bundle-like aggregates. Bundles are comprised of a core of backbone chains surrounded by a surface layer of charged anionic headgroups and a diffuse halo of counterions. Parametric studies of bundle properties explored the role of backbone hydrophobicity, strength of electrostatic interactions between charged moieties, side chain content, and counterion valence. Expectedly, the size of bundles increases with backbone hydrophobicity. The aggregate size depends nonmonotonically on the value of the Bjerrum length. Increasing the grafting density of pendant side chains results in smaller bundles and the counterion valence exerts a strong effect on bundle size and counterion localization in the near-bundle area. Results are interpreted in terms of the interplay of the surface energy of hydrophobic chains and the electrostatic repulsion among the anionic headgroups. The findings are discussed within the context of experimental studies on the formation of rodlike structures in ionomer solution.

**8:12AM A33.00002 Electrostatic Effect on the Solution Structure and Dynamics of PEDOT:PSS** , MICHAEL LEAF, MURUGAPPAN MUTHUKUMAR, Department of Polymer Science and Engineering, University of Massachusetts at Amherst, Amherst MA 01003 — Poly(3,4-ethylenedioxythiophene):poly(styrene sulfonic acid) (PEDOT:PSS) is a popular material used in organic electronic devices as a conductor. It consists of PEDOT polycations complexed with PSS polyanions which are initially suspended in aqueous solution and eventually cast into a film. Various annealing and doping methods dramatically enhance PEDOT:PSS film conductivity. To understand the physical interactions at play, we explore structural and dynamic aspects of PEDOT:PSS solutions through scattering and rheology techniques. We highlight several aspects of the phase behavior of PEDOT:PSS, and the significance of electrostatic interactions.

**8:24AM A33.00003 Ion Correlation and Transport in Polymer Electrolytes at Finite Salt Concentrations; Coarse-Grained Simulation Study** , UMI YAMAMOTO, ZHEN-GANG WANG, California Institute of Technology — We present results from coarse-grained simulation for ion dynamics and structures in dry polymer electrolytes. To capture the thermodynamic, kinetic, and system-specific aspects of ion solvation and clustering, cation-monomer complexation is modeled via functionalized physical bonds whose functionality and lifetime vary due to local availability of binding monomers and competition with Coulombic interaction. By varying salt concentration, cation-monomer binding energy, dielectric constant, and maximal functionality of the physical bonds, we systematically study the growth of ion clustering activity as characterized by packing structures, and associated changes in electric conductivity via single-ion and collective charge mobility. Deviations from Nernst-Einstein predictions, and comparisons with existing experiments for concentration dependence of conductivity will be discussed.

**8:36AM A33.00004 Explicit-ion Effects in the Coil-Globule Transition of Weak Polyelectrolytes** , BENJAMIN J. SIKORA, JONATHAN K. WHITMER, University of Notre Dame — The first-order coil-globule transition in weak (annealed) polyelectrolytes involves a subtle balance of pH, charge strength, and solvation forces. In this work, we utilize a coarse-grain hybrid grand-canonical Monte Carlo and Molecular Dynamics approach to explore the free energetic topography of a model hydrophobic polybase [representing poly(2-vinylpyridine) (P2VP)] and explore the role of salt concentration/valency in influencing polyelectrolyte conformations using both an implicit Debye-Hückel and explicit salt approach. Our simulations reproduce the experimentally measured behavior for dilute annealed polyelectrolytes, and present a solid foundation for understanding pH responsive polyelectrolyte materials.

**8:48AM A33.00005 The effect of ionic correlations on ion distribution across polyelectrolyte blend interfaces<sup>1</sup>** , HA-KYUNG KWON, MONICA OLVERA DE LA CRUZ, Department of Materials Science and Engineering, Northwestern University, Evanston, Illinois 60208 — Recent developments in high-density energy storage and generation devices have identified as polyelectrolyte blends and copolymers as suitable candidate materials for use in these applications, as they combine the low volatility and high flexibility of polymers with ion-selective conductivity of the charge-carrying backbone. It has been shown that in polyelectrolyte melts, where the dielectric constant is relatively low, ionic correlations can significantly reduce miscibility, inducing phase separation even at negative values of  $\chi_N$ . At selected values of ionic coupling strengths, the polyelectrolyte blend exhibits a triple point, where coexistence is observed between phases with different concentrations and ordering of ions. When salt is added, the system undergoes re-entrant behavior as electrostatic effects are screened out. Using a hybrid of self-consistent field and liquid state theories (SCFT-LS), we investigate the distribution of ions across the interface in polyelectrolyte blends. We demonstrate that the inclusion of ionic correlations induces complex charge-dependent adsorption behavior at the interface, leading to changes in the interfacial width and miscibility of the blend.

<sup>1</sup>This work was performed under the following financial assistance award 70NANB14H012 from U.S. Department of Commerce, National Institute of Standards and Technology as part of the Center for Hierarchical Materials Design (CHiMaD).

**9:00AM A33.00006 Effect of Charge Patterning on the Phase Behavior of Polymer Coacervates for Charge Driven Self Assembly** , MITHUN RADHAKRISHNA, CHARLES E. SING, University of Illinois at Urbana-Champaign — Oppositely charged polymers can undergo associative liquid-liquid phase separation when mixed under suitable conditions of ionic strength, temperature and pH to form what are known as 'polymeric complex coacervates'. Polymer coacervates find use in diverse array of applications like microencapsulation, drug delivery, membrane filtration and underwater adhesives. The similarity between complex coacervate environments and those in biological systems has also found relevance in areas of bio-mimicry. Our previous works have demonstrated how local charge correlations and molecular connectivity can drastically affect the phase behavior of coacervates. The precise location of charges along the chain therefore dramatically influences the local charge correlations, which consequently influences the phase behavior of coacervates. We investigate the effect of charge patterning along the polymer chain on the phase behavior of coacervates in the framework of the Restricted Primitive Model using Gibbs Ensemble Monte Carlo simulations. Our results show that charge patterning dramatically changes the phase behavior of polymer coacervates, which contrasts with the predictions of the classical Voorn-Overbeek theory. This provides the basis for designing new materials through charge driven self assembly by controlling the positioning of the charged monomers along the chain.

**9:12AM A33.00007 Connectivity and Excluded Volume Effects in Polymeric Complex Coacervates** , CHARLES SING, MITHUN RADHAKRISHNA, University of Illinois at Urbana-Champaign — Oppositely-charged polyelectrolytes in salt solutions can undergo phase separation to form complex coacervates. This charge-driven phase behavior is the basis for emerging motifs in self-assembly. Traditional uses for coacervates are in food and personal care products, while applications in technologies for drug delivery and sensory materials are being developed. One of the primary theories driving understanding of complex coacervates is the Voorn-Overbeek (V-O) theory, which is a precursor to more sophisticated field theories. We present both theory and simulation that provides an alternate picture of coacervates, specifically addressing the limitations of V-O. Our theoretical approach is based on PRISM, which is a liquid-state theory that specifically accounts for connectivity. This is compared with Monte Carlo-based simulations, which likewise provide a molecular picture of coacervation. We demonstrate that a combination of connectivity-based correlations and excluded volume has a profound effect on coacervation phase behavior, suggesting that favorable comparison of V-O to experiment benefits from a cancellation of errors. The influence of connectivity on coacervate phase behavior hints at new opportunities for molecular-based design in electrostatically-driven self-assembly.

**9:24AM A33.00008 Salting-out and Salting-in in Polyelectrolyte Solutions**, PENGFEI ZHANG, Division of Chemistry & Chemical Engineering, California Institute of Technology, JIANZHONG WU, Department of Chemical and Environmental Engineering, University of California, Riverside, ZHEN-GANG WANG, Division of Chemistry and Chemical Engineering, California Institute of Technology — The phase behavior of polyelectrolyte (PE) solutions is governed by complicated interplay involving the mixing entropy, excluded volume, chain connectivity, and electrostatic interactions. Here we study the phase behavior of PE solutions in both salt-free condition and with added salt using a liquid-state (LS) theory based thermodynamic model. The LS model accounts for the hard-core repulsion by the Canahan-Starling equation of state, correlations due to chain connectivity by the first-order thermodynamic perturbation theory, and electrostatic correlations by the mean-spherical approximation. In comparison to the prediction from the well-known Voorn-Overbeek theory, the LS model predicts loop-type binodal curves in the salt-PE concentration diagram at temperatures slightly above the critical temperature of PE solution in salt-free case, consistent with the experimental study. The phase separated region shrinks with increasing temperature. Three scenarios of salting-out and salting-in phenomenon are predicted with addition of salts based, depending on the PE concentration.

**9:36AM A33.00009 Influence of Higher Valence Ions on Flexible Polyelectrolytes Stiffness and Counter-ion Distribution**<sup>1</sup>, ALEXANDROS CHREMOS, JACK F. DOUGLAS, NIST - Natl Inst of Stds & Tech — We investigate the influence of counter-ion valency on the flexibility of highly charged flexible polymer chains by molecular dynamics simulations that include both salt and an explicit solvent. A theoretical understanding of solutions of these molecules (e.g., DNA, RNA, and sulfonate polystyrene) has been slow to develop due to the complex coupling between the polyelectrolyte conformation and the ionic species in solution due to their long range Coulomb interactions. As observed experimentally, we find that divalent counter-ions greatly reduce the chain persistence length, in comparison to monovalent counter-ions, an effect correlated with the tendency of the polyelectrolyte chain to become distorted by divalent counter-ions. We rationalize these results by with the substantial increase of counter-ion population at the interface with the polyelectrolyte, which not only leads to a more effective screening of the bare charge, but also leads to charge inversion in the trivalent counter-ion case. These conformational changes with counter-ion valency are also associated with a drastic increase of the number of contacts the counter-ions have at the interface with polyelectrolyte, an effect associated with polyelectrolyte chain coiling around the counter-ions.

<sup>1</sup>NIST Postdoctoral Fellowship

**9:48AM A33.00010 Understanding and Controlling Transitions in Polyelectrolyte Complex Materials**, SARAH PERRY, LI-WEI CHANG, YALIN LIU, BRIAN MOMANI, JON VELEZ, H. HENNING WINTER, University of Massachusetts Amherst — Polyelectrolyte complexation can be used in the self-assembly of a wide range of responsive soft materials ranging from dehydrated thin film and bulk solids to dense, polymer-rich liquid complex coacervates, and more complex hierarchical structures such as micelles and hydrogels. This responsivity can include swelling and dissolution, or liquid-to-solid transitions, typically as a function of ionic strength and/or pH. The patterning or presentation of charges and other chemical functionalities represents a powerful strategy for the design and manipulation of this type of responsiveness and the corresponding material properties. We utilize polypeptides and polypeptide derivatives as a model platform for the study of sequence and patterning effects on materials self-assembly. We also utilize rheology to understand the nature of the solid-to-liquid transition that has been observed in some systems. The goal of this systematic investigation of the effects of charge patterning is to elucidate design rules that facilitate the tailored creation of materials based on polyelectrolyte complexation with defined properties for a wide range of applications.

**10:00AM A33.00011 Complexation of two oppositely charged polyelectrolytes**, HAMIDREZA SHOJAEI, MURUGAPPAN MUTHUKUMAR, University of Massachusetts Amherst — Existence of both polycation and polyanion in a solution will lead to complexation. We investigate both dynamics and the steady state solution for complexation of two oppositely charged polyelectrolytes in a salty solution. By use of Smoluchowski equation, both dynamic and steady-state properties of a complexation event occurring were studied.

**10:12AM A33.00012 Morphology-induced low temperature conductivity in ionic liquids**.<sup>1</sup>, AYKUT ERBAS, MONICA OLVERA DE LA CRUZ, Northwestern University, OLVERA DE LA CRUZ TEAM — Ionic liquids exhibit nano-scale liquid crystalline order depending on the polymeric details of salt molecules. The resulting morphology and temperature behavior are key factors in determining the room temperature conductivity of ionic liquids. Here we discuss the phase behavior and related ionic conductivities of dry ionic liquids with volume fractions close to unity by using extensive molecular dynamics simulations. Temperature dependence, effective persistence length of tails, and excluded volume symmetry of amphiphilic ionic liquid molecules are investigated in large scale systems with short and long-range electrostatics. Our results suggest that by adjusting stiffness of the amphiphilic molecules and excluded volume interactions, lamellar or interconnected 3D phases can be obtained. Resulting phases have significant effects on the conductive properties. If there is no excluded volume asymmetry along the molecules, mostly lamellar phases with anisotropic conductivities emerge. If the excluded volume interactions become asymmetric, lamellar phases are replaced by interconnected phases consist of charged groups. Within temperature ranges that morphological phases are observed, conductivities exhibit low-temperature maxima in accord with experiments of ionic liquid-based liquid

<sup>1</sup>Center of Bio-inspired Energy Center (CBES)

**10:24AM A33.00013 Structural Dynamics of Star-Shaped Weak Polyelectrolytes in Dilute Aqueous Solution**, CHEN QU, Univ of Notre Dame, Y. ELAINE ZHU, Wayne State University — Weak polyelectrolyte (PE) bearing tunable charges along their backbones show great potential as “smart” polymer materials for diverse applications from drug delivery to energy storage. With the introduction of branched topology, the local counterion distribution in the vicinity to the polyelectrolyte segments becomes highly inhomogeneous. To experimentally investigate the interplay between structural dynamics and local electric environment of a branched polyelectrolyte, in this work we custom synthesized star-shaped poly(2-vinylpyridine) (P2VP) using reversible addition fragmentation chain transfer (RAFT) polymerization and labeled P2VP stars with pH-sensitive fluorophore precisely either in the center or periphery. By employing fluorescence correlation spectroscopy (FCS) with photon counts histogram (PCH) analysis, we observed gradual stretched-to-collapses conformational transition with increasing solution pH for both P2VP stars of different fluorophore labeling locations. However, the measured local pH, or local proton concentration, shows strong dependence of the fluorophore labeling locations. Higher electric potential yet lower ionization degree was observed in the core of P2VP star than that in the periphery. Ongoing work is carried out to examine the scaling behaviors of P2VP star sizes with varied number of arms, arm lengths and counterion concentrations in dilute aqueous solutions.

**10:36AM A33.00014 Thermodynamics and Phase Behavior of Phosphonated Block Copolymers Containing Ionic Liquids**, HA YOUNG JUNG, Pohang Univ of Sci & Tech, MOON JEONG PARK, Pohang Univ of Sci Tech — Charge-containing copolymers have drawn intensive attention in recent years for their uses in wide range of electrochemical devices such as fuel cells, lithium batteries and actuators. Particularly, the creation of microphase-separated morphologies in such materials by designing them in block and graft configurations has been the subject of extensive studies, in order to establish a synergistic means of optimizing ion transport properties and mechanical integrity. Interest in this topic has been further stimulated by intriguing phase behavior from charge-containing polymers, which was not projected from conventional phase diagrams of non-ionic polymers. Herein, we investigate thermodynamics and phase behavior of a set of phosphonated block copolymers. By synthesizing low-molecular weight samples with degree of polymerization ( $N$ ) < 35, we observed order-disorder transition that enabled us to estimate effective Flory-Huggins interaction parameters ( $\chi$ ) by using random phase approximation. We further examined the systems by adding various ionic liquids, where noticeable increases in  $\chi$  values and modulated microphase separation behavior were observed. The morphology-conductivity relationship has been elucidated by taking into account the segmental motion of polymer chains, volume of conducting phases, and the molecular interactions between phosphonated polymer chains and cations of ionic liquids.

**Monday, March 14, 2016 8:00AM - 10:48AM —**

**Session A34 GSOFD DBIO GSNP/DFD: Active Matter I** 337 - Joern Dunkel, Massachusetts Institute of Technology

**8:00AM A34.00001 And yet it moves - propulsion of colloidal clusters under reciprocal actuation<sup>1</sup>**, GABI STEINBACH, Technische Universität Chemnitz, SIBYLLE GEMMING, ARTUR ERBE, Helmholtz-Zentrum Dresden-Rossendorf — In the regime of low Reynolds numbers, the challenge of torque-based magnetic actuation lies in the conversion of torque into an effective force via symmetry breaking without inertial effects. Most reported systems rely on the hydrodynamic coupling between rotation and translation by an asymmetry in the environment (surfaces/interfaces) or the object shape. There, net translation can be realized only under non-reciprocal actuation given by precessing and rotating fields. In contrast, under oscillating fields, which are easier to realize, hydrodynamic coupling intrinsically leads to cyclic, reciprocal translation (Scallop theorem) unless the object has a certain flexible shape such as a flagellum. We present an alternative approach where symmetry breaking can be realized by magnetically interacting colloids which have been effectively modeled by spheres with shifted dipoles. If such colloids self-assemble, they form rigid clusters. We show how the collective, non-equilibrium dynamics of the colloids under oscillating fields propel the cluster. Depending on the configuration of the cluster it can rotate, translate and perform screw-like motion.

<sup>1</sup>Grants funding by DFG: FOR 1713 GE 1202/9-1 and ER 341/9-1

**8:12AM A34.00002 Hyperuniformity in periodically sheared dilute suspensions**, SAM WILKEN, RO-DRIGO GUERRA, DAVID J PINE, PAUL M CHAIKIN, New York University — Periodically sheared dilute, non-Brownian suspensions explore new configurations through collisions in an otherwise reversible flow. Below a critical strain, the particles remain active until they find a configuration with no collisions and reach an absorbing state. Recent simulations by Hexner and Levine have shown that the configuration of particles in the critically absorbing state is hyperuniform. The particle number fluctuations of hyperuniform systems decrease with counting box size more rapidly than random systems (like the same suspension that is not in a critically absorbing state). We built a compact, lightweight uni-axial shear cell where particle coordinates can be measured while shearing with a confocal microscope. We have identified hyperuniform structures with density fluctuation measurements in colloidal suspensions of up to 40% volume fraction in the critically absorbing state with a strain ramp down protocol and find hyperuniform scaling of the density fluctuations.

**8:24AM A34.00003 Convection-driven aggregation of micron sized capsules**, OLEG SHKLYAEV, HENRY SHUM, ANNA BALAZS, Department of Chemical Engineering, The University of Pittsburgh — Collective dynamics of microcapsules often serve as a model for understanding behavior observed in colonies of biological cells. Using computer simulations, we explore the capability of chemically generated convection to assemble microcapsules into a colony with neighbors close enough to facilitate chemical communication. The microcapsules are assumed to carry a supply of chemical fuel. When this fuel, leaking out of the capsules, reacts at enzyme-covered sites of the chamber, the reaction generates fluid density variations driving flows. These flows carry the microcapsules, which tend to aggregate into colonies on and near the enzyme-covered sites. This aggregation continues until the reagent has been depleted and convection stops. We show that capsule colonies of predesigned shapes can be assembled by patterning the enzyme-covered surface.

**8:36AM A34.00004 Electric-field mediated propulsion in binary colloidal suspensions**, LAURA COLON-MELENDEZ, MATTHEW SPELLINGS, SHARON C. GLOTZER, MICHAEL J. SOLOMON, University of Michigan — We observe propulsion of pairs of unequally sized dielectric colloidal spheres in a plane perpendicular to the applied AC electric field. The fully reversible and reconfigurable effect is observed at different applied voltages and frequencies. Using confocal microscopy and particle tracking methods, we study the degree of active motion as a function of the number of particles in the dynamic clusters. The observed phenomenon is consistent with previous observations of asymmetric dumbbell propulsion in electric fields attributed to asymmetric electrohydrodynamic flow (Ma et al, PNAS 2015 112 (20) 6307-6312).

**8:48AM A34.00005 Self-assembly of active colloidal molecules with dynamic function**, RODRIGO SOTO, Universidad de Chile, RAMIN GOLESTANIAN, University of Oxford — Catalytically active colloids maintain non-equilibrium conditions in which they produce and deplete chemicals at their surface. While individual colloids that are symmetrically coated do not exhibit dynamical activity, the concentration fields resulting from their chemical activity decay as  $1/r$  and produce gradients that attract or repel other colloids depending on their surface chemistry and ambient variables. This results in a non-equilibrium analogue of ionic systems, but with the remarkable novel feature of action-reaction symmetry breaking. In dilute conditions these active colloids join up to form molecules via generalized ionic bonds. Colloids are found to join up to form self-assembled molecules that could be inert or have spontaneous activity in the form of net translational velocity and spin depending on their symmetry properties and their constituents. As the interactions do not satisfy detailed-balance, it is possible to achieve structures with time dependent functionality. We study a molecule that adopts spontaneous oscillations and another that exhibits a run-and-tumble dynamics similar to bacteria. Our study shows that catalytically active colloids could be used for designing self-assembled structures that possess dynamical functionalities.

**9:00AM A34.00006 Optimal Navigation of Self-Propelled Colloids in Microstructured Mazes**, YUGUANG YANG, MICHAEL BEVAN, Johns Hopkins University — Controlling navigation of self-propelled microscopic 'robots' subject to random Brownian motion in complex microstructured environments (e.g., porous media, tumor vasculature) is important to many emerging applications (e.g., enhanced oil recovery, drug delivery). In this work, we design an optimal feedback policy to navigate an active self-propelled colloidal rod in complex mazes with various obstacle types. Actuation of the rods is modelled based on a light-controlled osmotic flow mechanism, which produces different propulsion velocities along the rod's long axis. Actuator-parameterized Langevin equations, with soft rod-obstacle repulsive interactions, are developed to describe the system dynamics. A Markov decision process (MDP) framework is used for optimal policy calculations with design goals of colloidal rods reaching target end points in minimum time. Simulations show that optimal MDP-based policies are able to control rod trajectories to reach target regions order-of-magnitudes faster than uncontrolled rods, which diverges as maze complexity increases. An efficient multi-graph based implementation for MDP is also presented, which scales linearly with the maze dimension.

**9:12AM A34.00007 Active colloids that slosh through passive matrices.**, JIE ZHANG, University of Illinois at Urbana-Champaign, STEVE GRANICK, IBS Center for Soft & Living Matter — Studies of natural and artificial active matter have focused on systems with a large mismatch of the time and length scales for active and passive elements, but in a variety of non-equilibrium condensed matter systems, including numerous biological processes, actively driven elements have a crowded environment of surrounding passive "solvent" elements of comparable size. Here we study self-propelled colloidal particles in a passive matrix of comparable size. Particles with high activity take straight lines and sharp turns through the soft 2-D crystal matrix to ensure rapid healing of the crystal structure. Effective attraction between active particles arises when the concentration of active particles or the hardness of the matrix increases; active particles tend to segregate in the grain boundaries of the crystal matrix.

**9:24AM A34.00008 Diffusion of torqued active Brownian particles** , FRANCISCO J SEVILLA, Instituto de Física, Universidad Nacional Autónoma de México — An analytical approach is used to study the diffusion of active Brownian particles that move at constant speed in three-dimensional space, under the influence of passive (external) and active (internal) torques. The Smoluchowski equation for the position distribution of the particles is obtained from the Kramer-Fokker-Planck equation corresponding to Langevin equations for active Brownian particles subject to torques. In addition to giving explicit formulas for the mean square-displacement, the non-Gaussian behavior is analyzed through the kurtosis of the position distribution that exhibits an oscillatory behavior in the short-time limit. FJS acknowledges support from PAPIIT-UNAM through the grant IN113114

**9:36AM A34.00009 ABSTRACT WITHDRAWN** —

**9:48AM A34.00010 Motile Microbots from Dynamically Interacting and Self-Reconfiguring Assemblies of Metallo-Dielectric Janus Microcubes**<sup>1</sup> , KOOHEE HAN, North Carolina State Univ, C. WYATT SHIELDS IV, Duke University, BHUVNESH BHARTI, North Carolina State Univ, GABRIEL P. LOPEZ, Duke University, ORLIN D. VELEV, North Carolina State Univ — A new class of dynamically and reversibly reconfigurable active matter made by magnetic assembly and actuation of metallo-dielectric microcubes will be presented. We describe how magnetically responsive Janus microcubes can be assembled hierarchically into dynamically reconfiguring microclusters. Ferromagnetic cobalt patches of the cubes act as assembly directors. The residual magnetic polarization of the metal-coated facets leads to directional dipole-dipole and field-dipole interactions and reconfiguration of the neighboring cubic particles, which is directed by the conformational restrictions. Dynamic reconfiguration of assembled clusters can be achieved by on-demand switching between the dipole-field interaction and the residual dipole-dipole interaction when the field is turned on and off. We show how pre-assembled Janus microcube clusters can be directionally motile in non-Newtonian fluids by applying asymmetric magnetic fields. The modulation of the viscosity of non-Newtonian fluids upon varying the shear rate allowed demonstrating directional motion, resulting from time-asymmetric stroke patterns (e.g., rapid opening and slow closing). These motile clusters can serve as early prototypes of self-propelling microswimmers capable of *in-situ* assembly.

<sup>1</sup>NSF Grant DMR-1121107

**10:00AM A34.00011 Spontaneous Oscillations in an Active Matter System** , ROBERT HAYES, BOYCE TSANG, University of Illinois, STEVE GRANICK, IBS Center for Soft & Living Matter and UNIST — Active matter (which consumes energy to move about) can organize into dynamic structures more interesting than those possible at steady-state. Here we show spontaneous periodic self-assembly in a simple three-component system of water, oil phase, and surfactant at constant room temperature, with emphasis on one model system. Benchtop experiments show that liquid crystal oil droplets spontaneously and collectively oscillate like a 'beating heart' for several hours; contract, relax, and subsequently re-contract in a petri dish at a rate of a few 'beats' per minute. These oscillations, emergent from the cooperative interaction of the three components, are driven by the competition between positive and negative feedback processes. This illustration of feedback in action reveals a new way to program self-assembled structures to vary with time.

**10:12AM A34.00012 Catalytic particles induced Marangoni flow: motion, pumping and self-assembly** , PAOLO MALGARETTI, Max Planck Institute Stuttgart, ALVARO DOMINGUEZ, Universidad de Sevilla, MIHAIL N POPESCU, SIEGFRIED DIETRICH, Max Planck Institute Stuttgart — When catalytic particles, such as Janus particles, or enzymes are in the vicinity of a fluid-fluid interface, their behavior can be strongly modulated by the presence of the interface and/or by the inhomogeneity in the transport properties of the two fluid phases. Hence, the effective interaction with the interface can lead to novel dynamical regimes absent in homogeneous fluids. For example, if the by-products of the catalysis are surface active their spatial distribution will affect the local value of the surface tension. In such a scenario, when a catalytic particle approaches a fluid-fluid interface a Marangoni flow will set up as a response to the inhomogeneity in the surface tension induced by the byproducts of the catalysis. The onset of such a flow will attract the catalytic particle towards the interface. Interestingly the strength of such an effective attraction is strongly affected by the affinity of the byproduct to the interface as well as by the transport properties of the two fluid phases. In particular, for water-oil interfaces such an effect overwhelms other means of active transport such as self-diffusiophoresis and makes it suitable to enhance particle accumulation close to fluid-fluid interfaces. Finally I will discuss the onset of collective behavior.

**10:24AM A34.00013 Dynamics of fractal cluster colloidal gels with embedded active Janus particles** , MICHAEL SOLOMON, MEGAN SZAKASITS, WENXUAN ZHANG, University of Michigan — We find that fractal cluster gels of colloids in which platinum-coated Janus particles have been embedded exhibit enhanced mobility when the Janus particles are made active by the addition of hydrogen peroxide. Gelation is induced through addition of a divalent salt, magnesium chloride, to an initially stable suspension of Janus and polystyrene colloids, each of size about 1 micron. After the gels have been created, the embedded Janus colloids are activated by hydrogen peroxide, which is delivered to the system through a porous hydrogel membrane. We vary the ratio of active to passive colloids in the gels from about 1:20 to 1:8. Changes in structure and dynamics are visualized by two channel confocal laser scanning microscopy. By image analysis, we determine the particle positions and compute the mean squared displacement (MSD) of all particles in the gel. We measure the mobility enhancement in the fractal gels as a function of hydrogen peroxide concentration and Janus particle concentration and discuss the results in terms of the force provided by each active particle to the fractal gel network.

**10:36AM A34.00014 Rotation-translation hydrodynamic coupling of a particle in a gradient of viscosity** , NAOMI OPPENHEIMER, Princeton University, SHAHIN NAVARDI, Texas Tech University, HOWARD STONE, Princeton University — We study the translation-rotation hydrodynamic coupling of spherical particles in Stokes flow where there are gradients of viscosity. In particular, we examine cases in which symmetry is broken by temperature gradients in the fluid. Using the Lorentz reciprocal theorem, we derive analytical expressions for the coupling tensor when the viscosity variations caused by the temperature gradients are small. We examine two cases. In the first, the temperature gradient is external and the particle moves perpendicular to it. In the second the translating object is a Janus sphere that creates its own local temperature gradient. We find that in the first case, translation induces rotation, and in the second it suppresses it. Our results may illuminate recent experimental results of Janus particles activated by light.

**Monday, March 14, 2016 8:00AM - 11:00AM** —

**Session A35 DBIO GSOF GSNP: Active Matter: Collective Phenomena in Living Systems I**

338 - Karsten Kruse, Saarland University, Germany

**8:00AM A35.00001 Self-organization of stress patterns drives state transition in actin cortices** , NIKITA FAKHRI, Massachusetts Institute of Technology —

**8:36AM A35.00002 Spontaneous actin dynamics in contractile rings<sup>1</sup>**, KARSTEN KRUSE, Theoretical Physics, Saarland University, 66123 Saarbrücken, VIKTORIA WOLLRAB<sup>2</sup>, RAGHAVAN THIAGARAJAN, Laboratory of Cell Physics, Institut de Science et d'Ingénierie Supramoléculaires, 67083 Strasbourg, France, ANNE WALD, Theoretical Physics, Saarland University, 66123 Saarbrücken, DANIEL RIVELINE, Laboratory of Cell Physics, Institut de Science et d'Ingénierie Supramoléculaires, 67083 Strasbourg, France — Networks of polymerizing actin filaments are known to be capable to self-organize into a variety of structures. For example, spontaneous actin polymerization waves have been observed in living cells in a number of circumstances, notably, in crawling neutrophils and slime molds. During later stages of cell division, they can also spontaneously form a contractile ring that will eventually cleave the cell into two daughter cells. We present a framework for describing networks of polymerizing actin filaments, where assembly is regulated by various proteins. It can also include the effects of molecular motors. We show that the molecular processes driven by these proteins can generate various structures that have been observed in contractile rings of fission yeast and mammalian cells. We discuss a possible functional role of each of these patterns.

<sup>1</sup>The work was supported by Agence Nationale de la Recherche, France, (ANR-10-LABX-0030-INRT) and by Deutsche Forschungsgemeinschaft through SFB1027.

<sup>2</sup>present address: FOM Institute AMOLF, 1098 XG Amsterdam, The Netherlands

**8:48AM A35.00003 Fluctuations and nematic order in collective motion of filamentous bacteria<sup>1</sup>**, DAIKI NISHIGUCHI, The University of Tokyo, KEN H. NAGAI, JAIST, MASAKI SANO, The University of Tokyo — Although there are many numerical and theoretical studies on Vicsek-like models, there have been no convincing experiments that clearly observe predicted properties of collective motion such as giant number fluctuations. To realize such experiments with a biological system, we used filamentous bacteria, which are 20 times as long as usual bacteria. Due to strong alignment interactions arising from their elongated shapes, these bacteria exhibit a nematic state when their dense suspensions are confined in a quasi-two-dimensional plane. We have quantitatively evaluated the nematic order parameter in this ordered state and concluded that it has true long-range order, and we have obtained giant number fluctuations in this true long-range ordered state. All the obtained experimental results are consistent with a Vicsek-like model with the same symmetry as our experiments, namely, the Vicsek-like self-propelled rods model, in which each particle has polarity and their interactions are nematic.

<sup>1</sup>This work is supported by a Grant-in-Aid for Japan Society for Promotion of Science (JSPS) Fellows (Grant No. 26-9915) and KAKENHI (No. 25103004, Fluctuation & Structure) from MEXT, Japan.

**9:00AM A35.00004 Modeling flexible active nematics<sup>1</sup>**, MICHAEL VARGA, ROBIN SELINGER, Liquid Crystal Institute, Kent State University — We study active nematic phases of self-propelled flexible chains in two dimensions using computer simulation, to investigate effects of chain flexibility. In a “dry” phase of self-propelled flexible chains, we find that increasing chain stiffness enhances orientational order and correlation length, narrows the distribution of turning angles, increases persistence length, and increases the magnitude of giant density fluctuations. We further adapt the simulation model to describe behavior of microtubules driven by kinesin molecular motors in two different environments: on a rigid substrate with kinesin immobilized on the surface; and on a lipid membrane where kinesin is bonded to lipid head groups and can diffuse. Results are compared to experiments by L. Hirst and J. Xu. Lastly, we consider active nematics of flexible particles enclosed in soft, deformable encapsulation in two dimensions, and demonstrate novel mechanisms of pattern formation that are fundamentally different from those observed in bulk.

<sup>1</sup>Supported by NSF-DMR 1409658.

**9:12AM A35.00005 Active nematics confined within a shell**, RUI ZHANG, YE ZHOU, MOHAMMAD RAHIMI, JUAN DE PABLO, University of Chicago, DEPABLO TEAM — Active fluids exhibit many striking flow patterns when confined within complex geometries. For example, recent work has demonstrated that when a thin film of extensile microtubules is confined within a vesicle, the four  $+1/2$  defects periodically oscillate between a tetrahedral and a planar configuration (Keber, *et al.* Science (2014)). Here we employ hybrid lattice Boltzmann simulations to study the dynamics of active nematics confined between two concentric spherical surfaces. We find that in both extensile and contractile systems, the four defects are coupled with noticeable macroscopic velocities and they move along their symmetry axes, even though in different patterns. We observe that in extensile systems with moderate activity, defects repel each other due to elastic forces, and their collective motion leads to the same patterned dynamics as observed in the above experiment. We further show that this periodic dynamics is accompanied by oscillations of the defect velocity, system's elastic energy, and the emergence and annihilation of vortices. We also observe that with stronger activity, the extensile system evolves to chaos. In contrast, the contractile system remains passive for the entire activity range, with defects being attracted to each other in pairs.

**9:24AM A35.00006 Active Cellular Nematics**, GUILLAUME DUCLOS, CHRISTOPH ERLINKAEMPER, SIMON GARCIA, HANNAH YEVICK, JEAN-FRANÇOIS JOANNY, PASCAL SILBERZAN, Physico-Chimie Curie, UMR 168, UPMC, Institut Curie, BIOLOGY INSPIRED PHYSICS AT MESOSCALES TEAM, PHYSICAL APPROACH OF BIOLOGICAL PROBLEMS TEAM — We study the emergence of a nematic order in a two-dimensional tissue of apolar elongated fibroblast cells. Initially, these cells are very motile and the monolayer is characterized by giant density fluctuations, a signature of far-from-equilibrium systems. As the cell density increases because of proliferation, the cells align with each other forming large perfectly oriented domains while the cellular movements slow down and eventually freeze. Therefore topological defects characteristic of nematic phases remain trapped at long times, preventing the development of infinite domains. By analogy with classical non-active nematics, we have investigated the role of boundaries and we have shown that cells confined in stripes of width smaller than typically 500 nm are perfectly aligned in the stripe direction. Experiments performed in cross-shaped patterns show that both the number of cells and the degree of alignment impact the final orientation. *Reference:* Duclos G., Garcia S., Yevick H.G. and Silberzan P., “Perfect nematic order in confined monolayers of spindle-shaped cells”, *Soft Matter*, 10, 14, 2014

**9:36AM A35.00007 Defect dynamics and ordering in compressible active nematics.<sup>1</sup>**, PRASHANT MISHRA, Department of Physics, Syracuse University, PRAGYA SRIVASTAVA, The Francis Crick Institute, M. CRISTINA MARCHETTI, Department of Physics, Syracuse University — Active nematics, such as suspensions of biopolymers activated by molecular motors or bacteria swimming in passive liquid crystals, exhibit complex self-sustained flow, excitability and defect generation. Activity renders the defect themselves self-propelled particles, capable of organizing in emergent ordered structures. We have developed a minimal model of compressible active nematics on a substrate. We eliminate the flow velocity in favor of the nematic order parameter via the balance of frictional dissipation and active driving to obtain a dynamical description entirely in terms of the nematic alignment order parameter. Activity renormalizes the bend and splay elastic constants rendering them anisotropic and driving them to zero or even negative, resulting in the appearance of modulated states and defective structures. Using linear stability analysis and numerics we organize the various regimes into a phase diagram and discuss the relation to experiments.

<sup>1</sup>This work was supported by NSF-DMR-1305184.

**9:48AM A35.00008 Directed and persistent movement arises from mechanochemistry of the ParA/ParB system**, LONGHUA HU, National Heart, Lung, and Blood Institute, National Institutes of Health, ANTHONY G. VECCHIARELLI, KIYOSHI MIZUUCHI, National Institute of Diabetes and Digestive and Kidney Diseases, National Institutes of Health, KEIR C. NEUMAN, JIAN LIU, National Heart, Lung, and Blood Institute, National Institutes of Health — The segregation of DNA prior to cell division is essential for faithful genetic inheritance. In many bacteria, segregation of the low-copy-number plasmids involves an active partition system composed of ParA ATPase and its stimulator protein ParB. Recent experiments suggest that ParA/ParB system motility is driven by a diffusion-ratchet mechanism in which ParB-coated plasmid both creates and follows a ParA gradient on the nucleoid surface. However, the detailed mechanism of ParA/ParB-mediated directed and persistent movement remains unknown. We develop a theoretical model describing ParA/ParB-mediated motility. We show that the ParA/ParB system can work as a Brownian ratchet, which effectively couples the ATPase-dependent cycling of ParA-nucleoid affinity to the motion of the ParB bound cargo. Paradoxically, the resulting processive motion relies on quenching diffusive plasmid motion through a large number of transient ParA/ParB-mediated tethers to the nucleoid surface. Our work sheds light on a new emergent phenomenon in which non-motor proteins work collectively via mechanochemical coupling to propel cargos — an ingenious solution shaped by evolution to cope with the lack of processive motor proteins in bacteria.

**10:00AM A35.00009 Decoupling tissue and cell scale stresses using embedded oil microdroplets<sup>1</sup>**, ELIJAH SHELTON, FRIEDHELM SERWANE, ALESSANDRO MONGERA, ADAM LUCIO, OTGER CAMPÀS, University of California Santa Barbara — Embryonic development and organ morphogenesis require mechanical stresses to be patterned in space and time over length scales ranging from cellular to tissue level. While several approaches use 4D live-imaging to infer forces from the observed flow fields, few techniques allow direct measurements of stress in vivo and in situ. We use oil microdroplets injected in between cells as direct stress sensors. Through confocal imaging and custom software for high resolution 3D droplet surface reconstruction, we can directly measure the patterns of stress by looking at the deformations of the drop. This analysis allows us to decouple the stresses at the tissue scale from those generated at cellular scales by disentangling ellipsoidal drop deformation modes from higher order drop deformations. Using this technique we measure both tissue and cell scale stresses within aggregates of mesenchymal cells as well as within developing zebrafish embryonic tissues. The decoupling of mechanical stresses at cell and tissue scales makes our technique uniquely suited for understanding how tissue scale reorganizations emerge from cell scale interactions.

<sup>1</sup>This material is based upon work supported by the National Science Foundation Graduate Research Fellowship

**10:12AM A35.00010 Volume Changes During Active Shape Fluctuations in Cells**, CATERINA A. M. LA PORTA, ALESSANDRO TALONI, University of Milan, ELENA KARDASH, University of Geneva, OGUZ UMUT SALMAN, CNRS, Paris, LEV TRUSKINOVSKY, CNRS, Ecole Polytechnique, Palaiseau, STEFANO ZAPPERI, University of Milan — Cells modify their volume in response to changes in osmotic pressure but it is usually assumed that other active shape variations do not involve significant volume fluctuations. Here we report experiments demonstrating that water transport in and out of the cell is needed for the formation of blebs, commonly observed protrusions in the plasma membrane driven by cortex contraction. We develop and simulate a model of fluid-mediated membrane-cortex deformations and show that a permeable membrane is necessary for bleb formation which is otherwise impaired. Taken together, our experimental and theoretical results emphasize the subtle balance between hydrodynamics and elasticity in actively driven cell morphological changes <sup>1</sup>.

<sup>1</sup>A. Taloni et al. Phys. Rev. Lett. 114, 208101 (2015)

**10:24AM A35.00011 Probing the Dynamics of the Cellular Actomyosin Network with Magnetic Microposts**, YU SHI, Department of Physics and Astronomy, Johns Hopkins University, STEVEN HENRY, JOHN CROCKER, Department of Chemical and Biomolecular Engineering, University of Pennsylvania, DANIEL REICH, Department of Physics and Astronomy, Johns Hopkins University — The actomyosin network in living cells is commonly accepted as an archetypal example of an active matter system. To characterize the dynamic properties and the effects of non-thermal motion of such a system requires simultaneously measuring the fluctuation spectrum of internal stresses as well as its local viscoelasticity. Via use of PDMS micropost arrays with magnetic nanowires embedded in selected posts, we measure the local complex modulus of cells through mechanical actuation of the magnetic microposts using a dual magnetic tweezer system. The microposts are also used as passive probes to measure the force fluctuations inside the cytoskeleton. The active and passive responses of fibroblasts will be presented, together with measurements of correlations between different subcellular regions, and the influence of cytoskeletal and myosin inhibitors. Results on the anisotropy of internal stress fluctuations and their response to chemical perturbations will also be discussed.

**10:36AM A35.00012 Active Contraction of Microtubule Networks**, PETER FOSTER, John A. Paulson School of Engineering and Applied Sciences and FAS Center For Systems Biology, Harvard University, SEBASTIAN FRTHAUER, Courant Institute of Mathematical Science, New York University and Department of Molecular and Cellular Biology, Harvard University, MICHAEL SHELLEY, Courant Institute of Mathematical Science, New York University, DANIEL NEEDLEMAN, John A. Paulson School of Engineering and Applied Sciences, FAS Center For Systems Biology, Harvard University — Many cellular processes are driven by cytoskeletal assemblies. It remains unclear how cytoskeletal filaments and motor proteins organize into cellular scale structures and how molecular properties of cytoskeletal components affect the large scale behaviors of these systems. Here we investigate the self-organization of stabilized microtubules in *Xenopus* oocyte extracts and find that they can form macroscopic networks that spontaneously contract. We propose that these contractions are driven by the clustering of microtubule minus ends by dynein. Based on this idea, we construct an active fluid theory of network contractions which predicts a dependence of the timescale of contraction on initial network geometry, a development of density inhomogeneities during contraction, a constant final network density, and a strong influence of dynein inhibition on the rate of contraction, all in quantitative agreement with experiments. These results demonstrate that the motor-driven clustering of filament ends is a generic mechanism leading to contraction.

**10:48AM A35.00013 Collective dynamics during cell division**, STEFANO ZAPPERI, University of Milan, ZSOLT BERTALAN, ZOE BUDRIKIS, ISI Foundation, CATERINA A. M. LA PORTA, University of Milan — In order to correctly divide, cells have to move all their chromosomes at the center, a process known as congression. This task is performed by the combined action of molecular motors and randomly growing and shrinking microtubules. Chromosomes are captured by growing microtubules and transported by motors using the same microtubules as tracks<sup>1</sup>. Coherent motion occurs as a result of a large collection of random and deterministic dynamical events. Understanding this process is important since a failure in chromosome segregation can lead to chromosomal instability one of the hallmarks of cancer. We describe this complex process in a three dimensional computational model involving thousands of microtubules. The results show that coherent and robust chromosome congression can only happen if the total number of microtubules is neither too small, nor too large. Our results allow for a coherent interpretation a variety of biological factors already associated in the past with chromosomal instability and related pathological conditions<sup>2</sup>.

<sup>1</sup>Z. Bertalan et al. Navigation Strategies of Motor Proteins on Decorated Tracks PLoS One 10 e0136945 (2015)

<sup>2</sup>Z. Bertalan et al. Role of the Number of Microtubules in Chromosome Segregation during Cell Division, PLoS One, 10 e0141305 (2015)

**Monday, March 14, 2016 8:00AM - 11:00AM –**  
**Session A36 GSOF: Colloids: Interactions, Structure, Statistics** 339 - Xiang Cheng, University of Minnesota

**8:00AM A36.00001 Simultaneous three-dimensional imaging and manipulation of grain boundaries in colloidal crystals**, KAZEM V. EDMOND, YANYAN LIU, ARRAN CURRAN, DIRK G.A.L. AARTS, University of Oxford, STEFANO SACANNA, New York University, ROEL P.A. DULLENS, University of Oxford — Characterizing the properties of grains and grain boundaries is critical for understanding and controlling material properties. We investigate the dynamics of grain boundaries in crystalline materials using concentrated colloidal suspensions of microspheres. The micron-sized particles are suspended in a mixture of solvents whose refractive index and density nearly match those of the particles, enabling three-dimensional visualization and negating gravitational effects. Throughout the sample we disperse specially designed core-shell particles whose cores have a higher refractive index that can be optically trapped. Via optical tweezing, these core-shell particles enable us to directly interact with and probe grain boundaries in 3D within the colloidal crystal. We use a uniquely developed optical microscopy system that combines confocal imaging with holographic trapping, enabling quantitative imaging and precise manipulation simultaneously in three dimensions<sup>1</sup>. Our experiments provide direct insight into the properties of grain boundaries in crystals.

<sup>1</sup>A. Curran, S. Tuohy, D. G. A. L. Aarts, M. J. Booth, T. Wilson, and R. P. A. Dullens, "Decoupled and simultaneous 3D imaging and optical manipulation through a single objective" *Optica* **1**, 223 (2014)

**8:12AM A36.00002 Capturing "glasslites": structures and dynamics of colloidal liquids under spherical confinement**, BO ZHANG, XIANG CHENG, University of Minnesota-Twin Cities — Recent theories have predicted that when a supercooled liquid approaches the glass transition, "glasslites"-amorphously-ordered particle clusters-nucleate within the liquid, which lead to static correlations dictating the dramatic slowdown of liquid relaxation. The prediction, however, has yet to be verified in 3D experiments. Here, we design a 3D colloidal system, where particles are confined inside spherical cavities with an amorphous layer of particles pinned at boundary. Using this novel system, we capture the glasslites proposed in theories and demonstrate the development of a static correlation. Moreover, by investigating the dynamics of spherically confined samples, we reveal a profound and unexpected influence of the static correlation on the underlying colloidal glass transition. These measurements provide crucial information on how the configurational entropy of a confined supercooled liquid varies when approaching the glass transition.

**8:24AM A36.00003 Tunable Time-Dependent Colloidal Interactions**, ANDREW M. BERGMAN, W. BENJAMIN ROGERS, VINOTHAN N. MANOHARAN, Harvard University — Self-assembly of colloidal particles can be driven by changes in temperature, density, or the concentration of solutes, and it is even possible to program the thermal response and equilibrium phase transitions of such systems [1]. It is still difficult, however, to tune how the self-assembly process varies in time. We demonstrate control over the time-dependence of colloidal interactions, using DNA-functionalized colloidal particles with binding energies that are set by the concentration of a free linker strand in solution. We control the rate at which this free strand is consumed using a catalytic DNA reaction [2], whose rate is governed by the concentration of a catalyst strand. Varying the concentration of the linker, its competitor, and the catalyst at a fixed temperature, we can tune the rate and degree of the formation of colloidal aggregates and their following disassembly. Close to the colloidal melting point, the timescales of these out-of-equilibrium assembly and disassembly processes are determined by the rate of the catalytic reaction. Far below the colloidal melting point, however, the effects from varying our linker and competitor concentrations dominate. [1] Rogers and Manoharan, *Science* **347** (6222): 639-642 (2015). [2] Zhang, Turberfield, Yurke and Winfree, *Science* **318** (5853): 1121-1125 (2007).

**8:36AM A36.00004 Transitions in colloidal crystals induced by changes in interparticle interactions<sup>1</sup>**, BARTHOLOMEUS MACHIELSE, MATTHEW GRATALE, ZOIEY DAVIDSON, ARJUN YODH, Univ of Pennsylvania — We experimentally study the phase diagram of two-dimensional colloidal crystals as the interparticle interactions transition from weakly attractive to strongly attractive. Simulations have shown that crystals transition from a crystal phase into fluid-crystal coexistence at high attraction strengths. To control the interaction between colloids, we use temperature sensitive, rod-like surfactant micelles as depletants. As the temperature of the system increases, the rod length of the micelles grows, leading to an increase in both the range and strength of interparticle attractions. As the attraction strength increases we observe a decrease in the lattice constant of the crystal, and the creation of tears in the crystal structure. These tears allow a colloidal fluid to form, thus yielding the fluid-crystal coexistence phase predicted by previous simulations. These tears and their corresponding phase separation occur simultaneously with a peak in the susceptibility of the orientational order parameter. By creating colloidal systems with various packing fractions and slowly increasing the temperature, which increases the attraction strength between colloids, we attempt to accurately map out the phase diagram of two-dimensional colloidal crystals with attractive interactions.

<sup>1</sup>This work is supported by NSF grants DMR12-05463 and NSF RUI-1306990, Penn MRSEC grant DMR11-20901, and NASA grant NNX08AO0G.

**8:48AM A36.00005 Probing Dynamical Heterogeneity in Dense Colloidal Suspensions with Depletion Attraction<sup>1</sup>**, ZACHERY BROWN, GREGORY HOGAN, Department of Physics, Saint Joseph's University, MATTHEW GRATALE, ARJUN G. YODH, Department of Physics and Astronomy, University of Pennsylvania, PIOTR HABDAS, Department of Physics, Saint Joseph's University — We directly observe the particle dynamics in dense colloidal suspensions. Using depletion attraction, we vary inter particle potential to study the reentrant glass transition. Confocal microscopy and particle tracking allow us to follow particle trajectories over time. By varying inter particle attraction strength for a fixed volume fraction of colloidal suspensions, we observe three qualitatively different states. Mean square displacement and long time diffusion constant vary with the depletant concentration and indicate a glass state for low attraction strengths, ergodic liquid state for moderate attraction strengths, and attractive arrested state for the highest attraction strengths. Variance in the self overlap function gives the four point susceptibility, a measure of dynamical heterogeneity over a range of length scales and lag times. Results show that the lag times corresponding to the most heterogeneous dynamics are longer for arrested states than for fluid states. The length scale that maximizes four point susceptibility across a range of attraction strengths exhibits a reentrant glass behavior similar to that of the long time diffusion constant.

<sup>1</sup>Z.B., G.H., and P.H. acknowledge financial support of the NSF RUI-1306990. M.G. and A.G.Y. acknowledge financial support of the NSF Grant DMR-1205463, NSF MRSEC Grant DMR-1120901, and NASA Grant NNX08AO0G.

**9:00AM A36.00006 Particle dynamics and vibrational properties of disordered colloidal packings with varying interparticle attraction strength<sup>1</sup>**, PIOTR HABDAS, Department of Physics, Saint Joseph's University, MATTHEW GRATALE, ZOIEY DAVIDSON, TIM STILL, ARJUN G. YODH, Department of Physics and Astronomy, University of Pennsylvania — We experimentally study dynamical and vibrational properties of disordered colloidal packings as a function of the strength of the interparticle attraction. Specifically, we probe the structural and dynamical changes in disordered colloidal glasses as the interparticle interaction between constituent particles evolves from nearly hard-sphere repulsive to attractive. This increase of the interparticle attraction is achieved through use of temperature-tunable surfactant micelle depletants. The depletion-driven entropic attraction between particles in suspension grows with increasing temperature. Increasing temperature changes particle interactions in a dense colloidal packing from repulsive (weakly attractive) to strongly attractive, and accompanying variations in structure and dynamics is investigated. Preliminary experiments on these disordered systems show a continuous change in particle dynamics as attraction strength increases. Interestingly, vibrational properties show a more sudden change reflected in the behavior of the vibrational density of states.

<sup>1</sup>Z.B., G.H., and P.H. acknowledge financial support of the NSF Grant RUI-1306990. M.G., Z.D., T.S., and A.G.Y. acknowledge financial support of the NSF Grant DMR-1205463, NSF MRSEC Grant DMR-1120901, and NASA Grant NNX08AO0G.

**9:12AM A36.00007 On Determination of the Equation of State of Colloidal Suspensions<sup>1</sup>**, KRITTANON SIRORATTANAKUL, Department of Physics, Lehigh University, HAO HUANG, Department of Chemical and Biomechanical Engineering, Lehigh University, CHRISTOPHER UHL, Bioengineering Program, Lehigh University, DANIEL OU-YANG, Department of Physics, Lehigh University — Colloidal suspensions are the main ingredients for a variety of materials in our daily life, e.g., milk, salad dressing, skin lotions and paint for wall coatings. Material properties of these systems require an understanding of the equation of state of these materials. Our project aims to experimentally determine the equation of state of colloidal suspensions by microfluidics, dielectrophoresis (DEP) and optical imaging. We use fluorescent polystyrene latexes as a model system for this study. Placing semi-permeable membranes between microfluidics channels, which made from PDMS, we control the particle concentration and ionic strengths of the suspension. We use osmotic equilibrium equation to analyze the particle concentration distribution in a potential force field created by DEP. We use confocal optical imaging to measure the spatial distribution of the particle concentration. We compare the results of our experimental study with data obtained by computer simulation of osmotic equilibrium of interacting colloids.

<sup>1</sup>NSF DMR-0923299, Emulsion Polymer Institute, Department of Physics, Bioengineering Program of Lehigh University

**9:24AM A36.00008 Non-equilibrium steady-state distributions of colloids in a tilted periodic potential<sup>1</sup>**, XIAO GUANG MA, University of Pennsylvania, PIK-YIN LAI, National Central University, BRUCE ACKERSON, Oklahoma State University, PENDER TONG, Hong Kong University of Science and Technology — A two-layer colloidal system is constructed to study the effects of the external force  $F$  on the non-equilibrium steady-state (NESS) dynamics of the diffusing particles over a tilted periodic potential, in which detailed balance is broken due to the presence of a steady particle flux. The periodic potential is provided by the bottom layer colloidal spheres forming a fixed crystalline pattern on a glass substrate. The corrugated surface of the bottom colloidal crystal provides a gravitational potential field for the top layer diffusing particles. By tilting the sample with respect to gravity, a tangential component  $F$  is applied to the diffusing particles. The measured NESS probability density function  $P_{ss}(x, y)$  of the particles is found to deviate from the equilibrium distribution depending on the driving or distance from equilibrium. The experimental results are compared with the exact solution of the 1D Smoluchowski equation and the numerical results of the 2D Smoluchowski equation. Moreover, from the obtained exact 1D solution, we develop an analytical method to accurately extract the 1D potential  $U_0(x)$  from the measured  $P_{ss}(x)$ .

<sup>1</sup>Work supported in part by the Research Grants Council of Hong Kong SAR

**9:36AM A36.00009 Diffusing colloids in the vicinity of a surface: Anomalous yet Brownian diffusion?**, MAXIME IGNACIO, MYKYTA V. CHUBYNSKY, GARY W. SLATER, University of Ottawa — Anomalous yet Brownian diffusion refers to a process with a linear mean-square displacement coexisting with a non-Gaussian Displacement Distribution (DispD) [1]. Chubynsky and Slater [2] proposed a model of this phenomenon in which the diffusion coefficient varies randomly in time ("diffusing diffusivity"). Recently, Bechhoefer's group has showed experimentally that diffusion of colloids near a wall exhibits non-Gaussian DispD with exponential tails. Due to hydrodynamic interactions, the diffusivity  $D(r)$  is space-dependent and therefore varies in time as the particle moves in space. Qualitatively, the experimental results agree with the predictions of the diffusing diffusivity model. However, the two situations differ in details. First, space-dependent diffusivity implies the possibility of different interpretations of the stochastic term in the overdamped Langevin equation (i.e. the Ito-Stratonovich dilemma). Second, in the system of Bechhoefer et al, there is an external potential due to gravity and the electrostatic repulsion from the wall. Using Lattice Monte Carlo simulations, we explore the role of these effects. [1] B. Wang et al., PNAS 106, 15160 (2009), [2] M. V. Chubynsky and G. W. Slater, PRL 113, 098302 (2014)

**9:48AM A36.00010 Non-Gaussian yet normal diffusion of a bead near a wall<sup>1</sup>**, MPUMELELO MATSE, JOHN BECHHOEFER, Simon Fraser University — Brownian motion of microscopic particles in a simple fluid exhibits two key properties: the mean-squared displacement (MSD) increases linearly with time ( $\langle \Delta x^2 \rangle = 2D\Delta t$ , where  $D$  is the diffusivity) and the displacement distribution is Gaussian. Although linear MSD ("normal diffusion") was initially assumed to always imply Gaussian displacements, recent experiments by Granick et al. show that this is not so. Chubynsky et al. [PRL 113, 098302, 2014] have argued that such behavior arises when  $D$  has temporal and/or spatial fluctuations that are convoluted together and form a non-Gaussian distribution. Experiments to date have been in complex settings where direct measurements of  $D(x, t)$  have not been possible. Here, we report experiments on a simple system where  $D(x, t)$  is known: the Brownian motion of a colloidal sphere near a wall. By choosing the particle size carefully, we ensure that the bead explores a wide range of  $D$ . We observe a linear MSD curve and non-Gaussian displacements for vertical motion and directly confirm the proposed mechanism of Chubynsky et al. for such "diffusing diffusivity."

<sup>1</sup>Research funded by NSERC, Canada.

**10:00AM A36.00011 Structural relaxation of vapour-deposited colloidal glass<sup>1</sup>**, XIN CAO, HUIJUN ZHANG, YILONG HAN, Hong Kong Univ of Sci & Tech, YILONG GROUP COLLABORATION — Freshly made glasses by vapor deposition exhibit ultra-stability similar to fully aged glasses formed by quenching liquids. It has been suggested that the mobile surface layers in vapor deposition accelerates the aging process, but its mechanism is unclear. Here we study the vapor deposition process of colloidal glass by video microscopy and MD simulation with single-particle dynamics. We found that the structural relaxation near the surface, characterized by cooperative-rearrangement regions (CRRs), is much stronger during the deposition process than after deposition due to the perturbation of newly attached particles. Near the surface, a thermal-induced vacancy can triggered a large CRR which propagates from the vacancy to the surface. Deep inside the bulk, CRRs are rare, smaller and cannot propagate to the surface. By measuring the evolution of free-volume entropy, we found that the strong structural relaxation is accompanied by local free energy decreasing.

<sup>1</sup>The work was supported by grant RGC-GRF601613.

**10:12AM A36.00012 Assembly of colloidal strings in a simple fluid flow**, YU ABE, Toray Industries, Inc. University of Minnesota, LORRAINE FRANCIS, XIANG CHENG, University of Minnesota — Colloidal particles self-assemble into ordered structures ranging from face- and body-centered cubic crystals to binary ionic crystals and to kagome lattices. Such diverse micron-scale structures are of practical importance for creating photonic materials and also of fundamental interest for probing equilibrium and non-equilibrium statistical mechanics. As a particularly interesting example, 1D colloidal strings provide a unique system for investigating non-equilibrium dynamics of crystal lattices. Here, we report a simple experimental method for constructing 1D colloidal crystals, where colloidal particles self-assemble into flow-aligned string structures near solid boundary under unidirectional flows. Using fast confocal microscopy, we explore the degree of particle alignment as functions of flow rate, particle concentrations, wetting properties of solid boundary and ionic strength of solvent. Through our systematic experiments, we show that these colloidal strings arise from hydrodynamic coupling, facilitated by electrostatic attractions between particles and the boundary. Compared with previous methods, our work provides a much simpler experimental procedure for assembling a large number of colloidal strings.

**10:24AM A36.00013 Hiding in plain view: Colloidal self-assembly from polydisperse populations**, LUCAS GOEHRING, Max Planck Institute for Dynamics and Self-Organization, BERNARD CABANE, ESPCI ParisTech, JOAQUIM LI, Max Planck Institute for Dynamics and Self-Organization, FRANCK ARTZNER, University of Rennes, ROBERT BOTET, University Paris-Sud, CHRISTOPHE LABBEZ, GUILLAUME BAREIGTS, University of Bourgogne, MICHAEL SZTUCKI, ESRF – The European Synchrotron — We report small-angle x-ray scattering (SAXS) experiments on aqueous dispersions of colloidal silica with a broad monomodal size distribution (polydispersity 14%, size  $a = 8$  nm). This distribution of sizes was expected to destroy any long-range order of the particles. However, we found ordered states when the particles repelled each other with soft ionic potentials of range  $\sim a$ . Over a range of volume fractions the particles segregated to build first one, then two distinct sets of colloidal crystals. These dispersions thus demonstrate fractional crystallization and multiple-phase (bcc, Laves AB<sub>2</sub>, liquid) coexistence. Their remarkable ability to build complex crystal structures from a polydisperse population originates from the intermediate-range nature of interparticle forces, and suggests routes for designing self-assembling colloidal crystals from the bottom-up.

**10:36AM A36.00014 Controlling Chirality of Entropic Crystals<sup>1</sup>**, PABLO DAMASCENO, Applied Physics Program, University of Michigan, ANDREW KARAS, Chemical Engineering Department, University of Michigan, BENJAMIN SCHULTZ, Physics Department, University of Michigan, MICHAEL ENGEL, SHARON GLOTZER, Chemical Engineering Department, University of Michigan — Colloidal crystal structures with complexity and diversity rivaling atomic and molecular crystals have been predicted and obtained for hard particles by entropy maximization. However, thus far homochiral colloidal crystals, which are candidates for photonic metamaterials, are absent. Using Monte Carlo simulations we show that chiral polyhedra exhibiting weak directional entropic forces self-assemble either an achiral crystal or a chiral crystal with limited control over the crystal handedness. Building blocks with stronger faceting exhibit higher selectivity and assemble a chiral crystal with handedness uniquely determined by the particle chirality. Tuning the strength of directional entropic forces by means of particle rounding or the use of depletants allows for reconfiguration between achiral and homochiral crystals. We rationalize our findings by quantifying the chirality strength of each particle, both from particle geometry and potential of mean force and torque diagrams.

<sup>1</sup>Work supported by the National Science Foundation, Division of Materials Research Award No. DMR 1120923, U.S. Army Research Office under Grant Award No. W911NF-10-1-0518, and also by the DOD/ASD (RE) under Award No. N00244-09-1-0062

**10:48AM A36.00015 Realization of atomistic transitions with colloidal nanoparticles using an ultrafast laser**, GURSOY AKGUC, SERIM ILDAY, OMER ILDAY, OGUZ GULSEREN, GHAITH MAKEY, KORAY YAVUZ, ONUR TOKEL, IHOR PAVLOV, OZGUN YAVUZ, bilkent university — We report on realization of rapid atomistic transitions with colloidal nanoparticles in a setting that constitutes a dissipative far-from-equilibrium system subject to stochastic forces. Large colloidal crystals (comprising hundreds of particles) can be formed and transitions between solid-liquid-gas phases can be observed effortlessly and within seconds. Furthermore, this system allows us to form and dynamically arrest metastable phases such as glassy structures and to controllably transform a crystal pattern from square to hexagonal lattices and vice versa as well as to observe formation and propagation of crystal defects (i.e. line defects, point defects, planar defects). The mechanism largely relies on an interplay between convective forces induced by femtosecond pulses and strong Brownian motion; the former drags the colloids to form and reinforce the crystal and the latter is analogous to lattice vibrations, which makes it possible to observe phase transitions, defect formation and propagation and lattice transformation. This unique system can help us get insight into the mechanisms underlying various solid state phenomena that were previously studied under slowly evolving (within hours/days), near-equilibrium colloidal systems.

## Monday, March 14, 2016 8:00AM - 11:00AM —

Session A37 GSOF DBIO: Phase Transitions and Self-Assembly in Biological Systems I 340 -

Jens Glaser, University of Michigan

**8:00AM A37.00001 Study of the Effect of Ellipsoidal Shape on the Kern and Frenkel Patch Model<sup>1</sup>**, THIENBAO NGUYEN, JAMES GUNTON, JEFFREY RICKMAN, Lehigh University — In their work on the self-assembly of complex structures, Glotzer and Solomon (Nature Materials 6, 557 - 562 (2007)) identified both interaction and shape anisotropy as two of several means to build complex structures. Advances in fabricating materials and new insights into protein biology have revealed the importance of these types of interactions. The Kern and Frenkel (J. Chem. Phys. 118, 9882 (2003)) model of hard spheres carrying interaction patches of various sizes has been used extensively to describe interaction anisotropies important in protein phase transitions. However their model did not also account for shape anisotropy. We studied the role of both shape and interaction anisotropy by applying N=2 and N=4 attractive Kern and Frenkel patches with an interaction range to hard ellipsoids with various aspect ratios and patch coverages. Following Kern and Frenkel, we studied the liquid-liquid phase separation of our particles using a Monte Carlo simulation. We found the critical temperatures for our model using the approximate law of rectilinear diameter and compared them with the original results of Kern and Frenkel. We found that the critical temperatures increased both with aspect ratio and percent coverage.

<sup>1</sup>G Harold and Leila Y Mathers Foundation

**8:12AM A37.00002 Effects of Coulomb Repulsion on the Phase Diagram of the Asakura-Oosawa Model<sup>1</sup>**, JASON HAAGA, Lehigh University, ELIZABETH PEMBERTON, Drew University, JAMES GUNTON, JEFFREY RICKMAN, Lehigh University — We investigate the effect of adding a screened Coulomb charge to a model colloidal system interacting via the Asakura-Oosawa depletion potential. This model has previously been used to study the early stages of amelogenin self-assembly, a crucial process in the formation of dental enamel, by Li et al (Biophysical Journal 101, 2502 (2011)). By employing Monte Carlo simulations, we explore the role of interaction strengths and ranges on phase behavior. We find that charge strength and range have a strong influence on the stable, in the case of long range depletion potential, or metastable, in the case of short range depletion, fluid-fluid phase separation. Coulomb repulsion narrows and flattens the coexistence curve with increasing charge. This talk will also discuss solid-solid transitions present for certain interaction ranges.

<sup>1</sup>This work is supported by the G. Harold and Leila Y. Mathers Foundation

**8:24AM A37.00003 Mapping Liquid-liquid protein phase separation using ultra-fast-scanning fluorescence correlation spectroscopy.**, MING-TZO WEI, SHANA ELBAUM-GARFINKLE, CRAIG B. ARNOLD, RODNEY D. PRIESTLEY, CLIFFORD P. BRANGWYNNE, Princeton University — Intrinsically disordered proteins (IDPs) are an understudied class of proteins that play important roles in a wide variety of biological processes in cells. We've previously shown that the C. elegans IDP LAF-1 phase separates into P granule-like droplets in vitro. However, the physics of the condensed phase remains poorly understood. Here, we use a novel technique, ultra-fast-scanning fluorescence correlation spectroscopy, to study the nano-scale rheological properties of LAF-1 droplets. Ultra-fast-scanning FCS uses a tunable acoustic gradient index of refraction (TAG) lens with an oil immersion objective to control axial movement of the focal point over a length of several micrometers at frequencies of 70kHz. Using ultra-fast-scanning FCS allows for the accurate determination of molecular concentrations and their diffusion coefficient, when the particle is passing through an excitation volume. Our work reveals an asymmetric LAF-1 phase diagram, and demonstrates that LAF-1 droplets are purely viscous phases which are highly tunable by salt concentration.

**8:36AM A37.00004 Using Symmetry to Design Self-Assembling Protein Cages and Nanomaterials on the Mid-Nanometer Scale**, TODD YEATES, UCLA Department of Chemistry and Biochemistry — Self-assembling molecular structures having diverse cellular functions are widespread in nature. Some of the largest and most sophisticated types are built from many copies of the same or similar protein molecules arranged following principles of symmetry. A long-standing engineering goal has been to design novel protein molecules to self-assemble into geometrically specific structures similar to the extraordinary structures that have evolved in Nature. Practical routes to this goal have been developed by using ideas in symmetry to articulate the minimum design requirements for achieving various types of symmetric architectures, including cages, extended two-dimensional layers, and three-dimensional crystalline materials. The key requirement is that two distinct self-associating interfaces, each conferring one element of rotational symmetry, have to be engineered into the protein molecule (or molecules), following particular geometric specifications. The main principle is that combining two separate symmetry elements into a single molecular entity produces a molecule that necessarily assembles into an architecture dictated by a symmetry group that is the product of the two simpler contributing symmetries. Recent experiments have demonstrated success using a variety of symmetry-based strategies. Strategic variations are emerging that differ from each other with respect to biophysical features such as flexibility vs rigidity in the assembled structures, and with respect to design aspects such as whether the protein interfaces are inherited from natural oligomeric proteins or are designed de novo by advanced computational methods. The success of these strategies has been proven by determining crystal structures of several giant, self-assembling protein cages and clusters (10-25 nm in diameter), created by design. The ability to create sophisticated supramolecular structures from designed protein subunits opens the way to broad applications in synthetic biology and nanotechnology.

**9:12AM A37.00005 Hierarchical assembly of protein nanocrystals into macroscopic gels**, DANIEL GREENE, STANLEY SANDLER, NORMAN WAGNER, ABRAHAM LENHOFF, Univ of Delaware — From crystallization screens to downstream processing, protein gel phases are common during protein solution processing. While the structure of crystalline protein is well known, very little is known about the structure of these gel phases. We recently measured the microstructure of a salted-out ovalbumin dense phase and found that nanocrystalline protein clusters, which are only a few unit cells in size, percolate 5 micron gel beads. It is unclear if the behavior seen for ovalbumin is representative of a more general phenomenon. Here we present microstructural measurements on a salted-out monoclonal antibody (mAb) and salted-out ribonuclease-a that support this possibility. Using small-angle x-ray and neutron scattering (SAS) and transmission electron microscopy (TEM), we find both salted-out mAb and ribonuclease-a gels exhibit nanocrystalline regions. Within the mAb gel, the mAb aggregates into hollow tubular structures that are hundreds of nanometers long, have an inner diameter of approximately 15-20 nm and an outer diameter of approximately 20-30 nm. The SAS intensity from these structures contains a peak at high-q that is commensurate with scattering from idealized mAb nanocrystals that are 1-2 unit cells wide. Ribonuclease-a does not appear to form tubular structures, but the SAS intensity contains peaks at high-q that are consistent with the scattering from a nanocrystal 2-3 unit cells wide. Power-law scattering at low-q indicates the nanocrystals aggregate into a gel with fractal dimension 2.5. This research provides insight into the nanostructure and formation of protein gel phases.

**9:24AM A37.00006 The mechanical properties of phase separated protein droplets**, LOUISE JAWERTH, MAHDIYE IJAVI, AVINASH PATEL, SHAMBADITYA SAHA, Max Planck Institute of Molecular Cell Biology and Genetics, FRANK JLICHER, Max Planck Institute for the Physics of Complex Systems, ANTHONY HYMAN, Max Planck Institute of Molecular Cell Biology and Genetics — In vivo, numerous proteins associate into liquid compartments by de-mixing from the surrounding solution, similar to oil molecules in water. Many of these proteins and their corresponding liquid compartments play a crucial role in important biological processes, for instance germ line specification in *C. elegans* or in neurodegenerative diseases such as Amyotrophic lateral sclerosis (ALS). However, despite their importance, very little is known about the physical properties of the resulting droplets as well as the physical mechanisms that control their phase separation from solution. To gain a deeper understanding of these aspects, we study a few such proteins in vitro. When these proteins are purified and added to a physiological buffer, they phase separate into droplets ranging in size from a few to tens of microns with liquid-like behavior similar to their physiological counterparts. By attaching small beads to the surface of the droplets, we can deform the droplets by manipulating the beads directly using optical tweezers. By measuring the force required to deform the droplets we determine their surface tension, elasticity and viscosity as well as the frequency response of these properties. We also measure these properties using passive micro-rheology.

**9:36AM A37.00007 Phase separation and the formation of cellular bodies**, BIN XU, Department of Physics, Princeton University, CHASE P. BROEDERSZ, Faculty of Physics, Ludwig-Maximilians-University of Munich, YIGAL MEIR, Department of Physics, Ben-Gurion University, NED S. WINGREEN, Lewis-Sigler Institute for Integrative Genomics, Princeton University — Cellular bodies in eukaryotic cells spontaneously assemble to form cellular compartments. Among other functions, these bodies carry out essential biochemical reactions. Cellular bodies form micron-sized structures, which, unlike canonical cell organelles, are not surrounded by membranes. A recent in vitro experiment[1] has shown that phase separation of polymers in solution can explain the formation of cellular bodies. We constructed a lattice-polymer model to capture the essential mechanism leading to this phase separation. We used both analytical and numerical tools to predict the phase diagram of a system of two interacting polymers, including the concentration of each polymer type in the condensed and dilute phase.

## References

- [1] Li P, Banjade S, Cheng HC, Kim S, Chen B, Guo L, Llaguno M, Hollingsworth JV, King DS, Banani SF, Russo PS, Jiang QX, Nixon BT, Rosen MK *Phase transitions in the assembly of multivalent signalling proteins* Nature. 2012 Mar 7;483(7389):336-40.

**9:48AM A37.00008 Nucleic Acid-Peptide Complex Phase Controlled by DNA Hybridization**, JEFFREY VIEREGG, MICHAEL LUECKHEIDE, LORRAINE LEON, AMANDA MARCIEL, MATTHEW TIRRELL, University of Chicago — When polyanions and polycations are mixed, counterion release drives formation of polymer-rich complexes that can either be solid (precipitates) or liquid (coacervates) depending on the properties of the polyelectrolytes. These complexes are important in many fields, from encapsulation of industrial polymers to membrane-free segregation of biomolecules such as nucleic acids and proteins. Condensation of long double-stranded DNA has been studied for several decades, but comparatively little attention has been paid to the polyelectrolyte behavior of oligonucleotides. We report here studies of DNA oligonucleotides (10 - 88 nt) complexed with polylysine (10 - 100 aa). Unexpectedly, we find that the phase of the resulting complexes is controlled by the hybridization state of the nucleic acid, with double-stranded DNA forming precipitates and single-stranded DNA forming coacervates. Stability increases with polyelectrolyte length and decreases with solution salt concentration, with complexes of the longer double-stranded polymers undergoing precipitate/coacervate/soluble transitions as ionic strength is increased. Mixing coacervates formed by complementary single-stranded oligonucleotides results in precipitate formation, raising the possibility of stimulus-responsive material design.

**10:00AM A37.00009 The Ion-Specific, Non-Equilibrium Structural Behavior of DNA Hydrogels.** , DAN NGUYEN<sup>1</sup>, OMAR SALEH<sup>2</sup>, University of California Santa Barbara — The highly tunable, sequence-dependent hybridization of DNA has enabled construction of DNA hydrogels with applications ranging from drug delivery to responsive materials. Though many have examined the structural characteristics of DNA hydrogels at equilibrium, relatively little is known about their non-equilibrium behavior, apart from their degradation rates when delivering molecular payloads. Here, we examine the effect of changing salt concentration on the dynamic formation, ageing, and degradation of DNA hydrogels comprised of branched DNA nanostars with palindromic overhangs. First, we observe that hydrogel phase is sensitive to the presence of a single unpaired base on the overhang, resulting in either a percolated network or a liquid-liquid phase separated state at high salt concentrations. Particular to the percolated network, we can induce the system to either contract or relax by changing the salt concentration. Decreasing monovalent NaCl induces the network to irreversibly contract whereas decreasing divalent MgCl<sub>2</sub> induces the network to reversibly expand; this behavior runs counter to what is expected solely from electrostatic screening. We qualitatively understand these results by assuming that the monovalent salt modulates the dynamic hybridization between nanostar binding partners, whereas the divalent salt drives the dramatic/reversible induction of the 'stacked-X' conformation in the DNA nanostars.

<sup>1</sup>Biomolecular Science and Engineering Program

<sup>2</sup>Materials Department; Biomolecular Science and Engineering Program

**10:12AM A37.00010 Counterion Distribution Around Protein-SNAs probed by Small-angle X-ray scattering** , KURINJI KRISHNAMOORTHY, MICHAEL BEDZYK, SUMIT KEWALRAMANI, LIANE MOREAU, CHAD MIRKIN, Northwestern University — Protein-DNA conjugates couple the advanced cell transfection capabilities of spherical DNA architecture and the biocompatible enzymatic activity of a protein core to potentially create therapeutic agents with dual functionality. An understanding of their stabilizing ionic environment is crucial to better understand and predict their properties. Here, we use Small-angle X-ray scattering techniques to decipher the structure of the counterion cloud surrounding these DNA coated nanoparticles. Through the use of anomalous scattering techniques we have mapped the local concentrations of Rb<sup>+</sup> ions in the region around the Protein-DNA constructs. These results are further corroborated with simulations using a geometric model for the excess charge density as function of radial distance from the protein core. Further, we investigate the influence of solution ionic strength on the structure of the DNA corona and demonstrate a reduction in the extension of the DNA corona with increasing concentration of NaCl in solution for the case of both single and double stranded DNA shells. Our work reveals the distribution of counterions in the vicinity of Protein-DNA conjugates and decouples the effect of solution ionic strength on the thickness of the DNA layer.

**10:24AM A37.00011 Electrolyte-Mediated Assembly of Charged Nanoparticles** , SUMIT KEWALRAMANI, MICHAEL BEDZYK, GUILLERMO GUERRERO-GARCA, LIANE MOREAU, JOS ZWANIKKEN, CHAD MIRKIN, MONICA OLVERA DE LA CRUZ, Northwestern University — Solutions at high salt concentrations are used to crystallize or segregate colloids, proteins and polyelectrolytes via an unknown mechanism referred to as "salting-out". Here, we show salting-out is a long-range interaction controlled by electrolyte concentration and nanoparticle charge density. Small-angle X-ray scattering (SAXS) shows that DNA-coated Au nanoparticles designed to prevent inter-particle assembly via Watson-Crick hybridization undergo "gas" to FCC to "glass-like" transitions with increasing NaCl or CaCl<sub>2</sub> concentration. Simulations reveal that the crystallization is concomitant with inter-particle interactions changing from purely repulsive to a long-range potential well condition. Liquid-state theory explains this attraction as a sum of cohesive and depletion forces. Our work reveals the mechanism behind salting-out and suggests new routes for the successful crystallization of colloids and proteins using concentrated salts.

**10:36AM A37.00012 Modeling of DNA-Mediated Self-Assembly from Anisotropic Nanoparticles: A Molecular Dynamics Study** , JAIME MILLAN, MARTIN GIRARD, JEFFREY BRODIN, MATT O'BRIEN, CHAD MIRKIN, MONICA OLVERA DE LA CRUZ, Northwestern University — The programmable selectivity of DNA recognition constitutes an elegant scheme to self-assemble a rich variety of superlattices from versatile nanoscale building blocks, where the natural interactions between building blocks are traded by complementary DNA hybridization interactions. Recently, we introduced and validated a scale-accurate coarse-grained model for a molecular dynamics approach that captures the dynamic nature of DNA hybridization events and reproduces the experimentally-observed crystallization behavior of various mixtures of spherical DNA-modified nanoparticles. Here, we have extended this model to robustly reproduce the assembly of nanoparticles with the anisotropic shapes observed experimentally. In particular, we are interested in two different particle types: (i) regular shapes, namely the cubic and octahedral polyhedra shapes commonly observed in gold nanoparticles, and (ii) irregular shapes akin to those exhibited by enzymes. Anisotropy in shape can provide an analog to the atomic orbitals exhibited by conventional atomic crystals. We present results for the assembly of enzymes or anisotropic nanoparticles and the co-assembly of enzymes and nanoparticles.

**10:48AM A37.00013 Two-stages of chiral selectivity in the molecular self-assembly of tryptophan**<sup>1</sup> , NATHAN GUISSINGER, Argonne National Laboratory — Both chirality and molecular assembly are essential and key components to life. In this study we explore the molecular assembly of the amino acid tryptophan (both L- and D- chiralities) on Cu(111). Our investigation utilizes low temperature scanning tunneling microscopy to observe resulting assemblies at the molecular scale. We find that depositing a racemic mixture of both L- and D-tryptophan results in the assembly of basic 6 molecule "Lego" structures that are enantiopure. These enantiopure "Legos" further assemble into 1-dimensional chains one block at a time. These resulting chains are also enantiopure with chiral selectivity occurring at two stages of assembly. Utilizing scanning tunneling spectroscopy we are able to probe the electronic structure of the chiral Legos that give insight into the root of the observed selectivity.

<sup>1</sup>Two-stages of chiral selectivity in the molecular self-assembly of tryptophan

**Monday, March 14, 2016 8:00AM - 11:00AM –**

**Session A38 DPOLY FIAP GSOF: Polymer Nanocomposites, Active Particles and Applications**

341 - Michael Hore, Case Western Reserve University

**8:00AM A38.00001 Plasmonic Gold Nanorod Dispersions with Electrical and Optical Tunability** , CHRISTOPHER GRABOWSKI, CLARE MAHONEY, KYOUNGWEON PARK, ALI JAWAID, TIMOTHY WHITE, RICHARD VAIA, Air Force Research Laboratory, WPAFB — The transmissive, absorptive, electrical, and thermal properties of plasmonic gold nanorods (NRs) have led to their employment in a broad range of applications. These electro-optical properties - governed by their size, shape, and composition - are widely and precisely tunable during synthesis. Gold NRs show promise for large scale optical elements as they have been demonstrated to align faster than liquid crystal films ( $\mu$ s) at low fields (1 V/ $\mu$ m). Successfully dispersing a high volume fraction of gold NRs requires a strategy to control particle-particle separation and thus avoid aggregation. Herein, we discuss the role of theta temperature and the ability to swell or collapse the chains of polymer-grafted gold NRs to alter the interaction potential between particles. UV-Vis spectroscopy, scattering, and electrical susceptibility characterization methods were employed to determine nanoparticle dispersion along with the degree of gold NR alignment. The development of new agile photonic materials, controllable with both light and electric fields, will help address emerging needs in laser hardening (agile filters) and variable transmission visors.

**8:12AM A38.00002 Molecular dynamics study of reversible thermal stiffening in viscoelastic polymer blends and nanocomposites**, WEI PENG, RAGHAVAN RANGANATHAN, FIONA KINE, RAHMI OZISIK, PAWEL KEBLINSKI, Rensselaer Polytech Inst, STEVEN COLLEGE COLLABORATION — We use non-equilibrium molecular dynamics simulations to model stiffening mechanisms in viscoelastic polymer blends and nanocomposites with the overarching goal to understand the mechanisms for reversible thermal stiffening (stiffening while heating and softening up on cooling). The blend is comprised of two kinds of polymer chains with differing stiffness and glass transition temperatures ( $T_g$ ) and the nanocomposite consists of nanoparticles grafted to the high  $T_g$  polymer phase in addition to the soft matrix phase. We employ both constant shear-rate and oscillatory shear deformations to characterize stiffening. Upon heating above the  $T_g$  of both polymeric phases, we show that significant stiffening arises due to the coupled relaxation and dynamics of both polymeric phases. The effects of shear rate, interaction strength between phases and the corresponding structural changes and dynamics leading to reversible stiffening are studied and are corroborated with experimental findings.

**8:24AM A38.00003 Role of bound polymer mobility on multiscale dynamics of PEO in attractive nanocomposites**, ERKAN SENSES, Univ of Maryland-College Park & NIST Center for Neutron Research, ANTONIO FARAONE, NIST Center for Neutron Research, PINAR AKCORA, Stevens Institute of Technology — We study intermediate and large scale chain dynamics in nanocomposites where particle-bound polymer (PMMA) and matrix (PEO) chains are chemically different, miscible, and have very large  $T_g$  difference ( $\Delta T_g \approx 200$  K). These nanocomposites with dynamically asymmetric 'polymer blend interphases' were shown to exhibit an unusual reversible thermal-stiffening accompanied by vitreous-to-rubbery transition of PMMA.\* Using quasi-elastic neutron scattering, this work examines the impact of mobility of the bound-polymer on segmental and collective dynamics of the matrix chains at sub-ns to 100 ns range. While bare silica particles appear to slow down the segmental relaxation, in the composites with PMMA coated particles the Rouse dynamics of PEO is identical to its bulk behavior, possibly due to the negligible enthalpic interaction inherent to this blend system. On larger scale, we observed  $\approx 25\%$  increase in the apparent tube diameter of PEO when PMMA is glassy. Remarkably, the tube size recovers its bulk value as PMMA softens at elevated temperatures. The resulting disentanglement-entanglement transition of PEO under hard and soft confinement well relates to the macroscopic softening-stiffening transition of these composites as evidenced from the bulk rheology. (\*ACS Appl. Mater. Interfaces, 2015, 7 (27), pp 14682–14689)

**8:36AM A38.00004 Hierarchical Nanocomposites for Device Applications**, JAMES WATKINS, University of Massachusetts — We have outlined templating strategies for electronic and optical device fabrication that include self-assembly of well-ordered polymer/nanoparticle hybrids and nanoimprint lithography using novel materials sets. Using additive-driven self-assembly, for example, we demonstrate the formation of periodic nanocomposites with tunable magnetic and optical characteristics containing up to 70 wt. % of metal, metal oxide and/or semiconducting nanoparticles through phase specific interactions of the particles with either linear block copolymer or brush block copolymer (BBCP) templates. The BBCP templates provide direct access to large domain spacings for optical applications and spontaneous alignment within large volume elements. We have further developed highly filled nanoparticle/polymer hybrids for applications that require tailored dielectric constant or refractive index and a new imprinting process that allows direct printing of patterned 2-D and 3-D crystalline metal oxide films and composites with feature sizes of less than 100 nm. Applications in flexible electronics, light and energy management, and sensors and will be discussed.

**9:12AM A38.00005 Driving degradation within biodegradable polymers with embedded nanoparticles<sup>1</sup>**, RUSSELL GORGA, GABRIEL FIRESTONE, DANIELA FONTECHA, JASON BOCHINSKI, LAURA CLARKE, NC State University — The ability to controllably trigger breaking of chemical bonds enables a substance that has robust material properties during use but can be re-worked or deteriorated upon command. Photothermal heating creates intense local heat at isolated nanoparticle locations within a sample and can result in very different material responses than those achievable with conventional (uniform) heating. In this process, irradiation with visible light resonant with the nanoparticle's surface plasmon resonance results in dramatic local heating of the particles and the surrounding material. This work studies intentional thermal degradation of poly ethyl cyanoacrylate-starch composites doped with metal nanoparticles, and explores differences in degradation speed, efficiency, and resultant mechanical properties when heated via the photothermal effect.

<sup>1</sup>This work was supported by the National Science Foundation, Grant : CMMI-1462966

**9:24AM A38.00006 Waveguiding Actuators Based on Photothermally Responsive Hydrogels**, YING ZHOU, ADAM HAUSER, NAKUL BENDE, Univ of Mass - Amherst, MARK KUZYK, Washington State University, RYAN HAYWARD, Univ of Mass - Amherst — A simple means to achieve rapid and highly reversible photo-responsiveness in a hydrogel is to combine a thermally-responsive gel such as poly(N-isopropyl acrylamide) (PNIPAM), with the photothermal effect of gold nanoparticles. Relying on such composite gels, we fabricate micro-scale bilayer photoactuators by photolithographic patterning, and demonstrate their controlled bending/unbending behavior in response to visible light. In addition to actuation by flood exposure, 532 nm laser light can be waveguided through a plastic optical fiber to direct it into the photoactuator, providing the possibility for remotely controllable actuators that do not require line-of-sight access. The actuators show large magnitude responses within time-scales of  $\sim 1$  s, consistent with the small dimensions of the actuators, but also exhibit smaller-scale responses over much longer times, suggesting the possibility of slow internal relaxations within the network. Based on our study on this bilayer system, we further explore fabrication methods for cylindrical actuators that are able to bend in arbitrary directions.

**9:36AM A38.00007 In-situ curing of liquid epoxy via gold-nanoparticle mediated photothermal heating<sup>1</sup>**, GABRIEL FIRESTONE, JU DONG, JASON BOCHINSKI, RUSSELL GORGA<sup>2</sup>, LAURA CLARKE<sup>3</sup>, North Carolina State Univ — The ability to selectively alter material properties in-situ is important for many biological applications where an initially flexible part (needed for ease of placement) would ideally be rigidified once in position (for instance, within a broken bone as a tissue scaffold). Thermoset epoxies harden from viscous liquids into solid materials when heated. In this work, metal nanoparticle-epoxy-hardener composites are formed and utilized to enable in-situ crosslinking by drawing a pattern on a shallow bath of liquid epoxy with a laser. This approach capitalizes on the photothermal effect of metal nanoparticles where irradiation with light resonant with the nanoparticle surface plasmon resonance leads to dramatic local heating. We discuss challenges to incorporating metal particles into epoxy-hardener, observation of changes in the heat profile within the epoxy due to the intensity and rastering speed of the laser, and show that the mechanical properties of internally cured epoxy are the same as those cured conventionally. The ability to selectively fabricate a part from a liquid (with no mold or waste) may be an important alternative manufacturing approach.

<sup>1</sup>National Science Foundation CMMI-1069108

<sup>2</sup>Dept. of Textile Engineering, Chemistry, and Science

<sup>3</sup>Dept. of Physics

**9:48AM A38.00008 High Thermal Conductivity Aligned Polyethylene-Graphene Nanocomposites**, JIVTESH GARG, MORTAZA SAEIDIJAVASH, University of Oklahoma — We investigate enhancement of thermal conductivity in polyethylene-graphene nanocomposites. The effect of alignment of both the polymer chains and the dispersed graphene flakes on thermal conductivity enhancement will be reported. In this work nanocomposites are prepared through microextrusion of polyethylene pellets and graphene nanopowder. Alignment is achieved through mechanical stretching of the nanocomposites. Thermal conductivity is measured using both Angstrom method and Laser flash. Variables involved in the study are the draw ratio and the weight percentage of graphene nanopowder. Results will shed light on the role of alignment of graphene flakes on enhancing thermal transport and provide new avenues to achieve ultra-high thermal conductivity in polymeric materials.

**10:00AM A38.00009 Mechanical Properties of Polymeric Nanocomposites with Liquid Inclusions<sup>1</sup>**, HEYI LIANG, ZHEN CAO, ANDREY DOBRYNIN, Univ of Akron — We study mechanical properties of polymeric nanocomposites of liquid inclusions in network matrix using molecular dynamics simulations and analytical calculations. The shear modulus of nanocomposite is shown to be a non-monotonic function of the elastocapillary number  $\gamma_{SL}/(G_N R)$ , where  $\gamma_{SL}$  is the interfacial energy network/liquid interface,  $G_N$  is the shear modulus of network and  $R$  is the initial size of liquid inclusion. First, in the range of elastocapillary numbers,  $\gamma_{SL}/(G_N R) < 1$ , the composite shear modulus increases with increasing this parameter value. In this interval of elastocapillary numbers, a liquid inclusion softens the network such that the composite modulus  $G_{comp}$  is smaller than  $G_N$ . This is in agreement with the classical Eshelby theory. However, for elastocapillary numbers  $\gamma_{SL}/(G_N R) \approx 1$ , the liquid inclusions reinforces the network,  $G_{comp} > G_N$ . In this range of parameters the surface energy of the deformed liquid inclusions strengthens the composite. When the elastocapillary number increases further,  $\gamma_{SL}/(G_N R) \gg 1$ , the interfacial energy of network/liquid interface dominates the mechanical response of the composite resulting in composite weakening. Analysis of the elongation ratio of the liquid inclusion shows that it decreases with increasing elastocapillary number  $\gamma_{SL}/(G_N R)$ . The classical Eshelby's theory of inclusions fails to explain this phenomenon. We develop a new linear elasticity model of this class of nanocomposite materials capable to explain this unusual mechanical response of nanocomposite materials.

<sup>1</sup> NSF DMR-1409710

**10:12AM A38.00010 Tailoring the Structure of Polymer Networks with Photo-Controlled Radical Polymerization**, AWANEESH SINGH, OLGA KUKSENOK, Clemson University, JEREMIAH A. JOHNSON, Massachusetts Institute of Technology, ANNA C. BALAZS, Univ of Pittsburgh — Using dissipative particle dynamics (DPD) approach, we developed a novel computational model to study the photo-controlled radical polymerization (photo-CRP) within polymer networks with embedded iniferters. The polymerization process can be turned “on” or “off” in response to light and the polymerization rate can be modulated by altering the light intensity. This “photo-growth” approach allows us to impart changes in the gel network pore size and composition to form photo-tunable smart materials. For example, our approach allows us to design gel composites that are comprised of two distinct layers made of two compatible components at low photo-iniferter concentrations or gel composites that are comprised of two incompatible components that are relatively well intermixed at high photo-iniferter concentration.

**10:24AM A38.00011 Use Electrospinning to Introduce Graphene into Poly(4-Vinylpyridine) (P4VP) Polymer Fibers and Their Biocompatibility with Dental Pulp Stem Cells (DPSCs)<sup>1</sup>**, LINXI ZHANG, CHUNG-CHUEH CHANG, MIRIAM RAFAILOVICH, Stony Brook University — Graphene-polymer composite materials have been popularized in tissue engineering due to the outstanding thermal, electrical and mechanical properties of graphene. Most of the current studies, however, focus on 2-D structured films which hardly represent the real conditions of scaffolds in vivo environment and dispersion of graphene in polymer matrix has always been challenging since the graphene tends to aggregate. In our study, we have successfully introduced graphene nanoplatelets (GNPs) into poly(4-vinylpyridine) (P4VP) matrix and fabricated nano- and micro-scale size fibers by using electrospinning technique. SEM and TEM reveal uniform defect-free fiber structures and good dispersion of graphene; DSC and AFM indicate the enhancement of physical properties. The biocompatibility of the electrospun 3-D scaffolds with dental pulp stem cells (DPSCs) has been examined. Our results show that the cells can accelerate proliferation to respond to the existence of GNPs. SEM with EDAX reveals a deposition of mineralized calcium matrix on the fibers after 35-day incubation, which has possibly been caused by cell differentiation induced by fibrous scaffolds.

<sup>1</sup> Electrospinning Nano- and Micro-scale size Poly(4-vinylpyridine) Fibers Loaded with Graphene Nano Platelets (GNPs)

**10:36AM A38.00012 Studies of a new class of high electro-thermal performing Polyimide embedded with 3D scaffold in the harsh environment of outer space**, MANUELA LOEBLEIN, Nanyang Tech Univ, ASAF BOLKER, Soreq NRC, SIU HON TSANG, Temasek Laboratories@NTU, NURIT ATAR, Soreq NRC, CECILE UZAN-SAGUY, Technion - Israel Institute of Technology, RONEN VERKER, IRINA GOUZMAN, EITAN GROSSMAN, Soreq NRC, EDWIN HANG TONG TEO, Nanyang Tech Univ — The polymer class of Polyimides (PIs) has been wide-spread in the use of outer space coatings due to their chemical stability and flexibility. Nevertheless, their poor thermal conductivity and completely electrically insulating characteristics have caused severe limitations, such as thermal management challenges and spacecraft electrostatic charging, which forces the use of additional materials such as brittle ITO in order to completely resist the harsh environment of space. For this reason, we developed a new composite material via infiltration of PI with a 3D scaffold which improves PIs performance and resilience and enables the use of only a single flexible material to protect spacecraft. Here we present a study of this new material based on outer-space environment simulated on ground. It includes an exhaustive range of tests simulating space environments in accordance with European Cooperation for Space Standard (ECSS), which includes atomic oxygen (AO) etching, Gamma-ray exposure and outgassing properties over extended periods of time and under strenuous mechanical bending and thermal annealing cycles. Measurement methods for the harsh environment of space and the obtained results will be presented.

**10:48AM A38.00013 Biocompatible Silk-Poly(Pyrrole) Composite Trilayer Actuators**, CARLY FENGEL, NATHAN BRADSHAW, SEAN SEVERT, AMANDA MURPHY, JANELLE LEGER, Western Washington Univ — Biocompatible materials capable of controlled actuation are in high demand for use in biomedical applications such as dynamic tissue scaffolding, valves, and steerable surgical tools. Conducting polymers (CPs) have some desirable traits for use as an actuator, such as the ability to operate in biologically relevant fluids and responsiveness to low voltages. However CPs alone are limited due to their brittle nature and poor solubility. Recently we have shown that a composite material of silk and the CP poly(pyrrole) (PPy) shows promising characteristics as an actuator; it is mechanically robust as well as fully biocompatible. Initial proof-of-concept experiments demonstrated that these composites bend under an applied voltage (or current) using a simple bilayer device. Here we present trilayer devices composed of two silk-PPy composite layers separated by an insulating silk layer. This configuration results in more charge is passed in comparison to the analogous bilayer system, as well as a more sustainable current response through cycling, resulting in a larger angle of deflection per volt applied. In addition, the motion of the trilayer devices is more symmetric than that of the bilayer analogs, resulting in a more repeatable movement. We will discuss the fabrication and characterization of these devices, as well as their performance and future applications of this technology.

**Monday, March 14, 2016 8:00AM - 11:00AM —**

**Session A39 DBIO DPOLY DCOMP: Physics of Proteins: Bio Meets Quantum** 342 - Mark Tuominen, University of Massachusetts Amherst

**8:00AM A39.00001 Hidden Linear Quantum States in Proteins: Did Davydov Get the Sign Wrong?** , ROBERT AUSTIN, Princeton University, AIHUA XIE, Oklahoma State University, BRITTA REDLICH, LEX VAN DER MEER, Radboud University Nijmegen — A fair amount of time has been spent hunting down one prospective quantum mechanical model, namely the Davydov soliton along the  $\alpha$ -helix backbone of the protein. These experiments were challenging, we used a tunable ps mid-IR Free Electron Laser to try and observe the long-term (microsecond or greater) trapping of coherent excitation in proteins which had been proposed by a several theorists. These experiments were successful in the sense that we directly observed vibrational excited state population relaxation on the picosecond time scale, and transfer of coherent excitation into the incoherent thermal bath: but we did not see the trapping on the microsecond time scale of short (ps) coherent light pulses in the amide I band of a generic  $\alpha$ -helix rich protein, myoglobin. However, we would like to revisit that experiment one more time in this paper to analyze and try to understand something puzzling that we did observe, in the context a possible unusual “hidden” quantum phenomena in proteins which probably is of no biological consequences, but bears re-examination.

**8:12AM A39.00002 Single-Molecule Electronic Measurements of the Dynamic Flexibility of Histone Deacetylases** , JAMES FROBERG, SEUNGYONG YOU, Dept. Physics, North Dakota State Univ., USA, JUNRU YU, Dept. Chemistry, North Dakota State Univ., USA, MANAS HALDAR, Dept. Pharm. Sci, North Dakota State Univ., USA, ABBAS SEDIGH, Dept. Chemistry, North Dakota State Univ., USA, SANKU MALLIK, Dept. Pharm. Sci., North Dakota State Univ., USA, D.K. SRIVASTAVA, Dept. Chemistry, North Dakota State Univ., USA, YONGKI CHOI, Dept. Physics, North Dakota State Univ., USA — Due to their involvement in epigenetic regulation, histone deacetylases (HDACs) have gained considerable interest in designing drugs for treatment of a variety of human diseases including cancers. Recently, we applied a label-free, electronic single-molecule nano-circuit technique to gain insight into the contribution of the dynamic flexibility in HDACs structure during the course of substrates/ ligands binding and catalysis. We observed that HDAC8 has two major (dynamically interconvertible) conformational states, “ground (catalytically unfavorable)” and “transition (catalytically favorable)”. In addition, we found that its cognate substrates/ligands reciprocally catalyze the transition of the ground to the transition state conformation of HDAC8. Thus, we propose that both enzymes and their substrates/ligands serve as “catalysts” in facilitating the structural changes of each other and promoting the overall chemical transformation reaction. Such new information provides the potential for designing a new class of mechanism-based inhibitors and activators of HDAC8 for treating human diseases.

**8:24AM A39.00003 Single-Molecule Electronic Monitoring of DNA Polymerase Activity** , DENYS O. MARUSHCHAK, KAITLIN M. PUGLIESE, MACKENZIE W. TURVEY, YONGKI CHOI, O. TOLGA GUL, TIVOLI J. OLSEN, ARITH J. RAJAPAKSE, GREGORY A. WEISS, PHILIP G. COLLINS, Univ of California - Irvine — Single-molecule techniques can reveal new spatial and kinetic details of the conformational changes occurring during enzymatic catalysis. Here, we investigate the activity of DNA polymerases using an electronic single-molecule technique based on carbon nanotube transistors. Single molecules of the Klenow fragment (KF) of polymerase I were conjugated to the transistors and then monitored via fluctuations in electrical conductance. Continuous, long-term monitoring recorded single KF molecules incorporating up to 10,000 new bases into single-stranded DNA templates. The duration of individual incorporation events was invariant across all analog and native nucleotides, indicating that the precise structure of different base pairs has no impact on the timing of incorporation. Despite similar timings, however, the signal magnitudes generated by certain analogs reveal alternate conformational states that do not occur with native nucleotides. The differences induced by these analogs suggest that the electronic technique is sensing KF's O-helix as it tests the stability of nascent base pairs [1]. [1] K.M. Pugliese, et. al., "Processive Incorporation of Deoxynucleoside Triphosphate Analogs by Single-Molecule DNA Polymerase I (Klenow Fragment) Nanocircuits." JACS 137, 9587 (2015).

**8:36AM A39.00004 Observation of an electrical signal from a single molecule** , AROOJ ASLAN, NOOR SHAHEEN, KYLE DOBISZEWSKI, ALOKIK KANWAL, REGINALD FARROW, GORDON THOMAS, NJIT Physics — We have attached a folded protein molecule to the tip of a carbon nanotube using electrophoresis. We have then measured the electrons produced when the protein catalyzes a series of reactions. As an initial example of the reactions, we have used the catalysis by glucose-oxidase of glucose. We can show that the characteristic dynamic signals from the molecule scale with the glucose concentration. The molecule on the carbon nanotube tip is stable with respect to time under controlled conditions. The signals also indicate the glucose diffusion as its concentration is locally depleted at the nanotube by the catalysis. We use a second carbon nanotube with a laccase molecule on its tip to complete the circuit with an oxygen reaction. In a previous stage of this process, the other end of the nanotube is attached with a low-impedance electrical connection to a Ti thin film and the measuring circuitry. This work is an early step toward investigating the feasibility of an implantable glucose monitor to help treat diabetes.

**8:48AM A39.00005 Relevance of Aromatic Amino Acids for Electron Conduction along *Geobacter* Pili Protein.**<sup>1</sup> , RAMESH ADHIKARI, University of Massachusetts Amherst, NIKHIL MALVANKAR, Yale University, MARK TUOMINEN, DEREK LOVLEY, University of Massachusetts Amherst — It has been proposed that the charge transport through *Geobacter sulfurreducens* pili protein occurs through the aromatic amino acids forming helical conducting chain within pili.[1] X-ray studies of pili show that the aromatic amino acids are packed close enough (3-4 Å) for  $\pi$ -stacking to occur. Conductivity of the pili network increases with lowering temperature indicating metallic-like transport mechanism. [2] However due to the complexity of charge percolation path in 3D network, the intrinsic conductivity of an individual pili was not known. Here, we report transport measurements of individual pili of *G. sulfurreducens*. The conductivity, similar to that of organic polymers, shows that the pili may have implications in materials research. In addition, the conductivity value is sufficient to explain the respiration rate of the *G. sulfurreducens*. Further studies of pili from different natural and genetically modified species with varying amount of aromatic amino acid density demonstrate that it can play a decisive role on the magnitude of the conductivity. [1] Malvankar, N. S. et al. mBio 6, e00084-00015 (2015). [2] Malvankar, N. et al. Nature Nano. 6, 573-579 (2011).

<sup>1</sup>This research was supported by the Office of Naval Research (ONR) and National Science Foundation (NSF) Center for Hierarchical Manufacturing (CHM). Nikhil S. Malvankar holds a Career Award from the Burroughs Wellcome Fund.

**9:00AM A39.00006 Finite Difference Frequency Domain (FDFD) Band Structure Calculations of Diatom Frustules** , JONATHAN MISHLER, STEPHEN BAUMAN, SALVADOR BARRAZA-LOPEZ, Department of Physics, University of Arkansas, ANDREW ALVERSON, Department of Biology, University of Arkansas, JOSEPH HERZOG, Department of Physics, University of Arkansas — Diatoms are single-celled photosynthetic algae commonly known for their siliceous cell walls, called frustules. Over the last decade, the uncanny resemblance of their frustules to manufactured photonic crystals has led researchers to study their photonic properties with the hope of using them as self-constructing photonic crystals or biomimetic templates for artificial photonic crystals. The 2D photonic band structures of the foramen, areolae, and cribrum of the diatom species *Coscinodiscus* sp. were calculated using the finite difference frequency domain (FDFD) method in both water and air. These calculations revealed the effects of all three layers on a frustule's photonic properties, both in and out of their natural environment.

**9:12AM A39.00007 Protein separation using an electrically tunable membrane<sup>1</sup>**, INING JOU, DMITRIY MELNIKOV, MARIA GRACHEVA<sup>2</sup>, Clarkson University — Separation of small proteins by charge with a solid-state porous membrane requires control over the protein's movement. Semiconductor membrane has this ability due to the electrically tunable electric potential profile inside the nanopore. In this work we investigate the possibility to separate the solution of two similar sized proteins by charge. As an example, we consider two small globular proteins abundant in humans: insulin (negatively charged) and ubiquitin (neutral). We find that the localized electric field inside the pore either attracts or repels the charged protein to or from the pore wall which affects the delay time before a successful translocation of the protein through the nanopore. However, the motion of the uncharged ubiquitin is unaffected. The difference in the delay time (and hence the separation) can be further increased by the application of the electrolyte bias which induces an electroosmotic flow in the pore.

<sup>1</sup>NSF DMR and CBET Grant No. 1352218

<sup>2</sup>Corresponding Author

**9:24AM A39.00008 Investigating the Binding of Peptides to Graphene Surfaces for Biosensing Applications**, AMANDA GARLEY, NABANITA SAIKIA, University of Colorado - Boulder, STEPHEN BARR, GARY LEUTY, RAJIV BERRY, Air Force Research Laboratory, HENDRIK HEINZ, University of Colorado - Boulder — The Air Force Research Lab is focused on developing highly selective and sensitive graphene-based sensors functionalized with peptides for biomolecule detection. To achieve this there is a need to model interfacial binding interactions between the organic and inorganic components to complement ongoing experimental investigations. It is important to characterize the binding behavior of individual amino acids, with the goal of predicting binding of large peptides. Since polarization is important in graphene systems, a new force field which includes polarizability is used. This allows for an in depth exploration of pi-pi interactions, electrostatics and van der Waals forces involved with binding. The binding strength is determined via enthalpy and free energy calculations. Additionally, structural quantities are computed, such as how aromatic rings align with the graphene surface and the arrangement of various residue substituents in relation to the surface and water layers. Computational results are useful in guiding experimental methods focused on rapidly screening optimal peptide sequence for binding.

**9:36AM A39.00009 The formation of bio-corona on graphene and boron nitride**, ACHYUT RAGHAVENDRA, BISHWAMBHAR SENGUPTA, Clemson Nanomaterials Center, Dept., of Physics and Astronomy, Clemson University, JINGYI ZHU, Clemson Nanomaterials Center, Dept., of Physics and Astronomy, Clemson University, Clemson, SC USA 29634., APPARAO RAO, RAMAKRISHNA PODILA, Clemson Nanomaterials Center, Dept., of Physics and Astronomy, Clemson University, Clemson, Laboratory of Nano-biophysics and COMSET — The increase in applications of engineered two-dimensional (2D) materials has raised concerns over their discharge into the environment. The inadvertent fouling of 2D-materials with natural organic matter (NOM) results in the formation of biocorona, which in turn determines the transport and fate of 2D-materials. Our experiments showed that the physicochemical characteristics of 2D-materials play an important role in biocorona formation. In particular, the formation of biocorona is determined by: i) the amount of aromatic content in NOM, and ii) the distribution of pi-electrons in 2D-materials such as graphene and BN. More importantly, we found that the delocalized pi-electron cloud in NOM results in significant charge transfer while while the charge transfer does not occur for the case of BN wherein the electron cloud is centered near N atoms. A detailed analysis of 2D-material biocorona formation and the impacts on 2D-material transport and fate will be presented.

**9:48AM A39.00010 First principles simulations of nano-peptides on copper surfaces.<sup>1</sup>**, DUY LE, TALAT S. RAHMAN, University of Central Florida — Protein folding is the process in which a protein structure finds its stable conformation or functional shape. It is considered as a robust way for self-assembling proteins into conformations with desired functionalities. In this work, to obtain a microscopic understanding of the protein folding phenomenon, as influenced by a metallic environment, we perform density functional theory based simulations of the folding of a 9-amino-acid nano-peptide on various copper surfaces. We show that the considered nano-peptides fold into stable monomers or dimers with different conformations depending on the crystallographic orientation of the surface. Comparison of our simulated Scanning Tunneling Microscopy (STM) image with available experimental results [1] provides insights into the microscopic forces responsible for dimerization on Cu(100). [1] S. Rauschenbach et al., to be published

<sup>1</sup>This work is supported in part by NSF grant CHE-1310327

**10:00AM A39.00011 “Cold Denaturation” induces inversion of dipole and spin transfer in chiral peptide monolayers**, SOUMYAJIT SARKAR, MEITAL ECKSHAIN-LEVI, EYAL CAPUA, SIVAN REFAELY-ABRAMSON, YULIAN GAVRILOV, SHINTO MATHEW, Weizmann Institute of Science, YOSSIE PALTIEL, The Hebrew University, Jerusalem, YAAKOV LEVY, LEEOR KRONIK, RON NAAMAN, Weizmann Institute of Science — Using a combination of several experimental and computational techniques, we show that the  $\alpha$ -helix structure of oligopeptides based on alanine and aminoisobutyric acid is transformed to a more linear conformation upon cooling, due to interaction with neighboring molecules in a self-assembled monolayer (SAM) structure. This process is similar to the known “cold denaturation” in peptides, but here the SAM plays the role of the solvent. Our DFT-based first principles calculations show that the structural change results in a flip in the direction of the electrical dipole moment of the adsorbed molecules. The dipole flip is accompanied by an associated change in the spin channel that is preferred in electron transfer through the molecules. This is also experimentally observed via a new solid state hybrid organic-inorganic device that is based on the Hall effect, but operates with no external magnetic field or magnetic material.

[1] Boudiffa et al., Science, 87, 3 (2000)

[2] Sullivan et al., Phys Rev A, 68, 042708 (2002)

**10:12AM A39.00012 A New Apparatus for Studies of Nucleotide Molecules**, JESSICA DURON, LEIGH HARGREAVES, Cal State Univ — by-product of radiation cancer therapy, have been shown to be a strong driver of DNA damage. These challenges include the low-vapor pressure of commercial samples (which are powders at room temperature), and the need for high energy electron sources, required to establish the absolute scale of the measurements [2], a new apparatus is presently undergoing commissioning at the California State University. We will make the first cross-section measurements for slow ( $E_0 \leq 30$  eV) electron collisions with nucleotides. We will also make the commissioning of this new experiment.

**10:24AM A39.00013 Resonant soft X-ray scattering on protein solutions**, DAN YE, THINH LE, Department of Chemical Engineering, The Pennsylvania State University, CHENG WANG, Advanced Light Source, Lawrence Berkeley National Laboratory, PETER ZWART, Berkeley Center for Structural Biology, Lawrence Berkeley National Laboratory, ESTHER GOMEZ, Department of Chemical Engineering, Department of Biomedical Engineering, The Pennsylvania State University, ENRIQUE GOMEZ, Department of Chemical Engineering, Materials research institute, The Pennsylvania State University — Protein structure is crucial for biological function, such that characterizing protein folding and packing is important for the design of therapeutics and enzymes. We propose resonant soft X-ray scattering (RSOXS) as an approach to study proteins and other biological assemblies in solution. Calculations of the scattering contrast suggest that soft X-ray scattering is more sensitive than hard X-ray scattering, because of contrast generated at the absorption edges of constituent elements such as carbon, nitrogen and oxygen. We have examined the structure of bovine serum albumin (BSA) in solution by RSOXS. We find that by varying incident X-ray energies, we are able to achieve higher scattering contrast near the absorption edge. From our RSOXS scattering result we are able to reconstruct the structure of BSA in 3D. These RSOXS results also agree with hard X-ray experiments, including crystallographic data. Our study demonstrates the potential of RSOXS for studying protein structure in solution.

**10:36AM A39.00014 Strontium and Barium in aqueous solution and an ion channel blocking site.**, MANGESH CHAUDHARI, SUSAN REMPE, Sandia National Labs — Ion hydration structure and free energy establish criteria for understanding selective ion binding in potassium ( $K^+$ ) ion channels, and may be significant to understanding blocking mechanisms as well. Recently, we investigated the hydration properties of  $Ba^{2+}$ , the most potent blocker of  $K^+$  channels among the simple metal ions. Here, we use a similar method of combining ab-initio molecular dynamics simulations, statistical mechanical theory, and electronic structure calculations to probe the fundamental hydration properties of  $Sr^{2+}$ , which does not block bacterial  $K^+$  channels. The radial distribution of water around  $Sr^{2+}$  suggests a stable 8-fold geometry in the local hydration environment, similar to  $Ba^{2+}$ . While the predicted hydration free energy of  $-331.8$  kcal/mol is comparable with the experimental results of  $-334$  kcal/mol, the value is significantly more favorable than the  $-305$  kcal/mol hydration free energy of  $Ba^{2+}$ . When placed in an innermost  $K^+$  channel blocking site, the solvation free energies and lowest energy structures for both  $Sr^{2+}$  and  $Ba^{2+}$  are nearly unchanged compared with their respective hydration properties. That result suggests that difference in blocking behavior may arise due to kinetic properties associated with exchange of water ligands for channel ligands instead of equilibrium thermodynamic properties.

**10:48AM A39.00015 An Efficient Single-Molecule Resolution Method for Simulating Spatio-Temporal Dynamics of Protein Interaction Networks that Involve the Cell Membranes<sup>1</sup>**, OSMAN N. YOGURTCU, MARGARET E. JOHNSON, Johns Hopkins University — A significant number of the cellular protein interaction networks, such as the receptor mediated signaling and vesicle trafficking pathways, includes membranes as a molecular assembly platform. Computer simulations can provide insight into the dynamics of complex formation and help identify the principles that govern recruitment and assembly on the membranes. Here, we introduce the Free-Propagator Re-weighting (FPR) algorithm, a recently developed method that efficiently simulates the spatio-temporal dynamics of multiprotein complex formation both in the solution and on the membranes. In the FPR, the position of each protein is propagated using the Brownian motion and the reactions between pairs of proteins can occur upon collisions. Depending on the dimensionality of the interaction, the association probabilities are determined by solving the Smoluchowski diffusion equations in 2D or 3D and trajectory reweighting allows us to obtain the exact association rates for all the reactive pairs. Using the FPR, in this presentation, we investigate the interaction dynamics of the receptor mediated endocytic network as a case study and discuss the possible effects of membrane binding and molecular crowding on the formation of complexes.

<sup>1</sup>Supported by the NIGMS/NIH under R00GM098371

**Monday, March 14, 2016 8:00AM - 11:00AM –**

**Session A40 GSNP: Systems Far From Equilibrium** 343 - Michel Pleimling, Virginia Tech University

**8:00AM A40.00001 Jarzynski equality for non-Hamiltonian dynamics<sup>1</sup>**, DIBYENDU MANDAL, Department of Physics, University of California Berkeley, MICHAEL R. DEWEESE, Department of Physics, Redwood Center for Theoretical Neuroscience, and Helen Wills Neuroscience Institute, University of California Berkeley — Recent years have witnessed major advances in our understanding of nonequilibrium processes. The Jarzynski equality, for example, provides a link between equilibrium free energy differences and finite-time, nonequilibrium dynamics. We propose a generalization of this relation to non-Hamiltonian dynamics, relevant for active matter systems, continuous feedback, and computer simulation. Surprisingly, this relation allows us to calculate the free energy difference between the desired initial and final states using arbitrary dynamics. As a practical matter, this dissociation between the dynamics and the initial and final states promises to facilitate a range of techniques for free energy estimation in a single, universal expression.

<sup>1</sup>This material is based upon work supported in part by the U.S. Army Research Laboratory and the U.S. Army Research Office under contract number W911NF-13-1-0390.

**8:12AM A40.00002 Field Theoretic Description of Nonequilibrium Work Relations**, BENJAMIN VOLLMAYR-LEE, Bucknell University, ANDREW BAISH, UC Santa Barbara — We develop Doi-Peliti field theory for driven, interacting particles coupled to a thermal bath. This mapping of classical particles to a field theory does not require any assumption of large particle numbers or slow modes. As an application we consider nonequilibrium work relations. With the introduction of an auxiliary complex field, the Jarzynski relation emerges from the field theory as direct consequence of time reversal.

**8:24AM A40.00003 Extending Landauer's Bound from Bit Erasure to Arbitrary Computation**, DAVID WOLPERT, Santa Fe Institute — Recent analyses have calculated the minimal thermodynamic work required to perform any computation  $\pi$  whose output is independent of its input, e.g., bit erasure. First I extend these analyses to calculate the work required even if the output of  $\pi$  depends on its input. Next I show that if a physical computer  $C$  implementing a computation  $\pi$  will be re-used, then the work required depends only on the dynamics of the logical variables under  $\pi$ , independent of the physical details of  $C$ . This establishes a formal identity between the thermodynamics of (re-usable) computers and theoretical computer science. To illustrate this identity, I prove that the minimal work required to compute a bit string  $\sigma$  on a (physical) Turing machine  $M$  is  $k_B T \ln(2) [K(\sigma) + \log(\mu(\sigma)) + \log(h(M))]$ . I also prove that uncertainty about the distribution over inputs to the computer increases the minimal work required to run the computer. I end by using these results to relate the free energy flux incident on an organism / robot / biosphere to the maximal amount of computation that the organism / robot / biosphere can do per unit time.

### 8:36AM A40.00004 Average work measurement below the Landauer limit for memory erasure<sup>1</sup>

, MOMČILO GAVRILOV, JOHN BECHHOEFER, Simon Fraser University — Landauer's Principle states that erasing a one-bit memory requires an average work of at least  $kT \ln 2$ . Recent experiments have confirmed this prediction for a one-bit memory represented by a symmetric double-well potential. However, if a memory is represented by a non-equilibrium state in an asymmetric double-well potential, theoretical studies predict that one can measure work below  $kT \ln 2$ . Using a feedback trap, we have confirmed this prediction. Surprisingly, we found that two different erasure protocols give two different values for the asymptotic work. We can explain this result by noting that one protocol is symmetric with the respect to time reversal and the other is not.

<sup>1</sup>This work was supported by NSERC (Canada).

### 8:48AM A40.00005 Dynamics and thermodynamics of open chemical networks , MASSIMILIANO

ESPOSITO, University of Luxembourg — Open chemical networks (OCN) are large sets of coupled chemical reactions where some of the species are chemostated (i.e. continuously restored from the environment). Cell metabolism is a notable example of OCN. Two results will be presented. First, dissipation in OCN operating in nonequilibrium steady-states strongly depends on the network topology (algebraic properties of the stoichiometric matrix)<sup>1</sup>. An application to oligosaccharides exchange dynamics performed by so-called D-enzymes will be provided<sup>2</sup>. Second, at low concentration the dissipation of OCN is in general inaccurately predicted by deterministic dynamics (i.e. nonlinear rate equations for the species concentrations). In this case a description in terms of the chemical master equation is necessary. A notable exception is provided by so-called deficiency zero networks, i.e. chemical networks with no hidden cycles present in the graph of reactant complexes<sup>3</sup>.

<sup>1</sup>M. Poletti and M. Esposito, J. Chem. Phys. 141, 024117 (2014)

<sup>2</sup>R. Rao, D. Lacoste and M. Esposito, arxiv:1509.07446

<sup>3</sup>M. Poletti, A. Wachtel and M. Esposito, arxiv:1507.00058

### 9:00AM A40.00006 Cost and consequences of breaking the fluctuation dissipation relation in biochemical networks<sup>1</sup> , YUHAI TU, IBM — Living systems need to be highly responsive, and also to keep fluctuations low. These goals

are incompatible in equilibrium systems due to the Fluctuation Dissipation Theorem (FDT). Here, we show that biological sensory systems, driven far from equilibrium by free energy consumption, can reduce their intrinsic fluctuations while maintaining high responsiveness. By developing a continuum theory of the *E. coli* chemotaxis pathway, we demonstrate that adaptation can be understood as a non-equilibrium phase transition controlled by free energy dissipation, and it is characterized by a breaking of the FDT [1]. We show that the maximum response at short time is enhanced by free energy dissipation. At the same time, the low frequency fluctuations and the adaptation error decrease with the free energy dissipation algebraically and exponentially, respectively. [1] "Free Energy Cost of Reducing Noise while Maintaining a High Sensitivity", Pablo Sartori and Yuhai Tu, Phys. Rev. Lett. 2015. 115: 118102.

<sup>1</sup>This work is partly supported by a NIH grant (R01GM081747 to YT)

### 9:12AM A40.00007 Mimicking Nonequilibrium Steady States with Time-Periodic Driving ,

OREN RAZ, YIGIT SUBASI, CHRISTOPHER JARZYNSKI, Univ of Maryland-College Park — Under static conditions, a system satisfying detailed balance generically relaxes to an equilibrium state in which there are no currents: to generate persistent currents, either detailed balance must be broken or the system must be driven in a time-dependent manner. A stationary system that violates detailed balance evolves to a nonequilibrium steady state (NESS) characterized by fixed currents. Conversely, a system that satisfies instantaneous detailed balance but is driven by the time-periodic variation of external parameters - also known as a stochastic pump (SP) - reaches a periodic state with non-vanishing currents. In both cases, these currents are maintained at the cost of entropy production. Are these two paradigmatic scenarios effectively equivalent? For discrete-state systems we establish a mapping between NESS and SP. Given a NESS characterized by a particular set of stationary probabilities, currents and entropy production rates, we show how to construct a SP with exactly the same (time-averaged) values. The mapping works in the opposite direction as well. These results establish a proof of principle: they show that SP are able to mimic the behavior of NESS, and vice-versa, within the theoretical framework of discrete-state stochastic thermodynamics.

### 9:24AM A40.00008 The thermal vacuum for non-equilibrium steady state , RYOSUKE IMAI, YUKIRO

KUWAHARA, YUSUKE NAKAMURA, YOSHIYA YAMANAKA, Waseda Univ — Our purpose is to construct a theoretical description of non-equilibrium steady state (NESS), employing thermo field dynamics (TFD). TFD is the operator-based formalism of thermal quantum field theory, where every degree of freedom is doubled and thermal averages are given by expectation values of the thermal vacuum<sup>1</sup>. To specify the thermal vacuum for NESS is a non-trivial issue, and we attempt it on the analogy between the superoperator formalism and TFD<sup>2</sup>. Using the thermal vacuum thus obtained, we analyze the NESS which is realized in the two-reservoir model. It will be shown that the NESS vacuum of the model coincides with the fixed point solutions of the quantum transport equation derived by the self-consistent renormalization of the self-energy in non-equilibrium TFD<sup>3</sup>.

<sup>1</sup>H. Umezawa, *Thermo Field Dynamics and Condensed States* (Elsevier Science Ltd, 1982).

<sup>2</sup>M. Schmutz, Z. Phys. B **30**, 97 (1978); Y. Nakamura and Y. Yamanaka, Ann. Phys. (N.Y.) **331**, 51 (2013).

<sup>3</sup>H. Umezawa, *Advanced Field Theory: Micro, Macro, and Thermal Physics* (AIP, 1993); Y. Nakamura and Y. Yamanaka, Ann. Phys. (N.Y.) **331**, 51 (2013).

### 9:36AM A40.00009 Closed hierarchies and non-equilibrium steady states of driven systems ,

ISRAEL KLICH, University of Virginia — We present a class of tractable non-equilibrium dynamical quantum systems which includes combinations of injection, detection and extraction of particles interspersed by unitary evolution. We show how such operations generate a hierarchy of equations tying lower correlation functions with higher order ones. The hierarchy closes for particular choices of measurements and leads to a rich class of evolutions whose long time behavior can be simulated efficiently. In particular, we use the method to describe the dynamics of current generation through a generalized quantum exclusion process, and exhibit an explicit formula for the long time energy distribution in the limit of weak driving.

### 9:48AM A40.00010 Mechanical autonomous stochastic heat engines , MARC SERRA-GARCIA, ANDRE FOEHR,

MIGUEL MOLERO, Swiss Federal Institute of Technology (ETH), JOSEPH LYDON, jlydon@ethz.ch, CHRISTOPHER CHONG, Bowdoin College, CHIARA DARAIO, Swiss Federal Institute of Technology (ETH), . TEAM — Stochastic heat engines extract work from the Brownian motion of a set of particles out of equilibrium. So far, experimental demonstrations of stochastic heat engines have required extreme operating conditions or nonautonomous external control systems. In this talk, we will present a simple, purely classical, autonomous stochastic heat engine that uses the well-known tension induced nonlinearity in a string. Our engine operates between two heat baths out of equilibrium, and transfers energy from the hot bath to a work reservoir. This energy transfer occurs even if the work reservoir is at a higher temperature than the hot reservoir. The talk will cover a theoretical investigation and experimental results on a macroscopic setup subject to external noise excitations. This system presents an opportunity for the study of non equilibrium thermodynamics and is an interesting candidate for innovative energy conversion devices.

**10:00AM A40.00011 A dissipation bound for thermodynamic control** , BENJAMIN MACHTA, Princeton Univ — Biological and engineered systems operate by coupling function to the transfer of heat and/or particles down a thermal or chemical gradient. In idealized *deterministically* driven systems, thermodynamic control can be exerted reversibly, with no entropy production, as long as the rate of the protocol is made slow compared to the equilibration time of the system. Here we consider *fully realizable, entropically driven* systems where the control parameters themselves obey rules that are reversible and that acquire directionality in time solely through dissipation. We show that when such a system moves in a directed way through thermodynamic space, it must produce entropy that is on average larger than its generalized displacement as measured by the Fisher information metric. This distance measure is sub-extensive but cannot be made small by slowing the rate of the protocol.

**10:12AM A40.00012 Thermodynamic second law in a feedback process with time delay** , JAEGON UM, Korea Institute for Advanced Study, CHULAN KWON, Myongji University, HYUNGGYU PARK, Korea Institute for Advanced Study — We investigate a realistic feedback process repeated in multiple steps where a feedback protocol from measurement is applied with delay and maintains for a finite duration until next step. Unlike a feedback without delay, a composite system consists of the system and two memories where previous and present measurement outcomes are stored, leading to the 3-state Shannon entropy for the composite system. Then according to the thermodynamic second law, the change of the 3-state Shannon entropy provides the upper bound for heat flow from reservoir to system during the feedback and relaxation process. However, if the feedback protocol is depending on memory states sequentially, it turns out that the tighter bound for heat production can be obtained by integrating out the irrelevant memory state. We exemplify a cold damping case where a velocity of a particle is measured and a dissipative protocol is applied by feedback, and it is confirmed that the Shannon-entropy change of the reduced composite system gives the tighter bound for heat production.

**10:24AM A40.00013 Direct measurement of the Einstein relation in a macroscopic, non-equilibrium system of chaotic surface waves** , KYLE WELCH, ALEXANDER LIEBMAN-PELAEZ, ERIC CORWIN, University of Oregon — Equilibrium statistical mechanics is traditionally limited to thermal systems. Can it be applied to athermal, non-equilibrium systems that nonetheless satisfy the basic criteria of steady-state chaos and isotropy? We answer this question using a macroscopic system of chaotic surface waves which is, by all measures, non-equilibrium. The waves are generated in a dish of water that is vertically oscillated above a critical amplitude. We have constructed a rheometer that actively measures the drag imparted by the waves on a buoyant particle, a quantity entirely divorced in origin from the drag imparted by the fluid in which the particle floats. We also perform a separate, passive measurement, extracting a diffusion constant and effective temperature. Having directly measured all three properties (temperature, diffusion constant, and drag coefficient) we go on to show that our macroscopic, non-equilibrium case is wholly consistent with the Einstein relation, a classic result for equilibrium thermal systems.

**10:36AM A40.00014 Least action and entropy considerations of self-organization in Benard cells** , GEORGI GEORGIEV, WPI and Assumption College, GERMANO IANNACCHIONE, WPI — We study self-organization in complex systems using first principles in physics. Our approach involves the principle of least action and the second law of thermodynamics. In far from equilibrium systems, energy gradients cause internal ordering to facilitate the dissipation of energy in the environment. This internal ordering decreases their internal entropy in order to obey the principle of least action, minimizing the product of time and energy for transport through the system. We are considering the connection between action and entropy decrease inside Benard cells in order to derive some general features of self-organization. We are developing mathematical treatment of this coupling and comparing it to results from experiments and simulations.

**10:48AM A40.00015 Dissipation and irreversibility for models of mechanochemical machines** , AIDAN BROWN, DAVID SIVAK, Simon Fraser University — For biological systems to maintain order and achieve directed progress, they must overcome fluctuations so that reactions and processes proceed forwards more than they go in reverse. It is well known that some free energy dissipation is required to achieve irreversible forward progress, but the quantitative relationship between irreversibility and free energy dissipation is not well understood. Previous studies focused on either abstract calculations or detailed simulations that are difficult to generalize. We present results for mechanochemical models of molecular machines, exploring a range of model characteristics and behaviours. Our results describe how irreversibility and dissipation trade off in various situations, and how this trade-off can depend on details of the model. The irreversibility-dissipation trade-off points towards general principles of microscopic machine operation or process design. Our analysis identifies system parameters which can be controlled to bring performance to the Pareto frontier.

## Monday, March 14, 2016 8:00AM - 11:00AM —

Session A41 DBIO GSOF: Cellular Biophysics 344 - Bo Sun, Oregon State University

**8:00AM A41.00001 Effects of Matrix Alignment and Mechanical Constraints on Cellular Behavior in 3D Engineered Microtissues.**<sup>1</sup> , PRASENJIT BOSE, Johns Hopkins University, JEROEN EYCKMANS, CHRISTOPHER CHEN, Boston University, DANIEL REICH, Johns Hopkins University — The adhesion of cells to the extracellular matrix (ECM) plays a crucial role in a variety of cellular functions. The main building blocks of the ECM are 3D networks of fibrous proteins whose structure and alignments varies with tissue type. However, the impact of ECM alignment on cellular behaviors such as cell adhesion, spreading, extension and mechanics remains poorly understood. We present results on the development of a microtissue-based system that enables control of the structure, orientation, and degree of fibrillar alignment in 3D fibroblast-populated collagen gels. The tissues self-assemble from cell-laden collagen gels placed in micro-fabricated wells containing sets of elastic pillars. The contractile action of the cells leads to controlled alignment of the fibrous collagen, depending on the number and location of the pillars in each well. The pillars are elastic, and are utilized to measure the contractile forces of the microtissues, and by incorporating magnetic material in selected pillars, time-varying forces can be applied to the tissues for dynamic stimulation and measurement of mechanical properties. Results on the effects of varying pillar shape, spacing, location, and stiffness on microtissue organization and contractility will be presented.

<sup>1</sup>This work is supported by NSF CMMI-1463011

**8:12AM A41.00002 Dynamics of Cancer Cell near Collagen Fiber Chain** , JIHAN KIM, BO SUN, Oregon State University — Cell migration is an integrated process that is important in life. Migration is essential for embryonic development as well as homeostatic processes such as wound healing and immune responses. When cell migrates through connective extracellular matrix (ECM), it applies cellular traction force to ECM and senses the rigidity of their local environment. We used human breast cancer cell (MDA-MB-231) which is highly invasive and applies strong traction force to ECM. As cancer cell applies traction force to type I collage-based ECM, it deforms collagen fibers near the surface. Patterns of deforming collagen fibers are significantly different with pairs of cancer cells compared to a single cancer cell. While a pair of cancer cells within 60 um creates aligned collagen fiber chains between them permanently, a single cancer cell does not form any fiber chains. In this experiment we measured a cellular response and an interaction between a pair of cells through the chain. Finally, we analyzed correlation of directions between cancer cell migration and the collagen chain alignment.

**8:24AM A41.00003 The Characteristics of Force Production of Kinesin-5 on MCF7 Microtubules**, MITRA SHOJANIA FEIZABADI, Seton Hall University — Unlike neural mammalian microtubules with class II of beta tubulin as the major beta tubulin in their compositions, MCF7 microtubules composed of 0% class II beta tubulin isotype, 39.1% class I beta tubulin isotype, 2.5% class III beta tubulin isotype and 58.4% class IV beta tubulin isotype. Recent studies have revealed that function of some of motor proteins can be affected by the structural composition of microtubules. In this work, we will show how the function of mitotic kinesin (Kin-5) under external load changed when moving along bovine versus MCF7 microtubules. Along MCF7 microtubules, the detachment force was reduced and the force-velocity curve was different as compared to those related to bovine brain. We will also show that the elimination of the C-terminal tails made the transport almost similar to the two sets of microtubules. This suggests that the C-terminal tails of tubulin plays a regulatory role in Kinesin-5's function.

**8:36AM A41.00004 On the robustness of SAC silencing in closed mitosis<sup>1</sup>**, DONOVAN RUTH, JIAN LIU, Natl Inst of Health - NIH — Mitosis equally partitions sister chromatids to two daughter cells. This is achieved by properly attaching these chromatids via their kinetochores to microtubules that emanate from the spindle poles. Once the last kinetochore is properly attached, the spindle microtubules pull the sister chromatids apart. Due to the dynamic nature of microtubules, however, kinetochore-microtubule attachment often goes wrong. When this erroneous attachment occurs, it locally activates an ensemble of proteins, called the spindle assembly checkpoint proteins (SAC), which halts the mitotic progression until all the kinetochores are properly attached by spindle microtubules. The timing of SAC silencing thus determines the fidelity of chromosome segregation. We previously established a spatiotemporal model that addresses the robustness of SAC silencing in open mitosis for the first time. Here, we focus on closed mitosis by examining yeast mitosis as a model system. Though much experimental work has been done to study the SAC in cells undergoing closed mitosis, the processes responsible are not well understood. We leverage and extend our previous model to study SAC silencing mechanism in closed mitosis. We show that a robust signal of the SAC protein accumulation at the spindle pole body can be achieved. This signal is a nonlinear increasing function of number of kinetochore-microtubule attachments, and can thus serve as a robust trigger to time the SAC silencing. Together, our mechanism provides a unified framework across species that ensures robust SAC silencing and fidelity of chromosome segregation in mitosis.

<sup>1</sup>intramural research program in NHLBI at NIH

**8:48AM A41.00005 Stochastic model of profilin-actin polymerization**, BRANDON HORAN, DIMITRIOS VAVYLONIS, Lehigh University — A driving factor in cell motility and other processes that involve changes of cell shape is the rapid polymerization of actin subunits into long filaments. This process is regulated by profilin, a protein which binds to actin subunits and regulates elongation of actin filaments. Whether profilin stimulates polymerization by coupling to hydrolysis of ATP-bound actin is debated. Previous studies have proposed indirect coupling to ATP hydrolysis using rate equations, but did not include the effects of fluctuations that are important near the critical concentration. We developed stochastic simulations using the Gillespie algorithm to study single filament elongation at the barbed end in the presence of profilin. We used recently measured rate constants and estimated the rate of profilin binding to the barbed end such that detailed balance is satisfied. Fast phosphate release at the tip of the filament was accounted for. The elongation rate and length diffusivity as functions of profilin and actin concentration were calculated and used to extract the critical concentrations of free actin and of total actin. We show under what conditions profilin leads to an increase in the critical concentration of total actin but a decrease in the critical concentration of free actin.

**9:00AM A41.00006 Surface deformation and shear flow in ligand mediated cell adhesion<sup>1</sup>**, SARTHOK SIRCAR, ANTHONY ROBERTS, University of Adelaide, SARTHOK SIRCAR / ANTHONY ROBERTS COLLABORATION — We present a unified, multiscale model to study the attachment/detachment dynamics of two deforming, near spherical cells, coated with binding ligands and subject to a slow, homogeneous shear flow in a viscous fluid medium. The binding ligands on the surface of the cells experience attractive and repulsive forces in an ionic medium and exhibit finite resistance to rotation via bond tilting. The microscale drag forces and couples describing the fluid flow inside the small separation gap between the cells, are calculated using a combination of methods in lubrication theory and previously published numerical results. For a select range of material and fluid parameters, a hysteretic transition of the sticking probability curves (i.e., the function  $g^*$ ) between the adhesion phase (when  $g^* \geq 0.5$ ) and the fragmentation phase (when  $g^* < 0.5$ ) is attributed to a nonlinear relation between the total nanoscale binding forces and the separation gap between the cells. We show that adhesion is favored in highly ionic fluids, increased deformability of the cells, elastic binders and a higher fluid shear rate (until a critical value). Continuation of the limit points (i.e., the turning points where the slope of the function  $g^*$  changes sign within a select range of critical shear

<sup>1</sup>SS is supported by the Adelaide University startup funds and AR is supported by the Australian Research Council Discovery grant DP150102385.

**9:12AM A41.00007 Nanoparticle Distributions in Cancer and other Cells from Light Transmission Spectroscopy**, ALISON DEATSCH, NAN SUN, JEFFERY JOHNSON, SHARON STACK, CAROL TANNER, STEVEN RUGGIERO, University of Notre Dame — We have measured the optical properties of whole cells and lysates using light transmission spectroscopy (LTS). LTS provides both the optical extinction coefficient in the wavelength range from 220 to 1100 nm and (by spectral inversion using a Mie model) the particle distribution density in the size range from 1 to 3000 nm. Our current work involves whole cells and lysates of cultured human oral cells and other plant and animal cells. We have found systematic differences in the optical extinction between cancer and normal whole cells and lysates, which translate to different particle size distributions (PSDs) for these materials. We have also found specific power-law dependences of particle density with particle diameter for cell lysates. This suggests a universality of the packing distribution in cells that can be compared to ideal Apollonian packing, with the cell modeled as a fractal body comprised of spheres on all size scales.

**9:24AM A41.00008 Simulation of the effect of confinement in actin ring formation**, MARAL ADELI KOUDEHI, DIMITRIOS VAVYLONIS, Lehigh University, HAOSU TANG TEAM, DIMITRIOS VAVYLONIS TEAM — Actin filaments are vital for different network structures in living cells. During cytokinesis, they form a contractile ring containing myosin motor proteins and actin filament cross-linkers to separate one cell into two cells. Recent experimental studies have quantified the bundle, ring, and network structures that form when actin filaments polymerize in confined environments in vitro, in the presence of varying concentrations of cross-linkers. In this study, we performed numerical simulations to investigate the effect of actin spherical confinement and cross-linking in ring formation. We used a spring-bead model and Brownian dynamics to simulate semiflexible actin filaments that polymerize in a confining sphere with a rate proportional to the monomer concentration. Applying the model for different size of the confining spheres shows that the probability of ring formation decreases by increasing the radius (at fixed initial monomer concentration), in agreement with prior experimental data. We describe the effect of persistence length, orientation-dependent cross-linking, and initial actin monomer concentration. Simulations show that equilibrium configurations can be reached through zipping and unzipping of actin filaments in bundles and transient ring formation.

**9:36AM A41.00009 Signaling and Dynamic Actin Responses of B Cells on Topographical Substrates**, CHRISTINA KETCHUM, Biophysics Program, University of Maryland, XIAOYU SUN, JOHN FOURKAS, Department of Chemistry, University of Maryland, WENXIA SONG, Department of Biology and Molecular Genetics, University of Maryland, ARPITA UPADHYAYA, Department of Physics, University of Maryland — B cells become activated upon physical contact with antigen on the surface of antigen presenting cells, such as dendritic cells. Binding of the B cell receptor with antigen initiates actin-mediated spreading of B cells, signaling cascades and eventually infection fighting antibodies. Lymphocytes, including B cells and T cells, have been shown to be responsive to the physical parameters of the contact surface, such as antigen mobility and substrate stiffness. However the roll of surface topography on lymphocyte function is unknown. Here we investigate the degree to which substrate topography controls actin-mediated spreading and B cell activation using nano-fabricated surfaces and live cell imaging. The model topographical system consists of 600 nanometer tall ridges with spacing varying between 800 nanometers and 5 micrometers. Using TIRF imaging we observe actin dynamics, B cell receptor motion and calcium signaling of B cells as they spread on the ridged substrates. We show that the spacing between ridges had a strong effect on the dynamics of actin and calcium influx on B cells. Our results indicate that B cells are highly sensitive to surface topography during cell spreading and signaling activation.

**9:48AM A41.00010 Mechanisms of T Lymphocyte Activation Exposed by Super Resolution Microscopy<sup>1</sup>**, LEONARD CAMPANELLO, WOLFGANG LOSERT, Univ of Maryland-College Park, MARIA TRAVER, BRIAN SCHAEFER, Uniformed Services University of the Health Sciences, ANDREW YORK, HARI SCHROFF, National Institutes of Health — In order to avoid the deleterious consequences of an uncontrolled immune response, tight regulatory control of positive and negative regulators during lymphocyte activation is needed. Utilizing cutting-edge super-resolution imaging technologies in combination with quantitative image analysis we explore the interplay between positive and negative regulation in activated T lymphocytes and investigate whether intercellular signaling is possibly governed by the degradation of a complex intracellular structure called the POLKADOTS signalosome. In segmenting the POLKADOTS signalosome structure by the betweenness centrality of its 3D medial axis skeleton, it was discovered that autophagosomes, small degradative intracellular organelles, localize preferentially to the ends of the filamentous POLKADOTS signalosome. These results provide new insight into the mechanisms behind the complex regulatory process that govern T lymphocyte activation.

<sup>1</sup>This research was supported by an Irvington Postdoctoral Fellowship from the Cancer Research Institute (awarded to MT) and a U01 grant from the National Institutes of Health (GM109887-01, awarded to BS and WL).

**10:00AM A41.00011 Single molecule analysis of B cell receptor motion during signaling activation**, IVAN REY SUAREZ, Biophysics Program, University of Maryland, PETER KOO, SIMON MOCHRIE, Department of Physics, Yale University, WENXIA SONG, Dept. of Cell Biology and Molecular Genetics, University of Maryland, ARPITA UPADHYAYA, Department of Physics, University of Maryland — B cells are an essential part of the adaptive immune system. They patrol the body looking for signs of infection in the form of antigen on the surface of antigen presenting cells. The binding of the B cell receptor (BCR) to antigen induces signaling cascades that lead to B cell activation and eventual production of high affinity antibodies. During activation, BCR organize into signaling microclusters, which are platforms for signal amplification. The physical processes underlying receptor movement and aggregation are not well understood. Here we study the dynamics of single BCRs on activated murine primary B cells using TIRF imaging and single particle tracking. The tracks obtained are analyzed using perturbation expectation-maximization (pEM) a systems-level analysis that allows the identification of different short-time diffusive states from a set of single particle tracks. We identified five different diffusive states on wild type cells, which correspond to different molecular states of the BCR. By using actin polymerization inhibitors and mutant cells lacking important actin regulators we were able to identify the BCR molecule configuration associated with each diffusive state.

**10:12AM A41.00012 Targeting cancer cell invasiveness using homing peptide-nanocomplexes**, GIULIA SUARATO, Materials Science and Engineering, Stony Brook University, JILLIAN CATHCART, Molecular and Cellular Pharmacology, Stony Brook University, WEIYI LI, Materials Science and Engineering, Stony Brook University, JIAN CAO, Medicine, Cancer Prevention, Stony Brook University, YIZHI MENG, Materials Science and Engineering, Stony Brook University — Matrix metalloproteinase-14 (MMP-14) plays critical roles in digesting the basement membrane and extracellular matrix and inducing cancer migration. We recently unraveled a unique role in cell invasion of the hemopexin (PEX) domain of MMP-14. The minimal motif located at the outmost strand of the fourth blade of the PEX domain was identified to form homodimers of MMP-14. A peptide (IVS4) mimicking the binding motif was shown to interrupt MMP-14 dimerization and decrease MMP-14-mediated functions. Since most invasive cancer cells express upregulated MMP-14 at the surface, IVS4 could be used as a cancer homing peptide to specifically deliver cytotoxic drugs for cancer therapy. We developed cancer homing nanocarriers by linking IVS4 to polysaccharide-based micellar nanoparticles (NPs). To determine if conjugation of IVS4 to NPs maintains the IVS4 inhibition of MMP-14 function, substrate degradation and cell migration assays were performed. IVS4-NPs efficiently prevented MMP-14-mediated substrate degradation and cell migration, and were minimally uptaken by non-cancer cells. Importantly, IVS4 confers an uptake advantage compared to the control peptide in MMP-14-expressing cells. Taken together, our findings demonstrate the potential use of IVS4-NPs as novel cancer nanotherapeutics.

**10:24AM A41.00013 Gating mechanosensitive channels in bacteria with an atomic force microscope.**, RENATA GARCES, University of Goettingen, SAMANTHA MILLER, University of Aberdeen, CHRISTOPH F. SCHMIDT, University of Goettingen, THIRD INSTITUTE OF PHYSICS TEAM, SCHOOL OF MEDICAL SCIENCES COLLABORATION — The regulation of growth and integrity of bacteria is critically linked to mechanical stress. Bacteria typically maintain a high difference of osmotic pressure (turgor pressure) with respect to the environment. This pressure difference (on the order of 1 atm) is supported by the cell envelope, a composite of lipid membranes and a rigid cell wall. Turgor pressure is controlled by the ratio of osmolytes inside and outside bacteria and thus, can abruptly increase upon osmotic downshock. For structural integrity bacteria rely on the mechanical stability of the cell wall and on the action of mechanosensitive (MS) channels: membrane proteins that release solutes in response to stress in the cell envelope. We here present experimental data on MS channels gating. We activate channels by indenting living bacteria with the cantilever of an atomic force microscope (AFM). We compare responses of wild-type and mutant bacteria in which some or all MS channels have been eliminated.

**10:36AM A41.00014 Impedance spectroscopy of micro-Droplets reveals activation of Bacterial Mechanosensitive Channels in Hypotonic Solutions**, AIDA EBRAHIMI, MUHAMMAD A. ALAM, Purdue University — Rapid detection of bacterial pathogens is of great importance in healthcare, food safety, environmental monitoring, and homeland security. Most bacterial detection platforms rely on binary fission (i.e. cell growth) to reach a threshold cell population that can be resolved by the sensing method. Since cell division depends on the bacteria type, the detection time of such methods can vary from hours to days. In contrast, in this work, we show that bacteria cells can be detected within minutes by relying on activation of specific protein channels, i.e. mechanosensitive channels (MS channels). When cells are exposed to hypotonic solutions, MS channels allow efflux of solutes to the external solution which leads to release the excessive membrane tension. Release of the cytoplasmic solutes, in turn, results in increase of the electrical conductance measured by droplet-based impedance sensing. The approach can be an effective technique for fast, pre-screening of bacterial contamination at ultra-low concentration.

**10:48AM A41.00015 Physics of Bacteria During Osmotic Shock**, JORDAN PRICE, WILLIAM KLUG, Department of Mechanical and Aerospace Engineering, UCLA — Bacteria combat hypoosmotic shocks by opening mechanosensitive ion channels located within the inner membrane. These channels are believed to act as “emergency release valves, reducing transient pressure during the shock by regulating solute and water flux. Recent experiments have shown that cell survivability depends strongly on channel populations and the rate of osmotic shock. However, the understanding of the physical mechanisms behind osmotic protection remains unclear. We investigate how channel deletions, variations in shock rate, and cell envelope mechanics affect survivability by constructing theoretical elasticity and transport models. We find that reducing the number of channels and applying faster shocks significantly increases the time-dependent stress of the cell membrane and wall. This result provides insight into physical mechanisms that govern cell failure, including membrane rupture and wall fracture.

**Monday, March 14, 2016 8:00AM - 10:48AM —**

**Session A42 DPOLY: Polymer Thin Films: Patterning and Flow** 345 - Justin Pye, Emory University

**8:00AM A42.00001 Deformation of Thin Free-standing Films with Sessile Droplets Through the Glass Transition**, ADAM FORTAIS, RAFAEL SCHULMAN, KARI DALNOKI-VERESS, McMaster University — Droplets on a rigid substrate will form a contact angle determined by interfacial tensions according to Young's law. Likewise, the Laplace pressure of a droplet will deform a liquid substrate, and the contact line geometry can be determined through a Neumann construction. We explore the intermediate case of micro-droplets placed on thin, highly compliant, free-standing films. The Laplace pressure of the droplet deforms the free-standing film, creating a spherical bulge. The film's tension is modulated by changing temperature continuously from well below the glass transition into the melt state of the film. The contact angle of the liquid droplet with the undeformed film as well as the angle of the bulge with the film is measured and compared to the contact angles predicted by a force balance at the contact line.

**8:12AM A42.00002 Measuring spatially distributed rheology of thin polymer films by non-contact shearing.**, MITHUN CHOWDHURY, Chemical and Biological Engineering, Princeton University, NJ 08544, USA, YUNLONG GUO, University of Michigan Shanghai Jiao Tong University Joint Institute, Shanghai 200240, P.R. China, RODNEY D. PRIESTLEY, Chemical and Biological Engineering, Princeton University, NJ 08544, USA — For nearly two decades, a great deal of research has been devoted to understand the impact of nanoscale confinement on the glassy and viscoelastic properties of thin polymer films. Prior works in supported films mostly used indirect mechano-rheological means, due to the complexity associated to probe such small volume. Here we present a non-contact shearing method 'blow-off', induced by the laminar flow of an inert gas through a narrow channel in order to generate a well-defined shear stress on a rectangular edge of a properly placed polymer thin film on a solid substrate. By appropriate control of temperature/ time during shearing, we explored effective viscosity and shear mobility, spatially from free surface to the material interior. In general, we found film surface has higher shear mobility and lower effective viscosity in comparison to its interior.

**8:24AM A42.00003 Photodirecting Marangoni Flow to Pattern Thin Polymer Films: Decoupling Viscosity and Diffusivity**, CHAE BIN KIM, AMANDA JONES, DUSTIN JANES, TALHA ARSHAD, ROGER BONNECAZE, CHRISTOPHER ELLISON, The University of Texas at Austin — The Marangoni effect causes liquids to flow towards localized regions of higher surface tension. In thin polymer films, this effect could offer a practically useful route to manufacture topographically patterned surfaces. In this presentation, we report a photochemical strategy to harness Marangoni flow as a versatile patterning method along with comparisons to a theoretical model that reveals the underlying physics of this process. The model agrees well with experiments with no adjustable parameters. It further indicates that higher aspect ratio features are favored by large surface tension gradients, low diffusivities and low viscosities. However, as described by the Rouse model, low viscosities are generally correlated with high diffusivities; diffusivity is also an important factor in the timescale by which the spatial surface tension patterns decay. This coupling between diffusivity and viscosity could critically limit feature aspect ratio for any given surface tension pattern. A potential strategy that decouples diffusivity and viscosity of the film components will be presented.

**8:36AM A42.00004 The Parametric Study of Focused Laser-Induced Marangoni Dewetting for Patterning Polymer Thin Films**, JONATHAN SINGER, TIANXING MA, Rutgers University, STEVEN KOOL, Massachusetts Institute of Technology, EDWIN THOMAS, Rice University — Highly-localized focused laser spike (FLaSk) heating of polymer thin films is a resist- and developer-free alternative to 2D laser direct write for creating patterns on the single micron or, by exploiting overlap effects, submicron scale. The massive temporal and spatial thermal gradients and resulting thermal Marangoni stresses generated by FLaSk are an effective means for the directed dewetting and patterning of such films. Here, the general applicability of this technique to glassy amorphous polymer thin film systems is investigated through systematic investigation of film thickness, glass transition temperature, and polymer mobility. The results reveal that the important parameters are the film thickness (coupled to the optical heating effects through anti-reflection coating effects) and the high-temperature polymer melt mobility, allowing for generation of single features with linewidths of down to 1  $\mu\text{m}$ . Further, the introduction of spatial mobility variations by using polymer brushes, bilayers, and microphase separated block copolymers leads to additional profile manipulation effects (*i.e.* spontaneous 2D pattern generation and flattened top profiles).

**8:48AM A42.00005 Degrafting of polymer brushes from substrates enables insight about the brush structure and facilitates surface patterning.**, ROHAN PATIL, North Carolina State Univ, SALOMON TURGMAN-COHEN, Kettering University, JIRI SROGL, North Carolina State Univ, DOUGLAS KISEROW, Army Research Office, JAN GENZER, North Carolina State Univ — Polymers end-grafted to surfaces or interfaces, commonly referred to as polymer brushes, enable tailoring physico-chemical properties of material surfaces. Many applications of polymer brushes require information about the molecular weight (MW) and grafting density (GD) of polymer brushes. For brushes synthesized by surface initiated polymerization (SIP) determining these attributes was always a challenge. We have developed a simple method of measuring MW and GD of these systems by degrafting SIP from silica-based surfaces by using tetrabutyl ammonium fluoride (TBAF), which attacks selectively Si-O bonds and enables complete degrafting of poly(methyl methacrylate) (PMMA) brushes from silica based substrates without damaging the backbone. The rate of PMMA degrafting decreases with reaction time and depends on the concentration of TBAF, temperature, and the initial GD of the system. The molecular weight distribution of the degrafted PMMA was measured using size exclusion chromatography. The GD was calculated from known MW and dry thickness of the PMMA brush. Spatial patterns of degrafted regions on the substrate can be prepared by either localizing the TBAF to certain regions or by gradually immersing homogeneous samples into TBAF solution.

**9:00AM A42.00006 Fabrication of Converging and Diverging Polymeric Microlens Arrays By A Thermocapillary Replication Technique<sup>1</sup>**, SOON WEI DANIEL LIM, KEVIN FIEDLER, SANDRA TROIAN, California Institute of Technology, 1200 E. California Blvd, MC 128-95, Pasadena, CA — Thermocapillary forces offer a powerful method for sculpting interfaces at microscale dimensions. Here we demonstrate how periodic arrays of cooled pins placed in close proximity to the surface of a molten polymer nanofilm can be used to fabricate various large area microlens arrays, which when solidified exhibit ultrasmooth surfaces and excellent focusing capability. This technique was used to fabricate both homogeneous converging and diverging microlens shapes by application of various thermal distributions. The converging arrays were incorporated into a Shack-Hartmann wavefront sensor able to image moving currents of airborne spray droplets. Feature overlap was also used to achieve hierarchical arrays comprising two superimposed patterns. By varying the width of the cooled pins, it was also possible to fabricate converging microlens structures featuring a caldera-like depression at the vertex able to focus collimated light into a sharp annulus. These demonstrations prove that with suitable microscale control over the thermal distributions projected onto molten nanofilms, a diverse set of micro-optical components can be fabricated by thermocapillary replication from a nearby mask without contact and in a single step.

<sup>1</sup>S. W. D. Lim acknowledges funding from the Toshi Kubota SURF fellowship. KRF is supported by a NASA Science and Technology Research Fellowship.

**9:12AM A42.00007 Ultrasmooth, Polydopamine Modified Surfaces for Block Copolymer Nanopatterning on Inert and Flexible Substrates**, REIKA KATSUMATA, JOON HEE CHO, SUNSHINE ZHOU, CHAE BIN KIM, AUSTIN DULANEY, The University of Texas at Austin, DUSTIN JANES, U.S. Food and Drug Administration, CHRISTOPHER ELLISON, The University of Texas at Austin — Nature has engineered universal, catechol-containing adhesives that can be synthetically mimicked in the form of polydopamine (PDA). We exploited PDA to enable block copolymer (BCP) nanopatterning on a variety of soft material surfaces in a way that can potentially be applied to flexible electrical devices. Applying BCP nanopatterning to soft substrates is challenging because soft substrates are often chemically inert and possess incompatible low surface energies. In this study, we exploited PDA to enable the formation of BCP nanopatterns on a variety of surfaces such as Teflon, poly(ethylene terephthalate) (PET), and Kapton. While previous studies produced a PDA coating layer too rough for BCP nanopatterning, we succeeded in fabricating conformal and ultra-smooth surfaces of PDA by engineering the PDA coating process and post-sonication procedure. This chemically functionalized, biomimetic thin film (3 nm thick) served as a reactive platform for subsequently grafting a surface treatment to perpendicularly orient a lamellae-forming BCP layer. Furthermore, we demonstrated that a perfectly nanopatterned PDA-PET substrate can be bent without distorting or damaging the nanopattern in conditions that far exceeds typical bending curvatures in roll-to-roll manufacturing.

**9:24AM A42.00008 Adsorption and Pattern Recognition of Polymer at Complex Heterogeneous Surfaces**, LEILA RAJABIBONAB, Victoria University of Wellington, SHAUN HENDY, University of Auckland, SHAUN HENDY TEAM, LEILA RAJABI TEAM — The statistical mechanics of polymer adsorption on a substrate has been well studied. However, there has been recent interest in the conformational behaviour of polymer chains on patterned heterogeneous surfaces, where absorption strength varies. Here we report on Monte Carlo simulations of the adsorption of homo-polymer chains on patterned surfaces. One difficulty in studying polymer self-assembly on a patterned surface is the fluctuation of polymer conformations, which can make calculating the free energy a challenge. To overcome this we apply an expanded ensemble method to compute free energy differences. Applying this approach enables us to identify different adsorbed phases at a range of temperatures. The simplest case of heterogeneous surface is striped pattern, but we consider heterogeneous surfaces with four other that are structured on different length scales. At low temperatures we find that the polymer chain will recognise the pattern, by conformationally adapting as it adsorbs before eventually becoming fully relaxed on the surface. Polymers are found to adsorb on simple patterns at higher temperatures than on complex patterns.

**9:36AM A42.00009 Wake and wave resistance on viscous thin films**, RENE LEDESMA-ALONSO, MICHAEL BENZAQUEN, THOMAS SALEZ, ELIE RAPHAEL, Gulliver UMR 7083, ESPCI, PHYSICO-CHIMIE THEORIQUE TEAM — The effect of an external pressure disturbance, which is displaced with constant speed along the free surface of a viscous thin film, is studied theoretically in the lubrication approximation in one- and two-dimensional geometries. In the comoving frame, the imposed pressure field creates a stationary deformation of the interface - a wake - that spatially vanishes in the far region. The shape of the wake and the way it vanishes depend on both the speed  $v$  and size  $a$  of the external source and the properties of the film: density  $\rho$ , air-liquid surface tension  $\gamma$ , shear viscosity  $\mu$ , and film thickness  $h_0$ . The wave resistance, namely the force that has to be externally furnished in order to maintain the disturbance speed and the stationary wake, is analyzed in detail. For finite-size pressure disturbances, it increases with the speed, up to a certain transition value above which a monotonic decrease occurs. The role of the horizontal extent of the pressure field is studied as well, revealing that for a smaller disturbance the latter transition occurs at a higher speed. Eventually, for a Dirac pressure source, the wave resistance either saturates for a 1D geometry, or diverges for a 2D geometry.

**9:48AM A42.00010 Plug flow in a viscous freely-suspended film**, KARI DALNOKI-VERESS, MARK ILTON, MILES COUCHMAN, Department of Physics and Astronomy, McMaster University, Hamilton, Ontario, Canada, L8S 4M1, THOMAS SALEZ, MICHAEL BENZAQUEN, Laboratoire de Physico-Chimie Théorique, UMR CNRS Gulliver 7083, ESPCI ParisTech, PSL Research University, 75005 Paris, France, PAUL FOWLER, Department of Physics and Astronomy, McMaster University, Hamilton, Ontario, Canada, L8S 4M1, ELIE RAPHAEL, Laboratoire de Physico-Chimie Théorique, UMR CNRS Gulliver 7083, ESPCI ParisTech, PSL Research University, 75005 Paris, France — The flow of viscous polymer liquids supported by a solid substrate has been well characterized by a variety of experimental techniques. Previous studies found that the velocity profile within a flowing liquid film depends strongly on the friction at the liquid-substrate interface. For the case of low interfacial friction, liquid molecules can slide along the solid substrate. This is the “slip” boundary condition. Here we probe flow in a system with no interfacial friction: a viscous polymer film suspended at its edges. Using AFM, we measure the capillary-driven relaxation of freestanding polymer films with an initially stepped film thickness profile. The time evolution of the profile is consistent with plug flow. A freely-suspended viscous polymer film provides a physical realization of an idealized infinite slip boundary condition. Interestingly, in such a context, the profile evolution satisfies a diffusion-like equation, thus allowing for the use of a broad mathematical and physical toolbox by analogy.

**10:00AM A42.00011 Understanding and Improving the Quality of Inter-Layer Interfaces in FDM 3-D Printing**, EDWARD DURANTY, BRANDON SPRADLIN, MADELINE STARK, University of Tennessee, MARK DADMUN, University of Tennessee, Oak Ridge National Laboratory — We have studied the effect of thermal history and material diffusion on inter-filament bonding in FDM 3D printed parts and developed methods to improve interlayer adhesion in 3D printed samples. The available thermal energy during the FDM print environment was determined quantitatively by tracking the temperature of the bottom most printed layer using a thermocouple attached to the print bed. The role of the thermal history of the filaments during the deposition process on the quality of inter-layer bonding in an FDM ABS part was monitored using a T-peel test and an innovative sample design. Additionally, the interfacial adhesion between 3D printed layers was improved by the addition of a chemical cross-linking agent 4,4'-diaminodiphenylmethane (DADPM). These studies have increased our understanding of the importance of the complex thermal history of a filament in the 3D printing process and its impact on the interfaces that form during the fused deposition modeling print process. Furthermore, the chemical crosslinking process demonstrates a potential method to covalently link layers in FDM printed parts, improving the bulk strength of the part. The insight provided in this work may aid in the development of techniques that can produce FDM parts that could be used as replacement parts in structural applications, or as completely standalone products.

**10:12AM A42.00012 Modelling Polymer Deformation during 3D Printing**, CLAIRE MCILROY, PETER OLMSTED, Georgetown University — Three-dimensional printing has the potential to transform manufacturing processes, yet improving the strength of printed parts, to equal that of traditionally-manufactured parts, remains an underlying issue. The fused deposition modelling technique involves melting a thermoplastic, followed by layer-by-layer extrusion to fabricate an object. The key to ensuring strength at the weld between layers is successful inter-diffusion. However, prior to welding, both the extrusion process and the cooling temperature profile can significantly deform the polymer micro-structure and, consequently, how well the polymers are able to “re-entangle” across the weld. In particular, polymer alignment in the flow can cause de-bonding of the layers and create defects. We have developed a simple model of the non-isothermal extrusion process to explore the effects that typical printing conditions and material rheology have on the conformation of a polymer melt. In particular, we incorporate both stretch and orientation using the Rolie-Poly constitutive equation to examine the melt structure as it flows through the nozzle, the subsequent alignment with the build plate and the resulting deformation due to the fixed nozzle height, which is typically less than the nozzle radius.

**10:24AM A42.00013 Fundamental characterization of soft matter 3D printing processes**, KALMAN MIGLER, JONATHAN SEPPALA, CHELSEA DAVIS, KAITLYN HILLGARTNER, NIST — In fused filament fabrication (FFF), a material extrusion 3D printing method, thermoplastic filament is extruded through a rastering nozzle on the previous layer. The resulting strength of the FFF produced part is limited by the strength of the weld between each layer. While numerous factors can affect the weld strength, the temperature of the extrudate and the previous layer dictate the amount of interdiffusion and thus the weld strength. Temperature measurements were performed using forward looking infrared imaging. Interdiffusion estimates were calculated from temperature profiles, normalized using horizontal shift factors from offline rheological measurements of the neat polymer. Weld strength was measured directly by Mode III Fracture using a simplified geometry limiting the measurement to a single weld. Since the processing conditions are known a priori this approach provides the data needed to estimate the final build strength at time of design. The resulting agreement between interdiffusion estimates and weld strength for a range of printing conditions are discussed.

**10:36AM A42.00014 Pinch-off dynamics, extensional viscosity and relaxation time of dilute and ultradilute aqueous polymer solutions**, MADELEINE BIAGIOLI, JELENA DINIC, LEIDY NALLELY JIMENEZ, VIVEK SHARMA, Chemical Engineering, University of Illinois at Chicago — Free surface flows and drop formation processes present in printing, jetting, spraying, and coating involve the development of columnar necks that undergo spontaneous surface-tension driven instability, thinning, and pinch-off. Stream-wise velocity gradients that arise within the thinning neck create an extensional flow field, which induces micro-structural changes within complex fluids that contribute elastic stresses, changing the thinning and pinch-off dynamics. In this contribution, we use dripping-onto-substrate (DoS) extensional rheometry technique for visualization and analysis of the pinch-off dynamics of dilute and ultra-dilute aqueous polyethylene oxide (PEO) solutions. Using a range of molecular weights, we study the effect of both elasticity and finite extensibility. Both effective relaxation time and the transient extensional viscosity are found to be strongly concentration-dependent even for highly dilute solutions.

**Monday, March 14, 2016 8:00AM - 11:00AM —**

**Session A43 GSNP GSOF: Avalanches in Granular and Other Particle-based Materials I** 346 -  
Corey O'Hern, Yale University

**8:00AM A43.00001 Critical Dynamics Near the Erosion Onset**, LE YAN, Kavli Institute for Theoretical Physics, UCSB, MATTHIEU WYART, Ecole Polytechnique Federale de Lausanne, Switzerland — Erosion shapes the Earth's landscape. Experiments reveal that there is an erosion threshold of a granular bed sheared by a viscous fluid. The granular particles start to flow when the shearing force is above the threshold  $\theta_c$ . Near  $\theta_c$ , the particle flux grows linearly  $J \sim \theta - \theta_c$ . The stationary state is reached after a transient time  $t_{conv}$ , which diverges as  $t_{conv} \sim |\theta - \theta_c|^{-z}$ . We theoretically study this dynamical transition by introducing a model capturing both the drainage effect of the disordered landscape and the interactions among the granular particles. Based on the model, we make the first time quantitative testable predictions for the drainage pattern — how the granular flux is spatially distributed and correlated. Our model enables us to rationalize the critical dynamics of erosion, which may also apply to the plastic depinning transition of vortex lattices in dirty superconductors.

**8:12AM A43.00002 Critical scaling with strain rate in overdamped sheared disordered solids<sup>1</sup>**, JOEL CLEMMER, Johns Hopkins University, KENNETH SALERNO, Sandia National Laboratories, MARK ROBBINS, Johns Hopkins University — In the limit of quasistatic shear, disordered solids demonstrate non-equilibrium critical behavior including power-law distributions of avalanches<sup>2</sup>. Using molecular dynamics simulations of 2D and 3D overdamped binary LJ glasses, we explore the critical behavior in the limit of finite strain rate. We use finite-size scaling to find the critical exponents characterizing shear stress, kinetic energy, and measures of temporal and spatial correlations. The shear stress of the system rises as a power  $\beta$  of the strain rate. Larger system size extends this power law to lower rates. This behavior is governed by a power law drop of the dynamic correlation length with increasing shear stress defined by the exponent  $\nu$ . This finite-size effect also impacts the scaling of the RMS kinetic energy with strain rate as avalanches begin nucleating simultaneously leading to continuous deformation of the solid. As system size increases, avalanches begin overlapping at lower rates. The correlation function of non-affine displacement exhibits novel anisotropic power law scaling with the magnitude of the wave vector. Its strain rate dependence is used to determine the scaling of the dynamic correlation length.

<sup>1</sup>Support provided by: DMR-1006805; NSF IGERT-0801471; OCI-0963185; CMMI-0923018

<sup>2</sup>K. M. Salerno and M. O. Robbins, Phys. Rev. E **77**, 062206 (2013)

**8:24AM A43.00003 Scaling theory of the process zone of quasibrittle materials: an avalanche crossover analysis**, JARON KENT-DOBIAS, Physics, Cornell University, ASHVINI SHEKHAWAT, Materials Science and Engineering, Berkeley, JAMES SETHNA, Physics, Cornell University — We present progress towards a natural theory of the process zone surrounding cracks in quasibrittle materials using renormalization group methods. Quasibrittle or disordered brittle materials like concrete evade usual fracture analysis because of strong finite-size effects and a large disordered process zone. Unlike metals, where the process zone is relatively small and dominated by plasticity, microcracking relieves stress around the tip of quasibrittle cracks, a process that is not well understood. Recently, a scaling crossover theory was developed by Sethna and Shekhawat to explain the influence of finite size on the fracture mechanism and avalanche precursors. We extend this theory to model the scaling of stress and distribution of microcracking in the process zone.

**8:36AM A43.00004 Avalanches and local force evolution in a granular stick-slip experiment<sup>1</sup>**, AGHIL ABED ZADEH, JONATHAN BARES, ROBERT BEHRINGER, Duke University — We carry out experiments to characterize stick-slip for granular materials. In our experiment, a constant speed stage pulls a slider which rests on a vertical bed of circular photoelastic particles in a 2D system. The stage is connected to the slider by a spring. We measure the force on the spring by a force sensor attached to the spring. The distributions of energy release and time duration of avalanches during slip obey power laws. We analyze the power spectrum of the force signal to understand the effect of the loading speed and of the spring stiffness on the statistical behavior of the system. From a more local point of view and by using a high speed camera and the photoelastic properties of our particles, we characterize the internal granular structure during avalanches. By image processing and analyzing the skeleton of force network inside the media, we try to understand the flow of particles and evolution of force chains inside the media and during avalanches.

<sup>1</sup>NSF DMR1206351, NASA NNX15AD38G, and the W. M. Keck Foundation.

**8:48AM A43.00005 Avalanche-like fluidization of a non-Brownian particle gel<sup>1</sup>**, AIKA KUOKAWA, Earthquake Research Institute, VALÉRIE VIDAL, ENS Lyon, KEI KURITA, Earthquake Research Institute, THIBAUT DIVOUX, CNRS, CRPP - Bordeaux, SÉBASTIEN MANNEVILLE, ENS Lyon — We report on the fluidization dynamics of an attractive gel composed of non-Brownian particles made of fused silica colloids. Extensive rheology coupled to ultrasonic velocimetry allows us to characterize the global stress response together with the local dynamics of the gel during shear startup experiments. In practice, after being rejuvenated by a preshear, the gel is left to age during a time  $t_w$  before being submitted to a constant shear rate  $\dot{\gamma}$ . We investigate in detail the effects of both  $t_w$  and  $\dot{\gamma}$  on the fluidization dynamics and build a detailed state diagram of the gel response to shear startup flows. The gel may either display transient shear banding towards complete fluidization, or steady-state shear banding. In the former case, we unravel that the progressive fluidization occurs by successive steps that appear as peaks on the global stress relaxation signal. Flow imaging reveals that the shear band grows up to complete fluidization of the material by sudden avalanche-like events which are distributed heterogeneously along the vorticity direction and correlated to large peaks in the slip velocity at the moving wall.

<sup>1</sup>PRC CNRS/JSPS RheoVolc, IUF & ERC Grant Agreement No. 258803

**9:00AM A43.00006 Spatiotemporal stick-slip phenomena in a coupled continuum-granular system**, ROBERT ECKE, Los Alamos National Laboratory — In sheared granular media, stick-slip behavior is ubiquitous, especially at very small shear rates and weak drive coupling. The resulting slips are characteristic of natural phenomena such as earthquakes and well as being a delicate probe of the collective dynamics of the granular system. In that spirit, we developed a laboratory experiment consisting of sheared elastic plates separated by a narrow gap filled with quasi-two-dimensional granular material (bi-dispersed nylon rods). We directly determine the spatial and temporal distributions of strain displacements of the elastic continuum over 200 spatial points located adjacent to the gap. Slip events can be divided into large system-spanning events and spatially distributed smaller events. The small events have a probability distribution of event moment consistent with an  $M^{-3/2}$  power law scaling and a Poisson distributed recurrence time distribution. Large events have a broad, log-normal moment distribution and a mean repetition time. As the applied normal force increases, there are fractionally more (less) large (small) events, and the large-event moment distribution broadens. The magnitude of the slip motion of the plates is well correlated with the root-mean-square displacements of the granular matter. Our results are consistent with mean field descriptions of statistical models of earthquakes and avalanches. We further explore the high-speed dynamics of system events and also discuss the effective granular friction of the sheared layer. We find that large events result from stored elastic energy in the plates in this coupled granular-continuum system.

**9:36AM A43.00007 Tuning Parameters and Scaling For Avalanches On A Slowly-Driven Conical Bead Pile with Cohesion**<sup>1</sup>, SUSAN LEHMAN, D. T. JACOBS, PAROMA PALCHOUDHURI, AVI VAJPEYI, JUSTINE WALKER, College of Wooster, KARIN DAHMEN, MICHAEL LEBLANC, University of Illinois at Urbana-Champaign, JONATHAN UHL, Retired — Slip avalanches on a slowly driven pile are investigated experimentally using a 3D conical pile built from uniform 3 mm steel beads. Beads are added to the pile by dropping them onto the apex one at a time; avalanches are measured through changes in pile mass. We investigate the dynamic response of the pile by recording avalanches from the pile over the course of tens of thousands of bead drops. The statistical properties of the avalanches, including probability of particular avalanche sizes and the time between avalanches of given size, are well-characterized by universal power laws and scaling functions. By adding a uniform magnetic field, we may systematically vary the cohesion between the beads and tune the critical behavior of the system. As the cohesion increases we observe an increase in both size and number for very large avalanches and decreases in the mid-size avalanches, causing a deviation from the power law. A full study of the effect of cohesion on the size and time distributions is in process, combining the experimental results with predictions from an analytical mean-field model [Dahmen, Nat Phys 7, 554 (2011)].

<sup>1</sup>Research supported by NSF CBET 1336116 and 1336634

**9:48AM A43.00008 Universality and depinning models for plastic yield in amorphous materials.**, ZOE BUDRIKIS, ISI Foundation, via Alassio 11/c 10126 Torino, Italy, DAVID FERNANDEZ CASTELLANO, STEFAN SANDFELD, MICHAEL ZAISER, 8-Materials Simulation, FAU University of Erlangen-Nuremberg, Germany, STEFANO ZAPPERI, Dipartimento di Fisica, Università di Milano, Italy — Plastic yield in amorphous materials occurs as a result of complex collective dynamics of local reorganizations, which gives rise to rich phenomena such as strain localization, intermittent dynamics and power-law distributed avalanches. While such systems have received considerable attention, both theoretical and experimental, controversy remains over the nature of the yielding transition. We present a new fully-tensorial coarsegrained model in 2D and 3D, and demonstrate that the exponents describing avalanche distributions are universal under a variety of loading conditions, system dimensionality and size, and boundary conditions. Our results show that while depinning-type models in general are apt to describe the system, mean field depinning models are not.

**10:00AM A43.00009 Atomic-scale reversibility in sheared glasses**, MENG FAN, MINGLEI WANG, YANHUI LIU, JAN SCHROERS, Department of Mechanical Engineering and Materials Science, Yale University, MARK SHATTUCK, Department of Physics and Benjamin LeVich Institute, The City College of the City University of New York, New York, COREY O'HERN, Department of Mechanical Engineering and Materials Science, Yale University — Systems become irreversible on a macroscopic scale when they are sheared beyond the yield strain and begin flowing. Using computer simulations of oscillatory shear, we investigate atomic scale reversibility. We employ molecular dynamics simulations to cool binary Lennard-Jones liquids to zero temperature over a wide range of cooling rates. We then apply oscillatory quasistatic shear at constant pressure to the zero-temperature glasses and identify neighbor-switching atomic rearrangement events. We determine the critical strain  $\gamma^*$ , beyond which atoms in the system do not return to their original positions upon reversing the strain. We show that for more slowly cooled glasses, the average potential energy is lower and the typical size of atomic rearrangements is smaller, which correlates with larger  $\gamma^*$ . Finally, we connect atomic- and macro-scale reversibility by determining the number of and correlations between the atomic rearrangements that occur as the system reaches the yield strain.

**10:12AM A43.00010 Multiscale minimal modeling of microscale crystal plasticity: Finite-size scaling and stochastic plastic flow**, STEFANOS PAPANIKOLAOU, Johns Hopkins University, PETER ISPANOVITY, Eötvös University — We investigate the multiscale description from continuum to discrete modeling of crystal plasticity in the context of a minimal model. We develop a continuum plasticity description of discrete edge dislocations moving athermally in a single slip system; Our continuum modeling not only matches the statistical behavior of the model, but also the onset of emergent length scales as load increases. We perform quasistatic stress-controlled simulations of our continuum model and compare it with the corresponding discrete dislocation dynamics model, which describes crystal plasticity at a smaller spatiotemporal discretization scale. We investigate the properties of strain bursts (dislocation avalanches) occurring during plastic deformation, as well as the onset of a dislocation patterning lengthscale, and compare in detail the continuum and discrete descriptions. Our approach provides a pathway to multiscale modeling of complex, multi-slip and three dimensional crystal plasticity.

**10:24AM A43.00011 The effectiveness of mean-field theory for avalanche distributions**, EDWARD LEE, ARCHISHMAN RAJU, JAMES SETHNA, Cornell University — We explore the mean-field theory of the pseudogap found in avalanche systems with long-range anisotropic interactions using analytical and numerical tools. The pseudogap in the density of low-stability states emerges from the competition between stabilizing interactions between spins in an avalanche and the destabilizing random movement towards the threshold caused by anisotropic couplings. Pazmandi et al. have shown that for the Sherrington-Kirkpatrick model, the pseudogap scales linearly and produces a distribution of avalanche sizes with exponent  $t=1$  in contrast with that predicted from RFIM  $t=3/2$ . Lin et al. have argued that the scaling exponent  $t$  of the pseudogap depends on the tail of the distribution of couplings and on non-universal values like the strain rate and the magnitude of the coupling strength. Yet others have argued that the relationship between the pseudogap scaling and the distribution of avalanche sizes is dependent on dynamical details. Despite the theoretical arguments, the class of RFIM mean-field models is surprisingly good at predicting the distribution of avalanche sizes in a variety of different magnetic systems. We investigate these differences with a combination of theory and simulation.

**10:36AM A43.00012 Elasto-plastic automata with realistic near field interactions: avalanches and diffusion**, CRAIG MALONEY, Northeastern, BOTOND TYUKODI, DAMIEN VANDEMBROUCQ, ESPCI — We present results on an elasto-plastic automaton model of an athermal amorphous solid under shear. We study four different variants of the model with two different loading geometries and two different stochastic prescriptions (random yield thresholds or random strain amplitudes). We perform a finite size scaling analysis for the avalanche size distribution and single-site displacement and strain statistics. The avalanche size distribution in all four cases is inconsistent with mean-field depinning results. For three of the four variants, the distribution is consistent with previous results from atomistic simulations and other related elasto-plastic models. The fourth seems to exhibit different scaling properties and may lie in a different universality class. The mean-squared displacement exhibits a pronounced dependence on the microscopic ingredients of the model and is completely non-universal. These results show that while certain microscopic ingredients of the model may be irrelevant for the individual avalanches, they may exhibit a profound impact on long-time correlations and long-lived shear localization.

**10:48AM A43.00013 Rearrangements in deformed foams near jamming**, MERLIJN VAN DEEN, VERA JANSSEN, ALEXANDER SIEMENS, MARTIN VAN HECKE, Huygens-Kamerlingh Onnes Lab, Leiden University — We deform two-dimensional foams at different densities and show there are two distinct regimes: a high density regime where bubbles deform affinely until the built up stress is released in rapid events (shear transformation zones), and a low density regime where bubbles are continuously in motion and rapid events are rare.

**Monday, March 14, 2016 8:00AM - 10:24AM —**

**Session A44 GQI: Quantum Information with Majorana Fermions & Parafermions** 347 - David Aasen, California Institute of Technology

**8:00AM A44.00001 Milestones toward Majorana-based quantum computing: Fusion rule detection and topological qubit validation**, RYAN V. MISHMASH, DAVID AASEN, Caltech, MICHAEL HELL, Lund University and NBI, Copenhagen, ANDREW HIGGINBOTHAM, Harvard and NBI, Copenhagen, JEROEN DANON, NBI, Copenhagen, MARTIN LEIJNSE, Lund University, THOMAS S. JESPERSEN, NBI, Copenhagen, JOSHUA A. FOLK, NBI, Copenhagen and UBC, CHARLES M. MARCUS, KARSTEN FLENSBERG, NBI, Copenhagen, JASON ALICEA, Caltech — We introduce a scheme for preparation, manipulation, and readout of Majorana zero modes in semiconducting wires coated with mesoscopic superconducting islands. Our approach synthesizes recent advances in materials growth with tools commonly used in quantum-dot experiments, including gate-control of tunnel barriers and Coulomb effects, charge sensing, and charge pumping. Recently, we have outlined a sequence of relatively modest milestones which interpolate between zero-mode detection and longer term quantum computing applications. In this talk, I will discuss two of these milestones: (1) detection of fusion rules for non-Abelian anyons using either proximal charge sensing or Majorana-mediated charge pumping and (2) validation of a prototype topological qubit via unconventional scaling relations between the time-averaged qubit splitting and its decoherence times  $T_1$  and  $T_2$ . Both of these proposed experiments require only a single wire with two islands—a hardware configuration already available in the laboratory. Furthermore, these pre-braiding experiments can be adapted to other manipulation and readout schemes as well.

**8:12AM A44.00002 Gate-controlled charging effects in superconducting nanowires: low-energy spectrum and time scales for Majorana manipulation**, MICHAEL HELL, Division of Solid State Physics and NanoLund, Lund Univ., Sweden / Center for Quantum Devices and Station Q Copenhagen, Univ. of Copenhagen, Denmark, JEROEN DANON, Center for Quantum Devices and Station Q Copenhagen and Niels Bohr International Academy, Univ. of Copenhagen, Denmark, MARTIN LEIJNSE, Division of Solid State Physics and NanoLund, Lund Univ., Sweden / Center for Quantum Devices and Station Q Copenhagen, Univ. of Copenhagen, Denmark, KARSTEN FLENSBERG, Center for Quantum Devices and Station Q Copenhagen, Univ. of Copenhagen, Denmark — In this talk, we investigate the gate-controlled crossover between different operating regimes of a superconducting nanowire segmented into two islands each Josephson-coupled to a bulk superconductor. This device may host two pairs of Majorana bound states and could be realized in the near future as a platform for testing Majorana fusion rules. We present a numerical study of the low-energy spectrum of this device covering both the charge-dominated regime utilizable for initialization and readout of the Majorana bound states as well as the Josephson-dominated transmon regime allowing for Majorana manipulations. Depending on the relative size of the energy scales associated with the Majorana coupling, the charging energy, and the transmon frequency, the fine structure of the low-energy spectrum differs. We finally discuss the associated time scales for implementing a fusion-rule testing protocol discussed in the talks by J. Alicea and R. V. Mishmash.

**8:24AM A44.00003 Demonstrating non-Abelian statistics of Majorana fermions using twist defects**, HUAIXIU ZHENG, ARPIT DUA, LIANG JIANG, Yale University — We study the twist defects in the toric code model introduced by Bombin [Phys. Rev. Lett. 105, 030403 (2010)]. Using a generalized 2D Jordan-Wigner transformation and a projective construction, we show explicitly the twist defects carry unpaired Majorana zero modes. In addition, we propose a quantum non-demolition measurement scheme of the parity of Majorana modes. Such a scheme provides an alternative avenue to demonstrate the non-Abelian statistics of Majorana fermions. The braiding operation is simulated by an efficient measurement-based approach that removes the uncertainty associated with the previous forced measurement scheme.

**8:36AM A44.00004 Parafermions in spin lattices**, ARPIT DUA, HUAIXIU ZHENG, LIANG JIANG, Yale Univ — We investigate the twist defects in the  $Z_N$  Toric code model first introduced by Bombin [Phys. Rev. Lett. 105, 030403 (2010)] for the  $Z_2$  model and then generalized and studied by You et al. [Phys. Rev. B 86, 161107(R) (2012)]. Using topological entanglement entropy (TEE) and generalized Jordan-Wigner transformation, we show explicitly that the twist defects carry unpaired Parafermion zero modes. We also demonstrate the fusion rules of these Parafermion modes using the TEE calculation. In addition, we propose a scheme for quantum non-demolition measurement of the topological charge of these modes. This scheme can be used to implement measurement-based braidings (MBBs) on Parafermions to implement gates for quantum computing.

**8:48AM A44.00005 Odd-frequency superconductivity in a nanowire coupled to Majorana zero modes<sup>1</sup>**, SHU-PING LEE, University of Alberta, ROMAN M. LUTCHYN, Microsoft Station Q, JOSEPH MACIEJKO, University of Alberta — Odd-frequency superconductivity, originally proposed by Berezinskii in 1974, is an exotic phase of matter in which pairing is entirely dynamical in nature. The pair potential is an odd function of frequency, leading to a vanishing static superconducting order parameter and exotic types of pairing seemingly inconsistent with Fermi statistics, such as spin triplet (singlet) pairing in an s-wave (p-wave) superconductor. Motivated by recent experimental progress in the realization of Majorana zero modes in semiconducting nanowires, we show that a spin-polarized nanowire coupled to a one-dimensional array of Majorana zero modes becomes an odd-frequency superconductor.

<sup>1</sup>This work was supported by NSERC, CRC, CIFAR, and the University of Alberta.

**9:00AM A44.00006 Readout scheme for Majorana parity states using a quantum dot<sup>1</sup>**, DARRYL HOVING, KAVEH GHARAVI, JONATHAN BAUGH, University of Waterloo — We propose and numerically study a scheme for reading out the parity state of a pair of Majorana bound states using a tunnel coupled quantum dot. The dot is coupled to one end of the topological wire but isolated from any reservoir, and is capacitively coupled to a charge sensor for measurement. The combined parity of the MBS-dot system is conserved and charge transfer between MBS and dot only occurs through resonant tunnelling. Resonance is controlled by the dot potential through a local gate and by the MBS splitting due to the overlap of the MBS pair wavefunctions. The latter splitting can be controlled by changing the position of the spatially separated, uncoupled MBS via a set of keyboard gates. Our simulations show that the oscillatory nature of the MBS splitting versus separation does not prevent high-fidelity readout. Indeed, the scheme can also be applied to measure the splitting versus separation, which would yield a clear signature of the topological state. With experimentally realistic parameters we find parity readout fidelities  $>99\%$  should be feasible.

<sup>1</sup>This work was supported by the Natural Sciences and Engineering Research Council of Canada

**9:12AM A44.00007 Majorana Fermion Rides on a Magnetic Domain Wall<sup>1</sup>** , SE KWON KIM, Univ of California - Los Angeles, SUMANTA TEWARI, Clemson University, YAROSLAV TSERKOVNYAK, Univ of California - Los Angeles — Owing to the recent progress on endowing the electronic structure of magnetic nanowires with topological properties, the associated topological solitons in the magnetic texture—magnetic domain walls—appear as very natural hosts for exotic electronic excitations. Here, we propose to use the magnetic domain walls to engender Majorana fermions [1], which has several notable advantages compared to the existing approaches. First of all, the local tunneling density-of-states anomaly associated with the Majorana zero mode bound to a smooth magnetic soliton is immune to most of parasitic artifacts associated with the abrupt physical ends of a wire, which mar the existing experimental probes. Second, a viable route to move and braid Majorana fermions is offered by domain-wall motion. In particular, we envision the recently demonstrated heat-current induced motion of domain walls in insulating ferromagnets as a promising tool for nonintrusive displacement of Majorana modes. This leads us to propose a feasible scheme for braiding domain walls within a magnetic nanowire network, which manifests the non-Abelian exchange statistics within the Majorana subspace.

[1] S. K. Kim, S. Tewari, and Y. Tserkovnyak, Phys. Rev. B **92**, 020412(R) (2015)

<sup>1</sup>This work has been supported in part by the U.S. DOE-BES, FAME, and AFOSR grants.

**9:24AM A44.00008 Majorana Fermion Surface Code for Universal Quantum Computation** , SAGAR VIJAY, TIM HSIEH, LIANG FU, MIT — We introduce an exactly solvable model of interacting Majorana fermions realizing  $Z_2$  topological order with a  $Z_2$  fermion parity grading and lattice symmetries permuting the three fundamental anyon types. We propose a concrete physical realization by utilizing quantum phase slips in an array of Josephson-coupled mesoscopic topological superconductors, which can be implemented in a wide range of solid state systems, including topological insulators, nanowires or two-dimensional electron gases, proximitized by  $s$ -wave superconductors. Our model finds a natural application as a Majorana fermion surface code for universal quantum computation, with a single-step stabilizer measurement requiring no physical ancilla qubits, increased error tolerance, and simpler logical gates than a surface code with bosonic physical qubits. We thoroughly discuss protocols for stabilizer measurements, encoding and manipulating logical qubits, and gate implementations.

**9:36AM A44.00009 Physical Architecture for a Universal Topological Quantum Computer based on a Network of Majorana Nanowires<sup>1</sup>** , JAY SAU, University of Maryland, MAISSAM BARKESHLI, Station Q, Microsoft Research — The idea of topological quantum computation (TQC) is to encode and manipulate quantum information in an intrinsically fault-tolerant manner by utilizing the physics of topologically ordered phases of matter. Currently, the most promising platforms for a topological qubit are either in terms of Majorana fermion zero modes (MZMs) in spin-orbit coupled superconducting nanowires or in terms of the Kitaev  $Z_2$  surface code. However, the topologically robust operations that are possible in these systems are not sufficient for realizing a universal gate set for topological quantum computation. Here, we show that an array of coupled semiconductor/superconductor nanowires with MZM edge states can be used to realize a more sophisticated type of non-Abelian defect, a  $\pi$ -anyon in an Ising  $X$  Ising topological state. This leads to a possible implementation of the missing topologically protected  $\pi/8$  phase gate and thus paves a path for universal topological quantum computation based on semiconductor-superconductor nanowire technology. We provide detailed numerical estimates of the relevant energy scales, which we show to lie within accessible ranges. [1] Barkeshli, Sau, arXiv:1509.07135 (2015).

<sup>1</sup>J. S. was supported by Microsoft Station Q, startup funds from the University of Maryland and NSF-JQI-PFC

**9:48AM A44.00010 Braiding Majorana fermions in  $p+ip$  superfluids with particle number conservation** , YIRUO LIN, ANTHONY LEGGETT, University of Illinois at Urbana-Champaign — We discuss braiding statistics of Majorana zero modes localized in vortices in 2D spinless  $p+ip$  superfluids with conserved total particle number. In the standard particle non-conserved context, it has been argued that braiding these zero Majorana fermions yields non-abelian statistics. With particle number conservation, We show that in certain geometry, the Berry phase of interchanging two Majorana zero modes is proportional to angular momentum of the system with the presence of two vortices, which can then be calculated in the thermodynamic limit. The braiding statistics turns out to be consistent with the standard result. We then discuss the possible complication due to finite size effect. We'll argue that in a finite size system, the abelian phase of interchanging two vortices is non-topological. We'll finish the discussion by sketching out ongoing work in which we investigate the possible modification of BdG quasi-particle wave functions beyond the BdG mean-field approximation, which can have dramatic effect on topological properties of Majorana zero modes and their braiding statistics.

**10:00AM A44.00011 Beyond parafermions: Defects and zero-modes in non-Abelian phases** , NETANEL LINDNER, Technion - Israel Institute of Technology, EREZ BERG, ADY STERN, Weizmann Institute of Science — Non-Abelian topological phases of matter can be utilized to encode and manipulate quantum information in a non-local manner, such that it is protected from imperfections in the implemented protocols and from interactions with the environment. The condition that the non-Abelian statistics of the anyons supports a computationally universal set of gates sets a very stringent requirement which is not met by many topological phases. We consider the possibility to enrich the possible topological operations supported by a non-Abelian topological phase by introducing defects into the system. We show that such defects bind zero modes which form a unique algebra that goes beyond the algebra of parafermions which describes defects in Abelian phases. For the case of a bi-layer containing Ising anyons, we show that by coupling zero modes one can obtain a set of topological operations that implements a universal set of gates.

**10:12AM A44.00012 Tunable Splitting of the Ground-State Degeneracy in 1D Parafermionic Wires** , CHUN CHEN, FIONA BURNELL, Univ of Minn - Minneapolis — Systems with topologically protected ground-state degeneracies are currently of great interest due to their potential applications in quantum computing. In practise this degeneracy is never exact, and the magnitude of the ground-state degeneracy splitting imposes constraints on the timescales over which information is topologically protected. In this Letter we use an instanton approach to evaluate the splitting of topological ground-state degeneracy in quasi-1D systems with parafermion zero modes, in the specific case where parafermions are realized by inducing a superconducting gap in pairs of fractional quantum Hall (FQH) edges. We show that, like 1D topological superconducting wires, this splitting has an oscillatory dependence on the chemical potential, which arises from an intrinsic Berry phase that produces interference between distinct instanton tunneling events. These Berry phases can be mapped to chiral phases in a (dual) quantum clock model using a Fradkin-Kadanoff transformation. Comparing our low-energy spectrum to that of phenomenological parafermion models allows us to evaluate the real and imaginary parts of the hopping integral between adjacent parafermionic zero modes as functions of the chemical potential.

**Monday, March 14, 2016 8:00AM - 11:00AM –**

**Session A45 GQI: Semiconductor Qubits: Si/SiGe Quantum Dots** 348 - Jason Petta, Princeton University

**8:00AM A45.00001 Spin qubits in quantum dots – beyond nearest-neighbour exchange<sup>1</sup>**, LIEVEN VANDERSYPEN, QuTech and Kavli Institute of Nanoscience — The spin of a single electron is the canonical two-level quantum system. When isolated in a semiconductor quantum dot, a single electron spin provides a well-lived quantum bit. So far, two-qubit gates in this system have relied on the spin exchange interaction that arises when the wave functions of neighbouring electrons overlap. Furthermore, experimental demonstrations of controlled spin-exchange have been limited to 1D quantum dot arrays only. Here we explore several avenues for scaling beyond 1D arrays with nearest-neighbour coupling. First, we show that second-order tunnel processes allow for coherent spin-exchange between non-nearest neighbour quantum dots. The detuning of the intermediate quantum dot controls the frequency of the exchange-driven oscillations of the spins. Second, we demonstrate shuttling of electrons in quantum dot arrays preserving the spin projection for more than 500 hops. We use this technique to read out multiple spins in a way analogous to the operation of a CCD. Finally, we develop superconducting resonators that are resilient to magnetic field and with a predicted tenfold increase in vacuum electric field amplitudes. This makes coupling spin qubits via superconducting resonators in a circuit-QED approach a realistic possibility. [1] F.R. Braakman et al, Nature Nano 8, 432, 2013 [2] T.A. Baart et al, Nature Nano, accepted, see arXiv:1507.07991 [3] T.A. Baart et al, in preparation [4] N. Samkhardje et al, in preparation

<sup>1</sup>Supported by ERC, FOM, NWO, IARPA, ARO, EU

**8:36AM A45.00002 Characterization of accumulation-mode Si/SiGe triple quantum dots<sup>1</sup>**, T. M. HAZARD, D. M. ZAJAC, X. MI, S. S. ZHANG, J. R. PETTA, Department of Physics, Princeton University — The transition from quantum dots fabricated from doped Si/SiGe quantum wells to undoped accumulation-mode structures has greatly improved the performance of few-electron quantum dots. Our accumulation-mode devices<sup>2</sup> are reconfigurable and allow for operation as single, double, or triple quantum dots. In these devices, we measure typical charging energies  $E_c = 5.7$  meV, orbital excited state energies as large as  $E_o = 2.9$  meV, and valley splittings of up to  $E_v = 80$   $\mu$ eV. With the device configured as a triple quantum dot, we easily reach the (1,1,1) charge configuration. The gate architecture allows the interdot tunnel coupling to be tuned over a wide range, which is important for operation as an exchange-only spin qubit.<sup>3</sup>

<sup>1</sup>Research sponsored by ARO Grant No. W911NF-15-1-0149.

<sup>2</sup>D. M. Zajac *et al.*, Appl. Phys. Lett. **106**, 223507 (2015).

<sup>3</sup>J. Medford *et al.*, Phys. Rev. Lett. **111**, 050501 (2013).

**8:48AM A45.00003 Characterization of a gate-defined double quantum dot in a Si/SiGe nanomembrane<sup>1</sup>**, T. J. KNAPP, R. T. MOHR, YIZE STEPHANIE LI, BRANDUR THORGRIMSSON, RYAN H. FOOTE, XIAN WU, DANIEL R. WARD, D. E. SAVAGE, M. G. LAGALLY, MARK FRIESEN, S. N. COPPERSMITH, M. A. ERIKSSON, University of Wisconsin: Madison — We report the characterization of a gate-defined double quantum dot formed in a Si/SiGe nanomembrane. Previously, all heterostructures used to form quantum dots were created using the strain-grading method of strain relaxation, a method that necessarily introduces misfit dislocations into a heterostructure and thereby degrades the reproducibility of quantum devices. Using a SiGe nanomembrane as a virtual substrate eliminates the need for misfit dislocations but requires a wet-transfer process that results in a non-epitaxial interface in close proximity to the quantum dots. We show that this interface does not prevent the formation of quantum dots, and is compatible with a tunable inter-dot tunnel coupling, the identification of spin states, and the measurement of a singlet-to-triplet transition as a function of the applied magnetic field. This work was supported in part by ARO (W911NF-12-0607), NSF (DMR-1206915, PHY-1104660), and the United States Department of Defense. The views and conclusions contained in this document are those of the author and should not be interpreted as representing the official policies, either expressly or implied, of the US Government.

<sup>1</sup>T. J. Knapp, et al. (2015). arXiv:1510.08888 [cond-mat.mes-hall].

**9:00AM A45.00004 Gate-defined quantum dot devices in undoped Si/SiGe heterostructures for spin qubit applications<sup>1</sup>**, CHRISTIAN VOLK, FREDERICO MARTINS, CHARLES M. MARCUS, FERDINAND KUEMMETH, Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen, Denmark — Spin qubits based on few electron quantum dots in semiconductor heterostructures are among the most promising systems for realizing quantum computation. Due to its low concentration of nuclear-spin-carrying isotopes, silicon is of special interest as a host material. We characterize gate-defined double and triple quantum dot devices fabricated from undoped Si/Si<sub>0.7</sub>Ge<sub>0.3</sub> heterostructures. Our device architecture is based on integrating all accumulation and depletion mode gates in a single gate layer. This allows us to omit the commonly used global accumulation gate in order to achieve a more local control of the potential landscape in the device. We present our recent progress towards implementing spin qubits in these structures.

<sup>1</sup>Support through the EC FP7- ICT project SiSPIN no. 323841, and the Danish National Research Foundation is acknowledged.

**9:12AM A45.00005 Observation of multiple exchange oscillation frequencies in Si/SiGe spin qubits**, MATTHEW RAKHER, HRL Laboratories, LLC — An all-electrical approach to quantum information processing with spin qubits in Si/SiGe quantum wells relies on the ability to quickly turn on and off the exchange interaction between electrons in neighboring quantum dots [1]. The quality of gates enabled by this technique depends critically on reliably achieving a specific value of exchange coupling for a given control voltage. In recent experiments [2], we have observed multiple exchange oscillation frequencies at the same control bias for several different devices. In particular, Fourier transforms of exchange oscillations measured as a function of evolution time reveal the presence of multiple frequencies over a wide range of pulse amplitudes. The data are suggestive of unwanted population of an excited singlet-triplet manifold that behaves similarly with bias as the qubit ground state pair. The occupation of excited singlet-triplet states can degrade gate performance in exchange-based quantum devices and we outline methods to observe and investigate these states. [1] K. Eng et al, Science Advances 1 (2015) [2] M.D. Reed et al, arxiv:1508.01223 (2015)

**9:24AM A45.00006 Predicting the valley physics of silicon quantum dots directly from a device layout<sup>1</sup>**, JOHN KING GAMBLE, Sandia National Laboratories, PATRICK HARVEY-COLLARD, Sandia National Laboratories and Université de Sherbrooke, N. TOBIAS JACOBSON, ANDREW D. BACEWSKI, ERIK NIELSEN, INÉS MONTAÑO, MARTIN RUDOLPH, MALCOLM S. CARROLL, RICHARD P. MULLER, Sandia National Laboratories — Qubits made from electrostatically-defined quantum dots in Si-based systems are excellent candidates for quantum information processing applications. However, the multi-valley structure of silicon's band structure provides additional challenges for the few-electron physics critical to qubit manipulation. Here, we present a theory for valley physics that is predictive, in that we take as input the real physical device geometry and experimental voltage operation schedule, and with minimal approximation compute the resulting valley physics. We present both effective mass theory and atomistic tight-binding calculations for two distinct metal-oxide-semiconductor (MOS) quantum dot systems, directly comparing them to experimental measurements of the valley splitting. We conclude by assessing these detailed simulations utility for engineering desired valley physics in future devices. Sandia is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the US Department of Energy's National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

<sup>1</sup>The authors gratefully acknowledge support from the Sandia National Laboratories Truman Fellowship Program, which is funded by the Laboratory Directed Research and Development (LDRD) Program.

### 9:36AM A45.00007 Gate fidelity and coherence time of an electron spin in a Si/SiGe quantum dot

, ERIKA KAWAKAMI, THIBAUT JULLIEN, PASQUALE SCARLINO, Delft Univ of Tech, D. R. WARD, D. E. SAVAGE, M. G. LAGALLY, University of Wisconsin-Madison, V. V. DOBROVITSKI, Ames Laboratory, MARK FRIESEN, S. N. COPPERSMITH, M. A. ERIKSSON, University of Wisconsin-Madison, L. M. K. VANDERSYPEN, Delft Univ of Tech — Electron spins in Si/SiGe quantum dots are one of the most promising candidates for a quantum bit for their potential scalability and long dephasing time. We realized coherent control of an individual electron spin in a single quantum dot (QD), lithographically defined in a Si/SiGe 2D electron gas. Spin rotations are achieved by applying microwave excitation to one of the gates, which oscillates the electron wave function back and forth in the gradient field produced by cobalt micromagnets fabricated near the dot. Thanks to the long intrinsic dephasing time  $T_2^* = 900$  ns and Rabi frequency of 1.4 MHz, we were able to obtain an average single qubit gate fidelity of an electron spin in a Si/SiGe quantum dot of 99 %, measured via randomized benchmarking. The dephasing time is extended to 70  $\mu$ s using Hahn echo, and up to 400  $\mu$ s with multipulse dynamical decoupling (128  $\pi$  pulses). We extract the noise spectrum in the range of 5 kHz -1 MHz using dynamical decoupling and show that the gate fidelity is well explained by this noise characteristic. We discuss the mechanism that induces this noise and is responsible for decoherence.

### 9:48AM A45.00008 Epitaxial deposition of highly enriched $^{28}\text{Si}$ films with <1 nm roughness

, K. J. DWYER, HYUN-SOO KIM, A. N. RAMANAYAKA, D. S. SIMONS, VLADIMIR OLESHKO, J. M. POMEROY, National Institute of Standards and Technology — Low temperature epitaxial deposition of thin films with less than 1 nm rms roughness is achieved using a  $^{28}\text{Si}$  ion beam deposition source. These films are enriched *in situ* to <140 ppb  $^{29}\text{Si}$  isotope fraction for quantum computing devices. Removal of the 4.7 %  $^{29}\text{Si}$  nuclear spins in natural silicon allows for exceedingly long coherence ( $T_2$ ) times of qubits, making incorporation of highly enriched  $^{28}\text{Si}$  into devices critical for solid state quantum information. Low roughness epitaxial  $^{28}\text{Si}$  thin films are achieved by depositing in an island growth mode at temperatures of 300 C to 400 C, and the morphology is verified using scanning tunneling microscopy. Further, the crystalline quality of the films is shown using cross-sectional transmission electron microscopy. Finally, the chemical purity and broader electrical properties of the  $^{28}\text{Si}$  films are assessed by secondary ion mass spectroscopy as well as capacitance-voltage profiling, schottky diode measurements, and hall measurements.

### 10:00AM A45.00009 First measurements of charge carrier density and mobility of in-situ enriched $^{28}\text{Si}$ .

, A. N. RAMANAYAKA, Joint Quantum Institute, National Institute of Standards and Technology, K. J. DWYER, HYUN-SOO KIM, University of Maryland, M. D. STEWART, JR., J. M. POMEROY, National Institute of Standards and Technology — Magnetotransport in top gated Hall bar devices is investigated to characterize the electrical properties of in-situ enriched  $^{28}\text{Si}$ . Isotopically enriched  $^{28}\text{Si}$  is an ideal candidate for quantum information processing devices as the elimination of unpaired nuclear spins improves the fidelity of the quantum information. Using mass filtered ion beam deposition we, in-situ, enrich and deposit epitaxial  $^{28}\text{Si}$ , achieving several orders of magnitude better enrichment compared to other techniques. In order to explore the electrical properties and optimize the growth conditions of in-situ enriched  $^{28}\text{Si}$  we perform magnetotransport measurements on top gated Hall bar devices at temperatures ranging from 300 K to cryogenic temperatures and at moderate magnetic fields. Here, we report on the charge carrier density and mobility extracted from such experiments, and will be compared among different growth conditions of in-situ enriched  $^{28}\text{Si}$ .

### 10:12AM A45.00010 Thermal oxidation of Si/SiGe heterostructures for use in quantum dot qubits

, SAMUEL F. NEYENS, RYAN H. FOOTE, T. J. KNAPP, THOMAS MCJUNKIN, D. E. SAVAGE, M. G. LAGALLY, S. N. COPPERSMITH, M. A. ERIKSSON, Wisconsin Institute for Quantum Information, University of Wisconsin-Madison — Here we demonstrate dry thermal oxidation of a Si/SiGe heterostructure at 700°C and use a Hall bar device to measure the mobility after oxidation to be  $43,000 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$  at a carrier density of  $4.1 \times 10^{11} \text{ cm}^{-2}$ . Surprisingly, we find no significant reduction in mobility compared with an  $\text{Al}_2\text{O}_3$  device made with atomic layer deposition on the same heterostructure, indicating thermal oxidation can be used to process Si/SiGe quantum dot devices. This result provides a path for investigating improvements to the gate oxide in Si/SiGe qubit devices, whose performance is believed to be limited by charge noise in the oxide layer. This work was supported in part by ARO (W911NF-12-0607) and NSF (DMR-1206915 and PHY-1104660). Development and maintenance of the growth facilities used for fabricating samples is supported by DOE (DE-FG02-03ER46028). This research utilized NSF-supported shared facilities at the University of Wisconsin-Madison.

### 10:24AM A45.00011 Electrode-induced In-plane Strain Variation in Si Quantum Well

, JOONKYU PARK, YOUNGJUN AHN, DONALD SAVAGE, University of Wisconsin Madison, JONATHAN PRANCE, Lancaster University, CHRISTINE SIMMONS, MAX LAGALLY, SUSAN COPPERSMITH, University of Wisconsin Madison, MARTIN HOLT, Argonne National Laboratory, MARK ERIKSSON, PAUL EVANS, University of Wisconsin Madison — Silicon quantum devices are often formed in electrostatically defined quantum dots within Si/SiGe heterostructures incorporating a strained silicon quantum well. Structural variations within the quantum well arise from several sources, including the plastic relaxation of the SiGe substrate and stresses arising from electrodes. The residual stress in the electrode causes an elastic bending distortion of the quantum well that modifies the energy by which the two split-off conduction minima in the silicon quantum well are shifted by biaxial strain. We report a synchrotron hard x-ray nanobeam diffraction study of the quantum well distortion (i) near isolated Pd electrodes and (ii) within a complex quantum dot pattern. The strain difference between the two interfaces of the 10-nm-thick silicon quantum well has a magnitude of up to  $10^{-5}$  in (i) while it is as large as  $10^{-4}$  in (ii) which is far larger than the strain difference arising from the plastic relaxation of the SiGe substrate. Mechanical analysis using the edge-force model, shows that the residual stress in the Pd electrode was 350 MPa. We expect that similar effects will arise in all quantum electronic systems with metal-electrode-defined devices.

### 10:36AM A45.00012 Are quantum dots in unexpected locations due to strain?

, NEIL ZIMMERMAN, NIST, TED THORBECK, University of Wisconsin-Madison — It is a fairly common occurrence that, in top-gated Si quantum dots, the dots appear in reproducible but unexpected positions. For instance, sometimes a group will make gates in order to electrostatically generate tunnel barriers, but discover that the quantum dot is formed underneath the gate rather than between two barrier gates. We will discuss the possibility that such quantum dots arise from the mechanical strain induced by the gate. The model is simple: i) We simulate metal or polysilicon gates on top of a Si/SiO $_2$  wafer, and calculate the stress and strain from differential thermal contraction of the materials; ii) Using the fact that the energy of the Si conduction band depends on strain through the deformation potential, we then convert the strain modulation to a potential energy modulation. As an example, we find that, for a single Al gate, there is a potential well directly underneath the gate with the size of a few meV, in agreement with recent experimental results. We also show that polysilicon gates will not produce such strain-induced quantum dots.

### 10:48AM A45.00013 Atomic scale quantum circuits in Si

, A. DUSKO, IF, UFRJ, Brazil / DP, uOttawa, Canada, M. KORKUSINSKI, IMS, NRC, Canada, A. SARAIVA, IF, UFRJ, Brazil, A. DELGADO, DP, uOttawa, Canada, B. KOILLER, IF, UFRJ, Brazil, P. HAWRYLAK, DP, uOttawa, Canada — The atomic scale circuits in Si are now realized by manipulation of dangling bonds on Si surface or incorporating dopant atoms in Si by STM techniques. We describe the electronic properties of these atomic scale quantum dot circuits (QDC) by the extended Hubbard-Kanamori Hamiltonian (HK), including on site Coulomb repulsion ( $U$ ) and interdot hopping ( $t$ ), direct interaction ( $V$ ) and exchange ( $J$ ) terms. The interdot terms strongly depend on dopant position ( $R_D$ ) in Si lattice—small changes in  $R_D$  strongly impact  $t$ ,  $V$  and  $J$ . We study how disorder in  $R_D$  impacts QDC electronic properties, in particular the interplay of disorder and interactions. With no disorder in  $R_D$  the energy spectrum (ES) of quantum dot chain at half-filling as a function of  $U/t$  ( $V, J = 0$ ) shows a transition from ES dominated by kinetic energy ( $U/t \ll 1$ ) to ES dominated by Coulomb interactions for  $U/t \gg 1$ . The excited states group by single particle energy spacing (Hubbard bands) for weak (strong) interactions. In the weak interaction regime, disorder leads to localization, which strongly affects the electronic properties. We explore the effect of interactions and disorder on HK atomic scale circuits and potential many-body localized phases using Lanczos and Density Matrix Renormalization Group approaches.

**Monday, March 14, 2016 8:00AM - 11:00AM —**

**Session A46 GIMS: Advances in Scanning Probe Microscopy I: Novel Approaches and Ultra-sensitive Detection** 311 - Hongwoo Baek, National Magnet Laboratory

**8:00AM A46.00001 AFM cantilever vibration detection with a transmitted electron beam**, TAYLOR WOEHL, RYAN WAGNER, ROBERT KELLER, JASON KILLGORE, Material Measurement Laboratory, National Institute of Standards and Technology — Cantilever oscillations for dynamic atomic force microscopy (AFM) are conventionally measured with an optical lever system. The speed of AFM cantilevers can be increased by decreasing the size of the cantilever; however, the fastest AFM cantilevers are currently nearing the smallest size that can be detected with the current optical lever approach. Here we demonstrate an electron detection scheme in an SEM for detecting AFM cantilever oscillations. An oscillating AFM tip is positioned perpendicular to the propagation direction of a stationary  $\approx 1$  nm diameter electron probe, and the oscillatory change in electron scattering resulting from the changing thickness of the electron irradiated area of the AFM tip is detected with a transmitted electron detector positioned below the AFM tip. We perform frequency sweep and ring-down experiments to determine the first resonant frequency and Q factor of an AFM cantilever.

**8:12AM A46.00002 Innovative SPM Probes for Energy-Storage Science: MWCNT-Nanopipettes to Nanobattery Probes<sup>1</sup>**, JONATHAN LARSON, Dept. of Physics, Univ of Maryland-College Park, ALEC TALIN, Dept. of Mat Physics, Sandia National Labs-Livermore, ALEXANDER PEARSE, Dept. of Mat Sci Eng, Univ of Maryland-College Park, ALEXANDER KOZEN, Dept of Mat Sci Eng, Univ of Maryland-College Park, JANICE REUTT-ROBEY, Dept. of Chem and Biochem, Univ of Maryland-College Park — As energy-storage materials and designs continue to advance, new tools are needed to direct and explore ion insertion/de-insertion at well-defined battery materials interfaces. Scanned probe tips, assembled from actual energy-storage materials, permit SPM measures of local cathode-anode (tip-sample) interactions, including ion transfer. We present examples of “cathode” MWCNT-terminated STM probe tips interacting with Li(s)/Si(111) anode substrates. The MWCNT tip functions as both SPM probe and Li-nanopipette,<sup>[1]</sup> for controlled transport and manipulation of Li. Local field conditions for lithium ionization and transfer are determined and compared to electrostatic models. Additional lithium metallic and oxide tips have been prepared by thin film deposition on conventional W tips, the latter of which effectively functions as a nanobattery. We demonstrate use of these novel probe materials in the local lithiation of low-index Si anode interfaces, probing local barriers for lithium insertion. Prospects and limitations of these novel SPM probes will be discussed. [1] J.M. Larson et al, Small, 2015, DOI: 10.1002/sml.201500999

<sup>1</sup>U.S. Department of Energy Award Number DESC0001160

**8:24AM A46.00003 Carbon nanotube/carbon nanotube composite AFM probes prepared using ion flux molding<sup>1</sup>**, GRACE CHESMORE, Santa Clara University, CARROLLYN ROQUE, Carbon Design Innovations, RICHARD BARBER, Santa Clara University — The performance of carbon nanotube-carbon nanotube composite (CNT/CNT composite) atomic force microscopy (AFM) probes is compared to that of conventional Si probes in AFM tapping mode. The ion flux molding (IFM) process, aiming an ion beam at the CNT probe, aligns the tip to a desired angle. The result is a relatively rigid tip that is oriented to offset the cantilever angle. Scans using these probes reveal an improvement in image accuracy over conventional tips, while allowing higher aspect ratio imaging of 3D surface features. Furthermore, the lifetimes of CNT-CNT composite tips are observed to be longer than both conventional tips and those claimed for other CNT technologies. Novel applications include the imaging of embiid silk.

<sup>1</sup>Supported by the Clare Boothe Luce Research Scholars Award and Carbon Design Innovations

**8:36AM A46.00004 Nanometer-scale scanning magnetometry of spin structures and excitations using Nitrogen-vacancy centers**, YULIYA DOVZHENKO, Department of Physics, Harvard University — The development of increasingly sensitive scanning techniques has led to new insights into the physics of interacting condensed matter systems. Recently, Nitrogen-Vacancy (NV) centers in diamond emerged as a promising scanning magnetic imaging platform capable of operating in a broad range of temperatures and magnetic fields, with sensitivity and resolution capable of imaging a single electron spin with sub-nanometer resolution under ambient conditions [1,2]. In this talk we will review some of the recent developments in this new scanning platform. We will describe our recent progress in using a single NV center in a scanning diamond nano-pillar to study condensed matter magnetism at both room and low temperatures. In particular, we demonstrate the use of scanning NV magnetometry to image stray fields originating from static chiral spin structures, as well as to detect resonant and off-resonant low-energy spin excitations [3]. [1] Grinolds et al., Nature Phys 9, 215 (2013) [2] Grinolds et al., Nature Nanotech. 9, 279 (2014) [3] Van der Sar et al., Nature Comm. 6, 7886 (2015)

**9:12AM A46.00005 Nanoscale imaging of paramagnetic spin labels using a single spin in diamond.**, AMILA ARIYARATNE, BRYAN MYERS, MATTHEW PELLICIONE, ANIA JAYICH, University of California Santa Barbara — Spin-labeling molecules with paramagnetic species is a powerful technique for probing molecular structure. However, current techniques are ensemble measurements, inherently lacking the sensitivity to detect a single spin or the conformational properties of a single biomolecule. In this talk, we demonstrate an imaging technique that has the promise of single-spin imaging and ultimately molecular structure imaging. We present two-dimensional nanoscale imaging of a monolayer of gadolinium (Gd) atomic spin labels at ambient conditions. The sensing element is a single nitrogen-vacancy (NV) center in diamond. A patterned monolayer of Gd atoms self-assembled on a Si atomic force microscopy tip is controllably interacted with and detected by the NV center. The fluctuating magnetic field generated by GHz-scale Gd spin flips relaxes the NV center in a manner that depends strongly on the Gd-NV separation. Using this technique, we demonstrate a Gd-induced reduction of the T1 relaxation time of the NV center with nm spatial resolution. Our results indicate that nanometer-scale imaging of individual electronic spins at ambient conditions is within reach. This will ultimately enable the study of structural and functional studies of single biomolecules in their native, folded state.

**9:24AM A46.00006 ABSTRACT WITHDRAWN —**

**9:36AM A46.00007 How to simultaneously scan connected tips in a dual-tip STM**, WAN-TING LIAO, Univ of Maryland-College Park, MICHAEL DREYER, Laboratory for Physical Sciences, JAMES ANDERSON, CHRISTOPHER LOBB, FREDERICK WELLSTOOD, Univ of Maryland-College Park — Starting with a dual independent-tip scanning tunneling microscope (STM) design [1], we have connected the two tips by a short ( $\sim 3$  mm) flexible Nb foil strip that was patterned by a laser. To enable simultaneous imaging with both tips, we move both tips to within tunneling distance of a surface and modulate one tip's z-piezo at  $\sim 5$  kHz and the other at  $\sim 10$  kHz. The resulting combined tunneling current from the system has modulation at both frequencies, which we detect using two lock-in amplifiers. The two outputs ( $dI/dz_1$  and  $dI/dz_2$ ) are feedback to individual STM electronic controllers to allow simultaneous topographic imaging using both tips. We tested our setup at room temperature using Pt-Ir tips on Au/Mica and HOPG samples. The next step is to operate this dual-tip STM at 30 mK on a superconducting sample so that the device forms a novel type of scanning SQUID. Holding one of the tips fixed as a reference junction, the other tip will be scanned to image the gauge-invariant phase difference of a superconductor at the atomic scale [2]. [1] A. Roychowdhury, et al., Rev. Sci. Inst. 85, 04.706(2014) [2] D. F. Sullivan, et al., J. Appl. Phys. 113, 183905 (2013)

**9:48AM A46.00008 High-resolution imaging of interfacial water by noncontact atomic force microscopy**<sup>1</sup>, JINBO PENG, Peking University, JING GUO, School of Physics, Peking University, PROKOP HAPALA, Institute of Physics, Academy of Sciences of the Czech Republic, DUANYUN CAO, School of Physics, Peking University, PAVEL JELNEK, Institute of Physics, Academy of Sciences of the Czech Republic, LIMEI XU, ENGE WANG, YING JIANG, School of Physics, Peking University, COLLABORATIVE INNOVATION CENTER OF QUANTUM MATTER COLLABORATION — Resolving the hydrogen-bonding configuration of water on the solid surfaces with atomic-scale precision is crucial in water science yet it remains challenging. Recently we have shown the possibility of attacking this problem by STM based on the submolecular orbital imaging of water. However, STM mainly probes the spatial distribution of the density of states near the Fermi level, thus is not sensitive to the chemical structure of molecules. Here we report the ultrahigh resolution imaging of water molecules on a NaCl film by NC-AFM, which enables us to determine the topology of hydrogen-bonding network in unprecedented details. Comparison with the theoretical simulations reveals that the sharp features in the AFM images result from the relaxation of the tip apex mainly due to the electrostatic force between the tip and the water molecules. Our results shed new light on the underlying mechanism of the ultrahigh imaging with NC-AFM and highlight the importance of electrostatics in the imaging of polar molecules such as water.

<sup>1</sup>This work was supported by the National Basic Research Programs of China.

**10:00AM A46.00009 Tip relaxation in atomic force microscopy imaging simulations to resolve intermolecular bonds**<sup>1</sup>, ALEX LEE, YUKI SAKAI, JIM CHELIKOWSKY, The University of Texas at Austin — Experimental noncontact atomic force microscopy (AFM) studies have reported distinct lines in regions with no electron density for a variety of systems. The appearance of these lines is unexpected because Pauli repulsion is thought to be the dominant factor in the AFM imaging mechanism. These lines have been proposed to represent intermolecular bonding. Recent theoretical studies have shown that accounting for tip probe relaxation can sharpen images and highlight features that make simulations more comparable to experiment. We will apply a similar tip relaxation scheme to our computational method—which uses an *ab initio* real-space pseudopotential formalism with frozen density embedding theory added—to the study of dibenzo[a,h]thianthrene and an 8-hydroxyquinoline dimer to develop our interpretation of imaged intermolecular bonds.

<sup>1</sup>Work is supported by the DOE under DOE/DE-FG02-06ER46286 and by the Welch Foundation under grant F-1837. Computational resources were provided by NERSC and XSEDE.

**10:12AM A46.00010 First-principles AFM image simulation with frozen density embedding theory**<sup>1</sup>, YUKI SAKAI, ALEX J. LEE, JAMES R. CHELIKOWSKY, Univ of Texas, Austin — We present efficient first-principles method of non-contact atomic force microscopy (nc-AFM). Ordinary nc-AFM simulations based on density functional theory (DFT) require exhaustive computational cost because it involves thousands of total energy calculations. Regarding the sample as a fixed external potential can reduce the computational cost, and we adopt frozen density embedding theory (FDET) for this purpose. Simulated nc-AFM images with FDET using a carbon monoxide tip well reproduces the full DFT images of benzene, pentacene, and graphene, although optimized tip-sample distances and interaction energies in FDET are underestimated and overestimated, respectively. The FDET-based simulation method is promising for AFM image simulation of surfaces and two-dimensional materials.

<sup>1</sup>This work was supported by U.S. DOE under grant No. DE-FG02-06ER46286 and award No. DE-SC0008877, and by Welch Foundation under Grant F-1837. Computational resources are provided by NERSC and TACC.

**10:24AM A46.00011 Isotope-Resolved and Charge-Sensitive Force Imaging Using Scanned Single Molecules**, YAN SUN, DOMINIK RASTAWICKI, YANG LIU, WARREN MAR, HARI MANOHARAN, Stanford University, ANNA MIGLIO, SORIN MELINTE, JEAN-CHRISTOPHE CHARLIER, GIAN-MARCO RIGNANESI, Université catholique de Louvain, LIANHUA HE, FANG LIU, AIHUI ZHOU, Chinese Academy of Sciences — Originally conceived as surface imaging instruments, the scanning tunnelling microscope (STM) and the atomic force microscope (AFM) were recently used to probe molecular chemical bonds with exquisite sensitivity. Remarkably, molecule-functionalized scanning tips can also provide direct access to the inelastic electron tunneling spectrum (IETS) of the terminal molecule. Here we report atomic manipulation experiments addressing carbon monoxide (CO) isotopes at low temperatures. The unique and quantifiable dependence of the CO vibrational modes offers insight into tip-controlled force and charge sensing of surface adsorbates, subsurface defects, and quantum nanostructures. The specific behavior of the monitored vibrational modes originates from the interplay of interaction forces between the top electrode—a scanned tip functionalized with a single molecule—and the atomic scale force field surrounding the target atomically-assembled nanostructure. We also present density functional theory (DFT) computations that have been performed in order to scrutinize and visualize the vibrational spectroscopic fingerprints and local force fields.

**10:36AM A46.00012 A cryogen-free variable temperature scanning tunneling microscope capable for inelastic electron tunneling spectroscopy**, SHUAI ZHANG, DI HUANG, SHIWEI WU, Fudan University — While low temperature scanning tunneling microscope (STM) has become an indispensable research tool in surface science, its versatility is yet limited by the shortage or high cost of liquid helium. The makeshifts include the use of alternative cryogen (such as liquid nitrogen) at higher temperature or the development of helium liquefier system usually at departmental or campus wide. The ultimate solution would be the direct integration of a cryogen-free cryocooler based on GM or pulse tube closed cycle in the STM itself. However, the nasty mechanical vibration at low frequency intrinsic to cryocoolers has set the biggest obstacle because of the known challenges in vibration isolation required to high performance of STM. In this talk, we will present the design and performance of our home-built cryogen-free variable temperature STM at Fudan University. This system can obtain atomically sharp STM images and high resolution dI/dV spectra comparable to state-of-the-art low temperature STMs, but with no limitation on running hours. Moreover, we demonstrated the inelastic tunneling spectroscopy (STM-IETS) on a single CO molecule with a cryogen-free STM for the first time.

**10:48AM A46.00013 Cryogen free scanning probe microscope: the solution for atomic scale surface science below 10 Kelvin without liquid helium**, BYOUNG CHOI, MIGUEL VENEGAS, RHK Technology Inc., RHK TEAM — We present a cryogen free low temperature scanning probe microscope (LT-SPM) working at 9K on both tip and sample. The performance of the microscope was validated in various conditions such as noisy environment and modulated temperature as well as the long time elapsed measurements. Building on the stability and consistency of the closed cycle refrigerator, time extended measurements are available with this state-of-the-art LT-SPM. Studies can now be performed without interrupting the critical moment of the tip on the surface while refilling the conventional liquid cryogen tank. We will present the time evolution of the dopant induced topographic and spectroscopic properties of some topological insulators such as Bi<sub>2</sub>Se<sub>3</sub> and Bi<sub>2</sub>Te<sub>3</sub>. The compact and rigid design of the microscope also allows this instrument to work as a practical variable temperature microscope without the hassle of liquid cryogen consumption. We will present temperature dependent STM/STS results on a TiSe<sub>2</sub> surface at the temperature between 10K and 350K. Finally, we will discuss how the cryogen free LT-SPM will make the study of the atomic scale phenomenon at low temperature both economical and easy, opening promising new capabilities to surface scientists and researchers in nanotechnology.

**Monday, March 14, 2016 8:00AM - 11:00AM –**

**Session A47 DCMP: Surface and Thin Film Phase Transitions and Electronic Properties 312 -**

Daniel Dougherty, North Carolina State University

**8:00AM A47.00001 High  $T_{\text{IMT}}$  insulator-to-metal transition of the  $\text{VO}_2$  films on AlN/Si substrate.** , TETIANA SLUSAR, JIN-CHEOL CHO, BONG-JUN KIM, HYUN-TAK KIM, MIT Center in ETRI — Electrical and structural properties of the  $\text{VO}_2$  thin films are strongly affected by growth conditions and underlying substrate providing a flexibility of their functional parameters. We present a new  $\text{VO}_2/\text{AlN}/\text{Si}$  heterostructure, where  $\text{VO}_2$  is characterized by an excellent insulator-to-metal transition (IMT) occurred at a higher temperature  $T_{\text{IMT}}$  than that typical for single crystals. Mentioned characteristics are associated with growth mechanism of the film and its epitaxial alignment with respect to the substrate. In particular, the  $T_{\text{IMT}}$  upshift in  $\text{VO}_2/\text{AlN}/\text{Si}$  is explained by a stable crystallographic configuration in the plane of the  $\text{VO}_2$  film as well as a tensile deformation of a monoclinic  $a$ -axis formed by tilted and dimerized  $\text{V}^{4+}\text{-V}^{4+}$ , responsible for strong electron correlations. Moreover, proposed synergy of  $\text{VO}_2$  and Si is able to make new results for advanced materials fabrication and development of switching devices of new generation.

**8:12AM A47.00002 Ultrafast dynamics of  $\text{VO}_2$  thin films measured in pump-probe configuration**<sup>1</sup>, ELIZABETH RADUE, William and Mary College, SALINPORN KITTIWATANAKUL, JIWEI LU, S. A. WOLF, University of Virginia, ZHENGPING FU, MASASHI YAMAGUCHI, RPI, ENRICO ROSSI, R. A. LUKASZEW, IRINA NOVIKOVA, William and Mary College — The semiconductor-metal transition of  $\text{VO}_2$  continues to be a vigorously studied phenomenon due to complicated interplay between the structural change and the electronic bands. It is also potentially a very useful material, particularly because of its ultrafast transition to the metallic state excited with a femtosecond pulse. We have been exploring the effects of polarization of the pump in relation to the probe affects the sub-picosecond response of  $\text{VO}_2$  thin films, which will be important in designing ultrafast switches. We have also been looking at pumping our  $\text{VO}_2$  films with a THz source that directly pumps the lattice, and have found the film responds optically on a slower scale than when pumped with 800 nm, suggesting that there is an electronic response from disturbing the lattice.

<sup>1</sup>This project was sponsored by the NSF, DMR-1006013: Plasmon Resonances and Metal Insulator Transitions in Highly Correlated Thin Film Systems, and the NASA Virginia Space Grant Consortium. We also acknowledge support from the NRI/SRC sponsored ViNC center

**8:24AM A47.00003 Investigation of the Effect of Crystal Thickness on Free-Standing Vanadium Dioxide Nanocrystals**<sup>1</sup>, SERKAN KASIRGA, MUSTAFA FADLELMULA, Bilkent University- UNAM — The first-order metal-insulator transition (MIT) that vanadium dioxide exhibits at 65 °C has been extensively studied in the last decade thanks to the growth of single crystal nanobeams/plates smaller than characteristic domain size as well as the advances in epitaxial film growth techniques. The effect of crystal thickness has been studied extensively in epitaxially grown  $\text{VO}_2$  films yet not in free-standing nanocrystals[1]. This is mainly due to lack of control over the crystal thickness in physical vapor transport growth of the nanocrystals. Here, we report first observations on the MIT of  $\text{VO}_2$  nanocrystals grown on oxidized silicon substrate thinned using argon-ions. Among these observations AFM measurements reveal an etch rate of 4 nm/min for 1keV Ar-ion energy. Two terminal suspended nanobeam measurements reveal an intriguing phase transition properties below a threshold thickness. [1]Aetukuri, N.B. et al. Nature Phys. 9, 661-666 (2013).

<sup>1</sup>This work was supported by TUBITAK (project no. 114F273)

**8:36AM A47.00004 Cryogenic optical nano-imaging of phase coexistence in correlated oxides**, A. S. MCLEOD, University of California San Diego, E. VAN HEUMEN, University of Amsterdam, J. ZHANG, J. G. RAMIREZ, University of California San Diego, Z. HUANG, University of Science and Technology of China, Hefei, S. WANG, T. SAERBECK, S. GUENON, M. GOLDFLAM, L. ANDEREGG, P. KELLY, A. MUELLER, University of California San Diego, M. K. LIU, Stony Brook University, W. B. WU, University of Science and Technology of China, Hefei, R. D. AVERT, I. K. SCHULLER, D. N. BASOV, University of California San Diego — Correlated transition metal oxides exhibit a bevy of textbook electronic phases characterized by richly interacting lattice, spin, and orbital degrees of freedom. A broad array of accessible thermodynamic phases, ranging from Mott insulator to superconductor, enables abrupt transitions in physical and electronic properties under modest external stimuli, accompanied by spontaneous phase coexistence at the nano-scale. We present a novel near-field optical scanning probe capable of resolving the electronic character of such “switched” phases in the coexistent regime, even insulators, at 10 nm resolution and down to liquid helium temperatures. We demonstrate variable-temperature optical, structural, and magnetic imaging functionalities through studies of the insulator-metal transition in two prototypic correlated oxides under epitaxial strain. Structural and electronic attributes of the Mott transition are distinguished in a  $\text{V}_2\text{O}_3$  thin film, whereas metastable electronic and magnetic phase coexistence is revealed across a 200K range in the strained manganite  $\text{La}_{0.67}\text{Ca}_{0.33}\text{MnO}_3$

**8:48AM A47.00005 Collapse of the low temperature insulating state in Cr-doped  $\text{V}_2\text{O}_3$  thin films**, PIA HOMM, LEANDER DILLEMANS, MARIELA MENGHINI, BART VAN BILZEN, PETAR BAKALOV, CHEN-YI SU, RUBEN LIETEN, MICHEL HOUSSA, JIN WON SEO, JEAN-PIERRE LOCQUET, KU Leuven, DAVOUD NASR ESFAHANI, LUCIAN COVANI, FRANCOIS PEETERS, University of Antwerp — We have grown epitaxial Cr-doped  $\text{V}_2\text{O}_3$  thin films with Cr concentrations between 0 and 20% on (0001)- $\text{Al}_2\text{O}_3$  by oxygen-assisted molecular beam epitaxy. For the highly doped samples (> 3%), a regular and monotonous increase of the resistance with decreasing temperature is measured. Strikingly, in the low doping samples (between 1% and 3%), a collapse of the insulating state is observed with a reduction of the low temperature resistivity by up to 5 orders of magnitude. A vacuum annealing at high temperature of the films recovers the low temperature insulating state for doping levels below 3% and increases the room temperature resistivity towards the values of Cr-doped  $\text{V}_2\text{O}_3$  single crystals. It is well known that oxygen excess stabilizes a metallic state in  $\text{V}_2\text{O}_3$  single crystals. Hence, we propose that Cr doping promotes oxygen excess in our films during deposition, leading to the collapse of the low temperature insulating state at low Cr concentrations. These results suggest that slightly Cr-doped  $\text{V}_2\text{O}_3$  films can be interesting candidates for field effect devices.

**9:00AM A47.00006 Modified Young's equation for equilibrium dihedral angles of grain boundary grooves in thin films at the nanoscale**, MING-WEI LIU, SHANG-CHUN LIN, Department of Physics, National Tsing Hua University, Hsinchu, Taiwan, MOGADALAI GURURAJAN, Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology-Bombay, Powai Mumbai, India, KUO-AN WU, Department of Physics, National Tsing Hua University, Hsinchu, Taiwan — We derive the modified Youngs equation for the equilibrium dihedral angle at the triple junction of the grain boundary groove by taking into account the discrete structure of the low angle grain boundary. For low angle grain boundaries, the geometric relation that the misorientation of the bicrystal is inversely proportional to the dislocation spacing naturally gives rise to the variation in the misorientation when the grain boundary length changes (holding the number of dislocations constant). The fact that the grain boundary energy increases as the grain boundary length decreases due to a smaller dislocation spacing leads to a larger dihedral angle compared to that of the classical theory. Two atomistic continuum modelling tools, namely the phase field crystal model and the amplitude equations, are used to simulate the equilibrium dihedral angle. The numerical results are in quantitatively good agreement with the derived modified Youngs equation.

**9:12AM A47.00007 First measurements of bulk and shear mechanical loss in optical thin film materials**, MATTHEW ABERNATHY, Naval Research Lab, GREGORY HARRY, JONATHAN NEWPORT, HANNA FAIR, SAM HICKEY, American University, ANDRI GRETARSSON, Embry-Riddle Aeronautical University, STEVE PENN, Hobart and William Smith Colleges, LIGO COLLABORATION — As advanced gravitational wave detectors come online, and the possibility of the first gravitational wave detection nears, plans for the next generation of gravitational wave detectors are already in the works. These new detectors, and those already planned for the future, are expected to be limited in their most sensitive frequency bands by the Brownian thermal noise generated within the optical thin films used to produce the interferometer mirrors. In order to predict the level of this Brownian noise, it is necessary to know the two independent mechanical moduli (Young modulus and Poisson ratio, Bulk and Shear moduli, etc.) as well as their associated mechanical loss parameters. Traditional measurements of the mechanical loss of thin films has measured only one linear combination of these two loss parameters. Here, we present measurements of the bulk and shear mechanical loss of tantalum pentoxide (tantala) thin films made by taking advantage of the differing ratios of elastic deformation in the various resonant modes of a coated silica disc. These results may have immediate implications for the ultimate sensitivity of currently operated gravitational wave detectors.

**9:24AM A47.00008 Between Crystal and Glass: Thermal Transport in C60 Molecular Crystals<sup>1</sup>**, SIMON LU, SUSHANT KUMAR, ALAN MCGAUGHEY, Department of Mechanical Engineering, Carnegie Mellon University — Molecular crystals of the fullerene C60 and its derivatives [e.g., phenyl-C61-butyric acid methyl ester (PCBM)] are candidate materials for use in photovoltaics and thermoelectrics. In thermoelectrics, their usefulness is due in part to their exceptionally low thermal conductivities (0.4 W/m-K for C60 and 0.05 W/m-K for PCBM) at room temperature. Little is known regarding the microscopic physics underlying these low thermal conductivities. An important question is whether thermal transport in the C60 molecular crystal is (i) crystal-like, where energy is transported as collective vibrations of the centers of mass of the molecules, or (ii) amorphous-like, where energy diffuses from molecule to molecule. We use molecular dynamics (MD) simulations and the Green-Kubo method to probe this question by predicting the relative contributions of crystal-like and amorphous-like transport to the thermal conductivity of the C60 molecular crystal. To isolate crystal-like transport, we perform simulations on C60 crystals where molecular rotations and intra-molecular vibrations are prohibited. To isolate amorphous-like transport, we fix the centers of mass of the molecules. We compare the MD results to predictions from a fully diffusive network resistance model.

<sup>1</sup>This work is supported by the National Science Foundation (grant DMR-1507325).

**9:36AM A47.00009 C<sub>60</sub>-Induced Devil's Staircase Transformation on Pb/Si(111) Wetting Layer<sup>1</sup>**, LIN-LIN WANG, Ames Lab, DUANE D. JOHNSON, Ames Lab and Department of Materials Science and Engineering, Iowa State University, MICHAEL C. TRINGIDES, Ames Lab and Department of Physics, Iowa State University — Density functional theory is used to study structural energetics of Pb vacancy cluster formation on C<sub>60</sub>/Pb/Si(111) to explain the unusually fast and error-free transformations between the "Devil's Staircase" (DS) phases on the Pb/Si(111) wetting layer at low temperature (~110 K). The formation energies of vacancy clusters are calculated in C<sub>60</sub>/Pb/Si(111) as Pb atoms are progressively ejected from the initial dense Pb wetting layer. Vacancy clusters larger than 5 Pb atoms are found to be stable with 7 being the most stable, while vacancy clusters smaller than 5 are highly unstable, which agrees well with the observed ejection rate of ~5 Pb atoms per C<sub>60</sub>. The high energy cost (~0.8 eV) for the small vacancy clusters to form indicates convincingly that the unusually fast transformation observed experimentally between the DS phases, upon C<sub>60</sub> adsorption at low temperature, cannot be the result of single-atom random walk diffusion but correlated multi-atom processes.

<sup>1</sup>DOE Office of Science, Basic Energy Sciences from the Divisions of MSE (DE-AC02-07CH1135) and Ames Lab LDRD. Ames Laboratory is operated for DOE by Iowa State University under contract DE-AC02-07CH11358.

**9:48AM A47.00010 Competing length scales for the electronic structure of rings of C60**, JERRY TAN, University of Maryland, GARNETT BRYANT, National Institute of Standards and Technology — Recently, rings of C60 have been fabricated. This opens up the possibility of studying the electronic structure of complex nanosystems with competing length scales: here the length scale defined by individual C60 molecules, the length scale defined by moving along the inner edge of the ring of C60s, and the length scale for the outer edge. The effects of such competing length scales could be probed with a magnetic field B. We use a tight-binding model to study these effects theoretically. Noninteracting electrons are considered. B is included with a Peierls transformation. Calculated electronic spectrum for an isolated ring of carbons, here used as a simple model for C60, is compared with spectra for rings of carbon rings. Changes in spectra due to inter-ring hopping are identified. New structure in the density of states is correlated with the spatial distribution of states in rings of rings. A magnetic field is applied to access and couple different length scales. Calculated spectra for rings of full C60 molecules are compared with the model results to highlight the effects of competing length scales in C60 rings. Results are used to suggest possible experiments for rings of C60 molecules.

**10:00AM A47.00011 The Size and Shape dependence of the Surface Free Energy of Nanocrystals**, ESAM ABDUL-HAFIDH, Yanbu University College — Based on many recent reports, it became possible to control the synthesis of nanomaterials with certain sizes and shapes. A theoretical model to investigate the effect of size and shape on the surface free energy of nanocrystals is worked out in this research. The model is applied to a general shape and size nanocrystal designated by a shape factor. The model considers all nanocrystals with different morphologies (but with the same shape factor) to be the same. The results were tested for gold and silver. The surface free energy was found to decrease with size for spherical nanocrystals. On the other hand, the surface free energy is enhanced for non-spherical nanocrystals. These findings are in qualitative agreement with previous experimental and theoretical predictions. The results pave the road to manufacture controlled- mechanical properties materials.

**10:12AM A47.00012 Theory of Space Charge Limited Current in Fractional Dimensional Space**, MUHAMMAD ZUBAIR, L.K. ANG, Engineering Product Development, Singapore University of Technology and Design, East Coast Campus, 8 Somapah Road, Singapore 487372, Singapore — The concept of fractional dimensional space has been effectively applied in many areas of physics to describe the fractional effects on the physical systems. We will present some recent developments of space charge limited (SCL) current in free space and solid in the framework of fractional dimensional space which may account for the effect of imperfectness or roughness of the electrode surface. For SCL current in free space, the governing law is known as the Child-Langmuir (CL) law. Its analogy in a trap-free solid (or dielectric) is known as Mott-Gurney (MG) law. This work extends the one-dimensional CL Law and MG Law for the case of a *D*-dimensional fractional space with  $0 < D \leq 1$ ; where parameter *D* defines the degree of roughness of the electrode surface. Such a fractional dimensional space generalization of SCL current theory can be used to characterize the charge injection by the imperfectness or roughness of the surface in applications related to high current cathode (CL law), and organic electronics (MG law). In terms of operating regime, the model has included the quantum effects when the spacing between the electrodes is small.

**10:24AM A47.00013 Significantly enhanced giant Rashba splitting in a thin film of binary alloy.** , SHU-JUNG TANG, Department of Physics, National Tsing Hua University, WEI-CHUAN CHEN, National Synchrotron Radiation Research Center, Hsinchu, Taiwan, TAY-RONG CHANG, SUN-TING TSAI, JE-MING KUO, Department of Physics, National Tsing Hua University, SH. YAMAMOTO, Institute for Solid State Physics, the University of Tokyo, CHENG-MAW CHENG, KU-DING TSUEI, National Synchrotron Radiation Research Center, Hsinchu, Taiwan , KOICHIRO YAJI, Institute for Solid State Physics, the University of Tokyo, HSIN LIN, Graphene Research Centre and Department of Physics, National University of Singapore, HORNG-TAY JENG, CHUNG-YU MOU, Department of Physics, National Tsing Hua University, IWAO MATSUDA, Institute for Solid State Physics, the University of Tokyo — Dirac cones in a 2D environment have attracted much attention not only because of the massless Dirac fermions but also due to their capability to lock the spin direction with the momentum. Here we demonstrate that the Rashba effect within a single layer of a binary alloy composed of heavy atoms, Pb and Au, can be driven by and even tweaked with the adjacent top and bottom layers to yield cones-like structures and further enhance the Rashba coupling strength. Two cones are observed at the surface zone center  $\bar{\Gamma}$  with giant Rashba parameters 1.53 and 4.45 eV; an anisotropic giant Rashba splitting at the surface zone boundary  $\bar{M}$  has a great value, 6.26 eV, inferring the critical role of  $p$ - $d$  hybridization between Pb and Au. Our results reveal not only an interesting natural phenomenon but also a feasible method of tweaking the Rashba effect of a 2D system.

**10:36AM A47.00014 Photoemission from Shockley surface state on Ag(111)** , SIDDHARTH KARKARE, WEISHI WAN, JUN FENG, HOWARD PADMORE, Lawrence Berkeley National Lab — We present measurements of quantum yield and transverse momentum distributions of electrons emitted from the Shockley surface state on Ag(111) surface using near threshold photons. Our measurements shed light on the validity of the conservation of transverse momentum during photoemission when the kinetic energy of electrons is less than 0.1 eV. We also develop a one-step photoemission model that quantitatively explains photoemission from single crystal metal surfaces. This model accurately calculates the dependence of the electron yield on the angle of incidence and the polarization of incident light (vectorial photoelectric effect). We show excellent agreement between the measured and calculated photoemission properties of the Ag(111) surface. Our measurements show that Ag(111) surface can act as an excellent electron source for several applications like Free Electron Lasers and Ultra-fast Electron Diffraction.

**10:48AM A47.00015 A new approach to measure spatially resolved thermovoltage** , KAI SOTTHEWES, MARTIN SIEKMAN, HAROLD ZANDVLIET, University of Twente — We have recorded spatial maps of the thermovoltage of a Au(111) surface with a scanning tunneling microscope using a novel approach. The novel approach relies a method where we record quasisimultaneously the normal topography as well as the thermovoltage by switching the feedback and sample bias on and off. The thermovoltage, which arises from a temperature difference between scanning tunneling microscope tip and sample, is very sensitive to small variations of the local electronic density of states in vicinity of the Fermi level. Near step edges and defects we have observed well-defined Friedel oscillations.

**Monday, March 14, 2016 8:00AM - 11:00AM —**  
**Session A48 GQI: Quantum Computing and Quantum Simulations with Superconducting Circuits** 349 - David Schuster, University of Chicago

**8:00AM A48.00001 Digitized adiabatic quantum computing with a superconducting circuit, part I: Theory** , L. LAMATA, University of the Basque Country, Spain, R. BARENDT, Google, Santa Barbara, USA , A. SHABANI, Google, Venice, USA , J. KELLY, Google, Santa Barbara, USA, A. MEZZACAPO, U. LAS HERAS, University of the Basque Country, Spain, R. BABUSH, Google, Venice, USA, A. G. FOWLER, Google, Santa Barbara, USA, B. CAMPBELL, University of California, Santa Barbara, USA , YU CHEN, Google, Santa Barbara, USA, Z. CHEN, B. CHIARO, A. DUNSWORTH, University of California, Santa Barbara, USA, E. JEFFREY, E. LUCERO, Google, Santa Barbara, USA, A. MEGRANT, University of California, Santa Barbara, USA, J. Y. MUTUS, M. NEELEY, Google, Santa Barbara, USA, C. NEILL, P. J. J. OMALLEY, C. QUINTANA, University of California, Santa Barbara, USA, P. ROUSHAN, Google, Santa Barbara, USA, E. SOLANO, University of the Basque Country, Spain, and IKERBASQUE, Spain, H. NEVEN, Google, Venice, USA, JOHN M. MARTINIS, Google, Santa Barbara, USA, and University of California, Santa Barbara, USA — Adiabatic quantum computing (AQC) is a general-purpose optimization algorithm that in contrast to circuit-model quantum algorithms can be applied to a large set of computational problems. An analog physical realization of AQC has certain limitations that we propose can be overcome by a gate-model equivalence of the AQC. In this talk we discuss the hardware advantages of digitized AQC in particular arbitrary interactions, precision, and coherence. We could experimentally realize the principles of digitized AQC on a chain of nine qubits, and highlight the physics of adiabatic evolutions as well as the Kibble-Zurek mechanism.

**8:12AM A48.00002 Digitized adiabatic quantum computing with a superconducting circuit, part II: Experiment** , R. BARENDT, A. SHABANI, Google Inc., L. LAMATA, University of the Basque Country, Spain, J. KELLY, Google Inc., A. MEZZACAPO, U. LAS HERAS, University of the Basque Country, Spain, R. BABUSH, A.G. FOWLER, Google Inc., B. CAMPBELL, UC Santa Barbara, Y. CHEN, Z. CHEN, Google Inc., B. CHIARO, A. DUNSWORTH, UC Santa Barbara, E. JEFFREY, E. LUCERO, A. MEGRANT, J. MUTUS, M. NEELEY, Google Inc., C. NEILL, P. O'MALLEY, C. QUINTANA, UC Santa Barbara, P. ROUSHAN, Google Inc., E. SOLANO, University of the Basque Country, Spain, H. NEVEN, J. MARTINIS, Google Inc. — A major challenge in quantum computing is to solve general problems with limited physical hardware. We implement digitized adiabatic quantum computing, combining the generality of the adiabatic algorithm with the universality of the digital approach, using a superconducting circuit with nine qubits. We probe the adiabatic evolutions, explore the scaling of errors with system size, and quantify the success of the algorithm for random spin problems. We find that the system can approximate the solutions to both frustrated Ising problems and non-stoquastic problem Hamiltonians with a performance that is comparable.

**8:24AM A48.00003 Digital quantum simulations with superconducting circuits** , URTZI LAS HERAS, LAURA GARCIA-ALVAREZ, LUCAS LAMATA, University of the Basque Country, Spain, ENRIQUE SOLANO, University of the Basque Country and IKERBASQUE, Spain — Superconducting circuits are a promising quantum technology for the implementation of quantum information protocols. In particular, digital quantum simulations are an efficient method for reproducing dynamics that are not produced naturally in the simulating system. We propose a method for simulating efficiently the dynamics of prototypical spin and fermionic models in circuit quantum electrodynamics architectures with either qubit-qubit pairwise interactions or resonators acting as quantum buses. We show how to implement Ising and Heisenberg spin models, and the Fermi-Hubbard model, making use of the Jordan-Wigner mapping and Mølmer-Sørensen gates.

**8:36AM A48.00004 Quantum simulation of micro and macro frustrated quantum magnetism with superconducting circuits.**<sup>1</sup> , JOYDIP GHOSH, BARRY C. SANDERS, Univ of Calgary — We devise a scalable scheme for simulating a quantum phase transition from paramagnetism to frustrated magnetism in a superconducting flux-qubit network, and show how to characterize this system experimentally both macroscopically and microscopically. The proposed macroscopic characterization of the quantum phase transition is based on the transition of the probability distribution for the spin-network net magnetic moment with this transition quantified by the difference between the Kullback-Leibler divergences of the distributions corresponding to the paramagnetic and frustrated magnetic phases with respect to the probability distribution at a given time during the transition. Microscopic characterization of the quantum phase transition is performed using the standard local-entanglement-witness approach. Simultaneous macro and micro characterizations of quantum phase transitions would serve to verify in two ways a quantum phase transition and provide empirical data for revisiting the foundational emergentist-reductionist debate regarding reconciliation of macroscopic thermodynamics with microscopic statistical mechanics especially in the quantum realm for the classically intractable case of frustrated quantum magnetism.

<sup>1</sup>NSERC, AITF and University of Calgarys Eyes High Fellowship Program

**8:48AM A48.00005 Engineering artificial Hamiltonians with parametric superconducting circuits** , YAO LU, SRIVATSAN CHAKRAM, NELSON LEUNG, RAVI NAIK, NATHAN EARNEST, James Franck Institute and Department of Physics, University of Chicago, PETER GROSZKOWSKI, JENS KOCH, Department of Physics & Astronomy, Northwestern University, ELIOT KAPIT, Department of Physics & Engineering Physics, Tulane University, DAVID SCHUSTER, James Franck Institute and Department of Physics, University of Chicago — One major challenge in building a large scale quantum computer is to generate and manipulate interactions between its many qubits. One promising approach is to use parametric flux or voltage modulation to realize effective interactions between different components of superconducting circuits, generating artificial Hamiltonians that are suitable for various quantum computation tasks, which might be difficult to achieve through other means. We propose a parametric superconducting circuit where transmon qubits and resonators are coupled to a flux-modulated parametric coupler. We show that with this device, arbitrary pairs of qubits or resonators in the circuit can be selectively and simultaneously brought into resonance with each other and swap excitations at a controllable rate. This allows for the creation of various artificial circuit Hamiltonians that are suitable for a number of applications such as single qubit state stabilization, parametric qubit state readout, autonomous error correction and so on.

**9:00AM A48.00006 Strongly interacting photons in a synthetic magnetic field** , PEDRAM ROUSHAN, Google, Inc., C. NEILL, UCSB, A. MEGRANT, Y. CHEN, R. BARENDS, Google, Inc., B. CAMBELL, Z. CHEN, B. CHIARO, A. DUNSWORTH, UCSB, A. FOWLER, E. JEFFREY, J. KELLY, E. LUCERO, J. MUTUS, Google, Inc., P. O'MALLEY, UCSB, M. NEELEY, C. QUINTANA, D. SANK, Google, Inc., A. VAINSENCER, J. WENNER, UCSB, T. WHITE, Google, Inc., E. KAPIT, Tulane University, J. MARTINIS, Google, Inc. — Interacting electrons in the presence of magnetic fields exhibit some of the most fascinating phases in condensed matter systems. Realizing these phases in an engineered platform could provide deeper insight into their. Using three superconducting qubits, we synthesize artificial magnetic fields by modulating the inter-qubit coupling. In the closed loop formed by the qubits, we observe the directional circulation of a microwave photon as well as chiral groundstate currents, the signatures of broken time-reversal symmetry. The existence of strong interactions in our system is seen via the creation of photon vacancies, or "holes", which circulate in the opposite direction from the photons. Our work demonstrates an experimental approach for engineering quantum phases of strongly interacting bosons.

**9:12AM A48.00007 Emulating the 1-Dimensional Fermi-Hubbard Model with Superconducting Qubits** , JAN-MICHAEL REINER, MICHAEL MARTHALER, GERD SCHN, Karlsruhe Institute of Technology — A chain of qubits with both  $ZZ$  and  $XX$  couplings is described by a Hamiltonian which coincides with the Fermi-Hubbard model in one dimension. The qubit system can thus be used to study the quantum properties of this model. We investigate the specific implementation of such an analog quantum simulator by a chain of tunable Transmon qubits, where the  $ZZ$  interaction arises due to an inductive coupling and the  $XX$  interaction due to a capacitive coupling.

**9:24AM A48.00008 Cavity-assisted cooling of Bose-Hubbard model simulator with superconducting circuits** , XIUHAO DENG, School of Natural Sciences, University of California Merced, CHUNJING JIA, Department of Applied Physics, Stanford University; Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator — Interesting progress have been made in using superconducting circuits to simulate Bose-Hubbard model (BHM). However, studying ground state feature of BHM calls for effective cooling process, where the cooling mechanism must preserve total number of simulated bosons and cooling rate has to be much stronger than decay rate. Here, we propose a cooling scheme that satisfies these two conditions by coupling an array of transmission line resonators with an assisted cavity. The quantum simulator we modelled here can be used to study generic BHM, which include both repulsive and attractive on-site interaction and hopping strength. We evaluate the cooling rate in all these regime analytically. And numerical simulation in time domain gives further supports. Our results present a promising cooling scheme for experiments.

**9:36AM A48.00009 Simulating chemical energies to high precision with fully-scalable quantum algorithms on superconducting qubits** , PETER O'MALLEY, UC Santa Barbara, RYAN BABBUSCH, Google Inc., Venice, CA, IAN KIVLICHAN, JHONATHAN ROMERO, Harvard University, JARROD MCCLEAN, Lawrence Berkeley National Lab, ANDREW TRANTER, Tufts University, RAMI BARENDS, JULIAN KELLY, YU CHEN, Google Inc., Santa Barbara, CA, ZIJUN CHEN, UC Santa Barbara, EVAN JEFFREY, AUSTIN FOWLER, Google Inc., Santa Barbara, CA, ANTHONY MEGRANT, UC Santa Barbara, JOSH MUTUS, Google Inc., Santa Barbara, CA, CHARLES NEILL, CHRISTOPHER QUINTANA, UC Santa Barbara, PEDRAM ROUSHAN, DANIEL SANK, Google Inc., Santa Barbara, CA, AMIT VAINSENCER, JAMES WENNER, UC Santa Barbara, THEODORE WHITE, Google Inc., Santa Barbara, CA, PETER LOVE, Tufts University, ALAN ASPURU-GUZIK, Harvard University, HARTMUT NEVEN, Google Inc., Venice, CA, JOHN MARTINIS, UC Santa Barbara and Google Inc. — Quantum simulations of molecules have the potential to calculate industrially-important chemical parameters beyond the reach of classical methods with relatively modest quantum resources. Recent years have seen dramatic progress both superconducting qubits and quantum chemistry algorithms. Here, we present experimental demonstrations of two fully-scalable algorithms for finding the dissociation energy of hydrogen: the variational quantum eigensolver and iterative phase estimation. This represents the first calculation of a dissociation energy to chemical accuracy with a non-precompiled algorithm. These results show the promise of chemistry as the "killer app" for quantum computers, even before the advent of full error-correction.

**9:48AM A48.00010 Hybrid Quantum-Classical Approach to Molecular Excited States On Superconducting Qubits** , JARROD MCCLEAN, Computational Research Division, Lawrence Berkeley National Laboratory, MOLLIE SCHWARTZ, CHRIS MACKLIN, IRFAN SIDDIQI, Quantum Nanoelectronics Laboratory, University of California, Berkeley, JONATHAN CARTER, WIBE DE JONG, Computational Research Division, Lawrence Berkeley National Laboratory — Quantum computers promise to dramatically advance our understanding of correlated quantum systems. Unfortunately, many proposed algorithms have resource requirements not yet suitable for near-term quantum devices. The variational quantum eigensolver (VQE) is a recently proposed hybrid quantum-classical method for solving eigenvalue problems and more generic minimizations on a quantum device leveraging classical resources to minimize coherence time requirements. However, this algorithm has so far focused only on the quantum ground state and has almost exclusively been studied in ideal closed system conditions. We briefly review the original VQE approach and introduce a simple extension requiring no additional coherence time to approximate excited states. Moreover, we show how the same method can be used to mitigate the effects of noise in a real system and how this algorithm can be applied in practice on a superconducting qubit architecture.

**10:00AM A48.00011 Implementation of a Quantum Variational Eigensolver in Superconducting Qubits**, MOLLIE SCHWARTZ, Quantum Nanoelectronics Laboratory, UC Berkeley, JARROD MCCLEAN, Computational Research Division, Lawrence Berkeley National Laboratory, CHRIS MACKLIN, Quantum Nanoelectronics Laboratory, UC Berkeley; Computational Research Division, Lawrence Berkeley National Laboratory, JONATHAN CARTER, WIBE ALBERT DE JONG, Computational Research Division, Lawrence Berkeley National Laboratory, IRFAN SIDDIQI, Quantum Nanoelectronics Laboratory, UC Berkeley; Materials Sciences Division, Lawrence Berkeley National Laboratory — The quantum variational eigensolver (QVE) represents an efficient implementation of quantum simulation that relies on a synergy between classical and quantum computing components. In this approach, a classical computer is used to map the target Hamiltonian onto a fermionic Hilbert space and to perform a variational update of the estimated ground state. This test state is then prepared in the quantum system, enabling an efficient estimation of the expectation value of the Hamiltonian and reducing the requirements for coherent qubit evolution. We present experimental progress toward implementing a QVE in superconducting qubits, capitalizing on the flexibility and scalability of the transmon cQED architecture.

**10:12AM A48.00012 Cavity-assisted dynamical quantum phase transition in superconducting quantum simulators<sup>1</sup>**, LIN TIAN, School of Natural Sciences, University of California, Merced, CA 95343 — Coupling a quantum many-body system to a cavity can create bifurcation points in the phase diagram, where the many-body system switches between different phases. Here I will discuss the dynamical quantum phase transitions at the bifurcation points of a one-dimensional transverse field Ising model coupled to a cavity. The Ising model can be emulated with various types of superconducting qubits connected in a chain. With a time-dependent Bogoliubov method, we show that an infinitesimal quench of the driving field can cause gradual evolution of the transverse field on the Ising spins to pass through the quantum critical point. Our calculation shows that the cavity-induced nonlinearity plays an important role in the dynamics of this system. Quasiparticles can be excited in the Ising chain during this process, which results in the deviation of the system from its adiabatic ground state.

<sup>1</sup>This work is supported by the National Science Foundation under Award Number 0956064.

**10:24AM A48.00013 Visualizing singularities of a groundstate landscape using superconducting circuits**, ERIK LUCERO, Google, Inc., A. DUNSWORTH, UCSB, P. ROUSHAN, A. MEGRANT, Google, Inc., C. NEILL, UCSB, T. SOUZA, M. TOMKA, M. KOLODRUBETZ, Boston University, Y. CHEN, R. BARENDT, Google, Inc., B. CAMPBELL, Z. CHEN, B. CHIARO, UCSB, E. JEFFREY, J. KELLY, J. MUTUS, Google, Inc., P. O'MALLEY, C. QUINTANA, UCSB, D. SANK, Google, Inc., J. WENNER, UCSB, T. WHITE, Google, Inc., A. POLKOVNIKOV, Boston University, J. MARTINIS, Google, Inc. — The defining properties of condensed matter phases are set by their groundstate wavefunctions. The adiabatic theorem provides an experimental approach for realizing such states. However, a general protocol for applying this theorem is experimentally unexplored, in particular when the energy gap is small. Using two superconducting qubits, we adiabatically prepare the entire groundstate manifold in a region of the parameter-space where degeneracies are present. We prepare these states by varying the Hamiltonian along 'geodesics' in parameter-space, obtained by minimizing the local non-adiabatic error. From the measured total magnetization of the final state, we compute the Berry curvature, where degeneracies appear as singular points, allowing us to directly visualize the degeneracies in the groundstate landscape.

**10:36AM A48.00014 Observation of the correspondence between Landau-Zener transition and Kibble-Zurek mechanism with a superconducting qubit system<sup>1</sup>**, MING GONG, DONG LAN, YUHAO LIU, XINSHENG TAN, HAIFENG YU, YANG YU, SHILIANG ZHU, School of Physics, Nanjing University, China, GUOZHU SUN, YU ZHOU, YUNYI FAN, PEIHENG WU, School of Electronic Science and Engineering, Nanjing University, China, XUEDA WEN, Department of Physics, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA, DANWEI ZHANG, Guangdong Provincial Key Laboratory of Quantum Engineering and Quantum Materials, SPTE, South China Normal University, Guangzhou 510006, China, SIYUAN HAN, Department of Physics and Astronomy, University of Kansas, Lawrence, KS 66045, USA — We present a direct experimental observation of the correspondence between Landau-Zener transition and Kibble-Zurek mechanism with a superconducting qubit system. We develop a time resolved approach to study quantum dynamics of the Landau-Zener transition. By using this method, we observe the key features of the correspondence between Landau-Zener transition and Kibble-Zurek mechanism, e.g., the boundary between the adiabatic and impulse regions, the freeze out phenomenon in the impulse region. Remarkably, the scaling behavior of the population in the excited state, an analogical phenomenon originally predicted in Kibble-Zurek mechanism, is also observed in the Landau-Zener transition.

<sup>1</sup>This work was partly supported by the SKPBR of China (2011CB922104), NSFC (91321310, 11125417, 11474153, 11474154, 61521001), and the PCSIRT (Grant No. IRT1243)

**10:48AM A48.00015 Artificial Quantum Thermal Bath**, ALIREZA SHABANI, HARTMUT NEVEN, Google Quantum AI Lab — In this talk, we present a theory for engineering the temperature of a quantum system different from its ambient temperature, that is basically an analog version of the quantum metropolis algorithm. We define criteria for an engineered quantum bath that, when couples to a quantum system with Hamiltonian  $H$ , drives the system to the equilibrium state  $\frac{e^{-H/T}}{\text{Tr}(e^{-H/T})}$  with a tunable parameter  $T$ . For a system of superconducting qubits, we propose a circuit-QED approximate realization of such an engineered thermal bath consisting of driven lossy resonators. We consider an artificial thermal bath as a simulator for many-body physics or a controllable temperature knob for a hybrid quantum-thermal annealer.

**Monday, March 14, 2016 8:00AM - 11:00AM –**

**Session A51 FIAP: Nanomanufacturing and Optical/Laser/High Frequency Devices** Hilton Baltimore Holiday Ballroom 2 - Nicholas Charipar, Naval Research Lab

**8:00AM A51.00001 Laser printed interconnects for flexible electronics<sup>1</sup>**, ALBERTO PIQUE, IYOEL BENIAM, SCOTT MATHEWS, NICHOLAS CHARIPAR, Naval Research Laboratory — Laser-induced forward transfer (LIFT) can be used to generate microscale 3D structures for interconnect applications non-lithographically. The laser printing of these interconnects takes place through aggregation of voxels of either molten metal or dispersed metallic nanoparticles. However, the resulting 3D structures do not achieve the bulk conductivity of metal interconnects of the same cross-section and length as those formed by wire bonding or tab welding. It is possible, however, to laser transfer entire structures using a LIFT technique known as lase-and-place. Lase-and-place allows whole components and parts to be transferred from a donor substrate onto a desired location with one single laser pulse. This talk will present the use of LIFT to laser print freestanding solid metal interconnects to connect individual devices into functional circuits. Furthermore, the same laser can bend or fold the thin metal foils prior to transfer, thus forming compliant 3D structures able to provide strain relief due to flexing or thermal mismatch. Examples of these laser printed 3D metallic bridges and their role in the development of next generation flexible electronics by additive manufacturing will be presented.

<sup>1</sup>This work was funded by the Office of Naval Research (ONR) through the Naval Research Laboratory Basic Research Program.

**8:12AM A51.00002 Expanding the Range and Utility of Atomic Calligraphy<sup>1</sup>**, LAWRENCE BARRETT, THOMAS STARK, JEREMY REEVES, RICHARD LALLY, DAVID BISHOP, Boston University — Due to the many potential applications of nanotechnology, there is a drive for new methods of nanomanufacturing. Atomic calligraphy has shown promise, not only as faster and as more economical than conventional methods, but also more precise, potentially being able to place single atoms with nanometer resolution [1]. Atomic calligraphy utilizes nanoscale apertures to define where material is deposited during evaporation. Microelectromechanical systems (MEMS) allow the aperture to be moved with nanometer precision. The technique has been demonstrated, but only over a small range of several microns and structures were written on the same substrate as the MEMS. We have moved from this to a system where structures can be written on any surface over a range of centimeters. To achieve this, first a process for etching through the substrate without damaging the delicate MEMS was developed. Then a scheme for making electrical contact to the MEMS with a low enough profile to still allow the aperture to be brought in contact with the writing surface was devised. Finally, a system of piezo stages was installed to quickly and precisely move the aperture from one area to another. [1] M. Imboden, H. Han, J. Chang, F. Pardo, C. A. Bolle, E. Lowell, and D. J. Bishop, Nano Lett. 13, 3379 (2013).

<sup>1</sup>This work is funded by the DARPA A2P Program.

**8:24AM A51.00003 3D Alignment of nanowriters using fringe capacitance<sup>1</sup>**, RICHARD LALLY, THOMAS STARK, JEREMY REEVES, LAWRENCE BARRETT, DAVID BISHOP, Boston University — With the introduction of atomic calligraphy, high resolution nanoscale structures can be fabricated rapidly over a large surface area [1]. This reliable, chemically stable and cost effective nanoscale writing method can be applied to a number of interesting applications. One specific application of this writing approach is to fabricate metamaterials, a process that requires precise alignment of the MEMS and substrate. Here we present a MEMS based solution coupling the well-studied comb drive capacitance effects [2] with the less predictable close order fringe effects. The combined capacitance allows for precise measurements in the nanometer range. Using two sets of orthogonal static MEMS comb drives, the capacitance is used to discern the x, y, and z spatial displacement from the substrate. The unique SOI wafer is prepared creating a periodic array of silicon pillars. Placement of additional MEMS comb drives at the MEMS device edges will allow stage corrections for tip, tilt and rotational alignment thereby reducing the effects generated by variations in wafer thickness and surface smoothness. [1] Imboden, M. and Bishop. D. Physics Today. 2014, 67 (12), 45-50. [2] Elshurafa, A. and El-Masry, E. J. Micromech. Microeng. 2010, 20(4), 045027

<sup>1</sup>This work is funded by the DARPA A2P Program

**8:36AM A51.00004 Monolayer Tungsten Disulfide Laser**, YU YE, ZI JING WONG, UC Berkeley, XIUFANG LU, University of Science and Technology of China, XINGJIE NI, HANYU ZHU, UC Berkeley, XIANHUI CHEN, University of Science and Technology of China, YUAN WANG, XIANG ZHANG, UC Berkeley — Two-dimensional van der Waals materials have opened a new paradigm for fundamental physics exploration and device applications because of their emerging physical properties. Unlike gapless graphene, monolayer transition-metal dichalcogenides are two-dimensional semiconductors that undergo an indirect-to-direct band gap transition, creating new optical functionalities for next-generation ultra-compact photonics and optoelectronics. Here, we report the realization of a two-dimensional excitonic laser by embedding monolayer tungsten disulfide in a microdisk resonator.

**8:48AM A51.00005 Guided-Wave Plasmon Polariton Modes in High-Index Dielectric Structures**, RACHEL OWEN, JANELLE LEGER, BRAD JOHNSON, Western Washington University — Interest in subwavelength waveguides has increased as the need to interface between optical signals and increasingly small electronic components grows. Surface plasmon polaritons (SPPs) are surface charge density oscillations localized to a metal-dielectric interface that confine energy to a structure that is not diffraction limited. Thus, structures that support SPPs are promising candidates for subwavelength waveguides. However, most of the electric field propagates along the metal interface, causing Ohmic damping to restrict use to short-range applications. Here we present an architecture that supports high index dielectric plasmon polariton modes (HID-PPMs). These structures utilize the metal-dielectric-metal-substrate structure of typical SPP waveguides. However, the core dielectric layer has a higher refractive index than the substrate. This small structural change causes the bulk of the electric field to be concentrated in the dielectric region resulting in a dramatic reduction of damping effects. Here we present experimental evidence of HID-PPMs in a simple trilayer structure. Our results match model predictions with remarkable accuracy using minimal parameter modifications. We discuss these results as well as the potential applications of these devices.

**9:00AM A51.00006 Efficient directional excitation of surface plasmons by a single-element nanoantenna**, WENJIE YAO, SHANG LIU, HUIMIN LIAO, ZHI LI, CHENGWEI SUN, JIANJUN CHEN, QIHUANG GONG, Peking University — Directional light scattering is important in basic research and real applications. This area has been successfully downscaled to wavelength and subwavelength scales with the development of optical antennas, especially single-element nanoantennas. Here we show, by adding an auxiliary resonant structure to a single-element plasmonic nanoantenna, the highly efficient lowest-order antenna mode can be effectively transferred into inactive higher-order modes. Based on this mode conversion, scattered optical fields can be well manipulated by utilizing the interference between different antenna modes. Both broadband directional excitation of surface plasmon polaritons (SPPs) and inversion of SPP launching direction at different wavelengths are experimentally demonstrated as typical examples. The proposed strategy based on mode conversion and mode interference provides new opportunities for the design of nanoscale optical devices, especially directional nanoantennas.

**9:12AM A51.00007 Enhanced performance in SnO<sub>2</sub> thin film UV photodetectors via self-assembled CuO/SnO<sub>2</sub> nanoheterojunctions**, BOTONG QIU, Johns Hopkins Univ, TING XIE, MD HASAN, National Institute of Standards and Technology, EBUKA ARINZE, Johns Hopkins Univ, NHAN NGUYEN, ABHISHEK MOTAYED, National Institute of Standards and Technology, SUSANNA THON, Johns Hopkins Univ, RATAN DEBNATH, National Institute of Standards and Technology — Low-cost visible-blind ultraviolet (UV) photodetectors (PDs) are of interest for versatile applications in digital imaging, optical communications, and biomedical sensing. We report on the use of CuO/SnO<sub>2</sub> *p-n* nanoscale heterojunctions to enhance the performance of SnO<sub>2</sub> thin film UV PDs. Our method produces robust structures that operate at low bias without complex fabrication processes. The nanoheterojunctions are self-assembled by sputtering Cu clusters that oxidize in ambient to form CuO nanoparticles. The chemical identity, morphology and distribution of the nanoparticles are investigated through high-resolution XPS and AFM characterization. Enhanced UV absorption is demonstrated both experimentally and using optical simulations after addition of the CuO/SnO<sub>2</sub> nanoheterojunctions. The device performance improvements are attributed to the strong absorption in the CuO nanoparticles and electron transfer facilitated by the nanoheterojunctions. The PDs show a five-fold increase in peak responsivity at 0.2 V bias. The photoresponse factor, defined as the wavelength-dependent ratio between the photocurrent and dark current, was estimated to be 592 for the CuO-SnO<sub>2</sub> PD under 290 nm illumination.

**9:24AM A51.00008 Influence of cavity optomechanics on Kerr frequency combs**, RYO SUZUKI, AKITOSHI JINNAI, TAKUMA NAGANO, TOMOYA KOBATAKE, TAKUMI KATO, TAKASUMI TANABE, Keio University — The Kerr frequency comb has the potential for applications in, for example, spectroscopy, optical communication, waveform shaping and astronomy. Recently, the mechanism of soliton pulse generation in a microcavity has been studied numerically and experimentally. Silicon nitride ring and magnesium fluoride microcavities are commonly used in experimental research, because of their high nonlinearity, dispersion and other advantageous characteristics. On the other hand, silica toroid microcavities are not much used for Kerr comb research in the time domain (e. g. pulse generation/measurement). This is because toroid microcavities are prone to cavity optomechanical vibration, and the cavity dispersion of the fundamental mode of a small radius microcavity is normal. To fabricate a toroid microcavity with a large radius, we need to use a particular fabrication process. In this research, by controlling the detuning of the resonance and pump laser frequencies, we suppressed the noise of optomechanical vibration and obtained pulses with low background noise using higher order resonance modes. In addition, we observed optical pulses with repetition frequencies of up to 3.7 THz.

**9:36AM A51.00009 Open optical microcavities for CQED experiments and devices**, JASON SMITH, AURELIEN TRICHET, University of Oxford, PHILIP DOLAN, DAVID COLES, LUCAS FLATTEN, SAM JOHNSON, ROBIN PATEL, University of Oxford, UK, STEFAN SCHWARZ, FENG LI, DIMITRII KRIZHANOVSKII, ALEXANDER TARTAKOVSKII, MAURICE SKOLNICK, University of Sheffield, UK, CLAIRE VALLANCE, University of Oxford, DAVID HUNGER, Ludwig Maximilians Universitaet, Germany — Open microcavities have emerged in recent years as flexible tools for quantum optics and engineered light matter coupling. Fabry Perot resonators with concave mirrors on the micrometre scale, highly resonant optical modes can be generated with volumes of order  $1-10\lambda^3$ , along with facile tunability and efficient external coupling. Here we will describe our latest advances in open cavity fabrication using focused ion beam milled templates on which high reflectivity mirrors can be deposited providing measured finesse up to 50,000 with surfaces that deviate by less than 2 nm rms from the design. This degree of control provides opportunities for engineering optical modes to suit a wide variety of applications. We will describe the fabrication of cavities with radius of curvature from  $2\ \mu\text{m}$  to 1 mm, and the realisation of coupled cavities with controlled mode overlap. We will further describe some of the applications of these open cavity devices to particle sensing, exciton-polariton physics with quantum wells and 2D materials, tunable lasers, and spin-photon interfaces using diamond colour centres.

**9:48AM A51.00010 Vanadium dioxide for terahertz devices<sup>1</sup>**, NICHOLAS CHARIPAR, HEUNGSOO KIM, SCOTT MATHEWS, ALBERTO PIQUE, Naval Research Lab — We investigate  $\text{VO}_2$  as a material for ultrafast sub-millimeter wave devices. This material exhibits a semiconductor to metal transition (SMT) at  $\sim 68^\circ\text{C}$  which results in a dramatic increase in carrier density ( $\sim 10^{19} - 10^{23}\text{ cm}^{-3}$ ). The SMT transition can be induced thermally, electrically, or optically enabling strong interactions and unique device operation. This transition has been exploited for numerous microwave/terahertz devices such as tunable filters and modulators. However due to its low carrier mobility ( $\sim 0.1\text{ cm}^2/\text{V-s}$ ) and long recovery times ( $\sim\text{ns}$ ),  $\text{VO}_2$  has been largely ignored as a possible material for millimeter wave and terahertz pulse generation even though the SMT can occur within 100 fs.  $\text{VO}_2$  thin film devices were fabricated and characterized. These devices were capable of generating  $\sim 1\text{ ps}$  electrical pulses. We will present details on the ultrafast switching behaviors of  $\text{VO}_2$  along with the design and fabrication of terahertz emitter based on the SMT of  $\text{VO}_2$ .

<sup>1</sup>This work was funded by the Office of Naval Research (ONR) through the Naval Research Laboratory Basic Research Program

**10:00AM A51.00011 Comparative electrochemical studies of a nanostructured vanadium oxide electrode material in aqueous electrolyte<sup>1</sup>**, VICTORIA SOGHOMONIAN, QIFAN YUAN, SHAOLA REN, JULIA ZUKOWSKI, Virginia Tech, Department of Physics — Electrochemical energy storage plays an increasing role in energy solutions. We report on a new hydrothermally synthesized vanadium oxide nanostructured material and study its performance as electrode material for insertion of various ions from aqueous solutions. The as-synthesized product is in the form of nanosheets forming quasi-spherical 3-dimensional objects. Variable temperature resistivity measurements indicate a thermally activated behavior. Electrodes are constructed, and comparative electrochemical insertion reactions of Li, Na, K and  $\text{NH}_4$  cations, over different cycle numbers, investigated. Concomitantly, morphological and microstructural changes are characterized by scanning electron microscopy, providing physical input to the observed electrochemical behavior. Specific charge is calculated. For Li and K, the specific charge decreases as the cycle number increases, while the reverse is observed for Na and  $\text{NH}_4$  cations. The trends are correlated to the morphological changes observed. The specific charge in the case of ammonium reaches 180 mAh/g after 20 cycles and continues increasing, indicating that ammonium cations may be considered as viable charge carriers for electrical energy storage system, and moreover in an aqueous electrolyte.

<sup>1</sup>We acknowledge support from the National Science Foundation, Grant No. DMR- 1206338.

**10:12AM A51.00012 High efficiency on-chip three wave parametric frequency conversion and its applications in both classical and quantum optics**, XIANG GUO, CHANGLING ZOU, CARSTEN SCHUCK, HOJOONG JUNG, RISHENG CHENG, HONG X. TANG, Yale Univ — Second order nonlinearity ( $\chi^{(2)}$ ) is one of the most widely explored properties in photonics. Integrating nonlinear devices on a photonic chip attracts more and more attention due to the devices small foot-print and large scalability. However,  $\chi^{(2)}$  nonlinearity in a scalable platform is normally believed to be weak due to difficulties in finding a suitable material with both high nonlinearity and compatibility with advanced nanofabrication technologies. Aluminum nitride is newly developed as a material combining such two properties: high nonlinearity in low-loss, small foot-print waveguide circuits. In experiment, we fabricate microring resonator devices supporting both telecom and visible modes and achieve exceptionally large second harmonic generation efficiency. High quality photon pair generation is further demonstrated with a generation rate of 3 MHz/mW for degenerate photon pair and 5.8 MHz/mW for non-degenerate photon pair. Furthermore, the strong nonlinearity results in coherent interaction between two spectrally far-away modes which manifest as a nonlinear optic induced transparency and efficient frequency converter. We envision more interesting and important applications in the AlN platform combining its outstanding linear and nonlinear properties.

**10:24AM A51.00013 Highly Stable Nanolattice Structures using Nonlinear Laser Lithography**, OZGUN YAVUZ, ONUR TOKEL, Department of Physics, Bilkent University, 06800 Ankara, Turkey, EMRE ERGECEN, Department of Physics, Massachusetts Institute of Technology, Cambridge Massachusetts MA 02139, IHOR PAVLOV, GHAITH MAKEY, FATIH OMER ILDAY, Department of Physics, Bilkent University, 06800 Ankara, Turkey — Periodic nanopatterning is crucial for multiple technologies, including photovoltaics and display technologies. Conventional optical lithography techniques require complex masks, while e-beam and ion-beam lithography require expensive equipment. With the Nonlinear Laser Lithography (NLL) technique, we had recently shown that various surfaces can be covered with extremely periodic nanopatterns with ultrafast lasers through a single-step, maskless and inexpensive method. Here, we expand NLL nanopatterns to flexible materials, and also present a fully predictive model for the formation of NLL nanostructures as confirmed with experiments. In NLL, a nonlocal positive feedback mechanism (dipole scattering) competes with a rate limiting negative feedback mechanism. Here, we show that judicious use of the laser polarisation can constrain the lattice symmetry, while the nonlinearities regulate periodicity. We experimentally demonstrate that in addition to one dimensional periodic stripes, two dimensional lattices can be produced on surfaces. In particular, hexagonal and square lattices were produced, which are highly desired for display technologies. Notably, with this approach, we can tile flexible substrates, which can find applications in next generation display technologies.

**10:36AM A51.00014 Adaptive quantum well/dot IR photodetector with modulated optical bias**, ANDREI SERGEEV, KIMBERLY SABLON, U.S. Army Research Laboratory, Adelphi, MD 20783, USA — Low doping of optical nanostructures leads to a weak electron coupling to radiation, because the radiation is absorbed due to electron transitions in nanoblocks (quantum wells and dots). High doping levels strongly enhance the absorption, but lead to high dark current and high noise current. This tradeoff is inevitable in traditional detector design and with conventional operating regimes, because the radiation absorption and dark current are both proportional to the number of electrons in nanoblocks. To overcome limitations related to the tradeoff between IR absorption and dark current, we propose and study the “nonequilibrium” IR quantum well or quantum dot photodetectors with modulated optical bias. Here we present design of the detector and results of modelling of key detector characteristics, such as responsivity, operating time, and noise equivalent power.

**10:48AM A51.00015 Multi-terminal Two-color ZnCdSe/ZnCdMgSe Based Quantum-well Infrared Photodetector**, YASIN KAYA, Princeton Univ, ARVIND RAVIKUMAR<sup>1</sup>, GUOPENG CHEN, Department of Electrical Engineering, The City College of New York, NY 10031, USA, MARIA C. TAMARGO, Department of Chemistry, The City College of New York, NY 10031, USA, AIDONG SHEN, Department of Electrical Engineering, The City College of New York, NY 10031, USA, CLAIRE GMACHL, Department of Electrical Engineering, Princeton University, Princeton, NJ 08544, USA — Target recognition and identification applications benefits from two-color infrared (IR) detectors in the mid and long-wavelength IR regions. Currently, InGaAs/AlGaAs and GaAs/AlGaAs multiple quantum wells (QWs) grown on GaAs substrate are the most commonly used two-color QW IR photodetectors (QWIPs). However, the lattice-mismatch and the buildup of strain limit the number of QWs that can be grown, in turn increasing the dark current noise, and limiting the device detectivity.

In this work, we report on two-color QWIPs based on the large conduction band offset ( $\sim 1.12\text{eV}$ ) ZnCdSe/ZnCdMgSe material system lattice matched to InP. QWIPs were designed based on a bound to quasi-bound transition, centered at  $4\text{ }\mu\text{m}$  and  $7\text{ }\mu\text{m}$  and each QW is repeated 50 times to eliminate the high dark current and a contact layer is inserted between the two stacks of QWs for independent electrical contacts. Wafers are processed into two step rectangular mesas by lithography and wet etching. Experiments showed absorption spectra centered at  $4.9\text{ }\mu\text{m}$  and  $7.6\text{ }\mu\text{m}$  at 80 K and the full width at half maximums were  $\Delta\lambda/\lambda = 21\%$  and  $\Delta\lambda/\lambda = 23\%$ , respectively. Current work studies the Johnson and the background noise limited detectivities of these QWIPs.

<sup>1</sup>Current address: School of Earth, Energy and Environmental Sciences, Stanford, CA 94305, USA

**Monday, March 14, 2016 8:00AM - 10:36AM –**  
**Session A53 DFD: Instabilities and Turbulence** Hilton Baltimore Holiday Ballroom 4 -

**8:00AM A53.00001 Oil Induced Spontaneous Flow in Water- Bis(2-ethylhexyl)Sulfosuccinat (AOT) system**, PARVATHALU KALAKONDA, King Abdulla University of Science and Technology — Instability and evaporation rates of oils within the layers of vesicles of a surfactants trigger the spontaneous (second flow) flow. The incorporation of oils into bis(2-ethylhexyl)sulfosuccinat (AOT) system remains incompletely characterized. We show that the second flow has a finite size that show a minimum at a particular concentration (mM) of surfactant solution. As a result, the layers are destabilized lead to explode and create the second flow. The fluorescence emission spectra and evaporation rates show that the oil diffuses into the layers of vesicles of a surfactant. We have characterized evaporation rates of oils on various concentrations (mM) of surfactant solution and observed that oils evaporation rates depend on volume and remain constant as the function of concentration of surfactant. We believe that second flow is new feature and brings a new insight into the fluid flow dynamics.

**8:12AM A53.00002 Joule Heating Effects on Electrokinetic Flow Instabilities in Ferrofluids.**<sup>1</sup>, CHRISTIAN BRUMME, RYAN SHAW, YILONG ZHOU, RAMA PRABHAKARAN, XIANGCHUN XUAN, Clemson University — We have demonstrated in our earlier work that the application of a tangential electric field can draw fluid instabilities at the interface of a ferrofluid/water co-flow. These electrokinetic flow instabilities are produced primarily by the mismatch of electric conductivities of the two fluids. We demonstrate in this talk that the Joule heating induced fluid temperature rises and gradients can significantly suppress the electrokinetic flow instabilities. We also develop a two-dimensional depth-averaged numerical model to predict the fluid temperature, flow and concentration fields in the two-fluid system with the goal to understand the Joule heating effects on electric field-driven ferrofluid flow instabilities.

<sup>1</sup>This work was supported by the Honors and Creative Inquiry programs at Clemson University.

**8:24AM A53.00003 Wall mode instability driven transition to turbulence in a soft microchannel**<sup>1</sup>, SAGAR SRINIVAS, KUMARAN V, Indian Institute of Science — Transition to turbulence has been triggered due to structure fluid interaction at Reynolds number (Re) much lower than hard wall transition Re, in a soft walled micro channel of dimensions  $40\text{mm} \times 1.5\text{mm} \times 0.16\text{mm}$ . Mixing index analysis indicates high degree of mixing accompanied by lower pressure drop as the channel deforms. Flow after transition velocity statistics has been extensively studied using Particle Imaging Velocimetry (PIV) along streamwise-wallnormal direction. The reduced plots of streamwise mean velocity are shown with the absence of viscous sublayer and presence of logarithmic layer with von Karman constants different from rigid wall channel. The one-point cross correlation between velocity fluctuations is non-zero at the soft surface which is in contrast to flow in hard walled channel. This indicates that the additional fluid stress exerted on the soft surface by the fluid velocity fluctuations result in net energy transfer due to shear work done at the interface. The structure fluid interface acts as a source of energy for the mean turbulent kinetic energy which is typically zero at the interface for hard walled channel. We also detect the onset of wall-oscillations primarily tangential to the surface at the transition Re.

<sup>1</sup>Department of Science and Technology (DST), Govt. of India

**8:36AM A53.00004 The effect of viscosity variation on the stability of a buoyantly unstable miscible layer in vertical porous media**<sup>1</sup>, SATYAJIT PRAMANIK, TAPAN KUMAR HOTA, MANORANJAN MISHRA, Indian Institute of Technology Ropar, India — We numerically show that in the absence of displacement a buoyantly unstable miscible layer with variable viscosity is less unstable than the constant viscosity layers. With the help of scaling analysis, we proved that the dynamics of variable viscosity layers with stable as well as unstable viscosity contrasts are identical in the absence of displacement. When the heavier fluid displaces the lighter one, the influence of viscosity contrast on the buoyantly unstable miscible layer is analogous to that in neutrally buoyant fluids. These findings of direct numerical simulations (DNS) in the fully nonlinear regime are consistent with the linear stability analysis (LSA). Furthermore, we perform a non-modal stability analysis of the linearized equations, which depicts the qualitative agreement with both LSA and DNS. In addition, the response of the linearized operator to external excitation has been studied through pseudospectra. The present findings are of great importance to understand the hydrodynamic mechanisms involved in geologic carbon sequestration.

<sup>1</sup>SP gratefully acknowledges the financial support from the National Board for Higher Mathematics through a Ph.D. fellowship

**8:48AM A53.00005 Untying vortex knots in fluids and superfluids**, DUSTIN KLECKNER, UC Merced, MARTIN SCHEELER, HRIDESH KEDIA, WILLIAM T. M. IRVINE, University of Chicago — Recent work has demonstrated that vortex knots appear to always untie in fluids and superfluids. Should we expect the same behavior from these two very different systems? I will discuss this unknotting behavior, both quantitatively – through helicity – and qualitatively through the geometry and topology of the vortex lines as they evolve.

**9:00AM A53.00006 Relaxation of Anisotropy in Superfluid Turbulence**, RENA ZIEVE, OWEN DIX, University of California - Davis — We simulate superfluid turbulence on a 3-sphere rather than using the more common periodic boundary conditions. We find that our topology naturally leads to anisotropy in a steady-state vortex tangle. A fundamental assumption in turbulence studies is that any large-scale anisotropy due to a driving velocity can be ignored at small length scales. However, there are practical concerns over how quickly the anisotropy decreases with length scale, and whether isotropic turbulence is attained above the dissipation scale. Here we examine how the anisotropy decreases upon moving from large to small length scales.

**9:12AM A53.00007 Simulating transitional hydrodynamics of the cerebrospinal fluid at extreme scale** , KARTIK JAIN, Simulation Techniques and Scientific Computing, Univ., of Siegen, Germany and Center for Biomedical Computing, Simula Research Lab., Lysaker Norway, SABINE ROLLER, Simulation Techniques and Scientific Computing, University of Siegen, Germany, KENT-ANDRE MARDAL, Center for Biomedical Computing, Simula Research Lab., Lysaker, Norway and Dept., of Mathematics, Univ., of Oslo, Norway — Chiari malformation type I is a disorder characterized by the herniation of cerebellar tonsils into the spinal canal through the foramen magnum resulting in obstruction to cerebrospinal fluid (CSF) outflow. The flow of pulsating bidirectional CSF is of acutely complex nature due to the anatomy of the conduit containing it - the subarachnoid space. We report lattice Boltzmann method based direct numerical simulations on patient specific cases with spatial resolution of  $24\mu\text{m}$  amounting meshes of up to 2 billion cells conducted on 50000 cores of the Hazelhen supercomputer in Stuttgart. The goal is to characterize intricate dynamics of the CSF at resolutions that are of the order of Kolmogorov microscales. Results unfold velocity fluctuations up to  $\sim 10KHz$ , turbulent kinetic energy  $\sim 2$  times of the mean flow energy in Chiari patients whereas the flow remains laminar in a control subject. The fluctuations confine near the cranio-vertebral junction and are commensurate with the extremeness of pathology and the extent of herniation. The results advocate that the manifestation of pathological conditions like Chiari malformation may lead to transitional hydrodynamics of the CSF, and a prudent calibration of numerical approach is necessary to avoid overlook of such phenomena.

**9:24AM A53.00008 Numerical Simulation of Parachutist Generated Turbulence on Parachute Inflation** , XIAOLEI CHEN, XIAOLIN LI, Stony Brook University — Using the front tracking computational platform, we couple parachutists as rigid bodies with the spring-mass model for the parachute system. The rigid body generates turbulent flow which affect the parachute inflation and stability. In this talk, we will present our numerical method to solve the complex system and study the effect of the turbulence at the wake of the parachutist on the canopy opening and parachute descent. Several different turbulence models are used and compared with experiments.

**9:36AM A53.00009 ABSTRACT WITHDRAWN** —

**9:48AM A53.00010 ABSTRACT WITHDRAWN** —

**10:00AM A53.00011 Tailoring boundary geometry to optimize heat transport in turbulent convection** , SRIKANTH TOPPALADODDI, Yale University, University of Oxford, SAURO SUCCI, Istituto per le Applicazioni del Calcolo "Mauro Picone" (C.N.R.), JOHN WETTLAUFER, Yale University, University of Oxford, NORDITA — Turbulent Rayleigh-Bénard convection between planar horizontal boundaries is a classical example of the challenge posed by multiple interacting scales in fluid dynamics. Here, by tailoring the geometry of the upper boundary we manipulate the boundary layer – turbulent interior flow interaction, and study the turbulent transport of heat in two-dimensional Rayleigh-Bénard convection with numerical simulations using the Lattice Boltzmann method. By fixing the roughness amplitude of the upper boundary and varying the wavelength  $\lambda$ , we find that the exponent  $\beta$  in the Nusselt-Rayleigh scaling relation,  $Nu - 1 \propto Ra^\beta$ , is maximized at  $\lambda \equiv \lambda_{max} \approx (2\pi)^{-1}$ , but decays to the planar value in both the large ( $\lambda \gg \lambda_{max}$ ) and small ( $\lambda \ll \lambda_{max}$ ) wavelength limits. The changes in the exponent originate in the nature of the coupling between the boundary layer and the interior flow. We present a simple scaling argument embodying this coupling, which describes the maximal convective heat flux. Results from simulations with both top and bottom rough boundaries showing a further enhancement of heat transport will also be presented.

**10:12AM A53.00012 Tracking Coherent Structures and Source Localization in Geophysical Flows<sup>1</sup>** , ERIC FORGOSTON, Montclair State University, ANI HSIEH, Drexel University, IRA SCHWARTZ, US Naval Research Laboratory, PHILIP YECKO, Cooper Union — There has been a steady increase in the deployment of autonomous underwater and surface vehicles for applications such as ocean monitoring, tracking of marine processes, and forecasting contaminant transport. The underwater environment poses unique challenges since robots must operate in a communication and localization-limited environment where their dynamics are tightly coupled with the environmental dynamics. This work presents current efforts in understanding the impact of geophysical fluid dynamics on underwater vehicle control and autonomy. The focus of the talk is on the use of collaborative vehicles to track Lagrangian coherent structures and to localize contaminant spills.

<sup>1</sup>Research supported by the National Science Foundation and the Office of Naval Research.

**10:24AM A53.00013 Neutral equivalent surface stress** , CHERYL KLIPP, US Army Research Laboratory — In laboratory turbulent flows, it has been observed that the eigen axes of the Reynolds stress tensor are oriented 17 deg from the streamwise coordinate system. This has also been observed in atmospheric flows over relatively flat terrain under thermally neutral conditions. The reliability of this relationship is examined, especially for locations very near the surface. The relationship is then used as the basis for a neutral equivalent momentum transport which can be calculated in complex environments, such as urban canyons, where the influence of multiple wall normals makes more conventional measurement of momentum transport problematic.

**Monday, March 14, 2016 8:00AM - 11:00AM** —

**Session A54 FIAP DMP: Optical Properties of Semiconductor Nanostructures I** Hilton Baltimore Holiday Ballroom 5 - Yong Zhang, UNC - Charlotte

**8:00AM A54.00001 Detection and characterization of semiconductor thin film domains in non linear nearfield regime<sup>1</sup>** , FARBOD SHAFIEI, The University of Texas at Austin, TOMMASO ORZALI, ALEXEY VERT, SEMATECH, MICHAEL DOWNER, The University of Texas at Austin — High carrier mobility in III-V semiconductor films is attractive for electro-optic devices based on Si substrate. The mismatch between thin film and substrate crystal creates defects that affect electron transport in the film. Optical nonlinear (second harmonic generation) technique has been used in search of domains and boundaries that might have connection to these defects. Fiber based nonlinear nearfield scanning optical microscope (NSOM) was used to detect sub-micron domains at surfaces of the films. This local nearfield optical information was compared with bulk farfield optical information and suppression of the domains was observed and studied by controlling the substrate-film interface. Anti phase boundaries, strain, local charge and cavities in connection with these domains are under study.

<sup>1</sup>Supporting Organization: Welch Foundation

**8:12AM A54.00002 Interfacial Stresses and Strains Effect on Band-Gap Emission from Silicon** , SUFIAN ABEDRABBO, The Petroleum Institute and The University of Jordan, ANTHONY FIORY, New Jersey Institute of Technology — Czochralski silicon wafer materials were interfaced with silica films formed by sol-gel deposition and thermal annealing. Under optimal annealing conditions ( $\sim 700^\circ\text{C}$ ), stresses in the silica films induce variations in elastic strains on the order of 1% in the silicon. Concomitantly, emission of band-gap photons at 1.1 eV observed by photoluminescence is increased by two orders of magnitude relative to unperturbed silicon. The enhancement in photon emission is produced by band-gap modulations estimated as  $\sim 0.1$  eV. Elastic reversibility of the strains is inferred from recovery of relatively weak photon emission for annealing above the glass reflow temperature of deposited silica films ( $\sim 950^\circ\text{C}$ ). Films with largest stress variations exhibit enhanced absorption signatures in the infrared and broadening of Si-O-Si stretching vibrations. Examples of Si-based photonics based on the observed effect will be presented.

**8:24AM A54.00003 Electronic Raman Scattering as an Ultra-Sensitive Probe of Strain Effects in Semiconductors.**<sup>1</sup> , ANGELO MASCARENHAS, BRIAN FLUEGEL, DAN BEATON, National Renewable Energy Laboratory — Semiconductor strain engineering has become a critical feature of high-performance electronics due to the significant device performance enhancements it enables. These improvements that emerge from strain induced modifications to the electronic band structure necessitate new ultra-sensitive tools for probing strain in semiconductors. Using electronic Raman scattering, we recently showed that it is possible to measure minute amounts of strain in thin semiconductor epilayers. We applied this strain measurement technique to two different semiconductor alloy systems, using coherently strained epitaxial thin films specifically designed to produce lattice-mismatch strains as small as  $10^{-4}$ . Comparing our strain sensitivity and signal strength in  $\text{Al}_x\text{Ga}_{1-x}\text{As}$  with those obtained using the industry-standard technique of phonon Raman scattering we found a sensitivity improvement of 200, and a signal enhancement of  $4 \times 10^3$  thus obviating key constraints in semiconductor strain metrology. The sensitivity of this approach rivals that of contemporary techniques and opens up a new realm for optically probing strain effects on electronic band structure.

<sup>1</sup>We acknowledge the financial support of the DOE Office of Science, BES under DE-AC36-80GO28308

**8:36AM A54.00004 Excitation mechanisms of Er optical centers GaN epilayers** , MATTHEW HAWKINS, Department of Physics, Virginia Tech, Blacksburg, Virginia 24061, HONGXING JIANG, JINGYU LIN, Department of Electrical and Computer Engineering, Texas Tech University, Lubbock, Texas 79409, JOHN ZAVADA, Department of Electrical and Computer Engineering, NYU Polytechnic School of Engineering, Brooklyn, New York 11201, NGUYEN VINH, Department of Physics, Virginia Tech, Blacksburg, Virginia 24061 — We report direct evidence of two mechanisms responsible for the excitation of optically active  $\text{Er}^{3+}$  ions in GaN epilayers grown by metal-organic chemical vapor deposition. These mechanisms, resonant excitation via the higher-lying inner 4f shell transitions and band-to-band excitation of the semiconductor host, lead to narrow emission lines from isolated and the defect-related Er optical centers. However, these centers have different photoluminescence spectra, local defect environments, decay dynamics, and excitation cross sections. The photoluminescence at 1.54 micrometer from the isolated Er optical center which can be excited by either mechanism has the same decay dynamics, but possesses a much higher excitation cross-section under band-to-band excitation. In contrast, the photoluminescence at 1.54 micrometer from the defect-related Er optical center can only be observed through band-to-band excitation but has the largest excitation cross-section. These results explain the difficulty in achieving gain in Er doped GaN and indicate approaches for realization of optical amplification, and possibly lasing, at room temperature.

**8:48AM A54.00005 Spectroscopic characterization of Er optical center in multiple quantum wells  $\text{AlN}/\text{GaN}:\text{Er}$**  , VINH HO, MATTHEW HAWKINS, Department of Physics, Virginia Tech, Blacksburg, Virginia 24061, HONGXING JIANG, JINGYU LIN, Department of Electrical and Computer Engineering, Texas Tech University, Lubbock, Texas 79409, JOHN ZAVADA, Department of Electrical and Computer Engineering, NYU Polytechnic School of Engineering, Brooklyn, New York 11201, NGUYEN VINH, Department of Physics, Virginia Tech, Blacksburg, Virginia 24061 — Er doped GaN material is known to result in the formation of luminescent centers suitable for applications in optoelectronic devices. We report here a significant enhancement of photoluminescence from the Er optical center at 1.5 micrometer in multi-nanolayer structures  $\text{AlN}/\text{GaN}:\text{Er}$  synthesized by metal organic chemical vapor deposition. The enhancement of photoluminescence from Er optical center can be explained via the carrier confinement and strain engineering of multi-nanolayer structures. We study the influence of the quantum wells and barrier width on the photoluminescence at 1.5 micrometer using time-resolved and high-resolution photoluminescence spectroscopy at a large range of temperature. The ability of controlling the carrier confinement in multi-nanolayer structures provides us the possibility of engineering Er doped GaN photonic devices with enhanced optical characteristics at 1.54 micrometer.

**9:00AM A54.00006 Observation of magnetic non-reciprocity for mobile excitons bound to stacking-fault potentials**<sup>1</sup> , KAI-MEI FU, TODD KARIN, XIAYU LINPENG, Univ of Washington, ARNE LUDWIG, ANDREAS WIECK, Ruhr-Universitat Bochum, MIKHAIL GLAZOV, Ioffe Institute — We show that single stacking faults in high-purity GaAs provide the most homogeneous two-dimensional potential for excitons yet reported. The ultra-narrow excitonic transitions enable us to directly observe the microscopic properties of the exciton, including a 0 transverse component of the hole g-factor, which are determined by the  $C_{3v}$  symmetry of the system. A surprising magnetic non-reciprocity effect, in which the energy of the detected excitonic emission depends on the sign of the magnetic field, is also observed. This effect is due to conservation of the exciton two-dimensional momentum in the process of light emission and provides direct evidence that excitons are mobile in this novel potential.

<sup>1</sup>This material is based upon work supported by the NSF under Grant Number 1150647 and the NSF Graduate Research Fellowship under grant number DGE-1256082.

**9:12AM A54.00007 Exploration of exciton delocalization in organic crystalline thin films**<sup>1</sup> , KIM HUA, LANE MANNING, NAVEEN RAWAT, VICTORIA AINSWORTH, MADALINA FURIS, Material Science Program and the Department of Physics, University of Vermont — The electronic properties of organic semiconductors play a crucial role in designing new materials for specific applications. Our group recently found evidence for a rotation of molecular planes in phthalocyanines that is responsible for the disappearance of a delocalized exciton in these systems for  $T > 150\text{K}$ .....<sup>1</sup> In this study, we attempt to tune the exciton delocalization of small organic molecules using strain effects and alloying different molecules in the same family. The exciton behavior is monitored using time- and polarization resolved photoluminescence (PL) spectroscopy as a function of temperature. Specifically, organic crystalline thin films of octabutoxy phthalocyanine ( $\text{H}_2\text{OBPC}$ ), octyloxy phthalocyanines and H-bonded semiconductors such as the quinacridone and indigo derivatives are deposited on flexible substrates (i.e. Kapton and PEN) using an in-house developed pen-writing method.....<sup>2</sup> that results in crystalline films with macroscopic long range order. The room temperature PL studies show redshift and changes in polarization upon bending of the film. Crystalline thin films of alloyed  $\text{H}_2\text{OBPC}$  and octabutoxy naphthalocyanine with ratios ranging from 1:1 to 100:1 fabricated on both sapphire and flexible substrates are also explored using the same PL spectroscopy to elucidate the behaviors of delocalized excitons. .<sup>1</sup>N. Rawat, et al., J Phys Chem Lett **6**, 1834 (2015). <sup>2</sup>R. L. Headrick, et al., Applied Physics Letters **92**, 063302 (2008).

<sup>1</sup>NSF DMR - 1056589, NSF DMR - 1062966

**9:24AM A54.00008 Collective magneto-polariton excitation in a terahertz photonic cavity** , QI ZHANG, MINHAN LOU, XINWEI LI, Rice University, ANDREY CHABANOV, University of Texas at San Antonio, JOHN RENO, WEI PAN, Sandia National Laboratory, JOHN WATSON, MICHAEL MANFRA, Purdue University, JUNICHIRO KONO, Rice University — Collective excitations in solids offer new opportunities for quantum optical studies. Many-body interactions inherent to condensed matter systems can lead to novel phenomena that cannot be achieved in traditional atomic systems. Here, we report collective ultrastrong light-matter coupling in a two-dimensional electron gas in a high- $Q$  terahertz photonic-crystal cavity in a magnetic field. We directly observed time-domain vacuum Rabi oscillations, whose frequency was found to be proportional to the square root of  $N$  (where  $N$  is the carrier density), evidence for the *collective* nature of ultrastrong coupling. In addition, a small but definite blue shift due to the diamagnetic term in the Hamiltonian was observed for the polariton frequencies, which is another signature of ultrastrong light-matter coupling. Furthermore, the high- $Q$  cavity suppressed the superradiant decay of cyclotron resonance, which resulted in unprecedentedly narrow intrinsic cyclotron resonance linewidths ( $\sim 5.6$  GHz at 2 K). Our method is also applicable to many classes of strongly correlated systems with collective many-body excitations in the terahertz range, opening a door to the fascinating physics of terahertz many-body cavity QED.

**9:36AM A54.00009 Multidimensional spectroscopy of exciton polaritons in a microcavity** , BRIAN WILMER, Department of Physics, West Virginia University, FELIX PASSMANN, Experimentelle Physik 2, TU Dortmund, MICHAEL GEHL, GALINA KHITROVA, College of Optical Sciences, The University of Arizona, ALAN BRISTOW, Department of Physics, West Virginia University, WEST VIRGINIA UNIVERSITY COLLABORATION, TU DORTMUND COLLABORATION, UNIVERSITY OF ARIZONA COLLABORATION — Two-dimensional coherent spectra map the anticrossing associated with normal-mode splitting in a semiconductor microcavity [1]. For a 12-meV detuning range near zero detuning, it is observed that there are two diagonal features related to the intra-action of exciton-polariton branches and two off-diagonal features related to coherent interaction between the polaritons. A biexcitonic companion feature is observed, shifted from the exciton feature by the biexciton binding energy. Closer to zero detuning, all features are enhanced and the diagonal intra-action features become nearly equal in amplitude and linewidth. Off-diagonal interaction features are strongly modulated (and invert) at small positive detuning, as the lower polariton branch crosses the bound biexciton energy determined from negatively detuned spectra. This Feshbach type behavior is further evidenced by strong polarization dependence. By exploiting selection rules, the quantum pathways can be more rigorously controlled, allowing the Feshbach coupling to be switched on or off as well as elucidating the role spin and two-quantum states play in the exciton-polariton system.  
[1]. Wilmer et al, Phys. Rev. B 91, 201304(R) (2015)

**9:48AM A54.00010 Indentation-induced structural phase transformations of semiconductor materials and applications**<sup>1</sup> , MAHA KHAYYAT, KACST assignee, NORMA SOSA, IBM assignee, M. MUNAWAR CHAUDHRI, University of Cambridge, CAVENDISH LABORATORY, UNIVERSITY OF CAMBRIDGE TEAM, T. J. WATSON RESEARCH CENTER, IBM COLLABORATION — During hardness indentation materials are subjected to highly localized pressures. These pressures may cause a complete change of the crystal structure of the material within the indented zone. Such structural phase transformations were observed within Vickers indentations made at room temperature in single crystals and amorphous films of Si and Ge. However, when indentations were made at 77 K in Si and Ge, no phase transitions were observed in either. Measurements were also taken from indentations made in silicon single crystals at different temperatures namely 263, 243, 235 and 206 K, and they showed a strong correlation of phase transformation with temperature. It was suggested that during room temperature indentations there is a significant temperature rise approximately to 760 K, which may assist phase transformation. Raman spectroscopy was used as an *ex-situ* tool monitoring phase transformations in semiconductor materials. *In-situ* electrical characterizations of indentation-induced metallization in single crystals of silicon were performed using two- and four-contact measurements. The previous work has led to a technique relates to semiconductor device manufacturing, including solar cells, which is a method for controlling the removal of a surface layer from a base substrate utilizing low-temperature.

<sup>1</sup>KACST is acknowledged for support

**10:00AM A54.00011 Photon correlations through Raman virtual processes**<sup>1</sup> , REINALDO DE MELO E SOUZA, Univ Fed Rio de Janeiro, ANDRE SARAIVA, BELITA KOILLER, UFRJ — In Raman inelastic scattering phonons are either absorbed or created, in what is respectively called an anti-Stokes (aS) or a Stokes (S) process. While these two processes are generally uncorrelated, it is possible that the same phonon generated by S is subsequently absorbed by aS. This two photon process is referred to as SaS. In a standard Raman process, conservation of energy forbids virtual phonons to play a role. However, in a SaS process these virtual phonons may be relevant as long as their lifetimes exceed the interval between the two scatterings. We derive the effective photon-photon interaction mediated by the phonon field. The effective hamiltonian is analogue to the one present in BCS superconductivity. The difference lies in the nature of the particles involved – since photons are bosons, there is no Fermi sea instability and no pair condensation. Still it is possible to obtain an attractive photon-photon interaction. Finally, we propose an experiment to detect the correlated photons emerging from a semiconductor. We pinpoint the material properties that might enhance this effect and discuss the possible technological applications of this idea as a correlated photon source.

<sup>1</sup>This work is part of the Brazilian National Institute for Science and Technology on Quantum Information. We also acknowledge partial support from the Brazilian agencies FAPERJ, CNPq and CAPES.

**10:12AM A54.00012 Calculating Effect of Point Defects on Optical Absorption Spectra of III-V Semiconductor Superlattices Based on (8x8) k-dot-p Band Structures** , DANHONG HUANG, Air Force Rsch Lab-Kirtland, ANDRII IUROV, University of New Mexico, GODFREY GUMBS, Hunter College of the City University of New York, DAVID CARDIMONA, Air Force Rsch Lab-Kirtland, SANJAY KRISHNA, University of New Mexico — For a superlattice which is composed of layered zinc-blende structure III-V semiconductor materials, its realistic anisotropic band structures around the Gamma-point are calculated by using the (8x8)k-dot-p method with the inclusion of the self-consistent Hartree potential and the spin-orbit coupling. By including the many-body screening effect, the obtained band structures are further employed to calculate the optical absorption coefficient which is associated with the interband electron transitions. As a result of a reduced quasiparticle lifetime due to scattering with point defects in the system, the self-consistent vertex correction to the optical response function is also calculated with the help of the second-order Born approximation.

**10:24AM A54.00013 Many-body Effects and the Role of Indirect Excitons in Asymmetric InGaAs/GaAs Double Quantum Wells** , CHRISTOPHER SMALLWOOD, JILA, University of Colorado, NIST, TAKESHI SUZUKI, ROHAN SINGH, Dept. of Physics, University of Michigan, TRAVIS AUTRY, MATTHEW DAY, JILA, University of Colorado, NIST, FAUZIA JABEEN, Laboratory of Quantum Optoelectronics, cole Polytechnique Fdrale de Lausanne (EPFL), STEVEN CUNDIFF, Dept. of Physics, University of Michigan — In semiconductor research, a fundamental question is how excitons in nearby but distinct spatial locations interact and exchange energy. In quantum well heterostructures, these interactions can be conveniently probed via optical coherent multidimensional spectroscopy (CMDS). Recently, it has been shown using CMDS that reducing the GaAs barrier from 30 nm to 10 nm between two asymmetric InGaAs quantum wells results in interactions driven by many-body effects. Here, we use the technique to show that for narrower barrier thicknesses, the interactions are accompanied by an emergence of spatially indirect excitons. Quantitative measurements of the effects are presented, which will be useful in tailoring GaAs heterostructure devices, and may also inform the role that excitonic interactions play in more complicated systems like microcavity polariton structures and/or photosynthetic light harvesting complexes.

**10:36AM A54.00014 Coupled Plasmon Phonon Dynamics in GaP: an indirect gap polar semiconductor.**<sup>1</sup> , AVINASH RUSTAGI, EVAN M. THATCHER, CHRISTOPHER J. STANTON, Univ of Florida - Gainesville, KUNIE ISHIOKA, National Institute for Materials Science, Tsukuba, Japan, KRISTINA BRIXIUS, ULRICH HOFER, Philipps University, Germany, HRVOJE PETEK, Univ of Pittsburgh — Transient Depletion Field Screening (TDFS) is the dominant mechanism behind coupled plasmon-phonon oscillations in polar semiconductors for above gap photoexcitation. Here the surface field distorting the polar lattice is screened by photoexcited plasma initiating coupled oscillations. These oscillations modify the optical property of the material and are observed in reflectivity measurements. We model these oscillations via a set of coupled differential equations in electronic polarization and lattice polarization. We consider the effects of lateral inhomogeneity and diffusion of photoexcited carriers which is crucial to understand the experimental results. The spectrum shows an LO(Longitudinal Optical) phonon peak alongside a LOPC(Longitudinal Optical Plasmon Coupled) peak. Lateral inhomogeneity accounts for the beating phenomenon between these frequencies.

<sup>1</sup>Supported by NSF through grants DMR-1311849 and DMR-1311845.

**10:48AM A54.00015 GaAs Refractive Index Dependence On Carrier Density and Optimizing Terahertz Devices**, CHRISTOPHER KIM, DONG HO WU, BENJAMIN GRABER, US Naval Research Laboratory — GaAs is used for various applications, including high speed transistors, high-efficiency photovoltaic cells, electro-optics and terahertz (THz) emitters and detectors. To date, information on the refractive index of GaAs is available only over a limited wave spectrum of 0.2-17 $\mu$ m, where the refractive index varies from 1.3 to 5.0. As detailed information on the refractive index of GaAs at THz frequencies is not available or inadequate for our effort to develop an improved GaAs-based THz emitter, we experimentally investigated the behavior of the refractive index of GaAs for different charge carrier densities, especially with or without the presence of surface plasma. Using a Time Domain THz Spectrometer, which is capable of measuring THz pulses containing a wave spectrum over 100-3000 $\mu$ m with a time accuracy better than 6 femtoseconds, we measured the delay of THz pulses traversing through a GaAs substrate of known thickness while modulating the charge carrier concentration. From the experimental data we estimated the refractive index for THz frequencies to vary from 3.5 to 3.8 for different charge carrier concentrations. We will discuss details of our experiments and implications of our experimental results, especially for our GaAs-based THz devices.

**Monday, March 14, 2016 8:00AM - 11:00AM –**

**Session A55 DBIO: Quantitative Immunology** Hilton Baltimore Holiday Ballroom 6 - Anton Zilman, University of Toronto

**8:00AM A55.00001 Signaling reactions on membrane surfaces: breaking the law of averages**, JAY T. GROVES, Dept. of Chemistry, UC Berkeley — Most intracellular signal transduction reactions take place on the membrane surface. The membrane provides much more than just a surface environment on which signaling molecules are concentrated. There is a growing realization that multiple physical and chemical mechanisms allow the membrane to actively participate in the signaling reactions. Using a combination of single molecule imaging and spectroscopic techniques, my research seeks to directly resolve the actual mechanics of signaling reactions on membrane surfaces both in reconstituted systems and in living cells. These observations are revealing new insights into cellular signaling processes as well as some unexpected functional behaviors of proteins on the membrane surface.

**8:36AM A55.00002 Physics of building an immunological synapse**, MICHAEL L. DUSTIN, New York University — The adaptive immune response depends upon interaction of T cell antigen receptor (TCR) and peptide-MHC complexes in the nanometer scale (15 nm) gap between the T cell and antigen presenting cells. This immunological synapse is built on a foundation of cell adhesion molecules (CAMs). Short CAM pairs (15 nm) and long CAM pairs (~30 nm) work in parallel to form immunological synapses under control of antigen receptor signaling. The engaged antigen receptor recruits tyrosine kinases to initiate formation of multicomponent signaling complexes that also incorporate F-actin foci. The physical process by which ligand binding to the TCR ligand in the context of the immunological synapse triggers the kinase cascade is not clear. Self-assembly of CAMs to form terraced junctions- with 15 nm and larger spacing between membranes in different positions, may contribute to triggering. We demonstrated segregation of the short and long CAMs in a model synapse in 1998, which was complementary to results from Kupfer demonstrating a bull's eye organization of TCR in the center surrounded by a ring of long CAMs- described as supramolecular activation clusters (SMACs), but corresponding to the predicted terraces. We can directly observe tyrosine kinase recruitment to the TCR complex and the dependence of this recruitment on the strength of interaction of TCR and peptide-MHC. Experimental manipulation of CAM length can predictably alter the effective 2D affinity, lateral mobility and the organization of other associated elements in a size dependent manner. We have developed a general model and will discuss supporting experimental data and implications for immunological synapse assembly in this talk and a related poster.

In collaboration with Christopher Peel, David Depoil and Omer Dushek Kennedy Institute of Rheumatology, The University of Oxford, Oxford, UK and Skirball Institute of Biomolecular Medicine, New York University School of Medicine, NY, USA

**9:12AM A55.00003 Lineage-tracking of stem cell differentiation: a neutral model of hematopoiesis in rhesus macaque<sup>1</sup>**, TOM CHOU<sup>2</sup>, Univ of California - Los Angeles — How a potentially diverse population of hematopoietic stem cells (HSCs) differentiates and proliferates to supply more than  $10^{11}$  mature blood cells every day in humans remains a key biological question. We investigated this process by quantitatively analyzing the *clonal* structure of peripheral blood that is generated by a population of transplanted lentivirus-marked HSCs in myeloablated rhesus macaques. Each transplanted HSC generates a clonal lineage of cells in the peripheral blood that is then detected and quantified through deep sequencing of the viral vector integration sites (VIS) common within each lineage. This approach allowed us to observe, over a period of 4-12 years, hundreds of distinct clonal lineages. Surprisingly, while the distinct clone sizes varied by three orders of magnitude, we found that collectively, they form a steady-state clone size-distribution with a distinctive shape. Our concise model shows that slow HSC differentiation followed by fast progenitor growth is responsible for the observed broad clone size-distribution. Although all cells are assumed to be statistically identical, analogous to a neutral theory for the different clone lineages, our mathematical approach captures the intrinsic variability in the times to HSC differentiation after transplantation. Steady-state solutions of our model show that the predicted clone size-distribution is sensitive to only two combinations of parameters. By fitting the measured clone size-distributions to our mechanistic model, we estimate both the effective HSC differentiation rate and the number of active HSCs.

<sup>1</sup>NSF and NIH

<sup>2</sup>Work done in collaboration with S. Goyal, S. Kim, and I. Chen

**9:48AM A55.00004 Specificity, cross-talk and adaptation in Interferon signaling**, ANTON ZILMAN, University of Toronto — Innate immune system is the first line of defense of higher organisms against pathogens. It coordinates the behavior of millions of cells of multiple types, achieved through numerous signaling molecules. This talk focuses on the signaling specificity of a major class of signaling molecules - Type I Interferons - which are also used therapeutically in the treatment of a number of diseases, such as Hepatitis C, multiple sclerosis and some cancers. Puzzlingly, different Interferons act through the same cell surface receptor but have different effects on the target cells. They also exhibit a strange pattern of temporal cross-talk resulting in a serious clinical problem - loss of response to Interferon therapy. We combined mathematical modeling with quantitative experiments to develop a quantitative model of specificity and adaptation in the Interferon signaling pathway. The model resolves several outstanding experimental puzzles and directly affects the clinical use of Type I Interferons in treatment of viral hepatitis and other diseases.

**10:24AM A55.00005 Within-host co-evolution of chronic viruses and the adaptive immune system**, ARMITA NOURMOHAMMAD, Princeton University — We normally think of evolution occurring in a population of organisms, in response to their external environment. Rapid evolution of cellular populations also occurs within our bodies, as the adaptive immune system works to eliminate infection. Some pathogens, such as HIV, are able to persist in a host for extended periods of time, during which they also evolve to evade the immune response. In this talk I will introduce an analytical framework for the rapid co-evolution of B-cell and viral populations, based on the molecular interactions between them. Since the co-evolution of antibodies and viruses is perpetually out of equilibrium, I will show how to quantify the amount of adaptation in each of the two populations by analysis of their co-evolutionary history. I will discuss the consequences of competition between lineages of antibodies, and characterize the fate of a given lineage dependent on the state of the antibody and viral populations. In particular, I will discuss the conditions for emergence of highly potent broadly neutralizing antibodies, which are now recognized as critical for designing an effective vaccine against HIV.

**Monday, March 14, 2016 9:30AM - 10:30AM –**

**Session A56 APS: Keynote Address: Secretary Moniz** Hilton Baltimore Key Ballroom 5-8 - Homer Neal, University of Michigan APS President

**9:30AM A56.00001 Keynote Address** , ERNEST MONIZ, United States Department of Energy —

**Monday, March 14, 2016 11:15AM - 2:15PM –**

**Session B1 DCMP: Condensed Matter Physics at NSF/DMR and DOE/BES: Challenges and Opportunities** Ballroom I - Tomasz Durakiewicz, Jim Horwitz, NSF/DMR , DOE/BES

**11:15AM B1.00001 Reflections on the past, present and future of condensed matter physics** , ANTHONY LEGGETT, Department of Physics, University of Illinois Urbana Champaign — I consider some of the ways in which the practice and even the definition of "condensed-matter physics" has evolved since its inception in the early twentieth century, with particular reference to its relationship to neighboring and even distant disciplines. I speculate on some possible directions in which the discipline may develop over the next few decades, emphasizing that there are still some very basic questions to which we currently have no satisfactory answers.

**11:51AM B1.00002 The NSF Condensed Matter Physics Program** , PAUL SOKOL, Division of Materials Research, National Science Foundation — The Condensed Matter Physics (CMP) program in the NSF Division of Materials Research (DMR) supports experimental, as well as combined experiment and theory projects investigating the fundamental physics behind phenomena exhibited by condensed matter systems. CMP is the largest Individual Investigator Award program in DMR and supports a broad portfolio of research spanning both hard and soft condensed matter. Representative research areas include: 1) phenomena at the nano- to macro-scale including: transport, magnetic, and optical phenomena; classical and quantum phase transitions; localization; electronic, magnetic, and lattice structure or excitations; superconductivity; topological insulators; and nonlinear dynamics. 2) low-temperature physics: quantum fluids and solids; 1D & 2D electron systems. 3) soft condensed matter: partially ordered fluids, granular and colloid physics, liquid crystals, and 4) understanding the fundamental physics of new states of matter as well as the physical behavior of condensed matter under extreme conditions e.g., low temperatures, high pressures, and high magnetic fields. In this talk I will review the current CMP portfolio and discuss future funding trends for the program. I will also describe recent activities in the program aimed at addressing the challenges facing current and future principal investigators.

**12:27PM B1.00003 DOE/BES Experimental Condensed Matter Physics program** , MICHAEL PECHAN, US Department of Energy — This talk will provide an overview of the Experimental Condensed Matter Physics Program in the Office of Basic Energy Sciences of the US Department of Energy. The role of ECMP within DOE, current priorities, highlights, and challenges will be discussed.

**1:03PM B1.00004 The NSF Condensed Matter and Materials Theory Program** , DARYL HESS, National Science Foundation — The Condensed Matter and Materials Theory (CMMT) Program in the Division of Materials Research is the home of condensed matter theory at the National Science Foundation. CMMT awards reflect a vibrant community with expanding scientific horizons and opportunities. I will present an overview of the CMMT program. Opportunities for theory and computation to open new directions and stimulate emerging frontiers will be discussed. Engaging research across disciplinary boundaries maintains the vitality of the field, leads to an agile next generation of theoretical and computational condensed matter physicists, and advances understanding of the world on the scale of life.

**1:39PM B1.00005 DOE/BES Theoretical Condensed Matter Physics Program** , JAMES DAVENPORT, US Department of Energy — This talk will provide an overview of the Theoretical Condensed Matter Physics Program in the Office of Basic Energy Sciences of the US Department of Energy. The role of theory in DOE, current priorities, highlights, and challenges will be discussed.

**Monday, March 14, 2016 11:15AM - 2:15PM –**

**Session B2 GSOF DPOLY GSNP: The Edwards Statistical Mechanics** Ballroom II - Fyl Pincus, University of California, Santa Barbara

**11:15AM B2.00001 Numerical calculation of granular entropy: counting the uncountable.** , DAAN FRENKEL, U. Cambridge — In 1989, Sir Sam Edwards introduced the concept of 'granular entropy', defined as the logarithm of the number of distinct packings of  $N$  granular particles in a fixed volume  $V$ . The proposal was rather controversial but much of the debate was sterile because the granular entropy could not even be computed for systems as small as 20 particles - hardly a good approximation of the thermodynamic limit. In my talk I will describe how granular entropies of much larger systems can now be computed, using a novel algorithm. Interestingly, it turns out the definition of granular entropy will have to be modified to guarantee that granular entropy is extensive.

**11:51AM B2.00002 Granular statistical mechanics – Building on the legacy of Sir Sam Edwards**<sup>1</sup> , RAPHAEL BLUMENFELD, National University of Defense Technology, Changsha and Imperial College London, UK, Co-Author, Shahar Amitai, Imperial College London, UK — When Sir Sam Edwards laid down the foundations for the statistical mechanics of jammed granular materials he opened a new field in soft condensed matter and many followed. In this presentation we review briefly the Edwards formalism and some of its less discussed consequences. We point out that the formalism is useful for other classes of systems - cellular and porous materials. A certain shortcoming of the original formalism is then discussed and a modification to overcome it is proposed. Finally, a derivation of an equation of state with the new formalism is presented; the equation of state is analogous to the PVT relation for thermal gases, relating the volume, the boundary stress and measures of the structural and stress fluctuations.

<sup>1</sup>NUDT, Changsha, China, Imperial College London, UK, Cambridge University, UK

**12:27PM B2.00003 Unifying Suspensions and Inertial Granular flows near Jamming**, WYART MATTHIEU, Institute of Theoretical Physics, Ecole Polytechnique Federale de Lausanne — Observations support that the fluid to solid transition in granular materials is a continuous transition, with diverging length scales and singular flow curves. I will introduce a framework that predict quantitatively scaling exponents near this transition when particles are frictionless. This framework captures both aerial granular flows and over-damped suspensions, phenomena traditionally studied by two distinct communities.

In this description, the dense fluid phase can be thought as a gas of excitations of the solid phase. Key aspects of the solid entering the description can be obtained by dynamical argument, and imply that the solid is marginally stable. Recent calculations in infinite spatial dimension support however that thermodynamics arguments a la Edwards also capture this marginality.

**1:03PM B2.00004 Soft active matter : a contemporary example of Edwardsian statistical mechanics**<sup>1</sup>, TANNIEMOLA LIVERPOOL, University of Bristol — Colonies of swimming bacteria, algae or spermatozoa are examples of active systems composed of interacting units that consume energy and collectively generate motion and mechanical stresses. Due to the anisotropy of their interactions, these active particles can exhibit orientational order at high concentrations and have been called living liquid crystals<sup>2</sup>. Biology at the cellular and multicellular scale provides numerous examples of these active systems. They provide a novel class of experimentally accessible system far from equilibrium. Their rich collective behaviour includes non-equilibrium phase transitions and pattern formation on mesoscopic scales. Interestingly however, some of the theoretical insights gained from field theories applied to equilibrium soft matter systems can be used to explain aspects of their behaviour, but with a number of surprising new twists. I will describe and summarise recent theoretical results characterising the behaviour of such soft active systems highlighting in particular the effects of their internal dynamics on their macroscopic behaviour.

<sup>1</sup>with support of the EPSRC Grant No. EP/G026440/1

**1:39PM B2.00005 Thinking Outside the Sandbox**, JASNA BRUJIC, New York Univ NYU — Theoretical approaches for inherently out-of-equilibrium systems, from granular to live matter, are at the forefront of soft condensed matter physics. Edwards pioneered a statistical mechanics framework to describe jammed particulate materials, which explains the slow compaction of granular materials towards a given density, the reversibility of such experiments, and the equilibration between shaken powders of different types. During my PhD, Edwards's theoretical work inspired me to develop a transparent emulsion system to test the microscopic distributions underlying granular thermodynamics. I will talk about what it was like to have Sir Sam as a PhD adviser and how he uniquely inspired my curiosity to design and build novel materials, which are not random, but assemble via mobile, multiflavored bonds that respond to environmental queues. I will give an overview of this kind of experimentally guided assembly these results call for new theories of emulsions with programmable architectures.

**Monday, March 14, 2016 11:15AM - 2:15PM —**

**Session B3 DCMF: Symmetry Breaking in Unconventional Superconductors** Ballroom III - Sauls James, Northwestern University

**11:15AM B3.00001 Signatures of time reversal symmetry breaking in multiband superconductors**, SAURABH MAITI, University of Florida — Multiband superconductors serve as natural host to several possible ground states that compete with each other. At the boundaries of such competing phases, the system usually compromises and settles for 'mixed' phases that can show intriguing properties like co-existence of magnetism and superconductivity or even co-existence of different superconducting phases. The latter is particularly interesting as it can lead to non-magnetic ground states that spontaneously break Time-Reversal symmetry. While the experimental verification of such states has proved to be challenging, the theoretical investigations have provided exciting new insights into the nature of the ground state and its excitations all of which have experimental consequences of some sort. These include extrinsic properties like spontaneous currents around impurity sites, and intrinsic properties in the form of collective excitations. These collective modes bear a unique signature and should provide clear evidence for time reversal symmetry broken state. While the results are general, in light of recent Raman scattering experiments, its direct relevance to extremely hole doped  $\text{Ba}_{(1-x)}\text{K}_x(\text{FeAs})_2$  will be presented where a strong competition of  $s$ -wave and  $d$ -wave ground state is expected.

**11:51AM B3.00002 Strain-tuning through a possible van Hove singularity in  $\text{Sr}_2\text{RuO}_4$** , CLIFFORD HICKS, Max Planck Institute for Chemical Physics of Solids — The superconducting transition temperature  $T_c$  of the tetragonal compound  $\text{Sr}_2\text{RuO}_4$  was recently shown to be strongly sensitive to  $\langle 100 \rangle$  orthorhombic distortion:  $T_c$  increases strongly both when  $\text{Sr}_2\text{RuO}_4$  is tensioned and compressed along a  $\langle 100 \rangle$  direction. This sensitivity was tentatively attributed to the proximity of one of its Fermi surface sheets to van Hove singularities (vHS): the sections of this sheet that pass closest to the Brillouin zone boundaries are also those perturbed most strongly by  $\langle 100 \rangle$  orthorhombic distortion. By increasing the applied orthorhombic distortion to 0.5–1.0% — a uniaxial pressure almost certainly above 1 GPa — we have now been able to tune through a sharp peak in both  $T_c$  and the upper critical field,  $H_{c2}$ . At the peak,  $T_c$  more than doubles. The peak is at a strain value consistent with predictions for when the Fermi surface contacts the zone boundary, i.e. the van Hove singularity, although concrete verification will require further measurement. The strength of the enhancement of  $H_{c2}$  may have bearing on the symmetry of the order parameter. The large change in properties at this peak mean that it can almost be considered as a new, unexplored material, opening avenues for future research.

**12:27PM B3.00003 Is  $\text{Sr}_2\text{RuO}_4$  a chiral p-wave superconductor? Insights from edge currents and uniaxial strain**, THOMAS SCAFFIDI, University of Oxford — The prevailing candidate for the superconducting order parameter in  $\text{Sr}_2\text{RuO}_4$  is chiral p-wave and signatures of this phase have been looked for experimentally. In this work, we discuss two of these experiments at the light of theoretical results obtained from a weak coupling RG calculation. First, we show that the most favored chiral superconducting order parameter in  $\text{Sr}_2\text{RuO}_4$  has Chern number  $C=7$  in the weak coupling limit, owing to a dominant longer range pairing. Since it was shown that the edge currents of a  $C=1$  superconductor vanish exactly in the continuum limit, and can be strongly reduced on the lattice, this form of order parameter could help resolve the conflict between experimental observation of time-reversal symmetry breaking and yet the absence of observed edge currents in  $\text{Sr}_2\text{RuO}_4$ . Second, the p-wave order parameter obtained from the RG calculation exhibits a large  $T_c$  enhancement under uniaxial strain along 100. This enhancement is symmetric for tensile and compressive strain, and shows no measurable cusp at zero strain, in agreement with experiments. The absence of such a cusp is therefore not incompatible with a chiral p-wave state. Finally, we make predictions about the evolution of the superconducting state as a Van Hove singularity is crossed at larger strain.

**1:03PM B3.00004 Study of the Topological-insulator-based Topological Superconductors<sup>1</sup>**, DONG QIAN, Shanghai Jiao Tong University — Three-dimensional topological insulators possess nontrivial spin-momentum locked surface states under the protection of time-reversal symmetry. The interplay between topological order and superconductivity can lead to topological superconducting state. In this talk, I will discuss our recent progress in topological-insulator-based topological superconductors. Using molecular beam epitaxy (MBE) method, we succeeded in fabricating very high quality TI/s-wave superconductor heterostructure by growing topological insulator thin films on the conventional superconductor niobium diselenide (NbSe<sub>2</sub>) substrate. Using low temperature scanning tunneling microscopy/spectroscopy (STM/STS) and angle-resolved photoemission spectroscopy (ARPES), we systematically studied its electronic structure and superconducting behavior. Through superconducting proximity effect, coexistence of Cooper pairs and topological surface states on the surface of topological insulator film was realized. By exploring the superconducting vortex core state as the function of film thickness, existing of nontrivial superconducting state on the TI's surface was proposed. Our topological insulator/superconductor heterostructure may host single zero-energy Majorana mode in the vortex core. In addition, I will also discuss STM and ARPES studies on the recently discovered superconducting Sr-doped Bi<sub>2</sub>Se<sub>3</sub> bulk crystals. Our results suggest that Sr-doped Bi<sub>2</sub>Se<sub>3</sub> could be an excellent candidate for exploring topological superconducting states.

<sup>1</sup>Supported by the Ministry of Science and Technology of China and NSFC

**1:39PM B3.00005 Proximity-induced Superconductivity in Topological Insulator/Superconductor Heterostructures<sup>1</sup>**, NITIN SAMARTH, Dept. of Physics, Penn State University, University Park PA 16802 — The exploration of superconductivity in helical Dirac fermions is strongly motivated by scenarios for realizing exotic quantum states in condensed matter. Examples include Majorana modes [1] and supersymmetry [2]. Motivated by such proposals, we are pursuing the development of epitaxially grown heterostructures wherein we attempt to induce superconductivity in the surface states of a three dimensional topological insulator thin film when interfaced with both conventional [3] and unconventional [4] superconductors. This talk will provide an overview of the materials synthesis challenges in this context and discuss the picture of induced superconductivity (or lack thereof) that emerges from angle-resolved photoemission spectroscopy [3,4], point contact Andreev reflection spectroscopy [5] and tunneling spectroscopy. Work done in collaboration with A. Richardella, S.-Y. Xu, M. Z. Hasan, M. Gilbert, F.-C. Chou, G. Gu, W.-Q. Dai and Qi Li.  
 1. X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. **83** 1057 (2011).  
 2. T. Grover, D. N. Sheng, A. Vishwanath, Science **344**, 280 (2014).  
 3. S.-Y. Xu *et al.*, Nature Physics **10**, 943 (2014).  
 4. S.-Y. Xu *et al.*, Phys. Rev. B **90**, 085128 (2014).  
 5. W.-Q. Dai *et al.*, in preparation.

<sup>1</sup>Supported by ARO/MURI grant W911NF-12-1-0461

## Monday, March 14, 2016 11:15AM - 2:15PM –

**Session B4 DPOLY: Macromolecular Assemblies: Structure and Dynamics** Ballroom IV - Nitash Balsara, Univ of California - Berkeley

**11:15AM B4.00001 Dynamics of Chain Exchange in Block Copolymer Micelles**, TIMOTHY LODGE, University of Minnesota — Block copolymer micelles are rarely at equilibrium. The primary reason is the large number of repeat units in the insoluble block,  $N_{core}$ , which makes the thermodynamic penalty for extracting a single chain ("unimer exchange") substantial. As a consequence, the critical micelle concentration (CMC) is rarely accessed experimentally; however, in the proximity of a critical micelle temperature (CMT), equilibration is possible. We have been using time-resolved small angle neutron scattering (TR-SANS) to obtain a detailed picture of the mechanisms and time scales for chain exchange, at or near equilibrium. Our model system is poly(styrene)-*block*-poly(ethylene-*alt*-propylene) (PS-PEP), in the PEP-selective solvent squalane (C<sub>30</sub>H<sub>62</sub>). Equivalent micelles with either normal (hPS) or perdeuterated (dPS) cores are initially mixed in a blend of isotopically substituted squalane, designed to contrast-match a 50:50 hPS:dPS core. Samples are then annealed at a target temperature, and chain exchange is revealed quantitatively by the temporal decay in scattered intensity. The rate of exchange as function of concentration, temperature,  $N_{core}$ ,  $N_{corona}$ , and chain architecture (diblock versus triblock) will be discussed.

**11:51AM B4.00002 Assemblies of Cellulose Nanocrystals.**, EUGENIA KUMACHEVA, University of Toronto — The entropically driven coassembly of nanorods (cellulose nanocrystals, CNCs) and different types of nanoparticles (NPs), including dye-labeled latex NPs, carbon dots and plasmonic NPs was experimentally studied in aqueous suspensions and in solid films. In mixed CNC-NP suspensions, phase separation into an isotropic NP-rich and a chiral nematic CNC-rich phase took place; the latter contained a significant amount of NPs. Drying the mixed suspension resulted in CNC-NP films with planar disordered layers of NPs, which alternated with chiral nematic CNC-rich regions. In addition, NPs were embedded in the chiral nematic domains. The stratified morphology of the films, together with a random distribution of NPs in the anisotropic phase, led to the films having close-to-uniform fluorescence, birefringence, and circular dichroism properties.

**12:27PM B4.00003 Mega-supramolecules for safer, cleaner fuel**, JULIE KORNFIELD, Invited Speaker — Guided by the statistical mechanics of ring-chain equilibrium, we designed and synthesized polymers that self-assemble into "mega-supramolecules" ( $\geq 5,000$  kg/mol) at low concentration ( $\leq 0.3\%$ wt) in hydrocarbon liquids. Experimental results accord with model predictions that end-functional polymers, which distribute among cyclic and linear supramolecules, can form a significant population of mega-supramolecules at low total polymer concentration—if, and only if, the backbones are long ( $>400$  kg/mol) and end-association strength is optimal ( $16-18kT$ ). Hydrocarbon liquid fuels are the world's dominant power source (34% of global energy consumption). Transportation relies heavily on such liquids, presenting the risk of explosive post-impact fires. The collapse of the World Trade Center on September 11, 2001 inspired us to revisit polymers for mist control to mitigate post-impact fuel explosions. Rheological and both light and neutron scattering measurements of long end-functional polymers having polycyclooctadiene backbones and acid or amine end groups verify formation of mega-supramolecules. Post-impact flame propagations experiments show that mega-supramolecules control misting. Turbulent flow measurements show that mega-supramolecules reduce drag like ultra-long covalent polymers. With individual building blocks short enough to avoid hydrodynamic chain scission ( $400 < M_w$  [kg/mol]  $\leq 1,000$ ) and reversible linkages that protect covalent bonds, they respond reversibly to flow through pumps and filters without degradation. Mega-supramolecules had no adverse effect on power output, fuel efficiency or emissions in diesel engines. In fact, they gave a 12% reduction in diesel soot. Thus, long end-associative polymers may open the way to fuel additives that reduce pollution and improve transportation safety and security.

**1:03PM B4.00004 Charge Effects on the Self-Assembly of Protein Block Copolymer Nanostructures**, BRADLEY OLSEN, MIT — Self-assembly of globular protein-polymer block copolymers into nanostructured phases provides a simple method for structural control in biomaterials. Electrostatics play a major role in the self-assembly of these structures from aqueous solutions. While the specific distribution of charge on the protein plays a relatively minor role in self-assembly, large changes in the total charge have a large impact on the concentration at which the proteins self-assemble. While for near-neutral proteins salt screening promotes disassembly and suggests that electrostatic interactions are attractive, proteins with a highly asymmetric charge have repulsive interactions that suppress self-assembly. Using a zwitterionic block in the bioconjugate was also explored as a means to promote self-assembly; however, zwitterionic fusions self-assemble over a narrower range of composition than fusions of any of the nonionic polymers explored. This suggests that dipolar attractions in charge-asymmetric protein-polymer materials play a significant role in the driving force for self-assembly. However, the sensitivity of zwitterionic materials to salt conditions in the buffer also provides a powerful handle for tuning polymer solubility, enabling salt to be used as a method to induce self-assembly.

**1:39PM B4.00005 Giant Surfactants based on Precisely Functionalized POSS Nano-atoms: Tuning from Crystals to Frank-Kasper Phases and Quasicrystals<sup>1</sup>**, STEPHEN Z. D. CHENG, University of Akron — In creating new functional materials for advanced technologies, precisely control over functionality and their hierarchical ordered structures are vital for obtaining the desired properties. Giant polyhedra are a class of materials which are designed and constructed via deliberately placing precisely functionalized polyhedral oligomeric silsesquioxane (POSS) and fullerene (C<sub>60</sub>) molecular nano-particles (MNPs) (so-called “nano-atoms”) at the vertices of a polyhedron. Giant surfactants are consisted of polymer tail-tethered “nano-atoms” which are deliberately and precisely functionalized POSS or C<sub>60</sub> molecular nano-particles (MNPs). The “nano-atom” heads and polymer tails thus have drastic chemical differences to impart amphiphilicity. These giant surfactants capture the essential structural features of their small-molecule counterparts in many ways but possess much larger sizes, and therefore, they are recognized as size-amplified versions of small molecule surfactants. Two of the most illustrating examples are a series of novel giant tetrahedra and a series of giant surfactants as building blocks to construct into hierarchical ordered super-lattice structures ranging from crystals, Frank-Kasper phases and quasicrystals in the condensed bulk states, reveals evidently the interconnections between soft matters and hard matters in sharing their common structures and fundamental knowledge.

<sup>1</sup>This work was supported by National Science Foundation (DMR-1409972).

**Monday, March 14, 2016 11:15AM - 2:15PM –**  
**Session B5 GMAG DMP: Frustrated Magnetism: Low Dimensional Magnets I** 301 - Oleg Starykh, University of Utah

**11:15AM B5.00001 Magnetic nanopantograph in the in SrCu<sub>2</sub>(BO<sub>3</sub>)<sub>2</sub> Shastry-Sutherland lattice**, ANDRES SAUL, CINaM/CNRS — Magnetostriction experiments of the frustrated spin dimer compound SrCu<sub>2</sub>(BO<sub>3</sub>)<sub>2</sub> have shown that its macroscopic physical dimensions change with the applied magnetic field mimicking the complicated structures, with discreet jumps and plateaus, observed in the magnetization. Using Density Functional based methods we find that the driving force behind the magnetoelastic coupling is the Cu-O-Cu superexchange angle which, thanks to the orthogonal Cu<sup>2+</sup> dimers acting as pantographs, can shrink significantly (0.44%) with minute (0.01%) variations in the lattice parameters. Our calculations show that the consequence is a reduction of the order of ~10% in the antiferromagnetic intra-dimer exchange integral *J*, sufficient to compensate the elastic energy loss in the deformation. This reduction should impact our reading of existing predictions of the magnetization versus field phase diagram and the effect of hydrostatic pressures on the ground state. Finally, our prediction of the dimer shrinking under applied magnetic field should appear as a modification of the optical Raman active modes compatible with the pantograph effect.

**11:51AM B5.00002 Hysteretic magnetoresistance and unconventional anomalous Hall effect in the frustrated magnet TmB<sub>4</sub>**, SAI SWAROOP SUNKU<sup>1</sup>, Div of Physics and Applied Physics, Nanyang Technological University, TAI KONG, Ames Laboratory and Dept of Physics and Astronomy, Iowa State University, TOSHIMITSU ITO, National Institute of Advanced Industrial Science and Technology (AIST), PAUL C. CANFIELD, Ames Laboratory and Dept of Physics and Astronomy, Iowa State University, B. SRIRAM SHASTRY, Physics Dept, University of California, Santa Cruz, PINAKI SENGUPTA, CHRISTOS PANAGOPOULOS, Div of Physics and Applied Physics, Nanyang Technological University — We study TmB<sub>4</sub>, a frustrated magnet on the Archimedean Shastry-Sutherland lattice, through magnetization and transport experiments. The lack of anisotropy in resistivity shows that TmB<sub>4</sub> is an electronically three-dimensional system. The magnetoresistance (MR) is hysteretic at low-temperature even though a corresponding hysteresis in magnetization is absent. The Hall resistivity shows unconventional anomalous Hall effect (AHE) and is linear above saturation despite a large MR. We suggest that both hysteretic MR and AHE arise from the formation of complex non-coplanar structures at magnetic domain walls.

<sup>1</sup>Current address: Department of Applied Physics and Applied Mathematics, Columbia University

**12:03PM B5.00003 Spin-lattice coupling of R<sub>1-x</sub>Lu<sub>x</sub>B<sub>4</sub> revealing anomalous weak ferromagnetism (R=Sm, Gd, Tb, Dy, Ho)**, B.Y. KANG, School of Materials Science and Engineering, Gwangju Institute of Science and Technology (GIST), Korea, SEONGSU LEE, Korea Atomic Energy Research Institute, Korea, SANG-YUN HWANG, SUNGDAE JI, Max Planck POSTECH/Korea Research Initiative, Korea, M.S. SONG, B.K. CHO, Gwangju Institute of Science and Technology (GIST), Korea — RB<sub>4</sub> (R=rare-earth elements) compounds exhibits antiferromagnetic ordering at low temperature and are classified as the Shastry-Sutherland lattice, which is a geometrically frustrated system. In previous study, it was reported that Y substitution in TbB<sub>4</sub> single crystals causes anomalous WF (weak ferromagnetism) even though Y<sup>3+</sup> is non-magnetic. The disturbance of a delicate equilibrium in a frustrated system can lead to new electronic and magnetic states. In this study, single crystals of R<sub>1-x</sub>Lu<sub>x</sub>B<sub>4</sub> (R=Sm, Gd, Tb, Dy, Ho), (x=0 ~0.8) were synthesized. WF is also observed. TbB<sub>4</sub> went through orthorhombic distortion below Néel temperature. To investigate the existence of orthorhombic distortion in TbLu<sub>x</sub>B<sub>4</sub> (x=0.1, 0.35), high resolution single crystal x-ray diffraction was performed at 5 K. It was confirmed that the distortion was vanished with Lu substitution. Interestingly, lattice constant *a* was increased with decreasing temperature below the T<sub>C</sub>. The strong correlation between spin-lattice coupling and WF will be discussed in detail.

**12:15PM B5.00004 Neutron Diffraction on  $\text{NaNi}_2\text{BiO}_6$ : Complex Interactions on a Honeycomb Lattice**<sup>1</sup>, ALLEN SCHEIE, Johns Hopkins University, KATE ROSS, Colorado State University, ELIZABETH SEIBEL, Princeton University, JOSE RODRIGUEZ-RIVERA, NIST, COLLIN BROHOLM, Johns Hopkins University, ROBERT CAVA, Princeton University, INSTITUTE FOR QUANTUM MATTER COLLABORATION — Magnetic crystals with a honeycomb lattice can have a very high degree of frustration when next-nearest neighbor interactions are strong. Such complex interactions can lead to Kitaev model physics, including a proposed spin liquid phase. Using neutron scattering, we studied the magnetic properties of a new spin-1/2 honeycomb compound,  $\text{NaNi}_2\text{BiO}_6$ , which was known to have heat capacity peaks indicative of a phase transition at 5 K. The magnetic order indicates beyond nearest-neighbor exchange as well as significant inter-plane interaction, which allows for a study of rich and complex structure. In this talk I report the magnetic structure of the compound as found with neutron powder diffraction, and discuss the exchanges necessary to lead to such a complex order.

<sup>1</sup>The work at IQM was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Material Sciences and Engineering, under Grant No. DEFG02-08ER46544.

**12:27PM B5.00005 Field-induced dynamical properties of the  $XXZ$  model on a honeycomb lattice**<sup>1</sup>, PAVEL MAKSIMOV, ALEXANDER CHERNYSHEV, Univ of California - Irvine — We present a comprehensive  $1/S$  study of the field-induced dynamical properties of the nearest-neighbor  $XXZ$  antiferromagnet on a honeycomb lattice using the formalism of the nonlinear spin-wave theory developed for this model. External magnetic field controls spin frustration in the system and induces non-collinearity of the spin structure, which is essential for the two-magnon decay processes. Our results include an intriguing field-evolution of the regions of the Brillouin zone where decays of spin excitations are prominent, a thorough analysis of the singularities in the magnon spectra due to coupling to the two-magnon continuum, the asymptotic behavior of the decay rates near high-symmetry points, and inelastic neutron-scattering spin-spin structure factor obtained in the leading  $1/S$  order.

<sup>1</sup>Supported by DOE

**12:39PM B5.00006 Featureless Quantum Insulator on the Honeycomb Lattice**<sup>1</sup>, SHENGHAN JIANG, Boston College, HYUNYONG LEE, PANJIN KIM, JUNG HOON HAN, Sungkyunkwan University, YING RAN, Boston College — We construct fully symmetric, gapped states without topological order on a spin-1/2's honeycomb lattice at half-filling in terms of projected entangled pair states (PEPS) Four distinct classes differing by lattice quantum numbers are found by applying the systematic classification scheme introduced by two of the authors [S. Jiang and Y. Ran, arXiv:1505.03171 (2015)]. Lack of topological degeneracy or other conventional form of symmetry breaking, and the existence of the energy gap in both wave functions are checked by numerical calculation of the entanglement entropy and various correlation functions.

<sup>1</sup>the Alfred P. Sloan fellowship and National Science Foundation under Grant No. DMR-1151440 and the NRF grant (No. 2013R1A2A1A01006430)

**12:51PM B5.00007 Possible spin liquid behavior in  $\text{Sc}_2\text{Ga}_2\text{CuO}_7$** , A.V. MAHAJAN, R. KUMAR, IIT Bombay, India, P. KHUNTIA, Ames Lab, Iowa State Univ, USA, D. SHEPTYAKOV, PSI, Switzerland, P.G. FREEMAN, H.M. RONNOW, EPFL, Switzerland, B. KOTESWARARAO, IIT Bombay, India, M. BAENITZ, MPICPFS, Germany, Y. FURUKAWA, Ames Lab, Iowa State Univ, USA, M. JEONG, EPFL, Switzerland — The title compound crystallizes in a hexagonal structure (space group  $P6_3/mmc$ ) containing edge-shared triangular planes as also triangular bi-planes. Our work establishes that the single triangular layers mainly have  $S = 0$   $\text{Ga}^{3+}$  (85% Ga, 15% Cu), while the bi-layers contain 43%  $\text{Cu}^{2+}$  and 57%  $\text{Ga}^{3+}$ , as far as the cations are concerned. Our  $\chi(T)$  data shows no spin-freezing or magnetic long-range order (LRO) down to 1.8 K. We infer an effective moment of  $1.79 \mu_B$  and a  $\theta_{CW}$  of about -50 K, suggesting AF interactions. In our specific heat data, no anomalies were found down to 0.35 K, in the field range 0-140 kOe. The magnetic specific heat has a nearly  $T^2$  power-law behavior at low- $T$  (for  $H > 90$  kOe). The  $^{71}\text{Ga}$  nuclear magnetic resonance (NMR) shift  $K(T)$  displays a broad maximum at  $T \sim 50$  K. The  $^{71}\text{Ga}$  spin lattice relaxation rate  $1/T_1$  displays a  $T^{3.2}$  power-law increase from 0.1 K to 2 K, then remains nearly unchanged up to 10 K, and increases thereafter. Once again, down to 100 mK there is no indication of LRO which is usually manifested as an anomaly in the  $T$ -dependence of  $K$  and  $1/T_1$ . Our data suggest the formation of a quantum spin liquid in the  $S = 1/2$  system  $\text{Sc}_2\text{Ga}_2\text{CuO}_7$ .

**1:03PM B5.00008 Phase diagram of weakly coupled Heisenberg spin chains subject to a uniform Dzyaloshinskii-Moriya interaction**<sup>1</sup>, WEN JIN, OLEG STARYKH, University of Utah — Motivated by recent experiments on spin chain materials  $\text{K}_2\text{CuSO}_4\text{Cl}_2$  and  $\text{K}_2\text{CuSO}_4\text{Br}_2$ , we theoretically investigate the problem of weakly coupled spin chains (chain exchange  $J$ , interchain  $J'$ ) subject to a *staggered between chains*, but *uniform* within a given chain, Dzyaloshinskii-Moriya interaction (DMI) of magnitude  $D$ . In the experimentally relevant limit  $J' \ll D \ll J$  of strong DMI the spins on the neighboring chains are forced to rotate in opposite directions, effectively resulting in a cancellation of the interchain interaction between components of spins in the plane normal to the vector  $D$ . This has the effect of promoting two-dimensional collinear spin density wave (SDW) state, which preserves  $U(1)$  symmetry of rotations about the  $D$ -axis. We also investigate response of this interesting system to an external magnetic field  $h$  and obtain the  $h - D$  phase diagrams for the two important configurations,  $h \parallel D$  and  $h \perp D$ . The transitions between various SDW-like phases are found to be of either a commensurate-incommensurate or a spin-flop kind.

<sup>1</sup>Supported by NSF DMR-1507054

**1:15PM B5.00009 Spin Liquid in the Triangular Lattice Heisenberg Model**<sup>1</sup>, IAN MCCULLOCH, SEYED SAADATMAND, University of Queensland — We report the results of a large-scale numerical study of the spin-1/2 Heisenberg model on the triangular lattice, with nearest- and next-nearest neighbor interactions. Using  $SU(2)$ -invariant iDMRG for infinite cylinders, we focus on the YC12 structure (with a circumference of 12 sites), and obtain 4 candidate groundstates, corresponding to even/odd spinon sectors, each with linear and projective representations of the cylinder geometry. The momentum-resolved entanglement spectrum reveals the structure of the low-lying spinon excitations. Contrary to some recent works, we find no evidence for chiral symmetry breaking.

<sup>1</sup>Supported by the ARC Centre for Engineered Quantum Systems

**1:27PM B5.00010 Anisotropic thermal conductivity of proton fluctuation-induced quantum spin liquid  $\kappa\text{-H}_3(\text{Cat-EDT-TTF})_2$** , MASAOKI SHIMOZAWA, YOSHITAKA SUZUKI, KAORI SUGII, AKIRA UEDA, SHOGO YAMADA, YUSUKE IMAI, KIYOSHI TORIZUKA, YOSHIYA UWATOKO, HATSUMI MORI, MINORU YAMASHITA, ISSP, University of Tokyo — We report the thermal transport properties of a quantum spin liquid candidate  $\kappa\text{-H}_3(\text{Cat-EDT-TTF})_2$  (H-CAT) with a two-dimensional nearly isotropic triangular lattice. Above 1.0 K, thermal conductivity of H-CAT is substantially smaller than that of a deuterated non-magnetic sample (D-CAT) despite no spin thermal conductivity in D-CAT. In the zero-temperature limit, a finite  $T$ -linear term of the thermal conductivity of H-CAT is clearly observed when the heat current is parallel to  $c$ -axis, while it is almost zero when the heat current is parallel to  $b$ -axis. These features would be attributed to anisotropic proton fluctuations present in H-CAT.

**1:39PM B5.00011 Theory of triplon dynamics in the quantum magnet  $\text{BiCu}_2\text{PO}_6$** , YONG BAEK KIM, KYUSUNG HWANG, Department of Physics and Centre for Quantum Materials, University of Toronto, Toronto, Ontario M5S 1A7, Canada — We provide a theory of triplon dynamics in the valence bond solid ground state of the coupled spin-ladders modeled for  $\text{BiCu}_2\text{PO}_6$ . Utilizing the recent neutron scattering experimental data as guides and a theory of interacting triplons via the bond operator formulation, we determine a minimal spin Hamiltonian for this system. It is shown that the splitting of the low energy triplon modes and the peculiar magnetic field dependence of the triplon dispersions can be explained by including substantial Dzyaloshinskii-Moriya and symmetric anisotropic spin interactions. Taking into account the interactions between triplons and the decay of the triplons to the two-triplon continuum via anisotropic spin interactions, we provide a theoretical picture that can be used to understand the main features of the recent neutron scattering experimental data.

**1:51PM B5.00012 Multi-Magnon Bound States in J1-J2 Model on a Triangular Lattice**, RINA TAKASHIMA, Kyoto University, HIROAKI ISHIZUKA, LEON BALENTS, KITP, UCSB — Competing exchange interactions in spin systems often give rise to unusual magnetic behavior, such as spiral orders and nematic orders in spin chains. Also, on classical triangular Heisenberg models, recent studies found skyrmion lattice phases in an applied magnetic field. Motivated by these studies, we investigate the magnetic phase diagram of a quantum J1-J2 XXZ model on a triangular lattice. In order to study the quantum phases close to the saturation field, we calculate the low energy excitation spectrum near the saturation field, and find the instability toward condensation of multi-magnon bound states, namely, multipolar order. A similar behavior is confirmed in the exact diagonalization of finite size clusters. We also discuss the relationship between the obtained quantum phases and the skyrmion lattice phase which is found in the classical counterpart of our model.

**2:03PM B5.00013 The  $S=1/2$  J1-J2 Heisenberg Model on the Triangular Lattice**, TSEZAR SEMAN, Northern Illinois University, Argonne National Laboratory, CHENG-CHIEN CHEN, Argonne National Laboratory, RAJIV SINGH, University of California, Davis, MICHEL VAN VEENENDAAL, Northern Illinois University, Argonne National Laboratory — We study the  $S=1/2$  triangular-lattice Heisenberg model using large-scale exact diagonalization. As a function of the next-nearest-neighbor exchange J2, the model shows different long-range magnetically ordered states and a potential quantum spin liquid phase. We compute the spin gap and static structure factors in different regions of the phase diagram. The spin-wave and two-magnon Raman spectra are also explored accordingly.

**Monday, March 14, 2016 11:15AM - 2:03PM –**

**Session B6 GMAG DMP FIAP: Dzyaloshinskii-Moriya Interaction** 302 - Emilie Jue, NIST

**11:15AM B6.00001 Proportionality of the interfacial Dzyaloshinskii-Moriya interaction and the Heisenberg exchange**, HANS NEMBACH, JUSTIN SHAW, National Institute of Standards and Technology, MATHIAS WEILER, Walther-Meissner Institut, EMILIE JU, TOM SILVA, National Institute of Standards and Technology — The Dzyaloshinskii-Moriya interaction (DMI) gives rise to chiral magnetic ordering and a shift of spin-wave frequencies, depending on their propagation direction. We employed Brillouin-Light-Scattering spectroscopy to measure this nonreciprocal frequency shift, which allowed us to directly determine the magnitude of the DMI in a series of  $\text{Ni}_{80}\text{Fe}_{20}(\text{t})/\text{Pt}$  thin film bilayers where the thickness t ranged from 1 to 13 nm. It has also been predicted by theory that the DMI is proportional to the Heisenberg exchange for bulk magnetic oxides and metallic spin-glasses. We tested this prediction for our metallic system by independently determining the Heisenberg exchange via fitting the Bloch  $T^{3/2}$ -law to the temperature dependence of the magnetization obtained from SQUID magnetometry. We find that the  $\text{Ni}_{80}\text{Fe}_{20}$  thickness dependence of the DMI and the Heisenberg exchange are identical, which is consistent with the notion that both effects share the same underlying physics. This result will lead us to a deeper understanding of the DMI and related spin-orbitronic effects.-/

**11:27AM B6.00002 Nonreciprocal magnon propagation in a noncentrosymmetric ferromagnet  $\text{LiFe}_5\text{O}_8$** , YUSUKE IGUCHI, SOICHIRO UEMURA, KAZUNORI UENO, YOSHINORI ONOSE, Department of Basic Science, University of Tokyo — In noncentrosymmetric materials, the relativistic effect extensively modifies the energy band of magnons as well as that of electrons. With use of microfabricated microwave antennae, we have demonstrated that the propagation of magnons with large momentum is nonreciprocal in a noncentrosymmetric ferromagnet  $\text{LiFe}_5\text{O}_8$ . The nonreciprocity is clearly explained by the effect of asymmetric magnon band originating from the relativistic Dzyaloshinskii-Moriya interaction. This result may pave a new path to designing magnonic device based on the relativistic band engineering.

**11:39AM B6.00003 A Dzyaloshinskii-Moriya Anisotropy in nanomagnets with in-plane magnetization<sup>1</sup>**, M. CUBUKCU, J. SAMPAIO, Unite Mixte de Physique, CNRS, Thales, Univ. Paris-Sud, Universite Paris-Saclay, Palaiseau, France, A. V. KHVALKOVSKIY, D. APALKOV, Samsung Electronics, Semiconductor RD Center (Grandis), San Jose, USA, V. CROS, N. REYREN, Unite Mixte de Physique, CNRS, Thales, Univ. Paris-Sud, Universite Paris-Saclay, Palaiseau, France — The Dzyaloshinskii-Moriya interaction (DMI) is known to be a direct manifestation of spin-orbit coupling in systems with broken inversion symmetry. We present a new anisotropy for in-plane-magnetized nanomagnets which is due to the interfacial DMI. This new anisotropy depends on the shape of the magnet, and is perpendicular to the demagnetization shape anisotropy [1]. The DMI anisotropy term that we introduce here results from the DMI energy reduction due to an out-of-plane tilt of the spins at the edges that are oriented perpendicular to the magnetization. For large enough DMI, the reduction of the DMI and anisotropy energies takes over the demagnetization energy cost when magnetization lies along the minor axis of a structure. Our experimental, numerical and analytical results demonstrate this prediction in magnets of elongated shape for small enough volume (and thus quasi-uniform magnetization). Our results also provide the first experimental evidence of the interfacial DMI-induced tilt of the spins at the borders. [1] M. Cubukcu *et al.*, *arXiv:1508.02961* (2015).

<sup>1</sup>This work was supported by the Samsung Global MRAM Innovation Program.

**11:51AM B6.00004 First principles study of the effective Hamiltonian for Dzyaloshinskii-Moriya interaction**, TAKASHI KORETSUNE, TORU KIKUCHI, RYOTARO ARITA, GEN TATARA, RIKEN CEMS — We propose a new formalism to calculate the Dzyaloshinskii-Moriya (DM) interaction by deriving an effective Hamiltonian for a spin gauge field. By treating the spin gauge field perturbatively, we obtain a physically intuitive result that the spin current density is related to the DM interaction. Using first-principles calculations, we confirm that our approach agrees well with the results using the energies of helical spin structures. We also discuss the relation between band structures and DM interaction for the B20 chiral magnets.

**12:03PM B6.00005 Torque, spin and energy Hall currents in magnets with Dzyaloshinskii-Moriya interactions**, VLADIMIR ZYUZIN, ALEXEY KOVALEV, University of Nebraska — Within a linear response theory, we study nonequilibrium magnonic torques as well as spin and energy Hall currents generated by thermal gradients in ferromagnetic and anti-ferromagnetic systems. We predict a contribution related to Berry curvature which arises in multiband systems with topologically non-trivial magnon bands. We identify symmetries that need to be broken in order to have non-vanishing nonequilibrium magnonic torques. As an example, we study kagome lattice of spins with various symmetries of Dzyaloshinskii-Moriya interactions.

**12:15PM B6.00006 Magnon Chirality Hall Effect in Antiferromagnet<sup>1</sup>**, RAN CHENG, NIKHIL SIVADAS, Carnegie Mellon University, SATOSHI OKAMOTO, Oak Ridge National Laboratory, DI XIAO, Carnegie Mellon University, CARNEGIE MELLON UNIVERSITY TEAM, OAK RIDGE NATIONAL LABORATORY COLLABORATION — In a collinear antiferromagnet with easy-axis anisotropy, symmetry dictates that the spin wave modes must be doubly degenerate with opposite chirality. We show that in the presence of the Dzyaloshinskii-Moriya interaction, there exist a magnon chirality Hall effect, where magnons with opposite chirality flow to opposite transverse edges when an in-plane temperature gradient is applied. Possible material candidates to realize this effect is also discussed.

<sup>1</sup>This work is supported by DOE BES (No. DE-SC0012509) and AFOSR (No. FA9550-12-1-0479)

**12:27PM B6.00007 Soliton-like magnetic domain wall motion induced by the interfacial Dzyaloshinskii-Moriya interaction**, TERUO ONO, Kyoto University — Topological defects such as magnetic solitons, vortices, Bloch lines, and skyrmions start to play an important role in modern magnetism due to their extraordinary stability which can be hailed as future memory devices. Recently, novel type of antisymmetric exchange interaction, namely the Dzyaloshinskii-Moriya interaction (DMI), has been uncovered and found to influence on the formation of topological defects. Exploring how the DMI affects the dynamics of topological defects is therefore an important task. Here we investigate the dynamics of the magnetic domain wall (DW) under a DMI by developing a time-of-flight measurement scheme which allows us to measure the DW velocity for magnetic fields up to 0.3T. For a weak DMI, the trend of DW velocity follows the Walker's model which predicts that the velocity of DW increases with field up to a threshold (Walker field) and decreases abruptly. On the other hand, for a strong DMI, velocity breakdown is completely suppressed and the DW keeps its maximum velocity even far above the Walker field. Such a distinct trend of the DW velocity, which has never been predicted, can be explained in terms of magnetic soliton, of which topology can be protected by the DMI. Importantly, such a soliton-like DW motion is only observed in two dimensional systems, implying that the vertical Bloch lines (VBLs) creating inside of the magnetic domain-wall play a crucial role. This work was partly supported by JSPS KAKENHI Grant Numbers 15H05702, 26870300, 26870304, 26103002, 254251, Collaborative Research Program of the Institute for Chemical Research, Kyoto University, and R & D Project for ICT Key Technology of MEXT from the Japan Society for the Promotion of Science (JSPS).

**1:03PM B6.00008 Magnetoelectric effects in the spin 1/2 XX chain with three spin interactions and Dzyaloshinskii-Moriya interaction<sup>1</sup>**, P DURGANANDINI, Department of Physics, SP Pune University, Pune - 411007, India — We consider the spin 1/2 XX chain with three spin interactions of the XZX+YXY and XZY-YZX types in an external magnetic field and with Dzyaloshinskii-Moriya (D-M) interaction. Interpreting the D-M interaction as a local electric polarization, we study the magnetoelectric effects in the system by using the exact solution of the problem. We obtain the ground state phase diagram by calculating the electric polarization, magnetization and entropies. There are various regimes of magnetic and electric polarization depending on the relative strengths of the three spin interaction as well as that of the external fields. For a certain range of three spin interaction strengths, the system shows the existence of finite magnetization and electric polarization even in the absence of any external fields. The external electric and magnetic fields modify the ground state phases and can be used to tune the various regimes. We also calculate the entropy and analyze the electrocaloric and magnetocaloric effects. We show that the electrocaloric and magnetocaloric effects can be used to obtain information about the magnetoelectric effects in the system.

<sup>1</sup>I thank DST, India for financial support through research grant.

**1:15PM B6.00009 Large anomalous Hall effect in a non-collinear antiferromagnet Mn<sub>3</sub>Sn at room temperature<sup>1</sup>**, TOMOYA HIGO, NAOKI KIYOHARA, ISSP, University of Tokyo, SATORU NAKATSUJI, ISSP, University of Tokyo and PRESTO, JST — Recent development in theoretical and experimental studies have provided a framework for understanding the anomalous Hall effect using Berry-phase concepts, and this perspective has led to predictions that, under certain conditions, a large anomalous Hall effect may appear in spin liquids and antiferromagnets [1, 2]. In this talk, we will present experimental results showing that the antiferromagnet Mn<sub>3</sub>Sn, which has a non-collinear 120-degree spin order, exhibits a large anomalous Hall effect [3]. The magnitude of the Hall conductivity is  $\sim 20 \Omega^{-1} \text{ cm}^{-1}$  at room temperature and  $> 100 \Omega^{-1} \text{ cm}^{-1}$  at low temperatures. We found that a main component of the Hall signal, which is nearly independent of a magnetic field and magnetization, can change the sign with the reversal of a small applied field, corresponding to the rotation of the staggered moments of the non-collinear antiferromagnetic spin order which carries a very small net moment of a few of  $m\mu_B$ . [1] N. Nagaosa *et al.*, Rev. Mod. Phys. **82**, 1539 (2010). [2] Y. Machida *et al.*, Nature **463**, 210 (2010). [3] S. Nakatsuji, N. Kiyohara and T. Higo, Nature, doi:10.1038/nature15723, (2015).

<sup>1</sup>Supported by PRESTO, JST, and Grants-in-Aid for Program for Advancing Strategic International Networks to Accelerate the Circulation of Talented Researchers (No. R2604) and Scientific Research on Innovative Areas (15H05882 and 15H05883) from JSPS.

**1:27PM B6.00010 Nanoscale and proximity effects on low-dimensional helical magnetic structures**, LEONID SANDRATSKII, J. FISHER, S. PARK, S. OUAZI, D. SANDER, J. KIRSCHNER, Max Planck Inst Microstructure — We combine symmetry arguments, first-principles calculations and spin-resolved STS measurements to study a 2D helical magnet of some nm extension in proximity to ferromagnetic Co and vacuum regions. Considering the prototypical helical 2D system, an Fe bilayer with intrinsic helical spin structure (1), we report a non-uniform distortion of the spin helix which depends on the lateral extension of the bilayer and on the proximity to either Co or vacuum. The proximity effect manifests itself in different modifications of the magnetic and electronic structures of Fe in vicinity of the interfaces with Co and vacuum. These nanosize and proximity effects have not been discussed before. We demonstrate that, in contrast to an ideal helix of infinite length, the lack of symmetry of the nm-long distorted Fe spin helix, induces an energy dependence of the direction of the electronic magnetization which is revealed in the measured energy dependence of the spin-asymmetry of the differential tunneling conductance. (1) Phark, S. H.; Fischer, J. A.; Corbetta, M.; Sander, D.; Nakamura, K. & Kirschner, J. Reduced-dimensionality-induced helimagnetism in iron nanoislands Nat Commun **5** (2014) 5183.

**1:39PM B6.00011 Emergence of magnetic order in ultra-thin pyrochlore iridate films<sup>1</sup>**, SURAJ CHEEMA, CLAUDY SERRAO, JULIA MUNDY, SHREYAS PATANKAR, ROBERT BIRGENEAU, JOSEPH ORENSTEIN, SAYEEF SALAHUDDIN, RAMAMOORTHY RAMESH, Univ of California - Berkeley — We report on thickness-dependent magnetotransport in (111) - oriented Pb<sub>2</sub>Ir<sub>2</sub>O<sub>7-x</sub> (Pb227) epitaxial thin films. For thicknesses greater than 4 nm, the magnetoresistance (MR) of metallic Pb227 is positive, linear and non-saturated up to 14 T. Meanwhile at 4 nm, the conduction turns nonmetallic and the MR becomes negative and asymmetric upon field-cooling; such traits are reminiscent of all-in-all-out (AIAO) magnetic order in the insulating pyrochlore iridates. Hysteretic low-field MR dips and trained-untrained resistivity bifurcations suggest the presence of magnetic conducting domain walls within the chiral AIAO spin structure. Beyond just AIAO order, angular-dependent MR indicates a magnetic phase space hosting 2-in-2-out (2I2O) spin ice order. Such anomalous magnetotransport calls for re-evaluation of the pyrochlore iridate phase diagram, as epitaxially strained Pb227 exhibits traits reminiscent of both the insulating magnetic and metallic spin-liquid members. Furthermore, these results open avenues for realizing topological phase predictions in (111) - oriented pyrochlore slabs of kagome-triangular iridate heterostructures.

<sup>1</sup>This work is supported by the Office of Basic Energy Sciences of the US Department of Energy under contract no. DE-AC02-05CH11231.

**1:51PM B6.00012 Modulated magnetic ground state and complex phase diagram in the chiral helimagnet  $\text{Cr}_{1/3}\text{NbS}_2$** , EM CLEMENTS, R DAS, Univ. of South Florida, L LI, Univ. of Tennessee, P LAMPEN-KELLEY, Univ. of Tennessee, Oak Ridge National Lab, MH PHAN, Univ. of South Florida, VEERLE KEPPENS, Univ. of Tennessee, D MANDRUS, Univ. of Tennessee, Oak Ridge National Lab, H SRIKANTH, Univ. of South Florida — The chiral helimagnetic ground state of noncentrosymmetric  $\text{Cr}_{1/3}\text{NbS}_2$  originates from competition between coexisting symmetric ferromagnetic (FM) exchange and the antisymmetric Dzyaloshinskii-Moriya (DM) interaction. Previously, it has been shown via Lorentz microscopy that a field induced chiral soliton lattice (SL) exists followed by an incommensurate-commensurate metamagnetic transition to a FM state. The high crystalline anisotropy as well as magnetic and temperature control of the c-axis oriented spin spiral has generated interest for spintronic applications. Currently, only a preliminary phase diagram has been proposed and details of the phase evolution, specifically from the paramagnetic (PM) to the helicoid HM and SL states, have not yet been determined. In this study, we exploit the magnetocaloric effect (MCE) to construct a phase diagram by determining the magnetic entropy change ( $\Delta S_M$ ) under the influence of applied field and temperature variations. Well below the Curie temperature ( $T_c \sim 131\text{K}$ ) we see the onset of SL formation at  $\sim 1\text{kOe}$  and a FM transition  $\sim 1.2\text{kOe}$ . A negative  $\Delta S_M$  value indicates that the system also shows weak FM behavior in a narrow region just below  $T_c$ , where thermal fluctuations destabilize the weaker DM coupling, before transitioning into the HM phase at lower temperatures.

**Monday, March 14, 2016 11:15AM - 2:15PM –**

**Session B7 APS SPS: Undergraduate Research/SPS II 303 - Daniel Golombek, Society of Physics Students**

**11:15AM B7.00001 Calibrating the High Density Magnetic Port within Tissue Expanders to Achieve more Accurate Dose Calculations for Postmastectomy Patients with Immediate Breast Reconstruction<sup>1</sup>**, JASMINE JONES<sup>2</sup>, RUI ZHANG<sup>3</sup>, DAVID HEINS<sup>4</sup>, Louisiana State University, KATHERINE CASTLE, Mary Bird Perkins Cancer Center — In postmastectomy radiotherapy, an increasing number of patients have tissue expanders inserted subpectorally when receiving immediate breast reconstruction. These tissue expanders are composed of silicone and are inflated with saline through an internal metallic port; this serves the purpose of stretching the muscle and skin tissue over time, in order to house a permanent implant. The issue with administering radiation therapy in the presence of a tissue expander is that the port's magnetic core can potentially perturb the dose delivered to the Planning Target Volume, causing significant artifacts in CT images. Several studies have explored this problem, and suggest that density corrections must be accounted for in treatment planning. However, very few studies accurately calibrated commercial TP systems for the high density material used in the port, and no studies employed fusion imaging to yield a more accurate contour of the port in treatment planning. We compared depth dose values in the water phantom between measurement and TPS calculations, and we were able to overcome some of the inhomogeneities presented by the image artifact by fusing the KVCT and MVCT images of the tissue expander together, resulting in a more precise comparison of dose calculations at discrete locations. We expect this method to be pivotal in the quantification of dose distribution in the PTV.

<sup>1</sup>Research funded by the LS-AMP Award

<sup>2</sup>Undergraduate Presenter

<sup>3</sup>Faculty Mentor

<sup>4</sup>Graduate Mentor

**11:27AM B7.00002 Theoretical Study of NaCl and LiCl Clusters**, BRIDGET ORTIZ, AJIT HIRA, JAMES MCKEOUGH, TED KOETTER, Northern New Mexico College — This research is a Quantum Mechanical study of molecular clusters that examines the chemical properties of small  $\text{Na}_n\text{Cl}_n$  and  $\text{Li}_n\text{Cl}_n$  clusters ( $n = 2 - 20$ ). The potentially important role of these molecular species in biochemical and medicinal processes is well known. This work applies the hybrid ab initio methods to derive the different alkali-halide ( $\text{M}_n\text{H}_n$ ) geometries. Of particular interest is the competition between hexagonal ring geometries and rock salt structures. Electronic energies, rotational constants, dipole moments, and vibrational frequencies for these geometries are calculated. Magic numbers for cluster stability are identified and are related to the property of cluster compactness. Mapping of the singlet, triplet, and quintet, potential energy surfaces is performed. Calculations were performed to examine the interactions of these clusters with some atoms and molecules of biological interest, including O, O<sub>2</sub>, and Fe. Potential design of new medicinal drugs is explored. We will also investigate model and material dependence of the results.

**11:39AM B7.00003 Anisotropic Magnetic Nanostructures For Enhanced Hyperthermia**, D. TORRES, Texas State Univ., R. DAS, J. ALONSO, M.H. PHAN, H. SRIKANTH, Univ. of South Florida — Magnetic nanoparticles assisted hyperthermia is one of the most promising techniques for cancer treatment. By the use of magnetic nanoparticles in an external AC magnetic field, one can target a specific tumor location and deliver toxic doses of heat to the tumor area without damaging the surrounding healthy tissue. Magnetite is typically used in biomedical applications due to its biocompatibility, but the heating efficiency of the commonly used magnetite nanoparticles is not enough to obtain the best results in cancer treatment. Therefore, novel magnetic nanostructures are required in order to improve the heating efficiency. Recently, it has been proposed by different groups that it is possible to increase the heating efficiency of the nanoparticles by tuning their effective anisotropy. Considering this, we have synthesized high aspect ratio magnetic nanorods with increased effective anisotropy. A thorough structural and magnetic characterization has revealed high crystallinity and optimal magnetic properties of these nanorods. The hyperthermia response shows that by increasing the aspect ratio from 5 to 11, their heating efficiency is increased by 150%. In addition, we have observed that a good alignment of the nanorods with the magnetic field ensures the best heating results. Hence, these nanorods appear to be promising candidates for cancer treatment with magnetic hyperthermia.

**11:51AM B7.00004 Layer-by-Layer Assembly Onto Gold Nanoparticles of Various Size**, ANDREW KILROY, SARAH KESSLER, TABBETHA DOBBINS, Rowan University, Dept. of Physics & Astronomy — This research focuses on the potential applications of coated gold nanoparticles in medicine. By coating gold nanoparticles in layers of polyelectrolytes, with a final layer of antibodies which targets chemicals uniquely exhibited by cancer cells, we eventually hope to selectively attach the nanoparticles to the cancer cells. The coated nanoparticles are assembled through layer-by-layer coulombic attraction due to the passive zeta potential of the particle and the charged nature of the polyelectrolytes. This poster will explore the potential usefulness of variously sized nanoparticles with various thickness of polyelectrolyte layers.

**12:03PM B7.00005 Formation and Cytotoxicity of Nanoparticles and Nanocubes Prepared from Gold and Silver Salts**, DANIEL BANKER, SKYLER DORRELL, PRESCOTT IVEY, JOSEPH SCURT, TABBETHA DOBBINS, Rowan University, Dept. of Physics & Astronomy — Photothermal therapy is the use of electromagnetic radiation as the treatment for medical conditions such as cancer. Noble metal nanoparticles and nanocubes are brought to an excited state with laser light and as a result they release vibrational energy in the form of heat, which can be used to kill targeted cancer cells. Wet chemistry gives the basics for the preparation of nanoparticles and nanocubes. Using  $\text{HAuCl}_4$ ,  $\text{AgNO}_3$ , tri-sodium citrate and other chemicals, we were able to successfully create gold and silver nanoparticles and nanocubes. The goal is to make sure that 3T3 cells can survive in a nanoparticle or nanocube doped medium so that we can then observe their reaction to photothermal effects. Cell culture techniques were done to 3T3 cells to keep them alive before the testing of cytotoxicity. Photothermal effect refers to the way that our nanoparticles or nanocubes can be photoexcited to release enough heat to kill the cells. We used a UV-Vis spectrophotometer to ensure that the correct wavelength laser. Assuming that the cells will survive living in the doped medium, a medium that has had nanomaterials introduced into it, we will use a high powered laser to observe what the excitation does to the cells since the photothermal effect should result in dead cells.

**12:15PM B7.00006 Implementation of Multiple Spectroscopic Techniques to Simultaneously Observe Native and Mutated Protein Unfolding**, BRENNAN CULL, KELTY BEN, JUSTIN LINK, Xavier University, Cincinnati, OH — A protein's natural, correctly folded structure can determine the protein's ability to carry out its function. If the unfolding process of proteins can be observed, then the relative stability can be better understood between native and mutated proteins. A global picture of the unfolding process may be completed through the studies of strategically mutated proteins using tryptophan as a probe. Horse heart cytochrome c, a thoroughly studied, model protein was used in our investigation to explore this idea. Various spectroscopic techniques such as circular dichroism (CD), absorbance, and fluorescence were simultaneously applied while slowly unfolding our protein by increasing the concentration of a chemical denaturant, guanidine hydrochloride. This provided us information about the thermodynamic properties of the protein and several mutants which can then be interpreted to gain relative stability information among mutations. Efforts to utilize these techniques on native and mutated proteins in comparison to current scientific unfolding theories will be presented in this session.

**12:27PM B7.00007 Transport of Motor Proteins along Microtubules: A Study by Optical Trapping Method and Analysis of Data<sup>1</sup>**, ANGELIQUE MCFARLANE, Seton Hall University — The cellular transportation is fundamental for cell function. Under this transportation, organelles bind to motor proteins. These proteins, then move along cellular microfilaments such as microtubules. The optical trapping technique is a method that allows us to monitor the movement of molecular motors along their tracks. In this method, motor proteins are absorbed by micro-sized beads. The beads are captured by the laser and placed close to the microfilaments. Consequently, the motor proteins bind to the track and move along them. This motion can be recorded and analyzed. In this work, we have analyzed many produced trajectories resulted from the motion of a single kinesin along microtubules. We present the design of the experiment, the method of recording and extracting data, as well as the factors that need to be considered to obtain accurate results. Finally, we calculated some of the physical properties resulted from kinesin movement in our experiment. Our outcomes are compatible with previously reported results.

<sup>1</sup>I acknowledge the support of NJSGC 2016 during this project. This work was conducted under the supervision of Dr. Mitra Feizabadi.

**12:39PM B7.00008 Olive Oil and its Potential Effects on Alzheimer's Disease**, SHAN ANTONY, Indiana State Univ, G.P. ZHANG, Indiana State University — Alzheimer's disease is a neuro-degenerative brain disease that is responsible for affecting the lives of hundreds of thousands of people every year. There has been no evidence to suggest a cure for the disease and the only existing treatments have very low rates of success in trial patients. This is largely due to the fact that the brain is one of the most undiscovered parts of the human body. Brain chemistry is highly complex and responds to its environment in random and radical ways. My research includes testing the reactionary outcomes of combining compounds of olive oil with the 20 basic amino acids. Regions around the world with olive oil based diets show a direct correlation to lower rates of Alzheimer's. Testing few compounds of olive oil with chemicals already found in the brain may yield to a better understanding as to why that is. I took the compounds tyrosol, hydroxytyrosol, and oleocanthal, and combined them with the 20 basic amino acids and calculated the total energy of the new molecule. The molecules produced with acceptably low energy values will be the center of further research. These molecules could lead to truly understanding olive oil's effect on the brain, and ultimately, the cure or prevention of Alzheimer's disease.

**12:51PM B7.00009 Optimization of Fe<sub>3</sub>O<sub>4</sub> Nanoparticle Synthesis**, E VILA, Baker University, K STOJAK REPA, H SRIKANTH, MH PHAN, University of South Florida — Magnetic nanoparticles have been of great interest for the past several decades due to the increasing demands of technology as a direct result of device miniaturization. Additionally, they are interesting for biomedical applications, such as magnetic hyperthermia, because of their controllable size and shape, which can make them compatible with biological entities such as cells or viruses. In this study, iron oxide nanoparticles were synthesized through a thermal decomposition process. The original recipe was altered by changing the type and amounts of reagents used; the reaction time was also changed. Specifically, the amount of surfactants and solvent were altered, and the typical co-surfactant, 1,2-hexadecanediol was substituted by 1,2-tetradecanediol. Finally, a systematic reflux time study was conducted to determine the importance of reaction time to the synthetic process. Each sample was analyzed structurally via XRD to confirm the Fe<sub>3</sub>O<sub>4</sub> phase and TEM to confirm their size. Several samples were also measured in a standard magnetometer to observe changes in their magnetic properties. Results from the systematic study will be presented here.

**1:03PM B7.00010 Study of gold nanoparticle synthesis by synchrotron x-ray diffraction and fluorescence<sup>1</sup>**, ZHONGYING YAN, XIAO WANG, LE YU, Bryn Mawr College, SINA MOEENDARBARI, YAOWU HAO, University of Texas at Arlington, ZHONGHOU CAI, Argonne National Laboratory, XUEMEI CHENG, Bryn Mawr College — Gold nanoparticles have a wide range of potential applications, including therapeutic agent delivery, catalysis, and electronics. Recently a new process of hollow nanoparticle synthesis was reported, the mechanism of which was hypothesized to involve electroless deposition around electrochemically evolved hydrogen bubbles. However, the growth mechanism still needs experimental evidence. We report investigation of this synthesis process using synchrotron x-ray diffraction and fluorescence measurements performed at beamline 2-ID-D of the Advanced Photon Source (APS). A series of gold nanoparticle samples with different synthesis time (50-1200 seconds) were deposited using a mixture electrolyte solution of Na<sub>3</sub>Au(SO<sub>3</sub>)<sub>2</sub> and H<sub>4</sub>N<sub>2</sub>NiO<sub>6</sub>S<sub>2</sub> on anodic aluminum oxide (AAO) membranes. The 2D mapping of fluorescence intensity and comparison of x-ray diffraction peaks of the samples have provided valuable information on the growth mechanism.

<sup>1</sup>Work at Bryn Mawr College and University of Texas at Arlington is supported by NSF grants (1207085 and 1207377) and use of the APS at Argonne National Laboratory is supported by the U. S. Department of Energy under Contract No. DE-AC02-06CH11357.

**1:15PM B7.00011 Softening and Hardening of a Micro-electro-mechanical systems (MEMS) Oscillator in a Nonlinear Regime**, SARAH JOHNSON, Hillsdale College, TERENCE EDMONDS, University of Florida — Micro-electro-mechanical systems or MEMS are used in a variety of today's technology and can be modeled using equations for nonlinear damped harmonic oscillators. Mathematical expressions have been formulated to determine resonance frequency shifts as a result of hardening and softening effects in MEMS devices. In this work we experimentally test the previous theoretical analysis of MEMS resonance frequency shifts in the nonlinear regime. Devices were put under low pressure at room temperature and swept through a range of frequencies with varying AC and DC excitation voltages to detect shifts in the resonant frequency. The MEMS device studied in this work exhibits a dominating spring softening effect due to the device's physical make-up. The softening effect becomes very dominant as the AC excitation is increased and the frequency shift of the resonance peak becomes quite significant at these larger excitations. Hardening effects are heavily dependent on mechanical factors that make up the MEMS devices. But they are not present in these MEMS devices. I will present our results along with the theoretical analysis of the Duffing oscillator model. This work was supported by NSF grant DMR-1461019 (REU) and DMR-1205891 (YL).

**1:27PM B7.00012 A Simple Memristor Model for Circuit Simulations**, FARRAH-AMOY FULLERTON, AALEYAH JOE, NADINE GERGEL-HACKETT, Mary Baldwin College, DEPARTMENT OF CHEMISTRY AND PHYSICS TEAM — This work describes the development of a model for the memristor, a novel nanoelectronic technology. The model was designed to replicate the real-world electrical characteristics of previously fabricated memristor devices, but was constructed with basic circuit elements using a free widely available circuit simulator, LT Spice. The modeled memristors were then used to construct a circuit that performs material implication. Material implication is a digital logic that can be used to perform all of the same basic functions as traditional CMOS gates, but with fewer nanoelectronic devices. This memristor-based digital logic could enable memristors' use in new paradigms of computer architecture with advantages in size, speed, and power over traditional computing circuits. Additionally, the ability to model the real-world electrical characteristics of memristors in a free circuit simulator using its standard library of elements could enable not only the development of memristor material implication, but also the development of a virtually unlimited array of other memristor-based circuits.

**1:39PM B7.00013 Cosmic Reionization: An Analysis of Various Contributable Cosmological Factors.** , ADAM BRYAN, MARCO FATUZZO, Xavier University, Cincinnati, OH — According to the most accepted model of cosmology, the  $\Lambda$ -CDM model, the intergalactic medium (IGM) slowly becomes ionized after the period of recombination. This span of ionization, deemed the epoch of reionization, has proven to be a pertinent chapter to the narrative of our evolving universe. Star-forming galaxies have been accredited as the driving force behind reionization, however, recent results suggest that they cannot be the only cause of reionization. The purpose behind this work was to incorporate other cosmological phenomena to reduce the amount of radiation needed from star-forming galaxies, while still meeting the observational criteria of reionization.

**1:51PM B7.00014 Alfvén Wave Propagation in Young Stellar Systems** , RAY HUMIENNY, MARCO FATUZZO, Xavier University, Cincinnati, OH — Young stellar systems have disks that are threaded by magnetic field lines with an hourglass geometry. These fields funnel ionizing cosmic rays (CRs) into the system. However, the effect is offset by magnetic mirroring. An previous analysis considered how the presence of magnetic turbulence moving outward from the disk would effect the propagation of cosmic-rays, and in turn, change the cosmic-ray ionization fraction occurring within the disk. This work indicated that turbulence reduces the overall flux of cosmic-rays at the disk, which has important consequences for both chemical processes and planet formation that occur within these environments. However, the analysis assumed ideal MHD condition in which the gas is perfectly coupled to the magnetic field. We explore here the validity of this assumption by solving the full equations governing the motion of both ions and neutral within the system.

**2:03PM B7.00015 Theoretically Investigating the Nature of Spacetime- A grand definition of what clocks measure<sup>1</sup>** , MERU EGIE<sup>2</sup>, None — Einstein's special theory of relativity established time as a dimension of reality, explaining physically the mathematical stipulations of Lorentz transformation equations that are required to keep the validity of Maxwell's equations of light and explain the null result of Michelson-Morley experiment. Our current understanding of time is relativistic, that is time is not absolute but runs differently depending on the frame of reference, yet this description uncovers so little about the fundamental reality of time. Using mathematical arguments derived from a simple thought experiment, both Lorentz transformation equations and Einstein's far reaching conclusions of his 1905 paper on the electrodynamics of moving bodies are obtained with arguments that suggest no prior knowledge of both Einstein and Lorentz works. This work attempts uncovering the fundamental nature of what clocks measure and a major implication of this is that the fourth dimension could just be a persistent illusion caused by the existence of space.

<sup>1</sup>gratitude to Mr. Jon Egie for his support and Aghogo Rita for her listening ears

<sup>2</sup>change permits all structures forms & proportion, whether cosmic or individual, organic or inorganic, optics or acoustics, it is evident with what clocks measure, leaving an undermine beauty in the clocks while noting their position and movement through space.

**Monday, March 14, 2016 11:15AM - 2:15PM —**

**Session B11 DMP: Superconductivity in Monolayer FeSe/SrTiO<sub>3</sub>** 307 - Douglas Scalapino, UCSB

**11:15AM B11.00001 ARPES of single layer iron pnictide on STO.** , ZHI-XUN SHEN, Stanford University — Quantum systems in confined geometries have been a very rich ground for discoveries. In this talk, I will discuss recent progresses in uncovering novel physics at ultra-thin limit, with focus on mono-unit-cell (UC) superconductor FeSe grown on SrTiO<sub>3</sub>, where the Cooper pairing temperature is reported to have dramatically enhanced from its bulk value of 8K to ~60K. Of interest are the cause of the enhanced pairing strength, and the nature of the superconducting state. We show angle-resolved photoemission spectroscopy (ARPES) data that provide clear evidence for strong cross-interface electron-phonon coupling in single UC limit, suggesting that pairing is significantly enhanced by the strong interface mode coupling. We will also show other results on the nature of the superconducting state in this system. [References: JJ Lee et al., Nature 515, 245 (2014)].

**11:51AM B11.00002 Enhanced superconductivity due to forward scattering in FeSe thin films on SrTiO<sub>3</sub> substrates** , STEVEN JOHNSTON, Univ of Tennessee, Knoxville, LOUK RADEMAKER, Kavli Institute for Theoretical Physics, University of California Santa Barbara, YAN WANG, Univ of Tennessee, Knoxville, TOM BERLIJN, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory — We examine the consequences of an electron-phonon (*e-ph*) interaction that is strongly peaked in the forward scattering ( $\mathbf{q} = 0$ ) direction in a two-dimensional superconductor. We find that strong forward scattering results in an enhanced  $T_c$  that is linearly proportional to the strength of the dimensionless *e-ph* coupling constant  $\lambda_m$  in the weak coupling limit. This is in stark contrast to the exponential dependence commonly derived in conventional BCS theory. This interaction also produces distinct replica bands in the single-particle spectral function, similar to those observed in recent angle-resolved photoemission experiments on FeSe monolayers on SrTiO<sub>3</sub> and BaTiO<sub>3</sub> substrates. By comparing our model to photoemission experiments, we infer an *e-ph* coupling strength that can provide a significant portion of the observed high  $T_c$  in these systems. [Reference: arXiv:1507.03967]

**12:03PM B11.00003 Electron-Phonon Couplings of the Interfacial Mode in FeSe Thin Films on SrTiO<sub>3</sub> and BaTiO<sub>3</sub>** , YAN WANG, Department of Physics and Astronomy, University of Tennessee, Knoxville, TOM BERLIJN, Oak Ridge National Laboratory, LOUK RADEMAKER, Kavli Institute for Theoretical Physics, University of California Santa Barbara, STEVE JOHNSTON, Department of Physics and Astronomy, University of Tennessee, Knoxville — Monolayers FeSe on SrTiO<sub>3</sub> or BaTiO<sub>3</sub> substrates possess highest superconducting transition temperatures in Fe-based superconductors with  $T_c \sim 70$  K measured by angle-resolved photoemission spectroscopy (ARPES) and other experiments. Furthermore, the high  $T_c$ 's concur with exact replica bands in ARPES spectra. A forward scattering mechanism with small momentum transfer through the electron-phonon interaction has been proposed to explain the high  $T_c$ 's and the replica bands.[1] We apply *ab initio* techniques to study such coupling in monolayer and bilayer FeSe thin films on SrTiO<sub>3</sub>, BaTiO<sub>3</sub>, and oxygen-vacant SrTiO<sub>3</sub> substrates. Our results confirm the forward scattering nature of electron-phonon coupling of the oxygen polar mode whose energy coincides with the off-set energy of the replica bands. [1]L. Rademaker, et al., arXiv:1507.03967.

**12:15PM B11.00004 Oxygen vacancy induced flat phonon mode at FeSe/STO interface.** , YUN XIE, HAI-YUAN CAO, YANG ZHOU, Fudan Univ, SHIYOU CHEN, East China Normal University, HONGJUN XIANG, XINGAO GONG, Fudan Univ, FUDAN UNIVERSITY TEAM — A high-frequency optical phonon mode of SrTiO<sub>3</sub>(STO) was found to assist the high-temperature superconductivity observed recently at the interface between monolayer FeSe and STO substrate. However, the origin of this mode is not clear. Through first-principles calculations, we find that there is a novel polar phonon mode on the surface layers of the STO substrate, which does not exist in the STO crystals. The oxygen vacancies near the FeSe/STO interface drives the dispersion of this phonon mode to be flat and lowers its energy, whereas the charge transfer between STO substrate and FeSe monolayer further reduces its energy to 81 meV. This energy is in good agreement with the experimental value fitted by Lee et al. for the phonon mode responsible for the observed replica band separations and the increased superconducting gap. The oxygen-vacancy-induced flat and polar phonon mode provides clues for understanding the origin of high  $T_c$  superconductivity at the FeSe/ STO interface.

**12:27PM B11.00005 ARPES Studies on the substrate effect on monolayer FeSe**, SLAVKO REBEC, Stanford, SIMES, TAO JIA, JAMES LEE, WEI LI, CHAOFAN ZHANG, SIMES, Stanford, ROBERT MOORE, SSRL, SIMES, Z.X. SHEN, SIMES, Stanford — For 2D films, interface interactions can play a critical role in determining the prevailing physics of the system. In the case of FeSe on SrTiO<sub>3</sub>, reducing the FeSe thickness to 1 monolayer (ML) from bulk leads to a significantly increased superconducting transition temperature (T<sub>c</sub>). To fully utilize and maximize this approach to increasing T<sub>c</sub> in FeSe and potentially apply it to other superconducting materials, the role which the substrate plays in this system must be understood. Here we present recent in-situ angle-resolved photo emission studies of the substrate effect on MBE grown 1 ML FeSe films.

**12:39PM B11.00006 The role of the  $\sqrt{13} \times \sqrt{13} - R33.7^\circ$  surface reconstruction on superconducting FeSe/SrTiO<sub>3</sub>**, STEPHEN D. ALBRIGHT, Department of Physics and Center for Research on Interface Structures and Phenomena (CRISP), Yale University, K. ZOU, SUBHASISH MANDAL, DIVINE KUMAR, Department of Applied Physics and CRISP, Yale University, OMUR DAGDEVIREN, G.H. SIMON, UDO SCHWARZ, Department of Mechanical Engineering & Materials Science and CRISP, Yale University, ERIC ALTMAN, Department of Chemical & Environmental Engineering and CRISP, Yale University, MYUNG-GEUN HAN, YIMEI ZHU, Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory, SOHRAB ISMAIL-BEIGI, F.J. WALKER, C.H. AHN, Department of Applied Physics and CRISP, Yale University — The creation of specific oxide surface structures is important to nucleating epitaxial growth. Here we show that the reconstructions of the SrTiO<sub>3</sub> (STO) surface impact the properties of monolayer FeSe grown on STO. We achieve high-quality epitaxial growth of FeSe on surfaces that feature a double TiO<sub>2</sub> termination, such as the  $\sqrt{13} \times \sqrt{13} - R33.7^\circ$  reconstructed STO surface prepared by high-temperature annealing in oxygen. Diffraction patterns characteristic of the reconstruction are observed with electron and synchrotron x-ray diffraction. The detailed structure of the FeSe/ $\sqrt{13} \times \sqrt{13} - R33.7^\circ$  interface is determined using crystal truncation rod analysis, and the double TiO<sub>2</sub> termination observed is consistent with previous transmission electron microscopy studies. We further demonstrate the significance of this particular interface structure on epitaxial growth and its implications for the resulting electronic structure using first principles theory.

**12:51PM B11.00007 Role of double TiO<sub>2</sub> layers at the FeSe/SrTiO<sub>3</sub> superconducting interface: A Density functional study<sup>1</sup>**, S. MANDAL, Department of Applied Physics, Yale University, R. PENG, Y. PU, D. FENG, Department of Physics and Advanced Materials Laboratory, Fudan University, X. HE, I. BOZOVIC, Brookhaven National Laboratory, K. ZOU, S. ALBRIGHT, G. SIMON, O. E. DAGDEVIREN, U. D. SCHWARZ, E. I. ALTMAN, D. KUMAR, F. J. WALKER, C. H. AHN, S. ISMAIL-BEIGI, Center for Research on Interface Structures and Phenomena (CRISP), Yale University — The recent discovery of high temperature superconductivity in monolayer FeSe on SrTiO<sub>3</sub> (STO) has drawn much attention. Since there is a strong enhancement of superconductivity compared to bulk FeSe, understanding the interfacial interactions between FeSe and STO is important. To date, density functional theory (DFT) studies have had difficulties explaining a key feature in the observed Fermi surface topology: namely the absence of a “hole pocket” about the  $\Gamma$  point in the Brillouin zone of the heterostructure. By combining DFT and experiment, we find that the STO surface termination is not the primitive  $1 \times 1$  single-layer TiO<sub>2</sub> assumed in most works but instead is a more complex double-layered TiO<sub>2</sub> structure. We find that the double layer facilitates epitaxial growth of monolayer FeSe. Our DFT calculations show that the hole pocket can be eliminated by the enhanced tendency of the double layer (compared to the single layer) termination to donate electrons to the FeSe when oxygen vacancies are present at the STO surface.

<sup>1</sup>NSF Grant MRSEC DMR-1119826

**1:03PM B11.00008 STM investigation of FeSe/STO binding<sup>1</sup>**, TATIANA A. WEBB, University of British Columbia, Harvard University, DENNIS HUANG, Harvard University, HARRIS PIRIE, JASON HOFFMAN, University of British Columbia, Harvard University, MOHAMMAD H. HAMIDIAN, Harvard University, Cornell University, CAN-LI SONG, Tsinghua University, CUI-ZU CHANG, JAGADEESH S. MOODERA, Massachusetts Institute of Technology, JENNIFER E. HOFFMAN, University of British Columbia, Harvard University — The electronic properties of monolayer FeSe grown on a SrTiO<sub>3</sub> (STO) substrate differ dramatically from bulk FeSe, with the superconducting transition temperature (T<sub>c</sub>) enhanced by an order of magnitude. This change in T<sub>c</sub> is accompanied by suppressed nematicity, electron doping, and possible coupling to substrate phonons. The first monolayer on the STO surface appears to be unique, and its electronic structure is tunable via sample preparation. We investigate the FeSe/STO binding and growth mechanism via scanning tunneling microscopy and spectroscopy, in order to understand the crucial role of the STO surface in modifying the electronic structure of FeSe.

<sup>1</sup>Work supported by the National Science Foundation DMR-1231319 (STC CIQM), and the Gordon & Betty Moore Foundation EPiQS GBMF4536.

**1:15PM B11.00009 Defects in Thin-Film FeSe/SrTiO<sub>3</sub>: STM and DFT Investigations<sup>1</sup>**, DENNIS HUANG, Harvard University, TATIANA A. WEBB, University of British Columbia, Harvard University, CAN-LI SONG, Tsinghua University, CUI-ZU CHANG, JAGADEESH S. MOODERA, Massachusetts Institute of Technology, EFTHIMIOS KAXIRAS, Harvard University, JENNIFER E. HOFFMAN, University of British Columbia, Harvard University — A single-layer of FeSe deposited on SrTiO<sub>3</sub> exhibits an order-of-magnitude enhancement of its superconducting transition temperature compared to bulk FeSe. This dramatic effect is curiously absent in a second layer of FeSe deposited on the heterostructure, leading to many questions concerning the role of the interface structure, electron doping and phonon coupling. Here, we approach these questions by using STM to characterize and compare native defects that appear in multi-layer and single-layer FeSe/SrTiO<sub>3</sub> grown by MBE under excess Se flux. We use DFT to explore candidate defect configurations, formation energies and diffusion barriers, in order to gain atomic-scale insights into the growth and structure of these film heterostructures.

<sup>1</sup>Work supported by NSF DMR-1231319 (STC CIQM) and Moore Foundation EPiQS GBMF4536. Computations run on Harvard RC Odyssey.

**1:27PM B11.00010 Impact of impurities on superconducting states of FeSe films on SrTiO<sub>3</sub><sup>1</sup>**, ZHUOZHI GE, DUSHYANT TOMER, SHIVANI RAJPUT, LIAN LI, Univ of Wisconsin, Milwaukee — Monolayer and bilayer FeSe films are grown on SrTiO<sub>3</sub> substrates by molecular beam epitaxy, and their surface atomic structure and electronic properties are studied using scanning tunneling microscopy/spectroscopy. Tunneling spectroscopy carried out at 6K reveals a superconducting gap of 20 meV for monolayer FeSe, while bilayer FeSe is found to be mostly semiconducting. However, a gap of 16 meV is observed within 1nm of impurity sites for the bilayer FeSe, indicating a superconducting state. This observation suggests that controlled doping can significantly change the electronic property of FeSe films on SrTiO<sub>3</sub>, which can even open a large superconducting gap. This research was supported by NSF DMR-1335215.

<sup>1</sup>This research was supported by NSF DMR-1335215.

**1:39PM B11.00011 Controlling superconductivity at the FeSe/SrTiO<sub>3</sub> interface by interfacial electron density<sup>1</sup>**, WEIWEI ZHAO, Pennsylvania State University, CUI-ZU CHANG, MIT, JUE JIANG, Pennsylvania State University, JAGADEESH MOODERA, MIT, MOSES CHAN, Pennsylvania State University — Single layer iron selenide (FeSe) on SrTiO<sub>3</sub> substrate with a possible superconducting transition temperature ( $T_c$ ) above 100K has attracted a great deal of attention recently. An important outstanding puzzle in this system is the inconsistency in  $T_c$  as measured by different techniques. Here we systematically study the dependence of  $T_c$  on the electron carrier density in this system and found that  $T_c$  can be most effectively enhanced by increasing the density of electron carriers directly at the FeSe/SrTiO<sub>3</sub> interface. We believe that our result resolves some of the puzzles in previous experiments, and open the possibility for further enhancement of  $T_c$  in this system even when taken outside the UHV chamber.

<sup>1</sup>This research is supported by the NSF grants (DMR-1420620, Penn State MRSEC; in MIT by DMR-1207469 and the STC Center for Integrated Quantum Materials under NSF grant DMR-1231319) and by ONR Grant N00014-13-1-0301.

**1:51PM B11.00012 Charge transfer effect of FeSe thin films on SrTiO<sub>3</sub><sup>1</sup>**, YUANJUN ZHOU, ANDREW MILLIS, Columbia University — Monolayer FeSe grown on SrTiO<sub>3</sub> substrate has shown a significant enhancement in the superconducting transition temperature ( $T_c$ ) relative to the bulk material. Monolayers of FeSe are electron doped relative to bulk; we propose that the doping comes from work-function-mismatch driven charge transfer from SrTiO<sub>3</sub> impurity bands, modified by out-of-plane polar distortions of the SrTiO<sub>3</sub>. We present a modified Schottky model combined with density functional calculations substantiating this picture for monolayer FeSe films on Nb doped SrTiO<sub>3</sub>. Physically relevant levels of Nb doping are shown to lead to doping of the FeSe compatible with observation. Adding polar fluctuations to the model leads to an electron-phonon interaction whose effect on the transition temperature is investigated.

<sup>1</sup>YZ is supported by National Science Foundation under grant No. DMR-1120296. AJM is supported by the Department of Energy under No. DOE-ER-046169.

**2:03PM B11.00013 Observation of Dirac cone band dispersions in FeSe thin films by photoemission spectroscopy.**, SHIYONG TAN, YUN FANG, DONGHUA XIE, WEI FENG, Institute of Materials, China Academy of Engineering Physics, CHENHAOPING WEN, QI SONG, Fudan university, QIYUN CHEN, WEN ZHANG, YUN ZHANG, LIUZHU LUO, Institute of Materials, China Academy of Engineering Physics, BINPING XIE, Fudan university, XINCHUN LAI, Institute of Materials, China Academy of Engineering Physics, DONGLAI FENG, Fudan university, FENG GROUP TEAM, LAI GROUP TEAM — The search for novel materials with Dirac cone band dispersion is one of the most challenging and important works for both fundamental physics and technological applications. Here, we studied the electronic structure of FeSe thin films grown on SrTiO<sub>3</sub> substrates by angle-resolved photoemission spectroscopy (ARPES). We reveal the existence of Dirac cone band dispersions in FeSe thin films thicker than 1 Unit Cell below the nematic transition temperature, whose apexes are located -10 meV below Fermi energy. The evolution of electronic structures for FeSe thin films as function of temperature, thickness and cobalt doping are systematically studied. The Dirac cones are found to be coexisted with the nematicity in FeSe, disappear when nematicity is suppressed. Our results provide useful guidelines for understanding the novel electronic structure, nematicity and superconductivity in FeSe system..

## Monday, March 14, 2016 11:15AM - 2:15PM —

Session B12 FIP DBIO: Large Scale Neuroscience Projects 308 - Maria Spiropulu, California Institute of Technology

**11:15AM B12.00001 Computational Neuroscience Today**, TERRY SEJNOWSKI, Salk Institute for Biological Studies — No abstract available.

**11:51AM B12.00002 The BRAIN Initiative**, MIYOUNG CHUN, Kavli Foundation — No abstract available.

**12:27PM B12.00003 Big neuron**, HANCHUAN PENG, Allen Institute for Brain Science — No abstract available.

**1:03PM B12.00004 The Global Brain (Simons Collaboration)**, DAVID TANK, Princeton — No abstract available.

**1:39PM B12.00005 Panel Discussion** —

## Monday, March 14, 2016 11:15AM - 2:15PM —

Session B13 GQI: Adiabatic Quantum Computation and Quantum Annealing 309 - Tameem Albash, Univ of Southern California

### 11:15AM B13.00001 Simulated annealing versus quantum annealing , MATTHIAS TROYER, ETH Zurich —

Based on simulated classical annealing and simulated quantum annealing using quantum Monte Carlo (QMC) simulations I will explore the question where physical or simulated quantum annealers may outperform classical optimization algorithms. Although the stochastic dynamics of QMC simulations is not the same as the unitary dynamics of a quantum system, I will first show that for the problem of quantum tunneling between two local minima both QMC simulations and a physical system exhibit the same scaling of tunneling times with barrier height. The scaling in both cases is  $O(\Delta^2)$ , where  $\Delta$  is the tunneling splitting. An important consequence is that QMC simulations can be used to predict the performance of a quantum annealer for tunneling through a barrier. Furthermore, by using open instead of periodic boundary conditions in imaginary time, equivalent to a projector QMC algorithm, one obtains a quadratic speedup for QMC, and achieve linear scaling in  $\Delta$  [1]. I will then address the apparent contradiction between experiments on a D-Wave 2 system that failed to see evidence of quantum speedup [2] and previous QMC results [3] that indicated an advantage of quantum annealing over classical annealing for spin glasses. We find that this contradiction is resolved by taking the continuous time limit in the QMC simulations which then agree with the experimentally observed behavior and show no speedup for 2D spin glasses. However, QMC simulations with large time steps gain further advantage: they “cheat by ignoring what happens during a (large) time step, and can thus outperform both simulated quantum annealers and classical annealers [4]. I will then address the question how to optimally run a simulated or physical quantum annealer. Investigating the behavior of the tails of the distribution of runtimes for very hard instances we find that adiabatically slow annealing is far from optimal. On the contrary, many repeated relatively fast annealing runs can be orders of magnitude faster for hard spin glass problems. The intuitive explanation is that hard instances, which are stuck in the wrong minimum can be solved faster by perturbing them [5]. I will finally discuss the consequences of these findings for designing better quantum annealers. [1] S.V. Isakov, G. Mazzola, V.N. Smelyanskiy, Z. Jiang, S. Boixo, H. Neven, and M. Troyer, arXiv:1510.08057. [2] T.F. Rønnow, Z. Wang, J. Job, S. Boixo, S.V. Isakov, D. Wecker, J.M. Martinis, D.A. Lidar, M. Troyer, Science **345**, 420 (2014). [3] G.E. Santoro, R. Martonak, E. Tönatti, and R. Car, Science **295**, 2427 (2002). [4] B. Heim, T. F. Rønnow, S. V. Isakov, and M. Troyer, Science **348**, 215 (2015). [5] D.S. Steiger, T.F. Rønnow, M. Troyer, Phys. Rev. Lett. (in press); arXiv:1504.07991

### 11:51AM B13.00002 Mean-field analysis of quantum annealing with XX-type terms , HIDETOSHI NISHIMORI, Tokyo Institute of Technology —

I analyze the role of XX-type terms in quantum annealing for a few mean-field systems including the Ising ferromagnet and the Hopfield model, both with many-body interactions. The XX-type terms are shown to be effective to remove first-order quantum phase transitions, which exist in the conventional implementation of quantum annealing using only transverse fields. This means an exponential increase in efficiency, and is suggestive for the design of quantum annealers. I will discuss how and why this phenomenon emerges and what may happen on realistic finite-dimensional lattices.

- [1] Y. Seki and H. Nishimori, J. Phys. A **48**, 335301 (2015).
- [2] B. Seoane and H. Nishimori, J. Phys. A **45**, 435301 (2012).
- [3] Y. Seki and H. Nishimori, Phys. Rev. E **85**, 051112 (2012).
- [4] S. Suzuki, H. Nishimori and M. Suzuki, Phys. Rev. E **75**, 051112 (2007).

### 12:27PM B13.00003 Error suppression and correction for quantum annealing , DANIEL LIDAR, Univ of Southern California —

While adiabatic quantum computing and quantum annealing enjoy a certain degree of inherent robustness against excitations and control errors, there is no escaping the need for error correction or suppression. In this talk I will give an overview of our work on the development of such error correction and suppression methods. We have experimentally tested one such method combining encoding, energy penalties and decoding, on a D-Wave Two processor, with encouraging results. Mean field theory shows that this can be explained in terms of a softening of the closing of the gap due to the energy penalty, resulting in protection against excitations that occur near the quantum critical point. Decoding recovers population from excited states and enhances the success probability of quantum annealing. Moreover, we have demonstrated that using repetition codes with increasing code distance can lower the effective temperature of the annealer.

References:

- K.L. Pudenz, T. Albash, D.A. Lidar, Error corrected quantum annealing with hundreds of qubits, Nature Commun. **5**, 3243 (2014).
- K.L. Pudenz, T. Albash, D.A. Lidar, Quantum annealing correction for random Ising problems, Phys. Rev. A. **91**, 042302 (2015).
- S. Matsuura, H. Nishimori, T. Albash, D.A. Lidar, Mean Field Analysis of Quantum Annealing Correction. arXiv:1510.07709.
- W. Vinci et al., in preparation.

### 1:03PM B13.00004 Precision and the approach to optimality in quantum annealing processors , MARK W JOHNSON, D-Wave Systems Inc —

The last few years have seen both a significant technological advance towards the practical application of, and a growing scientific interest in the underlying behaviour of quantum annealing (QA) algorithms [1]. A series of commercially available QA processors, most recently the D-Wave 2X™ 1000 qubit processor, have provided a valuable platform for empirical study of QA at a non-trivial scale. From this it has become clear that misspecification of Hamiltonian parameters is an important performance consideration, both for the goal of studying the underlying physics of QA, as well as that of building a practical and useful QA processor. The empirical study of the physics of QA requires a way to look beyond Hamiltonian misspecification.

Recently, a solver metric called ‘time-to-target’ was proposed [2] as a way to compare quantum annealing processors to classical heuristic algorithms. This approach puts emphasis on analyzing a solver’s short time approach to the ground state. In this presentation I will review the processor technology, based on superconducting flux qubits, and some of the known sources of error in Hamiltonian specification. I will then discuss recent advances in reducing Hamiltonian specification error, as well as review the time-to-target metric and empirical results analyzed in this way.

- [1] E.g. “Discussion and Debate: Quantum Annealing: The Fastest Route to Quantum Computation?”, S Suzuki and A Das eds., Eur. Phys. J. Special Topics, **224** (1), Feb 2015.
- [2] J. King, et al.; “Benchmarking a [QA] processor with the time-to-target metric”, arXiv:1508.05087 [quant-ph]

### 1:39PM B13.00005 Universal fault-tolerant adiabatic quantum computing with quantum dots or donors , ANDREW LANDAHL, Sandia National Laboratories —

I will present a conceptual design for an adiabatic quantum computer that can achieve arbitrarily accurate universal fault-tolerant quantum computations with a constant energy gap and nearest-neighbor interactions. This machine can run any quantum algorithm known today or discovered in the future, in principle. The key theoretical idea is adiabatic deformation of degenerate ground spaces formed by topological quantum error-correcting codes. An open problem with the design is making the four-body interactions and measurements it uses more technologically accessible. I will present some partial solutions, including one in which interactions between quantum dots or donors in a two-dimensional array can emulate the desired interactions in second-order perturbation theory. I will conclude with some open problems, including the challenge of reformulating Kitaev’s gadget perturbation theory technique so that it preserves fault tolerance. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

## Monday, March 14, 2016 11:15AM - 2:15PM —

Session B14 FHP: The History of Electrical Science 310 - Amy Fisher, University of Puget Sound

**11:15AM B14.00001 Electrical Enlightenment: Joseph Priestley's Historical and Experimental Studies of Electricity** , VICTOR BOANTZA, University of Minnesota — Joseph Priestley (1733–1804) was one of the most controversial public figures of the eighteenth century. A true Enlightenment polymath, he wrote more than two hundred books, pamphlets, sermons, and essays on subjects ranging from science to politics and from metaphysics to theology. He was a religious dissenter, political radical, vocal supporter of the French Revolution, and lifelong defender of the losing side in the Chemical Revolution. Priestley is best known for having "discovered" oxygen in the 1770s and for his lasting contributions to pneumatic chemistry. Yet his first scientific fascination, while teaching at Warrington Academy, was electricity—one of the greatest scientific fads of the Enlightenment. Priestley's work on electricity, both historical and experimental, culminated in his *History and Present State of Electricity* (1767), which became a standard textbook on the subject for nearly a century, and went through numerous editions and translations. Situating Priestley's electrical investigations against the background of eighteenth-century ideals of scientific theory and practice, especially concerning physics, experimental philosophy, and natural history, illuminates the relations between science, society, and epistemology in the Enlightenment.

**11:51AM B14.00002 Lomonosov's Electrical Experiments** , ROBERT CREASE, State Univ of NY- Stony Brook — No abstract available.

**12:27PM B14.00003 Priestley's Shadow and Lavoisier's Influence: Electricity and Heat in the Late Eighteenth and Early Nineteenth Centuries** , AMY FISHER, University of Puget Sound — In the late eighteenth century, Joseph Priestley argued that any complete theory of heat also had to explain electrical phenomena, which manifested many similar effects to heat. For example, sparking or heating a sample of trapped air caused a reduction in the volume of air and made the gas toxic to living organisms. Because of the complexity of electrical and thermal phenomena, Antoine Lavoisier did not address electrical action in his published works. Rather, he focused on those effects produced by heating alone. With the success of Lavoisier's caloric theory of heat, natural philosophers and chemists continued to debate the relationship between heat and electricity. In this presentation, I compare and contrast the fate of caloric in early-nineteenth-century electrical studies via the work of two scientists: Humphry Davy in Britain and Robert Hare in America.

**1:03PM B14.00004 Broken Circuits? International Scientific Communication on Galvanic Electricity During the Napoleonic Wars** , IAIN WATTS, University of Puget Sound — No abstract available.

**1:39PM B14.00005 The Bottom Line: Cable Telegraphy and the Rise of Field Theory in the Victorian British Empire** , BRUCE HUNT, Univ of Texas, Austin — The networks of telegraph wires and undersea cables that began to spread across the world in the 1840s and 1850s had far-reaching effects on commerce and the dissemination of news. They also had deep effects on electrical science. In this paper, I will argue that what might at first appear to be a prime example of pure science—the development of electromagnetic field theory in Britain in the middle decades of the 19th century—was in fact driven in important ways by developments in the telegraph industry, particularly British scientists' and engineers' encounters with puzzling new phenomenon of the 'retardation' of signals that turned up on underground wires and undersea cables in the early 1850s.

**Monday, March 14, 2016 11:15AM - 2:15PM —**

**Session B15 DCMP DMP: Graphene: Magnetotransport** 314 - Aubrey Hanbicki, Naval Research Laboratory

**11:15AM B15.00001 ABSTRACT WITHDRAWN —**

**11:27AM B15.00002 Magnetoresistance and Anti-Ferromagnetic Coupling in FM-Graphene-FM Trilayers** , ENRIQUE D. COBAS, OLAF M. J. VAN 'T ERVE, SHU-FAN CHENG, BEREND T. JONKER, US Naval Research Laboratory — Both high-magnetoresistance(MR) minority spin filtering[1] and anti-ferromagnetic (AFM) coupling[2-3] have been predicted for FM|Graphene|FM vertical heterostructures. Our previous experiments[4-5] demonstrated ordinary magnetoresistance in NiFe-Graphene-Co heterostructures and no evident AFM coupling. Here we present experimental results that confirm both MR minority spin filtering and AFM coupling in high-quality FM|Graphene|FM heterostructures. The heterostructures were fabricated by a combination of sputtering, chemical vapor deposition and electron beam evaporation. The stack was patterned into symmetric cross-bar structures using Ar ion milling. Measurements show negative magnetoresistance in excess of 10 percent, confirming spin-filtering, and weak anti-ferromagnetic coupling throughout the temperature range 15K to 300K. The temperature dependence of the MR was studied and found consistent with thermal excitation of spin waves in the ferromagnetic electrodes. Junction resistance-area products are in the range of  $10 \Omega\text{cm}^2$ . These heterostructures provide a fast and low-power magnetic field sensor in the sub-100 Oe range and are a step towards high-MR low RA-product MRAM junctions. [1] Karpan, et al. Phys. Rev. Lett 99, 176602, 2007. [2] Li et al., App. Phys. Lett 98 (13), 133111, 2011. [3] Kim, D. et al., App. Phys. Lett 102 (11), 112403, 2013 [4] Cobas et al., Nano Lett. 12, 3000, 2012. [5] Cobas et al., IEEE Trans. Mag., 49 (7), 4343, 2013.

**11:39AM B15.00003 Magneto Transport in Three Dimensional Carbon Nanostructures** , TIMIR DATTA, LEI WANG, University of South Carolina, JAN JAROSZYNSKI, National High Magnetic Field Lab, MING YIN, Benedict College, DHEYAA ALAMERI, University of South Carolina — Electrical properties of self-assembled three dimensional nanostructures are interesting topic. Here we report temperature dependence of magneto transport in such carbon nanostructures with periodic spherical voids. Specimens with different void diameters in the temperature range from 200 mK to 20 K were studied. Above 2 K, magnetoresistance,  $MR = [R(B) - R(0)] / R(0)$ , crosses over from quadratic to a linear dependence with the increase of magnetic field [Wang et al, APL 2015; DOI:10.1063/1.4926606]. We observe MR to be non-saturating even up to 18 Tesla. Furthermore, MR demonstrates universality because all experimental data can be collapsed on to a single curve, as a universal function of B/T. Below 2 K, magnetoresistance saturates with increasing field. Quantum Hall like steps are also observed in this low temperature regime. Remarkably, MR of our sample displays orientation independence, an attractive feature for technological applications.

**11:51AM B15.00004 Study on anisotropic quantum transport in graphene sheets by ESR** , LIQIN YAN, YOUNG SUN, JIAO HUANG, XIAOLONG CHEN, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100190, China — Quantum transport in graphene has attracted much attention due to its excellent thermal conductivity and high room-temperature electron mobility.[1] Using the electron spin resonance (ESR) spectrometer for studying weak localization (WL) and weak antilocalization (WAL) effects, except for having the obvious advantage of no need for electrical contacts, differs from the electric transport measurement technique also in the dominant signal from the surface of the layer not from the bulk substrate. [2] Here we have studied an experimental anisotropic quantum transport performed on an assemblage of vertical aligned graphene sheets from 5 to 300 K by a Bruker X-band (9.3 GHz). An anisotropic quantum transport is observed between b with WL and c with WAL axes at 5 - 50 K. With increasing temperature, the transport mechanism is changed along b and c axes. We use WL theory to fit all the spectra and obtain the coherence length  $L_\phi$ , long range scattering length  $L_{l\tau}$ , intervalley scattering length  $L_i$  and analyze the data. Our results indicate that ESR is a robust platform to study the intrinsic physical properties of graphene. [1] Y. Zhang, et al, Nature (London) 438, 201 (2005). [2] A. Drabinska, et al, Phys. Rev. B 86, 045421 (2012).

## 12:03PM B15.00005 Study of magnetotransport across the neutrality point in CVD graphene<sup>1</sup>

, RAMESH G. MANI, Georgia State University, Atlanta, GA 30303 — Hall effect compensation and a residual resistivity  $\rho_{xx} \approx h/4e^2$  are experimentally examined over the p $\leftrightarrow$ n transition about the nominal Dirac point in CVD graphene. The observed characteristics are reproduced in a model with a parabolic distribution  $f(V_N)$  of neutrality potentials,  $V_N$ , and simultaneous electron- and hole- conduction. The results suggest that, broadly about the gate-induced n  $\leftrightarrow$  p transition, charge transport is characterized by domain confined ambipolar currents, which leads to compensation in the global Hall effect and the observed residual resistivity.

<sup>1</sup>DOE-BES, Mat'l. Sci. & Eng. Div., DE-SC0001762; ARO W911NF-14-2-0076; ARO W911NF-15-1-0433

## 12:15PM B15.00006 Magnetotransport measurements in graphene/ferromagnetic insulator heterostructures

, AARON SHARPE, Stanford University, WENMIN YANG, Institute of Physics, Chinese Academy of Science, MENYOUNG LEE, DAVID GOLDBERGER-GORDON, Stanford University, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute of Material Science, Japan, ROBERT CAVA, Princeton University — Through proximity effects, it is possible for two-dimensional graphene sheets to inherit order parameters from another two-dimensional substrate. Specifically, graphene has been seen to exhibit ferromagnetism when placed on a ferromagnetic insulator. Ferromagnetic graphene is a very promising platform for devices potentially useful for spintronics applications. We present here magnetotransport measurements of graphene/ferromagnetic insulator heterostructures.

## 12:27PM B15.00007 Magnetotransport in Graphene on the Nano Scale measured by Scanning Tunneling Potentiometry<sup>1</sup>

, PHILIP WILLKE, THOMAS DRUGA, THOMAS KOTZOTT, RAINER ULBRICH, Univ Goettingen, ALEXANDER SCHNEIDER, Univ Erlangen-Nuernberg, MARTIN WENDEROTH, Univ Goettingen — The method of scanning tunneling potentiometry (STP) has been introduced by Muralt and Pohl [1] as a technique for mapping the electrochemical potential locally. Here we present a new home-built low-temperature STP setup with applicable magnetic field of up to 6T to study the spatial evolution of the voltage drop at extended defects in graphene with high-resolution.[2] We show that the voltage drop at a monolayer-bilayer boundary in graphene clearly extends spatially up to a few nanometers into the bilayer and hence is not located strictly at the structural defect. Moreover, different scattering mechanisms can be disentangled. Besides, we perform magnetotransport STP measurements mapping the local electrochemical potential as a function of the applied magnetic field. This allows us to identify localized and delocalized contributions to the magnetoresistance in epitaxial-grown graphene and to reveal the contribution of defects. [1] P. Muralt, D. W. Pohl, Scanning tunneling potentiometry, Appl. Phys. Lett., 48, 514 (1986) [2] P. Willke, et al. Spatial Extent of a Landauer Residual-Resistivity Dipole in Graphene quantified by Scanning Tunneling Potentiometry, Nature Commun. 6, 6399 (2015)

<sup>1</sup>This work was supported by the priority program 1459 Graphene of the German Science Foundation

## 12:39PM B15.00008 Universality of Effective Medium and Random Resistor Network models for disorder-induced linear unsaturating magnetoresistance<sup>1</sup>

, SILVIA LARA, YING TONG LAI, CAMERON LOVE, Yale-NUS College, NAVNEETH RAMAKRISHNAN, Department of Physics and Centre for Advanced 2D Materials, National University of Singapore, SHAFIQUE ADAM, Yale-NUS College — In recent years, the Effective Medium Theory (EMT) [1] and the Random Resistor Network (RRN) [2] have been separately used to explain disorder induced magnetoresistance that is quadratic at low fields and linear at high fields. We demonstrate that the quadratic and linear coefficients of the magnetoresistance and the transition point from the quadratic to the linear regime depend only on the inhomogeneous carrier density profile. We use this to find a mapping between the two models using dimensionless parameters that determine the magnetoresistance and show numerically that they belong to the same universality class. [1] J. Ping, I. Yudhistira, N. Ramakrishnan, S. Cho, S. Adam, and M. S. Fuhrer, Phys. Rev. Lett. 113, 047206 (2014). [2] M. Parish and P. Littlewood, Nature 426, 162 (2003)

<sup>1</sup>This work is supported by the Singapore National Research Foundation (NRF-NRFF2012-01) and the Singapore Ministry of Education and Yale-NUS College through grant number R-607-265-01312.

## 12:51PM B15.00009 Linear unsaturating magnetoresistance in disordered systems<sup>1</sup>

, YING TONG LAI, SILVIA LARA, CAMERON LOVE, Yale-NUS College, NAVNEETH RAMAKRISHNAN, Centre for Advanced 2D Materials, SHAFIQUE ADAM, Yale-NUS College — Theoretical works [1, 2] have shown that disordered systems exhibit classical magnetoresistance (MR). In this talk, we examine a variety of experimental systems that observe linear MR at high magnetic fields, including silver chalcogenides, graphene, graphite and Weyl semimetals. We show that a careful analysis of the magnitude of the MR, as well as the field strength at which the MR changes from quadratic to linear, reveal important properties of the system, such as the ratio of the root-mean-square fluctuations in the carrier density and the average carrier density. By looking at other properties such as the zero-field mobility, we show that this carrier density inhomogeneity is consistent with what is known about the microscopic impurities in these experiments. The application of this disorder-induced MR to a variety of different experimental scenarios underline the universality of these theoretical models. J. Ping, I. Yudhistira, N. Ramakrishnan, S. Cho, S. Adam, and M. S. Fuhrer, Phys. Rev. Lett. 113, 047206 (2014). M. Parish and P. Littlewood, Nature 426, 162 (2003)

<sup>1</sup>This work is supported by the Singapore National Research Foundation (NRF-NRFF2012-01) and the Singapore Ministry of Education and Yale-NUS College through grant number R-607-265-01312.

## 1:03PM B15.00010 Valley-symmetry-preserved transport in ballistic graphene layers with gate-defined carrier guiding

, MINSOO KIM, JI-HAE CHOI, SANG-HOON LEE, Department of Physics, Pohang University of Science and Technology, Korea, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Japan, SEUNG-HOON JHI, HU-JONG LEE, Department of Physics, Pohang University of Science and Technology, Korea — Zigzag graphene nanoribbons are predicted to exhibit interesting electronic properties stemming from its Dirac band structure. However, to date, investigation of them is highly limited because of the defects and the roughness at the edges, which mix different valley properties of graphene. Here, we report the signature of conservation of valley symmetry in two types of quasi-1D ballistic graphene transport devices; one is a quantum point contact (QPC) and another is an Aharonov-Bohm (AB) interferometer. In measurements, charge carriers were confined in a potential well formed by the dual gates operation and the four-terminal magnetoconductance (MC) was measured with varying the carrier density, dc bias, and temperature. It exhibits the conductance quantization in steps of  $\Delta G = 4e^2/h$  starting from  $G = (2, 6), 10 \times e^2/h$  in a constricted conducting channel of QPC-type devices. This behavior is similar to the one observed in zigzag graphene nanoribbons having edge localized channels. Our tight-binding calculation shows that quasi-1D charge flow on a graphene plane acts a zigzag-type nanoribbon, unless it is perfectly aligned along the armchair direction. In the AB interferometry, we observed  $h/e$  periodic modulation of MC and the zero-field conductance minimum with a negative MC background.

**1:15PM B15.00011 Visualization of phase-coherent electron interference in a ballistic graphene Josephson junction**, MONICA ALLEN, Harvard University, OLES SHTANKO, MIT, ION COSMA FULGA, Weizmann Institute, JOEL WANG, MIT, DANIYAR NURGALIEV, Harvard University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, ANTON AKHMEROV, TU Delft, PABLO JARILLO-HERRERO, LEONID LEVITOV, MIT, AMIR YACOBY, Harvard University — Graphene provides an appealing platform to explore electronic analogs of optics-like effects due to the nonclassical nature of ballistic charge transport. By coupling superconductors to a ballistic graphene sheet, we explore a new regime of superconducting transport in which phase-coherent interference of electron waves is a dominant feature. We employ Fraunhofer interferometry to achieve spatial imaging of cavity modes in a graphene Fabry-Perot resonator, embedded between two superconductors to form a Josephson junction. By visualizing current flow using Fourier methods, our measurements provide evidence of separate interference conditions for bulk and edge currents and elucidate the microscopic nature of interference at the crystal boundaries. We also observe modulation of the multiple Andreev reflection amplitude on and off resonance, a direct measure of cavity transparency. These results constitute a strong departure from conventional Josephson behavior and motivate further exploration of new effects at the intersection of superconductivity and electron-optics.

**1:27PM B15.00012 Magnetostrain-driven quantum engine on a grapheme flake<sup>1</sup>**, ENRIQUE MUNOZ, Pontificia Universidad Catolica de Chile, FRANCISCO PENA, Pontificia Universidad Catolica de Valparaiso — The concept of a quantum heat engine (QHE) has been discussed [1-3] as an alternative to efficiently recover, on a nanoscale device, thermal energy in the form of useful work. In a QHEN the working substance is in a mixed quantum state determined by a density matrix. Interesting examples of this concept are constituted by photosynthesis in plants as well as human-designed photocells [4]. In this work [1], we propose a graphene-based quantum engine, driven by a superposition of mechanical strain and an external magnetic field. Engineering of strain in a nanoscale graphene flake creates a gauge field with an associated uniform pseudo-magnetic field. The combination leads to the emergence of discrete relativistic Landau levels [1]. The inter-level distance and hence their statistical population can be modulated by quasi-statically tuning the imposed magnetic field along a sequence of reversible transformations that constitute a quantum mechanical analog of the classical Otto cycle. References [1] F. J. Pena and E. Munoz, Phys. Rev. E 91 (2015) 052152. [2] E. Munoz and F. J. Pena, Phys. Rev. E 89 (2014) 052107. [3] E. Munoz and F. J. Pena, Phys. Rev. E 86 (2012) 061108. [4] M. O. Scully, M. S. Zubairy, G. S. Agarwal, and H. Walther, Science 299 (2013) 862.

<sup>1</sup>Financial support from Fondecyt 1141146

**1:39PM B15.00013 Magnetotransport of Epitaxial Graphene on Hexagonal SiC Surface Grown with Metal Plate Capping<sup>1</sup>**, KIBOG PARK, HAN BYUL JIN, SUNGCHUL JUNG, JUNHYOUNG KIM, Ulsan Natl Inst of Sci & Tech, DONG-HUN CHAE, WAN-SEOP KIM, JAESUNG PARK, Korea Research Institute of Standards and Science — High quality epitaxial graphene (EG) was grown on a Si-face hexagonal SiC substrate by capping the surface with a metal plate (Molybdenum, Tungsten) during UHV annealing. The growth temperature was  $\sim 950$  degree C, significantly lower than the conventional UHV annealing. The crystallinity of EG film was examined with Raman spectrum measurements. Almost no D-peak and a large narrow 2D-peak ensure that a thin (mono- or bi-layer) EG film was grown with a negligible number of defects. The electrical properties of EG film were also characterized by performing magnetotransport measurements with Hall-bar structures. The carrier type was found to be n-type, the sheet carrier density be  $(3.6-9.2) \times 10^{12} / \text{cm}^2$ , and the Hall mobility be  $\sim 2100 \text{ cm}^2/\text{Vs}$ . Due to the relatively high carrier density, the Quantum Hall Effect was observed only for high filling factors up to 14 T. However, clear Shubnikov-de-Hass oscillations were observed, indicating that the random carrier scattering due to impurities or defects is minimal in the EG film grown with metal plate capping.

<sup>1</sup>Supported by NRF in South Korea (2014M2B2A9031944)

**1:51PM B15.00014 Thermal Smearing of the Magneto-Kohn Anomaly for Dirac materials and comparison with the Two-dimensional electron Liquid**, DIPENDRA DAHAL, Department of Physics and Astronomy, Graduate Center and Hunter College of the City University of New York, 695 Park Avenue, New York, NY 10065, ANTONIOS BALASSIS, Department of Physics, Fordham University, NY, USA, GODFREY GUMBS, Department of Physics and Astronomy, Hunter College of the City University of New York, 695 Park Avenue, New York, NY 10065, M. L. GLASSER, Department of Physics, Clarkson University, Potsdam, New York 13699-5820, USA, GRAPHENE PROJECTS COLLABORATION — We compute and compare the effects due to a uniform perpendicular magnetic field and the temperature on the static polarization functions for monolayer graphene (MLG) associated with the Dirac point with that for the two-dimensional electron liquid (2DEL). Previous results for the 2DEL are discussed and we point out a flaw in reported analytic derivation to exhibit the smearing of the Fermi surface for 2DEL. The relevance of our study to the Kohn anomaly in low-dimensional structures and the Friedel oscillations for the screening of the potential for a dilute distribution of impurities is reported.

**2:03PM B15.00015 Hofstadter butterfly and quantum transport in graphene on hexagonal boron nitride from multiscale lattice simulations**, NICOLAS LECONTE, University of Texas at Austin, US - Department of Physics, University of Seoul, Seoul 130-742, Korea, RAFAEL MARTINEZ-GORDILLO, Centre Interdisciplinaire de Nanoscience de Marseille, CINAM, CNRS and Aix Marseille University, Campus de Luminy, Case 913, 13288 Marseille Cedex 9, ALLAN MACDONALD, University of Texas at Austin, US, JEIL JUNG, Department of Physics, University of Seoul, Seoul 130-742, Korea — Clear signatures of the Hofstadter butterfly have been experimentally observed in graphene on hexagonal boron nitride (G/BN), thanks to an appropriate balance between the length scale and the quality of the moiré superlattices. During this talk, I will present a methodology to map the continuum moiré pattern of incommensurable G/BN crystals obtained from ab initio calculations onto supercell lattice tight-binding Hamiltonians. Using efficient Lanczos recursion techniques for simulating large scale systems containing millions of atoms, the density of states and the dc conductivity are obtained as a function of energy or carrier density and magnetic field. The calculated Hofstadter butterflies and Landau fan diagrams show that the site potential variations, the mass, and substantial virtual strain contributions that appear even in the absence of real strains in the band Hamiltonian sensitively affect the electron-hole asymmetry, the gaps at the secondary Dirac points, as well as the tertiary features that appear at high-carrier densities.

**Monday, March 14, 2016 11:15AM - 2:15PM –**  
**Session B16 DMP: 2D Devices: Plasmonics and Optoelectronics** 315 - Paola Barbara, Georgetown University

**11:15AM B16.00001 GRAPHENE PLASMONICS** , SHIN MOU, DON ABEYSINGHE, Air Force Research Laboratory, Materials & Manufacturing Directorate, Wright-Patterson AFB, OH, USA, NIMA NADER, JOSHUA HENDRICKSON, JUSTIN CLEARY, Air Force Research Laboratory, Sensors Directorate, Wright-Patterson AFB, OH, USA, SAID ELHAMRI, Department of Physics, University of Dayton, Dayton, OH, USA — Plasmon, the collective free charge carrier oscillation, has been a popular research theme recently mostly associated with surface plasmon in metal nanoparticles. After the discovery of graphene, researchers soon began to study plasmonic effects with or within graphene, for instance, decorating graphene with metal nanoparticles to enhance optical processes via plasmonic field enhancement. Following that, people also gained interests in studying the intrinsic plasmon of graphene. Graphene, a tunable semimetal under field effect, demonstrates tunable plasmon resonances at room temperature, which enables new capabilities beyond those of metal-nanoparticle surface plasmons. In this project, we would like to show intrinsic graphene plasmon resonances in that we experimentally demonstrated polarization dependent and gate-bias tunable plasmon-resonance absorption in the mid-infrared regime of 5-14  $\mu\text{m}$  by utilizing an array of graphene nanoribbon resonators. By scaling nanoribbon width and charge densities, we probed graphene plasmons with plasmon resonance energy as high as 0.26 meV ( $2100\text{ cm}^{-1}$ ) for 40 nm wide nanoresonators. The result reveals the intriguing nature of graphene plasmon in graphene nanoribbons where the nanoribbon edge plays critical roles by introducing extra doping and damping the graphene plasmon resonance.

**11:27AM B16.00002 Optical and Electronic Properties of 2D Graphitic Carbon-Nitride and Carbon Enriched Alloys** , JOEL THERRIEN, YANCEN LI, DANIEL SCHMIDT, MICHAEL MASAKI, ABDULMANNAN SYED, U. Massachusetts Lowell — The two-dimensional form of graphitic carbon-nitride (gCN) has been successfully synthesized using a simple CVD process. In its pure form, the carbon to nitrogen ratio is 0.75. By adding a carbon bearing gas to the growth environment, the C/N ratio can be increased, ultimately reaching the pure carbon form: graphene. Unlike attempts at making a 2D alloy system out of BCN, the CN system does not suffer from phase segregation and thus forms a homogeneous alloy. The synthesis approach and electronic and optical properties will be presented for the pure gCN and a selection of alloy compositions.

**11:39AM B16.00003 Infrared two-wave mixing technique for characterization of graphene THz plasmonic devices<sup>1</sup>** , DENNIS DREW, MOHAMMAD JADIDI, ANDREI SUSHKOV, XINGHAN CAI, RYAN SUESS, MARTIN MITTENDORFF, THOMAS MURPHY, University of Maryland, College Park, MD 20742, MICHAEL FUHRER, Monash University, Australia, KEVIN DANIELS, KURT GASKILL, U.S. Naval Research Laboratory, Washington, DC 20375 — We have studied the heterodyne mixing of two beams from infrared lasers on graphene plasmonic devices and detectors. The nonlinear thermal response of graphene allows us to measure a DC photovoltage that depends on the heterodyne difference frequency and gate voltage. The inversion symmetry of the graphene device is broken by using dissimilar metal contacts to allow a net photo-thermoelectric signal. The power, frequency, and temperature dependence of the photoresponse are used to probe the graphene hot-electron cooling rates and mechanisms. We will discuss the use of photothermal effects in graphene to excite surface plasmons at the difference frequency. The high mobility of the free carriers in graphene is important for this experiment. We have measured exfoliated graphene on SiO<sub>2</sub>/Si substrate detector and we are working on BN graphene and intercalated SiC graphene devices.

<sup>1</sup>This work was sponsored by the U.S. ONR (N000141310865) and the U.S. NSF (ECCS 1309750).

**11:51AM B16.00004 THz Plasmonics of Quasi-freestanding Bilayer Epitaxial Graphene via H-intercalation** , KEVIN DANIELS, NRC postdoc residing at US Naval Research Laboratory, ANTHONY BOYD, ASEE postdoc residing at US Naval Research Laboratory, ANINDYA NATH, U.S. Naval Research Laboratory, MOHAMMAD JADIDI, ANDREI SUSHKOV, DENNIS DREW, University of Maryland, RACHAEL MYERS-WARD, KURT GASKILL, U.S. Naval Research Laboratory — Graphene plasmonics has attracted attention as a suitable platform for tunable THz optoelectronics. THz plasmonic resonances in conventional large-area graphene, however, suffer from low quality factor (Q) because of high carrier scattering rate. This low Q is attributed to charge carrier induced scattering and lower carrier mobility caused by the partially covalent bonding between the silicon carbide (SiC) substrate and the  $6\sqrt{3}$  buffer layer between the substrate and EG. Improving the Q of plasmons makes stronger THz resonance effects and also enable THz optoelectronics with fine tunability in frequency via gating. EG on Si-face, semi-insulating 6H-SiC was intercalated in-situ by hydrogen (H<sub>2</sub>), releasing the buffer layer from SiC forming quasi-freestanding bilayer graphene. H-intercalation time was varied from 0 – 75 minutes and structural, electrical and optical properties were explored, revealing at long H-intercalation durations high carrier mobility ( $3000\text{-}4000\text{ cm}^2/\text{Vs}$ ) and high sheet carrier concentration ( $1\text{E}13\text{ cm}^{-2}$ ) independent of carrier mobility. Far IR simultaneous transmission/reflection measurements revealed a narrow frequency response with line widths ( $\gamma$ ) smaller in H-intercalated EG ( $30\text{cm}^{-1}$ ) than observed in pristine EG ( $>100\text{cm}^{-1}$ ) consistent with the improved mobility.

**12:03PM B16.00005 Graphene Josephson Junction Single Photon Detector** , EVAN D WALSH, Massachusetts Institute of Technology, Harvard University, Raytheon BBN Technologies, GIL-HO LEE, Harvard University, DMITRI K EFETOV, MIKKEL HEUCK, Massachusetts Institute of Technology, JESSE CROSSNO, Harvard University, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, Japan, THOMAS A OHKI, Raytheon BBN Technologies, PHILIP KIM, Harvard University, DIRK ENGLUND, Massachusetts Institute of Technology, KIN CHUNG FONG, Raytheon BBN Technologies — Single photon detectors (SPDs) have found use across a wide array of applications depending on the wavelength to which they are sensitive. Graphene, because of its linear, gapless dispersion near the Dirac point, has a flat, wide bandwidth absorption that can be enhanced to nearly 100% through the use of resonant structures making it a promising candidate for broadband SPDs. Upon absorbing a photon in the optical to mid-infrared range, a small ( $\sim 10\text{ }\mu\text{m}^2$ ) sheet of graphene at cryogenic temperatures can experience a significant increase in electronic temperature due to its extremely low heat capacity. At 1550 nm, for example, calculations show that the temperature could rise by as much as 500%. This temperature increase could be detected with near perfect quantum efficiency by making the graphene the weak link in a Josephson junction (JJ). We present a theoretical model demonstrating that such a graphene JJ SPD could operate at the readily achievable temperature of 3 K with near zero dark count, sub-50 ps timing jitter, and sub-5 ns dead time and report on the progress toward experimentally realizing the device.

**12:15PM B16.00006 Imaging height fluctuations in free-standing graphene membranes** , KYLE DORSEY, MARC MISKIN, ARTHUR BARNARD, PETER ROSE, ITAI COHEN, PAUL MCEUEN, Cornell University — We present a technique based on multi-wavelength interference microscopy to measure the heights of observed ripples in free-standing graphene membranes. Graphene membranes released from a transparent substrate produce interference fringes when viewed in the reflection mode of an inverted microscope (Blees et. al. Nature 524 (7564): 204-207 (2015)). The fringes correspond to corrugation of the membrane as it floats near an interface. A single set of fringes is insufficient to uniquely determine the height profile, as a given fringe spacing can correspond to an increase or decrease in height by  $\lambda/2$ . Imaging at multiple wavelengths resolves the ambiguities in phase, and enables unique determination of the height profile of the membrane (Schilling et. al. Phys. Rev. E, 69:021901, 2004). We utilize this technique to map out the height fluctuations in free-standing graphene membranes to answer questions about fundamental mechanical properties of two-dimensional materials.

**12:27PM B16.00007 Metal Ion Intercalated graphitic as Transparent Electrodes** , JIAYU WAN, Univ of Maryland-College Park, WENZHONG BAO, Fudan University, FENG GU, Univ of Maryland-College Park, MICHAEL FUHRER, Monash University, LIANGBIN HU, University of Maryland, UMD TEAM — To best utilize the performance of graphene based transparent electrodes, we novelized Li-ion intercalation in graphene, and achieved highest performance of carbon based transparent electrodes. Transmission as high as 91.7% with a sheet resistance of 3.0 ohm/sq is achieved for 19-layer LiC<sub>6</sub>, significantly higher than any other continuous transparent electrodes. The unconventional modification of ultrathin graphite optoelectronic properties is explained by the suppression of interband optical transitions and a small intraband Drude conductivity near the interband edge. To achieve low cost, large scale graphene-based transparent electrodes, we further developed Na-ion intercalated printed reduced graphene oxide (RGO) film. The larger layer-layer distance of RGO allows Na-ion intercalation, leading to simultaneously much higher DC conductivity and higher optical transmittance. Typical increase of transmittance from 36% to 79% and decrease of sheet resistance from 83 kohms/sq to 311 ohms/sq in the printed network was observed. This study demonstrated the great potential of metal-ion intercalation to improve the performance of graphene-based materials for transparent conductor applications.

**12:39PM B16.00008 Tunable Broadband Printed Carbon Transparent Conductor** , YUE XU, JIAYU WAN, Univ of Maryland-College Park — Transparent conductors have been widely applied in solar cells, transparent smart skins, and sensing/imaging antennas, etc. Carbon-based transparent conductor has attracted great attention for its low cost and broad range transparency. Ion intercalation has been known to highly dope graphitic materials, thereby tuning materials' optoelectronic properties. For the first time, we successfully tune the optical transmittance of a reduced graphene oxide (RGO)/CNT network from mid-IR range to visible range by means of Li-ion intercalation/deintercalation. We also observed a simultaneous increase of the electrical conductivity with the Li-ion intercalation. This printed carbon hybrid thin film was prepared through all solution processes and was easily scalable. This study demonstrates the possibility of using ion intercalation for low cost, tunable broadband transparent conductors.

**12:51PM B16.00009 Design Two-dimensional Materials with Superb Electronic and Optoelectronic Properties: The case of SiS** , SU-HUAI WEI, Beijing Computational Science Research Center, JI-HUI YANG, National Renewable Energy Laboratory, YUEYU ZHANG, Fudan University, WAN-JIAN YIN, Soochow University, X. G. GONG, Fudan University, BORIS I. YAKOBSON, Rice University — Two-dimensional (2D) semiconductors have many unique electronic and optoelectronic properties that is suitable for novel device applications. Most of the current study are focused on group IV or transition metal chalcogenides. In this study, using atomic transmutation and global optimization methods, we identified two group IV-VI 2D materials, Pma2-SiS and silicene sulfide that can overcome shortcomings encountered in conventional 2D semiconductor. Pma2-SiS is found to be both chemically, energetically, and thermally stable. Most importantly, Pma2-SiS has unique electronic and optoelectronic properties, including direct bandgaps suitable for solar cells, good mobility for nanoelectronics, good flexibility of property tuning by layer thickness and strain appliance, and good air stability as well. Therefore, Pma2-SiS is expected to be a very promising 2D material in the field of 2D electronics and optoelectronics. Silicene sulfide also shows similar properties. We believe that the designing principles and approaches used to identify these materials have great potential to accelerate future finding of new functional materials within the 2D families.

**1:03PM B16.00010 Tunable ambipolar polarization-sensitive photodetectors based on high anisotropy ReSe<sub>2</sub>** , ENZE ZHANG, Fudan University, PENG WANG, Shanghai Institute of Technical Physics, ZHE LI, CE HUANG, KAITAI ZHANG, SHIHENG LU, WEIYI WANG, SHANSHAN LIU, Fudan University, HEHAI FANG, XIAOHAO ZHOU, WEIDA HU, Shanghai Institute of Technical Physics, PENG ZHOU, FAXIAN XIU, Fudan University — Atomically-thin 2D layered transition metal dichalcogenides (TMDs) have been extensively studied recently because of their intriguing physical properties and promising applications in nanoelectronic devices. Among them, ReSe<sub>2</sub> is a material that exhibits a stable distorted 1T phase and strong in-plane anisotropy. Here, the anisotropic nature of ReSe<sub>2</sub> is revealed by Raman scattering under linearly polarized excitations. Utilizing high-quality ReSe<sub>2</sub> nanosheets, we are able to build top-gate ReSe<sub>2</sub> field-effect transistors which show an excellent on/off current ratio exceeding 10<sup>7</sup> and a well-developed current saturation at room temperature. Importantly, the successful synthesis of ReSe<sub>2</sub> directly onto hexagonal boron nitride substrates has effectively improved the electron motility over 100 times and the hole mobility over 50 times at low temperatures. Remarkably, the ReSe<sub>2</sub> based photodetectors show a polarization-sensitive photo-responsivity due to the intrinsic linear dichroism originated from high in-plane optical anisotropy. With a back gate the linear dichroism photodetection can be unambiguously tuned both in the electron and hole regime. The appealing physical properties of ReSe<sub>2</sub> demonstrated in this study identify it as an emerging candidate for electronic and optoelectronic applications.

**1:15PM B16.00011 Silicon-nitride photonic circuits interfaced with monolayer MoS<sub>2</sub>**<sup>1</sup> , TEODOR K. STANEV, GUOHUA WEI, NATHANIEL P. STERN, Department of Physics and Astronomy, Northwestern University, DAVID A. CZAPLEWSKI, IL WOONG JUNG, Center for Nanoscale Materials, Argonne National Laboratory — Monolayers of transition metal dichalcogenides exhibit interesting low-dimensional opto-electronic phenomena and large optical interactions. Harnessing these features for modulating light requires interfacing these monolayer semiconductors with photonic devices. Here, we show the integration of monolayer molybdenum disulphide (MoS<sub>2</sub>) with silicon nitride ring microresonators using a visco-elastic layer transfer<sup>2</sup>. Cavity transmission is used to measure the coupling of the monolayer evanescently coupled to the ring resonator. A linear absorption coefficient of 850 dB/cm is observed in this geometry, which is larger than that of graphene and black phosphorus with the same thickness. These assembly methods can be applied to a diverse catalog of monolayer materials for assembling hybrid optoelectronic devices over a wide spectral range.

<sup>1</sup>This work is supported by the DOE-BES (DE-SC0012130), ISEN, and the Center for Nanoscale Materials, DOE-BES (DE-AC02-06CH11357). N.P.S. is an Alfred P. Sloan Research Fellow.

<sup>2</sup>G. Wei, T. K. Stanev, D. A. Czaplewski, I. W. Jung, and N. P. Stern. *Appl. Phys. Lett.* **107**, 091112 (2015)

**1:27PM B16.00012 Plasmonic Hot Electron Induced Photocurrent Response at MoS<sub>2</sub>-Metal Junctions** , TU HONG, Vanderbilt University, BHIM CHAMLAGAIN, Wayne State University, SHUREN HU, SHARON WEISS, Vanderbilt University, ZHIXIAN ZHOU, Wayne State University, YAQIONG XU, Vanderbilt University — We investigate the photocurrent generation mechanisms at few-layer MoS<sub>2</sub>-metal junctions through wavelength- and polarization-dependent scanning photocurrent measurements. When laser energy is above the direct bandgap of MoS<sub>2</sub>, the maximum photocurrent response is observed when incident laser polarization direction is parallel to the metal electrode due to photovoltaic effect. On the contrary, when illuminated by laser with energy below the direct bandgap of MoS<sub>2</sub>, the strongest photocurrent response occurs when incident laser is polarized perpendicular to the metal electrode. Further studies demonstrate that light absorption by the plasmonic metal electrode is polarization-dependent, which creates hot electron-hole pairs and subsequently inject into MoS<sub>2</sub>. These studies shed light on future design rules of two-dimensional material based optoelectronic devices through surface plasmon resonances.

**1:39PM B16.00013 Spin-Polarized Transport on Photo-Assisted Bilayer Graphene Ribbons<sup>1</sup>**, DAVID ZAMBRANO, LUIS ROSALES, PEDRO ORELLANA, Departamento de Física, Universidad Técnica Federico Santa María, Casilla 110-V, Valparaíso, Chile, ANDREA LATGÉ, Instituto de Física, Universidade Federal Fluminense, 24210-340 Niterói-RJ, Brazil — We show how both transmission and spin polarization [1,2] behave in bilayer graphene ribbons in contact with a ferromagnetic insulator while a laser is applied to the ribbon. Using a  $\pi$ -orbital tight-binding model as a low energy approximation [1] and the Tien-Gordon [3] formalism we explore how these systems behave when the ribbon is photo-assisted with a laser. For particular values of the laser parameters, the Fano antiresonance are removed enhancing the transmission while for others spin-polarized transport will arise.

## References

- [1] P. A. Orellana, L. Rosales, L. Chico, and M. Pacheco, J. Appl. Phys. **113**, 213710 (2013).
- [2] J. F. Song, Y. Ochiai, and J. P. Bird, Appl. Phys. Lett. **82**, 4561 (2003).

<sup>1</sup>The authors acknowledge financial support from FONDECYT, under Grant 1140571 & 1140388 and from CONICYT, under Grant PAI-79140064

**1:51PM B16.00014 Graphene/MoS<sub>2</sub> heterostructures for optoelectronics applications<sup>1</sup>**, P HAN, Department of Physics, Georgetown University, Q WONG, Physics Department, University of Central Florida, A EL FATIMY, Department of Physics, Georgetown University, M ISHIGAMI, Physics Department and Nanoscience Technology Center, University of Central Florida, Orlando, FL 32816, P BARBARA, Department of Physics, Georgetown University, Washington DC, 20057 — Graphene and other atomically thin materials can be combined to make novel ultra-thin devices that are suitable for flexible substrates. However, fabricating these heterostructures is a challenge. Most previous work was done by stacking monolayers exfoliated from bulk materials [1], which is a very time-consuming, low-yield method. Large-area monolayer can also be grown by CVD and stacked, as demonstrated by the successful transfer of graphene on as-grown MoS<sub>2</sub> [2], yet the optical properties of some materials like MoS<sub>2</sub> may be degraded by the processing required to detach them from the growth substrate, thereby limiting options in device architecture. Here we develop a method to transfer, align and stack large flakes and films of MoS<sub>2</sub> and graphene after transferring both from the growth substrate onto an arbitrary substrate. The Raman and photoluminescence measurements show that the optical properties of the stacked monolayers are not degraded, making this method viable for fabrication of optoelectronics devices. [1] A.K. Geim, et al., Nature, 499 (2013) 419. [2] L.L. Yu, et al., Nano Letters, 14 (2014) 3055.

<sup>1</sup>Work supported by the U.S. ONR (award: N000141310865) and the NSF-REU (DMR-1358978)

**2:03PM B16.00015 Controlled growth, growth mechanism, and device applications of two-dimensional WSe<sub>2</sub>**, BILU LIU, CHONGWU ZHOU, University of Southern California — Atomically thin 2D transition metal dichalcogenides have attracted lots of attention recently. Here we will present our progress on the controlled growth of 2D WSe<sub>2</sub>. Vapor phase methods for the growth of large single crystalline WSe<sub>2</sub> with lateral sizes up to tens of micrometers will be discussed. Substrate atomic-step-guided nucleation and growth of aligned WSe<sub>2</sub> on single crystalline sapphire substrate will also be presented. In addition, by reducing the supply of source materials, we observed a novel screw-dislocation-driven growth of 2D few layer and pyramid-like WSe<sub>2</sub> flakes. Then, we will discuss device applications of CVD WSe<sub>2</sub>. We show that the device characteristics of CVD WSe<sub>2</sub> can be tuned into either p-type or ambipolar behavior, by changing the types of contact metals. We further developed an efficient method to convert as-grown semiconducting 2H-phase WSe<sub>2</sub> into metallic 1T-phase WSe<sub>2</sub>, by controlled reacting with n-butyl lithium (n-BuLi). By using metallic WSe<sub>2</sub> as contact regimes and intact semiconducting WSe<sub>2</sub> as channel regimes, we successfully made ohmic contacted WSe<sub>2</sub> transistors and achieved a hole mobility of 66 cm<sup>2</sup>/V.s and on/off ratio of 10<sup>7</sup> for monolayer CVD WSe<sub>2</sub>.

## Monday, March 14, 2016 11:15AM - 2:15PM —

**Session B17 DMP: Graphene: Synthesis, Properties, and Defects** 316 - Saptarshi Das, Pennsylvania State University

**11:15AM B17.00001 Synthesis and Properties of 2D Atomic Layers: from Graphene to 2D-GaN**, JOSHUA ROBINSON, The Pennsylvania State University — Beyond graphene, there is a huge variety of layered materials that range in properties from insulating to superconducting. Furthermore, heterogeneous stacking of 2D materials also allows for additional “dimensionality” for band structure engineering. In this talk, I will discuss recent breakthroughs in two-dimensional atomic layer synthesis and properties, including novel 2D heterostructures and novel 2D nitrides. Our recent works include development of an understanding of substrate impact on 2D layer growth and properties, doping of 2D materials with magnetic elements, selective area synthesis of 2D materials, and the first demonstration of 2D gallium nitride (2D-GaN). Our work and the work of our collaborators has lead to a better understanding of how substrate not only impacts 2D crystal quality, but also doping efficiency in 2D materials, and stabilization of nitrides at their quantum limit.

**11:51AM B17.00002 Line defects in Graphene: How doping cures the electronic and mechanical properties**, DANIEL BERGER, CHRISTIAN RATSCH, Department of Mathematics, UCLA — Graphene and carbon nanotubes have extraordinary mechanical properties. Intrinsic line defects such as local non-hexagonal reconstructions or grain boundaries, however, significantly reduce the tensile strength and destroy its unique electronic properties. Here, we address the properties of line defects in graphene from first-principles on the level of full-potential density functional theory, and assess doping as one strategy to strengthen such materials. We carefully disentangle the global and local effect of doping by comparing results from the virtual crystal approximation with those from local substitution of chemical species, in order to gain a detailed understanding of the breaking and stabilization mechanisms. We find that n-type doping or local substitution with electron rich species increases the ultimate tensile strength significantly. In particular, it can stabilize the defects beyond the ultimate tensile strength of the pristine material. We therefore propose that this should be a key strategy to strengthen graphenic materials. We find that doping can furthermore lead to semi-conducting behaviour along line defects, ultimately restoring the unique electronic properties of graphene.

**12:03PM B17.00003 Polycyclic carbon molecules with zigzag edges as sources of defects in graphene on a metal**, ALEXANDRE ARTAUD, CEA Grenoble, F-38000 Grenoble, France, LAURENCE MAGAUD, CNRS, Institut Néel, F-38000 Grenoble, France, KITTI RATTER, CNRS, SIMAP, F-38000 Grenoble, France, VALÉRIE GUISET, PHILIPPE DAVID, CNRS, Institut Néel, F-38000 Grenoble, France, BRUNO GILLES, CNRS, SIMAP, F-38000 Grenoble, France, JOHANN CORAUX, CNRS, Institut Néel, F-38000 Grenoble, France, CLAUDE CHAPÉLIER, CEA Grenoble, F-38000 Grenoble, France — Unlike the armchair edge, the zigzag edge of graphene breaks the equivalence of its two constituting carbon sub-lattices. Uncompensated magnetic moments are thus expected for such edges. For the same reason, dense polycyclic molecules (PCMs) terminated by zigzag edges are predicted to host net magnetic moments. Unfortunately, their synthesis is challenging. One approach relies on the pyrolysis of hydrocarbons, catalyzed by a transition metal. Here we investigate this little-explored approach, and put in evidence the formation of a series of highly symmetric zigzag edge PCMs onto Re(0001), among which phenalene, coronene and sumanene. We also address the relationship between the preparation of such molecules and graphene, which both form following hydrocarbon pyrolysis. We establish that the PCMs are unexpected obstacles towards high quality graphene.

**12:15PM B17.00004 Electronic Transport through linear strain defects in Graphene**, YONG WU, BIN CHENG, CHENG PAN, MARC BOCKRATH, University of California, Riverside — Strain-induced pseudo magnetic fields in Graphene have been studied by STM [1] as well as theoretically.[2] Such pseudo magnetic fields can confine electrons by the presence of magnetic barriers [3] or by the formation of closed cyclotron orbits. Here we report transport measurements through a nanometer-scale width, but micron-scale length linear strain defect in a graphene sheet. The transport data exhibits Coulomb blockade features, indicating the presence of a quantum dot. The charging energy and level spacing are consistent with the defect forming a one-dimensional quantum wire, similar to a carbon nanotube. This suggests the possibility that such defects can be used to confine or guide electrons in graphene. Our latest results will be discussed. [1].Strain? Induced PseudoMagnetic Fields Greater Than 300 Tesla in Graphene Nanobubbles ,N. Levy ,M. F. Crommie etc, Science [2].?Energy gaps and a zero? field quantum Hall effect in graphene by strain engineering, F. Guinea, A.Geim , Nature Physics [3].Magnetic Confinement of Massless Dirac Fermions in Graphene,A. De Martino, L. Dell'Anna, and R. Egger, Physical Review Letters

**12:27PM B17.00005 ABSTRACT WITHDRAWN —**

**12:39PM B17.00006 The Effect of Defects on Mechanical Properties and Failure Mechanisms of Graphene**, JONATHAN WILLMAN, JOSEPH GONZALEZ, University of South Florida, ROMAIN PERRIOT, Los Alamos National Laboratory, IVAN OLEYNIK, University of South Florida — Recent experiments involving nanoindentation of graphene have demonstrated counterintuitive increasing of Young's modulus with increasing concentrations of point defects in graphene. To fully resolve this controversy we perform large-scale molecular dynamics simulations of graphene nanoindentation. The reliable description of interatomic interactions is achieved by using recently developed screened environment-dependent bond order (SED-REBO) potential. The elastic properties of the defective graphene, the breaking strength and the mechanisms of fracture under indenter are investigated as a function of defect concentration and other factors specific to Atomic Force Microscopy (AFM) nanoindentation experiments.

**12:51PM B17.00007 Mechanical Behavior of Graphene Nanomeshes**, MENGXI CHEN, LIN HU, ASHWIN RAMASUBRAMANIAM, DIMITRIOS MAROUDAS, Univ of Mass - Amherst — Graphene nanomeshes (GNMs) are ordered, defect-engineered graphene nanostructures consisting of periodic arrays of nanopores in the graphene lattice with neck widths less than 10 nm. The electronic, transport, and mechanical properties of GNMs can be tuned by varying the structural, chemical, and architectural parameters of the nanomeshes, namely, their porosity, as well their pore lattice structure, pore morphology, and pore edge passivation. Here, we study the mechanical response of GNMs to uniaxial tensile straining and determine their mechanical properties based on molecular-dynamics simulations of dynamic deformation tests according to a reliable bond-order interatomic potential. We establish the dependences of the elastic modulus, fracture strain, ultimate tensile strength, and toughness on the nanomesh porosity and derive scaling laws for GNM modulus-density and strength-density relations. We also establish the dependence of the above properties on pore morphology, for GNMs with circular and elliptical pores over a range of aspect ratios, and on pore edge hydrogen passivation that causes elastic stiffening and strength reduction. The underlying mechanisms of crack initiation and propagation and nanomesh failure also are characterized.

**1:03PM B17.00008 Fe-catalyzed etching of graphene layers**, GUANGJUN CHENG, IRENE CALIZO, ANGELA HIGHT WALKER, NIST, PML, NIST TEAM — We investigate the Fe-catalyzed etching of graphene layers in forming gas. Fe thin films are deposited by sputtering onto mechanically exfoliated graphene, few-layer graphene (FLG), and graphite flakes on a Si/SiO<sub>2</sub> substrate. When the sample is rapidly annealed in forming gas, particles are produced due to the dewetting of the Fe thin film and those particles catalyze the etching of graphene layers. Monolayer graphene and FLG regions are severely damaged and that the particles catalytically etch channels in graphite. No etching is observed on graphite for the Fe thin film annealed in nitrogen. The critical role of hydrogen indicates that this graphite etching process is catalyzed by Fe particles through the carbon hydrogenation reaction. By comparing with the etched monolayer and FLG observed for the Fe film annealed in nitrogen, our Raman spectroscopy measurements identify that, in forming gas, the catalytic etching of monolayer and FLG is through carbon hydrogenation. During this process, Fe particles are catalytically active in the dissociation of hydrogen into hydrogen atoms and in the production of hydrogenated amorphous carbon through hydrogen spillover.

**1:15PM B17.00009 The Production of Graphene Coated Surface by PVD and Investigation of Its Electrical and Optical Properties**, MEHMET YUMAK, Bogazici University Lifescie Center, FATMA SIMSEK, OZGUR KOCATURK, Bogazici University Department of Biomedical Engineering — Graphene is used for a broad range of applications with unique properties such as lightweight, flexibility, mechanical strength, best electrical and thermal conductivity in industrial processes like electronics,medicine,energy,sensors, and other areas related with material usage variations. There are a few common methods to produce graphene. In this study PVD method was used to produce graphene. Many challenging issue was handled in this method like production temperature, growth surface, and mechanical effects. Produced graphene was studied by XRD, scanning electron microscopy (SEM), Raman spectroscopy, and AFM.

**1:27PM B17.00010 Defects, Strain, Incommensurability and Polymorphism in Graphene on Metals**, MICHAEL ALTMAN, KA MAN YU, FEIFEI WANG, Hong Kong University of Science and Technology — The prevalence of defects in large-area graphene fabricated on metal substrates may undermine the unique properties that are vital to its use in technological applications. Although efforts to mitigate these imperfections have met with some success, they may alternatively be harnessed to tailor graphene's properties or alter its functionality. We have studied the growth/defect structure of graphene/metals using low energy electron microscopy (LEEM) and micro-low energy electron diffraction ( $\mu$ -LEED). These investigations reveal the proliferation of small-angle lattice orientational disorder and small angle grain boundaries in graphene/Ru(0001) prepared by conventional ethylene CVD at high temperature. Although orientationally uniform graphene could be produced by a hybrid CVD/segregation method, this layer exhibits significant incommensurability and polymorphism, i.e. several commensurate structures. Two-dimensional strain mapping in graphene/Ir(111) obtained from scanning  $\mu$ -LEED measurements using a 250nm probe beam reveals inhomogeneous strain relaxation by wrinkles. This suggests that it may be possible to strain engineer the properties of graphene if wrinkling can be controlled to form desirable wrinkle networks. Coupling of lattice rotation and strain is also observed by the same approach in graphene on other metal substrates.

**1:39PM B17.00011 A single-step growth process of graphane using hydrogen plasma and observation of an induced bandgap.** , M.L. TEAGUE, D.A. BOYD, W.-S. TENG, C.-C. HSU, N.-C. YEH, Dept. of Physics, Caltech, Pasadena, CA 91125, M. GHARIB, Dept. of Aeronautics, Caltech, Pasadena, CA 91125 — There has been considerable interest in reliably opening up a bandgap in graphene for electronic applications. One promising method is the hydrogenation of graphene into graphane. We present Raman spectroscopy, scanning tunneling microscopy/spectroscopy (STM/STS) and x-ray photoemission spectroscopy (XPS) studies of hydrogenated multilayer graphene on Cu as a function of hydrogen exposure time ( $t$ ). Our growth process for hydrogenated graphene involved *in-situ* exposure of PECVD-grown graphene on Cu to hydrogen plasma. Raman measurements revealed an increase in intensity of a pronounced and narrow D-band with  $t$  when compared to pristine graphene. FTIR studies revealed the presence of C-H bonds on the surface of our samples post hydrogenation. STM topographic studies revealed a nanoscale Moiré pattern resulting from the hydrogenated graphene. For  $t = 120$ s, STS studies revealed an average gap of  $\Delta \sim (0.2750.050)$  eV, which increased to average value of  $\Delta \sim (0.3150.050)$  eV for  $t = 600$ s. Topographic and spectroscopic studies showed approximate hydrogen coverage of 20%, 50% and 80% for  $t = 30$ s, 60s and 120s, respectively. XPS studies of the C-1s state revealed an energy shift from the C-C peak (284.6 nm) towards a C-H peak (285.8 nm), consistent with the formation of carbon-hydrogen bonds. Our results have demonstrated the existence of a bandgap opening in graphene, induced by the adsorption of atomic hydrogen onto graphene.

**1:51PM B17.00012 Ion irradiation of graphene on Ir(111): From trapping to blistering** , CHARLOTTE HERBIG, Universität zu Köln, E. HARRIET ÅHLGREN, University of Helsinki, PHILIPP VALERIUS, ULRIKE A. SCHRÖDER, ANTONIO J. MARTÍNEZ-GALERA, Universität zu Köln, MOHAMMAD A. ARMAN, Lund University, JANI KOTAKOSKI, University of Vienna, JAN KNUDSEN, Lund University, ARKADY V. KRASHENINNIKOV, Aalto University and Helmholtz-Zentrum Dresden-Rossendorf, THOMAS MICHELY, Universität zu Köln — Graphene grown epitaxially on Ir(111) is irradiated with low energy noble gas ions and the processes induced by atomic collision and subsequent annealing are analyzed using scanning tunneling microscopy, low energy electron diffraction, X-ray photoelectron diffraction and thermal desorption spectroscopy. Upon room temperature ion irradiation graphene amorphizes and recovers its crystalline structure during annealing. The energetic noble gas projectiles are trapped with surprisingly high efficiency under the graphene cover up to extremely high temperatures beyond 1300K. The energy, angle, and ion species dependence of trapping are quantified. At elevated temperatures the trapped gas forms well developed and highly pressurized blisters under the graphene cover [1-3]. We use molecular dynamics simulations and ab initio calculations to elucidate the trapping mechanism and its thermal robustness. Similar trapping and blistering are observed after ion irradiation of a single layer of hexagonal boron nitride on Ir(111) and we speculate on the generality of the observed phenomena. [1] C. Herbig et al., ACS Nano 8, 12208 (2014). [2] C. Herbig et al., ACS Nano 9, 4664 (2015). [3] C. Herbig et al., PRB 92, 085429 (2015).

**2:03PM B17.00013 Visualizing Klein tunneling in graphene at the atomic limit** , CHRISTOPHER GUTIERREZ, Columbia University, LOLA BROWN, EDWARD B. LOCHOCKI, CHEOL-JOO KIM, KYLE M. SHEN, JIWOONG PARK, Cornell University, ABHAY N. PASUPATHY, Columbia University — Graphene has attracted much attention from both the solid-state and high-energy scientific communities because its elementary excitations mimic relativistic chiral fermions. This has allowed graphene to act as a table-top testbed for verifying certain longstanding theoretical predictions dating back to the very first formulation of relativistic quantum mechanics. One such prediction is Klein tunneling, the ability of chiral electrons to transmit perfectly through arbitrarily high potential barriers. Previous transport and point-spectroscopic studies confirmed Klein behavior of graphene electrons but lacked real-space resolution. Here we use scanning tunneling microscopy and spectroscopy (STM/STS) measurements to present the first real-space atomic images of Klein tunneling in graphene. In these CVD-grown samples, quasi-circular regions of the copper substrate underneath graphene act as potential barriers that can scatter and transmit electrons. At certain energies, the relativistic chiral fermions that Klein scatter from these barriers are shown to fulfill resonance conditions such that the transmitted electrons become trapped and form standing waves. These resonant modes are visualized with detailed spectroscopic images with atomic resolution that agree well with theoretical calculations. The trapping time is shown to depend critically on both the angular momenta quantum number of the resonant state and the radius of the trapping potential.

## Monday, March 14, 2016 11:15AM - 2:15PM –

Session B18 GMAG DCMP FIAP: Spin-orbit and Superconductivity: Majorana Modes 317 - Alex Matos-Abiague, University at Buffalo

**11:15AM B18.00001 Quantized Conductance in InSb nanowires at zero magnetic field** , JAKOB KAMMhuber, MAJA CASSIDY, HAO ZHANG, ÖNDER GÜL, FEI PEI, MICHIEL DE MOOR, Delft University of Technology, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Japan, DIANA CAR, ERIK BAKKERS, Eindhoven University of Technology, LEO KOUWENHOVEN, Delft University of Technology — We present measurements of InSb nanowires in the ballistic transport regime. In 1D materials such as nanowires, electron scattering has an increased chance of back-reflection, obscuring the observation of quantized conductance at low magnetic fields. By improving the contacts to the nanowire as well as its dielectric environment backscattering events are minimized and conductance quantization is observable at zero magnetic field with high device yield. We study the evolution of individual sub-bands in an external magnetic field, observing a degeneracy between the 2<sup>nd</sup> and 3<sup>rd</sup> sub-band when the magnetic field is orientated perpendicular to the nanowire axis.

**11:27AM B18.00002 Majorana fermions in charge carrier hole quantum wires<sup>1</sup>** , JINGCHENG LIANG, YULI LYANDA-GELLER, Purdue Univ — In order to realize Majorana fermions in a hybrid semiconductor- superconductor structure, spin helical order is needed, which prevents fermion doubling. A natural proposal for Majorana fermion setting is to utilize charge carrier hole systems, which have strong spin orbit couplings that can result in a spin helix. In this work, we demonstrate that transformation of heavy holes into light holes and vice versa upon reflection from the heterostructure boundaries crucially affects Luttinger hole spectrum in low dimensions, and most importantly, spin-orbit interactions in the ground sub-band of a hole quantum wire. Spin orbit interactions are dominated by several terms linear in the hole momentum. We show that the criterion for realizing proximity-induced topologically non-trivial superconducting phase and zero Majorana modes in a hole wire is similar to that for electrons, but an extra constraint should be satisfied. Due to their stronger spin-orbit coupling, the hole systems can be promising settings to study Majorana fermions experimentally.

<sup>1</sup>This research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-SC0010544.

**11:39AM B18.00003 Majorana modes in InSb nanowires (II): resolving the topological phase diagram**, HAO ZHANG, ÖNDER GÜL, MICHIEL DE MOOR, FOKKO DE VRIES, JASPER VAN VEEN, DAVID VAN WOERKOM, KUN ZUO, VINCENT MOURIK, MAJA CASSIDY, ATTILA GERESDI, Delft Univ. of Tech, DIANA CAR, Eindhoven Univ. of Tech, ERIK BAKKERS, Delft Univ. of Tech, Eindhoven Univ. of Tech, SRIJIT GOSWAMI, Delft Univ. of Tech, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, Japan, LEO KOUWENHOVEN, Delft Univ. of Tech — Majorana modes in hybrid superconductor-semiconductor nanowire devices can be probed via tunnelling spectroscopy which shows a zero bias peak (ZBP) in differential conductance (1). Majoranas are formed when the Zeeman energy  $E_Z$  and the chemical potential  $\mu$  satisfy the condition  $E_Z > \sqrt{\Delta^2 + \mu^2}$ , with  $\Delta$  the superconducting gap. This Majorana condition outlines the topologically non-trivial phase and predicts a particular dependence of ZBPs on the gate voltage and the external magnetic field. In this talk we show that the magnetic field range of ZBPs can be tuned by gate voltage and vice versa, consistent with these Majorana predictions. Supported by measurements in different external magnetic field orientations, these observations pave the way for exploring the topological phase diagram of spin-orbit coupled semiconductor nanowires with induced superconductivity.  
(1) V. Mourik, K. Zuo et al, *Science* **336**, 1003 (2012)

**11:51AM B18.00004 Majorana modes in InSb nanowires (I): zero bias peaks in hybrid devices with low-disorder and hard induced superconducting gap**, Ö. GÜL, H. ZHANG, M.W.A. DE MOOR, F. DE VRIES, J. VAN VEEN, D.J. VAN WOERKOM, K. ZUO, V. MOURIK, M. CASSIDY, A. GERESDI, Delft Univ. of Tech., D. CAR, Eindhoven Univ. of Tech., E.P.A.M. BAKKERS, Delft Univ. of Tech., Eindhoven Univ. of Tech., S. GOSWAMI, Delft Univ. of Tech., K. WATANABE, T. TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, Japan, L.P. KOUWENHOVEN, Delft Univ. of Tech. — Majorana modes in hybrid superconductor-semiconductor nanowire devices can be probed via tunnelling spectroscopy which shows a zero bias peak (ZBP) in differential conductance (1). However, alternative mechanisms such as disorder or formation of quantum dots can also give rise to ZBPs, and obscure experimental studies of Majoranas. Further, a soft induced superconducting gap commonly observed in experiments presents an outstanding challenge for the demonstration of their topological protection. In this talk we show that with device improvements, we reach low-disorder transport regime with clear quantized conductance plateaus and Andreev enhancement approaching the theoretical limit. Tunnelling spectroscopy shows a hard induced superconducting gap and no formation of quantum dots. Together with extremely stable ZBPs observed in large gate voltage and magnetic field ranges, we exclude various alternative theories besides the formation of localized Majorana modes for our observations.  
(1) V. Mourik, K. Zuo et al, *Science* **336**, 1003 (2012)

**12:03PM B18.00005 Investigation of semiconductor nanowires with shadow-evaporated epitaxial superconducting shells**, JOHN WATSON, MAJA CASSIDY, JAKOB KAMMHUBER, MICHIEL DE MOOR, LEO KOUWENHOVEN, Delft Technical University, PETER KROGSTROP, MINGTANG DENG, THOMAS JESPERSEN, JESPER NYGARD, CHARLES MARCUS, University of Copenhagen — We report progress on epitaxially grown InAs/Al core/shell nanowire heterostructures by molecular beam epitaxy with junctions in the Al shells formed in-situ by a crossed wire shadowing method during growth. Such wires allow the creation of superconductor-normal-superconductor (SNS) junctions with high quality superconductor-semiconductor interfaces without introducing damage in the junction by etching the Al. Shadowing is accomplished by a two-step growth process in which the nanowire growth direction is changed resulting in crossed networks of nanowires which shadow one another from the Al flux. We observe hard superconducting gaps and supercurrents in excess of 50 nA with in-plane critical fields above 1 T. We compare our results with shadowed devices to previous data from SNS junctions with wet-etched shells. Our experiments indicate that this crossed wire shadowing technique provides an interesting route to investigating induced superconductivity in semiconductor nanowires.

**12:15PM B18.00006 Wireless Majorana Fermions: From Magnetic Tunability to Braiding<sup>1</sup>**, GEOFFREY FATIN, ALEX MATOS-ABIAGUE, BENEDIKT SCHARF, IGOR ZUTIC, University at Buffalo - SUNY — We propose a versatile platform to investigate the existence of zero-energy Majorana fermions (MFs) and their non-Abelian statistics through braiding [1]. This implementation combines a two-dimensional electron gas formed in a semiconductor quantum well grown on the surface of an *s*-wave superconductor, with a nearby array of magnetic tunnel junctions (MTJs). The underlying magnetic textures produced by MTJs provide highly-controllable topological phase transitions to confine and transport MFs in two dimensions, overcoming the requirement for a network of wires.  
[1] G. Fatin, A. Matos-Abiague, B. Scharf, and I. Žutić, arXiv e-prints (2015), arXiv:1510.08182v1.

<sup>1</sup>This work has been supported by ONR Grant N000141310754 and U.S. DOE BES Award DE-SC0004890.

**12:27PM B18.00007 Spin-Orbit Coupling in Hybrid Semiconductor Structures: From Majorana Fermions to Topological Insulators**, BENEDIKT SCHARF, State Univ of NY - Buffalo — Hybrid semiconductor structures with strong spin-orbit coupling are responsible for many fascinating phenomena. Topological states in systems of reduced dimensionality, in particular, offer many intriguing possibilities, both for fundamental research as well as for potential applications. In this talk, we describe the importance of the interplay of spin-orbit coupling (SOC) and the sample geometry in realizing exotic Majorana fermions (MFs) in quantum dots and rings and discuss several schemes to detect MFs [1]. An effective SOC from the magnetic textures provided by magnetic tunnel junctions could enable a versatile control of MFs and their adiabatic exchange [2]. We show that in 2D topological insulators (TIs), such as inverted HgTe/CdTe QWs, helical quantum spin Hall (QSH) states persist even at finite magnetic fields below a critical magnetic field above which only quantum Hall (QH) states can be found [3]. We propose magneto-optical absorption measurements to probe the magnetic-field induced transition between the QSH and QH regimes. This measurement scheme is robust against perturbations such as additional SOC due to bulk or structure-inversion asymmetry [4]. Finally, tunnel junctions based on the surfaces of 3D TIs are presented. These junctions can exhibit giant tunneling anomalous Hall (TAH) currents and negative differential TAH conductance, which makes them an attractive and versatile system for spintronic applications [5]. [1] B. Scharf and I. Zutic, PRB **91**, 144505 (2015). [2] G. L. Fatin et al., arXiv:1510.08182. [3] B. Scharf et al., PRB **86**, 075418 (2012). [4] B. Scharf, et al., PRB **91**, 235433 (2015). [5] B. Scharf et al, preprint.

**1:03PM B18.00008 Wavefunction oscillations and fermion parity crossings in disordered Majorana wire**, SURAJ HEGDE, SMITHA VISHVESHVARA, Univ of Illinois - Urbana — We study aspects of decay and oscillations of Majorana wavefunctions in one dimensional topological superconducting chains, by employing Majorana transfer matrix technique. The phase transition separating the trivial phase and the topological phase associated with the Majorana end modes can be traced to the cancellation of the two parts (superconducting and normal) of the Lyapunov exponent of the transfer matrix. We find that the Majorana oscillations and related fermion parity flips can be completely determined by an underlying non-superconducting tight-binding model. Using this observation we pinpoint the behavior of Majorana mode oscillations within the topological phase diagram. For a disordered wire, these band oscillations are completely washed out, leading to a second localization length for the Majorana mode. The remnant oscillations are however manifested and completely randomized by disorder effects. As a result, the associated fermion parity flips depend heavily on the average of the disorder distribution and the number of lattice sites of the chain. We show that the transfer matrix technique offers a simple way of understanding the known log-normal distribution of mid-gap Majorana states.

**1:15PM B18.00009 Interfacial spin-orbit fields in ferromagnet/normal metal (FN) and ferromagnet/superconductor (FS) systems<sup>1</sup>**, PETRA HOEGL, University of Regensburg, ALEX MATOS-ABIAGUE, IGOR ZUTIC, University at Buffalo - SUNY, JAROSLAV FABIAN, University of Regensburg — Breaking of space-inversion symmetry at interfaces induces spin-orbit fields as an emergent phenomenon. Interfacial spin-orbit fields are believed to enable a wealth of new phenomena, not existent or fragile in the bulk, such as the tunneling anisotropic magnetoresistance (TAMR), interfacial spin-orbit torques, Skyrmions, or possible realization of topological superconductors. We theoretically investigate spin-polarized transport in FN and FS junctions in the presence of Rashba and Dresselhaus interfacial spin-orbit fields. The interplay of magnetism and spin-orbit fields leads to a marked magnetoanisotropy of the conductances. Remarkably, the anisotropy in FS systems—magnetoanisotropic Andreev reflection (MAAR)—is giant compared to TAMR, its normal-state counterpart in FN junctions [1]. We further report on the dependence of spin-flip probability currents on characteristic system parameters [2].

[1] P. Högl, A. Matos-Abiague, I. Žutić, J. Fabian, Phys. Rev. Lett. **115**, 116601 (2015)

[2] A. M. Kamerbeek, P. Högl, J. Fabian, T. Banerjee, Phys. Rev. Lett. **115**, 136601 (2015)

<sup>1</sup>This work has been supported by DFG SFB 689, International Doctorate Program Topological Insulators of the Elite Network of Bavaria, DOE-BES Grant No. DE-SC0004890, and ONR N000141310754.

**1:27PM B18.00010 An exactly solvable model for a strongly spin-orbit-coupled nanowire quantum dot<sup>1</sup>**, RUI LI, Beijing Computational Science Research Center, LIAN-AO WU, University of the Basque Country, XUEDONG HU, University at Buffalo, SUNY, J.Q. YOU, Beijing Computational Science Research Center — In the presence of spin-orbit coupling, quantum models for semiconductor materials are generally not exactly solvable. As a result, understanding of the strong spin-orbit coupling effects in these systems remains incomplete. Here we develop a method to solve exactly the one-dimensional hard-wall quantum dot problem for a single electron in the presence of a strong spin-orbit coupling and a finite magnetic field. This method allows us to obtain the exact eigenenergies and eigenstates for the single electron. With the help of this solution, we demonstrate unique effects from the strong spin-orbit coupling in a semiconductor quantum dot, in particular the anisotropy of the electron g-factor and its tunability.

<sup>1</sup>We thank financial support by NNSF China, NBRP China, NSAF China, Basque Country government, Spanish MICINN, US ARO, and US NSF-PIF.

**1:39PM B18.00011 Charge instability in double quantum dots in Ge/Si core/shell nanowires**, AZARIN ZARASSI, ZHAOEN SU, University of Pittsburgh, JENS SCHWENDERLING, RWTH Aachen University, SERGEY M. FROLOV, University of Pittsburgh, MORA HOCEVAR, Institutel Nel CNRS, BINH-MINH NGUYEN, HRL Labs, JINKYOUNG YOO, Los Alamos National Laboratory, SHADI A. DAYEH, University of California San Diego — Controlling dephasing times are of great challenge in the studies of spin qubit. Reported long spin coherence time and predicted strong spin-orbit interaction of holes in Ge/Si core/shell nanowires, as well as their weak coupling to very few nuclear spins of these group IV semiconductors, persuade electrical spin control. We have established Pauli spin blockade in gate-tunable quantum dots formed in these nanowires. The g-factor has been measured and evidence of spin-orbit interaction has been observed in the presence of magnetic field. However, electrical control of spins requires considerable stability in the double dot configuration, and imperfectly these dots suffer from poor stability. We report on fabrication modifications on Ge/Si core/shell nanowires, as well as measurement techniques to suppress the charge instabilities and ease the way to study spin-orbit coupling and resolve electric dipole spin resonance.

**1:51PM B18.00012 Electrically driven hole spin resonance in MOSFET nanowires**, DHARMRAJ KOTEKAR PATIL, ROMAIN MAURAND, ANDREA CORNA, XAVIER JEHL, CEA-INAC and Universit Grenoble Alpes, 17 Rue des Martyrs, 38054 Grenoble, France, ALEXEI ORLOV, Department of Electrical Engineering, University of Notre Dame, Notre Dame, IN 46556, USA, ROMAIN LAVIVILLE, SYLVAIN BARRAUD, LOUIS HUTIN, CEA-LETI and Universit Grenoble Alpes, 17 rue des Martyrs, 38054 Grenoble, France, MARC SANQUER, SILVANO DE FRANCESCHI, CEA-INAC and Universit Grenoble Alpes, 17 Rue des Martyrs, 38054 Grenoble, France — Hole spins in silicon represent a promising direction for solid-state quantum computation, possibly combining fast qubits with limited hyperfine interaction yielding long coherence times. Here we report on hole double quantum dots defined in dual-gate, p-type silicon nanowire MOSFETs. Devices are fabricated on 300-mm silicon-on-insulator wafers using an industry-standard CMOS platform. We show that a microwave frequency signal applied to one gate of the transistor can induce hole spin resonance leading to an enhanced electrical current through the device. The origin of the observed spin resonance is discussed. From the power dependence of the spin resonance signal we deduce Rabi frequencies as high as ~100 MHz. Our experiments suggest hole quantum dots in silicon as promising candidates for electrically controlled spin qubits.

**2:03PM B18.00013 Spin transistor based on pure nonlocal Andreev reflection in EuO-graphene/superconductor/EuO-graphene nanostructure**, YEE SIN ANG, LAY KEE ANG, Singapore University of Technology and Design, CHAO ZHANG, University of Wollongong, ZHONGSHUI MA, Peking University — In graphene-magnetic-insulator hybrid structure such as graphene-Europium-oxide, proximity induced exchange interaction opens up a spin-dependent bandgap and spin splitting in the Dirac band. We show that such band topology allows pure crossed Andreev reflection to be generated exclusively without the parasitic local Andreev reflection and elastic cotunnelling over a wide range of bias and Fermi levels. We model the charge transport in an EuO-graphene/superconductor/EuO-graphene three-terminal device and found that the pure non-local conductance exhibits rapid on/off switching characteristic with a minimal subthreshold swing of ~20 mV. Non-local conductance oscillation is observed when the Fermi levels in the superconducting lead is varied. The oscillatory behavior is directly related to the quasiparticle propagation in the superconducting lead and hence can be used as a tool to probe the subgap quasiparticle mode in superconducting graphene. The non-local current is 100% spin-polarized and is highly tunable in our proposed device. This opens up the possibility of highly tunable graphene-based spin transistor that operates purely in the non-local transport regime.

**Monday, March 14, 2016 11:15AM - 2:15PM—**

**Session B19 GMAG DMP: Magnetic Devices and Production Level Scaling** 318 - Joe Davies

**11:15AM B19.00001 Development of 22 T VSM System using Novel Improvements in HTS Conductor**, JEREMY GOOD, DARKO BRACANOVIC, Cryogenic Ltd — Current research has identified a need for greater magnetising fields during vibrating sample magnetometer (VSM) measurements and other measurement options. We present here the methodology involved in our development of a VSM system with 22 T superconducting magnet, a unique system and the highest field combined with a VSM anywhere in the world. Recent developments in HTS conductors have allowed greater reliability than previous coils made from YBCO and BISCO and thus facilitate the consistent achievement of higher magnetising fields at the sample with operation at 4.2 K rather than 2.2 K. Cryogenic Ltd wind HTS coils in both solenoid and pancake forms with an emphasis on solenoids, since they have been found to give a more reliable performance with less thermal transfer to the surrounding liquid helium. The 22T VSM system has been developed using 2G YBCO coated and BSSCO tape which exhibit critical currents up to 5 times greater than those seen in YBCO and BISCO at 4.2 K.

**11:27AM B19.00002 Write operation in MRAM with voltage controlled magnetic anisotropy**, KAMARAM MUNIRA, SUMEET PANDEY, GURTEJ SANDHU, Micron Technology, Inc. — In non-volatile Magnetic RAM, information is saved in the bistable configuration of the free layer in a magnetic tunnel junction (MTJ). New information can be written to the free layer through magnetic induction (Toggle MRAM) or manipulation of magnetization using electric currents (Spin Transfer Torque MRAM or STT-MRAM). Both of the writing methods suffer from a shortcoming in terms of energy efficiency. This limitation on energy performance is brought about by the need for driving relatively large electrical charge currents through the devices for switching. In STT-MRAM, the nonzero voltage drop across the resistive MTJ leads to significant power dissipation. An energy efficient way to write may be with the assistance of voltage controlled magnetic anisotropy (VCMA), where voltage applied across the MTJ creates an electric field that modulates the interfacial anisotropy between the insulator and free layer. However, VCMA cannot switch the free layer completely by 180 degree rotation of magnetization. It can lower the barrier between the two stable configurations or at best, cancel the barrier, allowing 90 degree rotation. A second mechanism, spin torque or magnetic field, is needed to direct the final switching destination.

**11:39AM B19.00003 Tunable Magnetic Resonance via Interlayer Exchange Interaction**, YUNPENG CHEN, University of Delaware, XIN FAN, University of Denver, YUNSONG XIE, University of Delaware, JEFFREY WILSON, RAINEE SIMONS, Electron and Opto-Electronic Devices Branch, NASA Glenn Research Center, SUI-TAT CHUI, JOHN XIAO, University of Delaware — Magnetic resonance is a critical property of magnetic materials for the applications in microwave devices and novel spintronics devices. The resonance frequency is commonly controlled with an external magnetic field generated by an energy-inefficient and bulky electromagnet. The search for tuning the resonance frequency without electromagnets has attracted tremendous attention. The voltage control of resonance frequency has been demonstrated in multiferroic heterostructures through magnetoelastic effect. However, the frequency tunable range is limited. We propose a paradigm to tune the magnetic resonance frequency by recognizing the huge interlayer exchange field and the existence of the high-frequency modes in coupled oscillators. We demonstrate the optical mode in exchange coupled magnetic layers which occurred at much higher frequencies than coherent ferromagnetic resonance. We further demonstrated a large resonance frequency tunable range from 11GHz to 21 GHz in a spin valve device by in-situ manipulating of the exchange interaction. The technique developed here is far more efficient than the conventional methods of using electromagnets and multiferroics. This new scheme will have an immediate impact on applications based on magnetic resonance.

**11:51AM B19.00004 Amplification effect of low-field magnetoresistance in silicon dual  $p-n$  junctions**, DEZHENG YANG, TAO WANG, MINGSU SI, FANGCONG WANG, Key Laboratory for Magnetism and Magnetic materials of Ministry of Education, Lanzhou University, Lanzhou 730000, China, SHIMING ZHOU, Department of physics, Tongji University, Shanghai 200092, China, DESHENG XUE, Key Laboratory for Magnetism and Magnetic materials of Ministry of Education, Lanzhou University, Lanzhou 730000, China — Nonmagnetic semiconductors with large magnetoresistance are identified as promising feature for the development of magnetoelectronics. However, to manipulate the magnetoresistance require the magnetic field of several Tesla. In this work, we realized an amplification effect of low-field magnetoresistance based on an elementary electronic building block: dual  $p-n$  junction. Analogous to the electrical amplification effect of transistor  $p-n-p$  junction, where the coupling current between  $p-n$  and  $n-p$  junctions is tuned by base current, in a silicon  $p+-n-n+$  device we demonstrate that the coupling strength of  $p+-n$  and  $n-n+$  junctions can be tuned by magnetic field. Owing to the amplification effect of magnetic-field-manipulated coupling, at a small magnetic field from 0 to 0.1 T the device is directly switched from conducting state "on" (10000 ohms) to blocking state "off" (5 megohm), yielding an magnetoresistance of 50,000 per cent and magnetic field sensitivity as high as 50 per cent  $\text{Oe}^{-1}$ . Such a combination of magnetoresistance and high sensitivity not only makes the semiconductor device available in the magnetic field sensing industry, but also permits a new kind of magnetic-field-manipulated semiconductor electronics.

**12:03PM B19.00005 Towards Atomic-Scale Data Storage in Topologically Protected Spin Structures**, RALPH SKOMSKI, BALA BALAMURUGAN, PRIYANKA MANCHANDA, University of Nebraska, GEORGE C HADJIPANAYIS, University of Delaware, D J SELLMYER, University of Nebraska — Model calculations are used to investigate prospects for atomic-scale data storage in topologically protected spin structures. The approach relies exclusively on exchange interactions, as contrasted to storage based on spin-orbit coupling. The latter category includes magnetocrystalline anisotropy, as in present-day ultrahigh-density recording media, and skyrmions involving Dzyaloshinski-Moriya (DM) interactions. Since spin-orbit coupling is a higher-order relativistic correction to the leading electrostatic terms, including exchange, the corresponding bit sizes are limited to about 5 nm at room temperature. Smaller bit sizes are possible at low temperatures, but cooling is not a practicable solution for most data-storage applications. Our mechanism relies on competing but not necessarily frustrated exchange interactions that realize topological protection through spin angles. The approach can also be considered a magnetic analog to cis-trans isomerism in chemistry and polymer science. The corresponding length scale is of the order of 1 nm, corresponding to an areal-density increase by a factor of order 25 compared to data storage based on spin-orbit coupling. Experimental realizations may involve elements in the middle of the iron transition-metal series, such as Cr, Mn, and Fe. - This research is supported by DOE (DE-FG02-04ER46152), ARO (W911NF-10-2-0099), and NCMN.

**12:15PM B19.00006 Stability of single skyrmionic bits.**<sup>1</sup>, OLENA VEDMEDENKO, JULIAN HAGEMEISTER, NIKLAS ROMMING, KIRSTEN VON BERGMANN, ROLAND WIESENDANGER, University of Hamburg — The switching between topologically distinct skyrmionic and ferromagnetic states has been proposed as a bit operation for information storage. While long lifetimes of the bits are required for data storage devices, the lifetimes of skyrmions have not been addressed so far. Here we show by means of atomistic Monte Carlo simulations that the field-dependent mean lifetimes of the skyrmionic and ferromagnetic states have a high asymmetry with respect to the critical magnetic field, at which these lifetimes are identical. According to our calculations, the main reason for the enhanced stability of skyrmions is a different field dependence of skyrmionic and ferromagnetic activation energies and a lower attempt frequency of skyrmions rather than the height of energy barriers. We use this knowledge to propose a procedure for the determination of effective material parameters and the quantification of the Monte Carlo timescale from the comparison of theoretical and experimental data [1]. [1] Nature Comms. 6, 8455 (2015)

<sup>1</sup>Financial support from the DFG in the framework of the SFB668 is acknowledged

**12:27PM B19.00007 Perpendicular reading of single confined magnetic skyrmions**<sup>1</sup>, DAX M. CRUM, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, and The University of Texas at Austin, MOHAMMED BOUHASSOUNE, JUBA BOUAZIZ, BENEDIKT SCHWEFLINGHAUS, STEFAN BLÜGEL, SAMIR LOUNIS, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA — We present the first fully self-consistent first-principles investigation of single chiral magnetic skyrmions as entire entities based on density functional theory. The work is tied to skyrmions with sub-5nm diameters embedded within thin ferromagnetic films stabilized through interfacial Dzyaloshinskii-Moriya interactions. We found that the non-collinearity of the magnetic texture inside the skyrmions leads to spin-mixing of the electronic structure, which can be probed as site-dependent tunneling spin-mixing magnetoresistance (TXMR). The conduction inhomogeneity can reach values up to 20% in Pd/Fe/Ir(111) samples [1]. The non-collinear component of the TXMR has been experimentally verified [2], validating our theoretical calculations and showing the capability of the TXMR to resolve complex nanoscale spin-textures. The work is carried out with the newly developed Jülich relativistic Korringa-Kohn Rostoker Green function method [3]. [1] Crum, D.M. et al. Perpendicular reading of single confined magnetic skyrmions. Nat. Commun. 6 8541 (2015). [2] Hanneken, C. et al. Electrical detection of magnetic skyrmions by tunnelling non-collinear magnetoresistance. Nat. Nanotech. doi:10.1038/nnano.2015.218 (2015). [3] Bauer, D.S.G., Schriften des Forschungszentrum, Key Technology 79 (2014).

<sup>1</sup>D.M.C. is supported by an NSF fellowship. Funding provided by the HGF-YIG Program VH-NG-717.

**12:39PM B19.00008 Reconfigurable magnetic logic combined with non-volatile memory in silicon.** , ZHAOCHU LUO, XIAOZHONG ZHANG, Tsinghua Univ — Silicon-based complementary metal-oxide-semiconductor (CMOS) transistors have achieved great success and become the mainstream of integrated logic circuits. However, the traditional pathway to enhance computational performance and decrease cost by continuous miniaturization is approaching its fundamental limits. The recent emergence of magnetic logic devices, especially magnetic-field-based semiconductor logic devices, shows promise for surpassing the development limits of CMOS logic and arouses profound attentions. Based on our Si based magnetoresistance (MR) device [1], we proposed a Si based reconfigurable magnetic logic device by coupling nonlinear transport effect and Hall effect in Si [2], which could do all four basic Boolean logic operations including AND, OR, NOR and NAND combined with non-volatile memory. Further, we developed a Si based current-mode magnetic logic device, which allowed direct communication between different logic devices by current-induced magnetization switch effect without external intermediate magnetic-electric converters. This may result in a memory-logic integrated system leading to a non von Neumann computer. [1] CH Wan, et al, Nature 477, 304, (2011). [2] ZC Luo et al. Adv. Funct. Mater. 25, 158, (2015)..

**12:51PM B19.00009 Toward spin-based Magneto Logic Gate in Graphene** , HUA WEN, Dept of Physics and Astronomy, Univ. of California, Riverside, HANAN DERY, Dept. of Electrical and Computer Engineering, University of Rochester, WALID AMAMOU, Dept. of Physics and Astronomy, University of California, Riverside, TIANCONG ZHU, Dept. of Physics, The Ohio State University, ZHISHENG LIN, Deptt. of Physics and Astronomy, University of California, Riverside, JING SHI, Dept. of Physics and Astronomy, University of California, Riverside, IGOR ZUTIC, Dept. of Physics, University at Buffalo, State University of New York, ILYA KRIVOROTOV, Dept. of Physics and Astronomy, University of California, Irvine, LU SHAM, Dept. of Physics, University of California, San Diego, ROLAND KAWAKAMI, Dept. of Physics, The Ohio State University — Graphene has emerged as a leading candidate for spintronic applications due to its long spin diffusion length at room temperature. A universal magnetologic gate (MLG) based on spin transport in graphene has been recently proposed as the building block of a logic circuit which could replace the current CMOS technology. This MLG has five ferromagnetic electrodes contacting a graphene channel and can be considered as two three-terminal XOR logic gates. Here we demonstrate this XOR logic gate operation in such a device. This was achieved by systematically tuning the injection current bias to balance the spin polarization efficiency of the two inputs, and offset voltage in the detection circuit to obtain binary outputs. The output is a current which corresponds to different logic states: zero current is logic '0', and nonzero current is logic '1'. We find improved performance could be achieved by reducing device size and optimizing the contacts.

**1:03PM B19.00010 Low Drift in Resistance of Plasma Oxidized, Cobalt Confined AlOx Tunnel Barriers** , Z. S. BARCIKOWSKI, Y. HONG, J. M. POMEROY, National Institute of Standards and Technology — Co/AlOx/Co tunnel junctions show <15% drift in resistance measured over the first three months. This long term stability is achieved using plasma oxidation and sandwiching the AlOx tunnel barrier between cobalt layers. Plasma oxidation of aluminum, when compared to thermal oxidation, has been shown to produce a more homogeneous and stoichiometric oxide. The confinement of the oxide between Co layers, which have higher oxide enthalpies of formation, is thought to provide a barrier against oxygen diffusion. Junction resistance and current-voltage (I-V) measurements are taken over a period of approximately 9 months. Barrier width (s) and asymmetric barrier heights ( $\varphi_1$ ,  $\varphi_2$ ) are extracted using Simmons/Chow transport model. Bottom barrier height ( $\varphi_2$ ) and barrier width (s) show near constant values in contrast to a rise in top barrier height ( $\varphi_1$ ) in time.

**1:15PM B19.00011 A Study of Morphology and Magnetic Properties of Doped Barium Ferrite Films Formed by Aerosol Deposition** , SCOTTER JOHNSON, Naval Research Laboratory, CHRISTOPHER GONZALEZ, California State University Long Beach, ZACHARY ROBINSON, College at Brockport SUNY, DAVID ELLSWORTH, MINGZHONG WU, Colorado State University — Aerosol deposition is a room-temperature thick film deposition technique that produces polycrystalline films that have > 95% of theoretical density and are up to several hundred microns thick. In addition to depositing films at room temperature another distinct advantage of aerosol deposition is the ability to produce films with the same resulting stoichiometry as the starting material. For this work, we deposited a proprietary doped barium ferrite (BaFe<sub>12</sub>O<sub>19</sub>) film from powder produced by *Temex Ceramics*. This material is designed for microwave absorption near 18 GHz via ferromagnetic resonance. We compare the structural and magnetic properties of the as-deposited film, bulk material, and starting powder. For this purpose, we employed scanning electron microscopy, x-ray photoemission spectroscopy, x-ray diffraction, vibrating sample magnetometry, and broad-band ferromagnetic resonance characterization techniques.

**1:27PM B19.00012 Large-area patterned substrates for micromagnetic actuation of superparamagnetic microbeads** , MINAE OUK, GEOFFREY S.D. BEACH, Massachusetts Inst of Tech-MIT — Superparamagnetic microbeads (SBs) have been used to capture and manipulate biological entities in a fluid environment. Chip-based magnetic actuation provides a means to transport SBs in lab-on-a-chip technologies. This is accomplished using the stray field from patterned magnetic microstructures [1], or domain walls in magnetic nanowires [2]. Recently many studies have focused on the submicron-size antidot array of magnetic materials because non-magnetic holes affect the micromagnetic properties. Here, we use photolithographic patterning to create periodic anti-dot arrays in Co thin films, show the transport of SBs across large distance by a rotating field. We describe the dynamics of bead motion, highlighting the key factors to control bead transport. We show there is a critical threshold for both in-plane and out-of-plane components that must be exceeded for bead motion to occur. The threshold values are different depending on direction, which allows for directionally-anisotropic transport across the chip surface. Hence the periodic magnetically-patterned substrates can be used to digitally separate magnetic beads and augment microfluidic actuation for long distance transport.[1]B. Yellen, et al., Lab Chip, 7, 1681 (2007) [2]E. Rapoport and G. S. D. Beach, APL 100, 082401 (2012)

**1:39PM B19.00013 Measurement of Nanoparticle Magnetic Hyperthermia Using Fluorescent Microthermal Imaging** , XIAOWAN ZHENG, EDWARD VAN KEUREN, Georgetown Univ — Nanoparticle magnetic hyperthermia uses the application of an AC magnetic field to ferromagnetic nanoparticles to elevate the temperature of cancer cells. The principle of hyperthermia as a true cell-specific therapy is that tumor cells are more sensitive to high temperature, so it is of great importance to control the locality and magnitude of the temperature differences. One technique to measure temperature variations on microscopic length scales is fluorescent microthermal imaging (FMI). Since it is the local temperature that is measured in FMI, effects such as heating due to nearby field coils can be accounted for. A dye, the rare earth chelate europium thenoyltrifluoroacetate (Eu:TTA), with a strong temperature-dependent fluorescence emission has been incorporated into magnetic nanoparticles dispersed in a polymer films. FMI experiments were carried out on these samples under an applied high frequency magnetic field. Preliminary results show that FMI is a promising technique for characterizing the local generation of heat in nanoparticle magnetic hyperthermia.

**1:51PM B19.00014 Optimization of magnetic refrigerators by tuning the heat transfer medium and operating conditions.** , MOHAMMADREZA GHAHREMANI, AMIR ASLANI, LAWRENCE BENNETT, EDWARD DELLA TORRE, George Washington University — A new reciprocating Active Magnetic Regenerator (AMR) experimental device has been designed, built and tested to evaluate the effect of the system's parameters on a reciprocating Active Magnetic Regenerator (AMR) near room temperature. Gadolinium turnings were used as the refrigerant, silicon oil as the heat transfer medium, and a magnetic field of 1.3 T was cycled. This study focuses on the methodology of single stage AMR operation conditions to get a higher temperature span near room temperature. Herein, the main objective is not to report the absolute maximum attainable temperature span seen in an AMR system, but rather to find the system's optimal operating conditions to reach that maximum span. The results of this work show that there is an optimal operating frequency, heat transfer fluid flow rate, flow duration, and displaced volume ratio in an AMR system. It is expected that such optimization and the results provided herein will permit the future design and development of more efficient room-temperature magnetic refrigeration systems.

**2:03PM B19.00015 Impact of DC Joule anneal treatment on the high-frequency magnetoimpedance response of Fe-rich FeCo ribbons with varying glass former content**, TATIANA EGGER, Department of Physics, University of South Florida, Tampa, FL, ALEX LEARY, MICHAEL MCHENRY, Materials Science and Engineering, Carnegie-Mellon University, Pittsburgh, PA, IVAN SKORVANEK, Institute of Experimental Physics, Slovak Academy of Sciences, Kosice, Slovakia, HARIHARAN SRIKANTH, MANH-HUONG PHAN, Department of Physics, University of South Florida, Tampa, FL — The Magnetoimpedance (MI) effect in 2 mm wide  $(\text{Fe}_{65}\text{Co}_{35})_{83.5-x}\text{B}_{13}\text{Nb}_x\text{Si}_2\text{Cu}_{1.5}$  rapidly quenched ribbons with varying glass former content ( $x = 0$  and  $x = 4$ ) has been studied in the frequency range of 1-1000 MHz. Two measurement techniques were used: auto-balancing bridge method in the frequency range of 1-110 MHz and transmission line technique for 20-1000 MHz. The impact of DC Joule heating treatments of varying current amplitude and annealing time on the MI effect of the amorphous ribbons was evaluated by examining the field and frequency dependence on the resistive and reactive components of the MI. To interpret the MI behavior, the domain structure of the ribbons in their as-quenched state and after heating treatment was imaged by magneto-optical Kerr effect microscopy. A significant improvement in the MI response from the as-quenched state was found for both compositions of ribbon with a 3 hour-500 mA Joule anneal treatment. The improvement is attributed to the development of a low anisotropy domain structure longitudinally and at an oblique angle between the longitudinal and transverse directions for the 0% and 4% Nb content, respectively.

**Monday, March 14, 2016 11:15AM - 2:15PM —**

**Session B20 DCOMP: Electronic Structure Methods I** 319 - Oliver Albertini, Georgetown University

**11:15AM B20.00001 An Accurate Density Functional from Exchange-Correlation Hole<sup>1</sup>**, JIANMIN TAO, YUXIANG MO, Temple Univ — The exchange-correlation hole is most fundamentally important in the development and understanding of density functional theory (DFT). However, due to the nonlocal nature of the exchange-correlation hole, development of DFT from the underlying hole presents a great challenge, and the works along this direction are limited. Here I will discuss a novel nonempirical DFT based on a semilocal hole, which is obtained from the density matrix expansion. Extensive tests on molecules and solids show that this functional can achieve remarkable accuracy for wide-ranging properties in condensed matter physics and quantum chemistry.

<sup>1</sup>This work was supported by NSF under Grant No. CHE-1261918.

**11:27AM B20.00002 Assessment of a New Semilocal Density Functional on Molecules and Solids<sup>1</sup>**, YUXIANG MO, JIANMIN TAO, Temple Univ — We have recently developed a new semilocal density functional based on the exchange hole (localized under a general coordinate transformation) from density matrix expansion, instead of imposing energy constraints to the functional or fitting it to a training set of properties. This functional is comprehensively evaluated on diverse properties of molecules and solids, including atomization energies for G2/97 (148 molecules), enthalpies of formation for G3-3 (75 molecules), ionization potentials for G3/99 (86 species), electron affinities for G3/99 (58 species), proton affinities (8 molecules), bond lengths for T-96R (96 molecules), vibrational frequencies for T-82F (82 molecules), 10 hydrogen bonded complexes, as well as lattice constants, bulk moduli, and cohesive energies for solids. Our tests show that the functional is remarkably accurate for these wide-ranging properties.

<sup>1</sup>This work was supported by NSF under Grant No. CHE-1261918.

**11:39AM B20.00003 Benchmarking Post-SCF Treatments of Spin-Orbit Coupling in Electronic Structure Theory**, WILLIAM PAUL HUHN, VOLKER BLUM, MEMS Department, Duke University, Durham, NC 27708 — Spin-orbit coupling (SOC) is an essential aspect of the electron band structures for all but the lightest-element materials. SOC is often incorporated into density-functional theory (DFT) calculations in a second-order variational approach, applying the SOC correction based on the orbitals from a scalar-relativistic self-consistent calculation. This talk compares the quality of non-self-consistent and self-consistent SOC corrections for a test set of over 100 different materials spanning the periodic table. We quantitatively compare entire DFT band structures from two benchmark-quality full-potential all-electron codes, i.e., the numeric atom-centered orbital code FHI-aims and the linearized augmented plane-wave code WIEN2k, based on the semilocal PBE functional. Few-meV agreement between non-self-consistent and self-consistent SOC is shown for elements up to row 4 of the periodic table, with agreement on the order of 10 meV for row 5 elements and differences exceeding 100 meV emerging for row 6 elements. We find little difference in SOC splittings between the PBE functional and the hybrid HSE06 functional.

**11:51AM B20.00004 Dielectric-dependent Density Functionals for Accurate Electronic Structure Calculations of Molecules and Solids<sup>1</sup>**, JONATHAN SKONE, Institute for Molecular Engineering, University of Chicago, MARCO GOVONI, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago & Argonne National Laboratory — Dielectric-dependent hybrid [DDH] functionals [1] have recently been shown to yield highly accurate energy gaps and dielectric constants for a wide variety of solids, at a computational cost considerably less than standard GW calculations. The fraction of exact exchange included in the definition of DDH functionals depends (self-consistently) on the dielectric constant of the material. In the present talk we introduce a range-separated (RS) version of DDH functionals [2] where short and long-range components are matched using material dependent, non-empirical parameters. Comparing with state of the art GW [3] calculations and experiment, we show that such RS hybrids yield accurate electronic properties of both molecules and solids, including energy gaps, photoelectron spectra and absolute ionization potentials. [1] See, e.g. Skone et. al. PRB 89 195112 (2014) [2] Skone et. al. PRB (to be submitted) [3] Govoni and Galli JCTC 11 2680 (2015)

<sup>1</sup>This work was supported by NSF-CCI grant number NSF-CHE-0802907 and DOE-BES

**12:03PM B20.00005 Quest for a semi-empirical MGGA functional with tight bound**, BERNARD DELLEY, Paul Scherrer Inst — A numerically robust parametrization for a meta-GGA exchange functional approximation has been obtained by optimization of bond energies in a database of 303 species. The variables, density, gradient and kinetic energy density, are useful to differentiate efficiently among the wide variety of bonding types in the database. The resulting MGGA rivals the thermochemistry accuracy of composite quantum chemistry approaches when applied to a wider data set of 592 species. Noticeable improvements over GGA's are also obtained for solid state properties. The present functional shows some similarities with the recently presented SCAN functional of Sun, Ruscinszky and Perdew. With the easily available semi-nonlocality through gradients and a kinetic energy density, this MGGA is widely applicable for molecular- as well as for extended systems and surface models.

**12:15PM B20.00006 Modeling Spin Fluctuations and Magnetic Excitations from Time-Dependent Density Functional Theory**, TOMMASO GORNI, IURI TIMROV, ANDREA DAL CORSO, STEFANO BARONI, SISSA, Trieste — Harnessing spin fluctuations and magnetic excitations in materials is key in many fields of technology, spanning from memory devices to information transfer and processing, to name but a few. A proper understanding of the interplay between collective and single-particle spin excitations is still lacking, and it is expected that first-principle simulations based on TDDFT may shed light on this interplay, as well as on the role of important effects such as relativistic ones and related magnetic anisotropies. All the numerical approaches proposed so far to tackle this problem are based on the computationally demanding solution of the Sternheimer equations for the response orbitals or the even more demanding solution of coupled Dyson equations for the spin and charge susceptibilities. The Liouville-Lanczos approach to TDDFT has already proven to be a valuable alternative, the most striking of its features being the avoidance of sums over unoccupied single-particle states and the frequency-independence of the main numerical bottleneck. In this work we present an extension of this methodology to magnetic systems and its implementation in the QUANTUM ESPRESSO distribution, together with a few preliminary results on the magnon dispersions in bulk Fe.

**12:27PM B20.00007 Symmetry-adapted Wannier Functions from  $L_1$  regularized Sparse Optimization**, JIATONG CHEN, KE YIN, YI XIA, VIDVUDS OZOLINS, STANLEY OSHER, RUSSEL CAFLISCH, Univ of California - Los Angeles — Wannier functions are widely used as real space representation of periodic solids in electronic structure calculation. We present a new approach to calculate symmetry-adapted Wannier functions which are directly obtained from variational principle of total energy plus an  $L_1$  regularization term,  $\frac{1}{\mu} \int |\psi| dr$ . The obtained compressed Wannier functions are only nonzero within a finite region. With the help of induced group representation theory, we only need to calculate Bloch functions (in Wannier gauge) within irreducible Brillouin zone, while point group symmetry is strictly enforced. Implementation in plane waves-pseudopotential codes and application to real material system will be demonstrated.

**12:39PM B20.00008 Free energy from stationary implementation of the DFT+EDMFT functional**, TURAN BIROL, KRISTJAN HAULE, Rutgers University — The workhorse of first principles calculations on crystalline solids is the Density Functional Theory at the level of Local Density Approximation (LDA). Despite its various successes, LDA is prone to an overbinding problem, which introduces an error in optimized lattice constants and other structural parameters. Various Generalized Gradient Approximations are introduced to correct for this problem, but they often fail to systematically correct it, in particular in correlated electron materials. We developed a stationary and functional derivable Embedded Dynamical Mean Field Theory combined with the DFT (EDMFT+DFT) to calculate the free energy and to optimize the structural parameters in correlated electron compounds. In our stationary formalism, the first order error in the density leads to a much smaller, second order error in the free energy. We consider the correlated metal  $\text{SrVO}_3$ , Mott insulating  $\text{FeO}$ , elemental Ce, and iron chalcogenide  $\text{FeSe}$  as examples to show that EDMFT predicts the lattice constants with high accuracy.

**12:51PM B20.00009 Relativistic Green's Functions in Full-Potential Multiple-Scattering Theory**, XIANGLIN LIU, Department of Physics, Carnegie Mellon University, YANG WANG, Pittsburgh Supercomputing Center, Carnegie Mellon University, MARKUS EISENBACH, G.MALCOLM STOCKS, Materials Science and Technology Division, Oak Ridge National Laboratory — The Greens functions play a central role in MST based KKR method. Obtaining the Greens functions by solving the Dirac equation is appealing since it naturally incorporated the electron spin and the spin-orbit coupling effects. Here we implemented the full-potential relativistic KKR method using a technique called the sine and cosine matrices formalism. The charge density and the density of states of some pure element crystals have been calculated. Different expressions of the Greens functions have been investigated for numerical benefits.

**1:03PM B20.00010 Understanding the Relativistic Generalization of Density Functional Theory (DFT) and Completing it in Practice.**, DIOLA BAGAYOKO, Department of Mathematics, Physics, and Science and Mathematics Education (MP-SMED) Southern University and AM College, Baton Rouge, LA 70813, USA — In 2014, 50 years following the introduction of density functional theory (DFT), a rigorous understanding of it was published [AIP Advances, 4, 127104 (2014)]. This understanding included necessary steps ab initio electronic structure calculations have to take if their results are to possess the full physical content of DFT. These steps guarantee the fulfillment of conditions of validity of DFT; not surprisingly, they have led to accurate descriptions of several dozens of semiconductors, from first principle, without invoking derivative discontinuity or self-interaction correction. This presentation shows the mathematically and physically rigorous understanding of the relativistic extension of DFT by Rajagopal and Callaway [Phys. Rev. B 7, 1912 (1973)]. As in the non-relativistic case, the attainment of the absolute minima of the occupied energies is a necessary condition for the corresponding current density to be that of the ground state of the system and for computational results to agree with corresponding, experimental ones. Acknowledgments: This work was funded in part by the US National Science Foundation [NSF, Award Nos. EPS-1003897, NSF (2010-2015)-RII-SUBR, and HRD-1002541], the US Department of Energy, National Nuclear Security Administration (NNSA, Award No. DE-NA0002630), LaSPACE, and LONI-SUBR.

**1:15PM B20.00011 Enhancing inter-tube conductivity in carbon nanotube networks<sup>1</sup>**, ARASH MOSTOFI, Departments of Materials and Physics and the Thomas Young Centre, Imperial College London, UK, ROBERT BELL, MIKE PAYNE, Cavendish Laboratory, University of Cambridge, UK — Retaining the remarkable electronic transport properties of individual carbon nanotubes (CNTs) when scaling up to macroscopic CNT networks for use in devices remains a significant challenge. As no single tube spans the device, electrons must travel between CNTs to contribute to the conductivity. Conductivity between CNTs of different chirality is suppressed due to the requirement of momentum conservation. Using a combination of analytic theory and tight-binding, I will show that this limitation can be overcome by supplying a weak perturbation to the system, resulting in order of magnitude increases of conductivity<sup>2</sup>. I will present practical realizations of such perturbations, which I will demonstrate using Landauer-Buttiker transport simulations based on large-scale density-functional theory calculations<sup>3</sup>.

<sup>1</sup>AM acknowledges support of the EPSRC under grant EP/J015059/1

<sup>2</sup>Phys. Rev. B 89, 245426 (2014)

<sup>3</sup>Comput. Phys. Commun. 193, 78 (2015); www.onetep.org

**1:27PM B20.00012 Data compression algorithms for electronic wave functions**, WILLIAM DAWSON, FRANCOIS GYGI, Univ of California - Davis — Large scale, First-Principles Molecular Dynamics (FPMD) simulations require an large amount of computational effort. Unfortunately, the size of the data they generate and the overhead cost of saving it result in the overwhelming majority of this potentially valuable data being lost. The rising gap between CPU and file I/O performance will restrict even further the amount of data saved during future FPMD simulations. The Recursive Subspace Bisection method for generating localized wavefunctions has recently been utilized to reduce the cost of computing Hartree-Fock exchange with controlled accuracy. We show that a variation of this method can be used to compress FPMD simulation data. Furthermore, we show that this method has controlled and predictable accuracy, and can be applied without concern for specific system properties. We demonstrate this method by compressing data from the simulation of liquid water, melting silicon, and other representative systems. Supported by: DE-SC0008938.

**1:39PM B20.00013 Nonorthogonal generalized hybrid Wannier functions for large-scale DFT simulations<sup>1</sup>**, ANDREA GRECO, Imperial College London, JOHN W. FREELAND, Argonne National Laboratory, ARASH A. MOSTOFI, Imperial College London — Semiconductor-based thin-films have applications in microelectronics, from transistors to nanocapacitors. Many properties of such devices strongly depend on the details of the interface between a metallic electrode and the thin-film semiconductor/insulator. Hybrid Wannier Functions (WFs), extended in the surface plane, but localized along the direction normal to the surface/interface, have been successfully used to explore the properties of such heterostructures layered along a given direction, and are a natural way to study systems that are at the same time a 2D conductor (in plane) and a 1D insulator (out of plane). Current state-of-the-art implementations of Hybrid WF's rely on first performing a traditional cubic-scaling density-functional theory (DFT) calculation. This unfavourable scaling precludes the applicability of this method to the large length scales typically associated with processes in realistic structures. To overcome this limitation we extend the concept of Hybrid WF's to nonorthogonal orbitals that are directly optimized in situ in the electronic structure calculation. We implement this method in the ONETEP large-scale DFT code and we apply it to realistic heterostructure systems, showing it is able to provide plane-wave accuracy but at reduced computational cost.

<sup>1</sup>The authors would like to acknowledge support from the EPSRC, the Centre for Doctoral Training in Theory and Simulation of Materials, and Argonne National Laboratory

**1:51PM B20.00014 Electronic correlation in magnetic contributions to structural energies<sup>1</sup>**, ROGER HAYDOCK, University of Oregon — For interacting electrons the density of transitions [see <http://arxiv.org/abs/1405.2288>] replaces the density of states in calculations of structural energies. Extending previous work on paramagnetic metals, this approach is applied to correlation effects on the structural stability of magnetic transition metals.

<sup>1</sup>supported by the H. V. Snyder Gift to the University of Oregon

**2:03PM B20.00015 Effective on-site Coulomb interaction and electron configurations in transition-metal complexes from constraint density functional theory**, KENJI NAWA, KOHJI NAKAMURA, TORU AKIYAMA, TOMONORI ITO, Mie University, MICHAEL WEINERT, University of Wisconsin-Milwaukee — Effective on-site Coulomb interactions ( $U_{\text{eff}}$ ) and electron configurations in the localized  $d$  and  $f$  orbitals of metal complexes in transition-metal oxides and organometallic molecules, play a key role in the first-principles search for the true ground-state. However, wide ranges of values in the  $U_{\text{eff}}$  parameter of a material, even in the same ionic state, are often reported. Here, we revisit this issue from constraint density functional theory (DFT) by using the full-potential linearized augmented plane wave method. The  $U_{\text{eff}}$  parameters for prototypical transition-metal oxides, TMO (TM=Mn, Fe, Co, Ni), were calculated by the second derivative of the total energy functional with respect to the  $d$  occupation numbers inside the muffin-tin (MT) spheres as a function of the sphere radius. We find that the calculated  $U_{\text{eff}}$  values depend significantly on the MT radius, with a variation of more than 3 eV when the MT radius changes from 2.0 to 2.7 a.u., but importantly an identical valence band structure can be produced in all the cases, with an approximate scaling of  $U_{\text{eff}}$ . This indicates that a simple transferability of the  $U_{\text{eff}}$  value among different calculation methods is not allowed. We further extend the constraint DFT to treat various electron configurations of the localized  $d$ -orbitals in organometallic molecules, TMCp<sub>2</sub> (TM=Cr, Mn, Fe, Co, Ni), and find that the calculated  $U_{\text{eff}}$  values can reproduce the experimentally determined ground-state electron configurations.

## Monday, March 14, 2016 11:15AM - 2:15PM –

Session B21 GMAG DMP: Single Molecule Magnets 320 - Janathan Friedman, Amherst College

**11:15AM B21.00001 Decoherence mechanisms in Mn3 single-molecule magnet<sup>1</sup>**, C ABEYWARDANA, Department of Chemistry, University of Southern California, Los Angeles CA 90089, USA, A. M. MOWSON, G. CHRISTOU, Department of Chemistry, University of Florida, Gainesville FL 32611, USA, S TAKAHASHI, Department of Chemistry, Department of Physics, University of Southern California, Los Angeles CA 90089, USA — In spite of wide interest in the quantum nature of SMMs, decoherence effects that ultimately limit such behavior have yet to be fully understood. Recent investigations have shown that there are three main decoherence mechanisms present in SMMs: spins can couple locally (i) to phonons (phonon decoherence); (ii) to many nuclear spins (nuclear decoherence); and (iii) to each other via dipolar interactions (dipolar decoherence)[1]. We have recently uncovered quantum coherence in a Mn3 SMM by quenching decoherence due to dipole interaction between SMMs using a high frequency electron paramagnetic resonance and low temperature [2]. In this presentation, we will discuss temperature dependence of spin relaxation times and the decoherence mechanisms in the Mn3 SMM. [1] S. Takahashi et al., Nature 476, 76 (2011). [2] C. Abeywardana et al. (2015), submitted.

<sup>1</sup>This work is supported by the National Science Foundation (DMR-1508661) and the Searle scholars program.

**11:27AM B21.00002 Controlling electronic access to the spin excitations of a single molecule in a tunnel junction**, CYRUS F. HIRJIBEHEDIN, BEN WARNER, FADI EL HALLAK, HENNING PRUESER, AFOLABI AJIBADE, TOBIAS G. GILL, ANDREW J. FISHER, UCL, MATS PERSSON, U. Liverpool and Chalmers University of Technology — Spintronic phenomena can be utilized to create new devices with applications in data storage and sensing. Scaling these down to the single molecule level requires controlling the properties of the current-carrying orbitals to enable access to spin states through phenomena such as inelastic electron tunneling. Here we show that the spintronic properties of a tunnel junction containing a single molecule can be controlled by their coupling to the local environment. For tunneling through iron phthalocyanine (FePc) on an insulating copper nitride (Cu<sub>2</sub>N) monolayer above Cu(001), we find that spin transitions may be strongly excited depending on the binding site of the central Fe atom. Different interactions between the Fe and the underlying Cu or N atoms shift the Fe  $d$ -orbitals with respect to the Fermi energy, and control the relative strength of the spin excitations, an effect that can be described in a simple co-tunneling model. This work demonstrates the importance of the atomic-scale environment in the development of single molecule spintronic devices.

**11:39AM B21.00003 Inelastic Neutron Scattering and Magnetisation Investigation of an Exchange-Coupled Dy<sub>2</sub> SMM<sup>1</sup>**, MICHAEL L. BAKER, City College of New York, CUNY and New York University, QING ZHANG, MYRIAM P. SARACHIK, City College of New York, CUNY, ANDREW D. KENT, YIZHANG CHEN, New York University, NICHOLAS BUTCH, NIST, EUFEMIO M. PINEDA, ERIC MCINNES, University of Manchester — The strong spin orbit coupling and weak crystal field energies of simple exchange-coupled rare earth SMMs makes the precise evaluation of their magnetic properties nontrivial. Here we report a detailed investigation of the single molecule magnet hqH<sub>2</sub>Dy<sub>2</sub>(hq)<sub>4</sub>(NO<sub>3</sub>)<sub>3</sub>MeOH. Inelastic neutron scattering is used to obtain direct access to several low energy crystal field excitations. The INS results display several features that are not found in earlier FIR absorption experiments [1], while other features found in the latter are absent. Based on the effective point charge model, numerical calculations are currently underway to resolve these apparent discrepancies using complementary magnetisation measurements to resolve the exchange between Dy ions. [1] E. M. Pineda et al. Nat. Commun. 5, 5243 (2014).

<sup>1</sup>Work supported by ARO W911NF-13-1-1025 (CCNY) and NSF-DMR- 1309202 (NYU)

**11:51AM B21.00004 Mechanisms of relaxation and spin decoherence in nanomagnets**, JOHAN VAN TOL, Florida State University, National High Magnetic Field Laboratory, Tallahassee, FL 32310 — Relaxation in spin systems is of great interest with respect to various possible applications like quantum information processing and storage, spintronics, and dynamic nuclear polarization (DNP). The implementation of high frequencies and fields is crucial in the study of systems with large zero-field splitting or large interactions, as for example molecular magnets and low dimensional magnetic materials. Here we will focus on the implementation of pulsed Electron Paramagnetic Resonance (ERP) at multiple frequencies of 10, 95, 120, 240, and 336 GHz, and the relaxation and decoherence processes as a function of magnetic field and temperature. Firstly, at higher frequencies the direct single-phonon spin-lattice relaxation (SLR) is considerably enhanced, and will more often than not be the dominant relaxation mechanism at low temperatures, and can be much faster than at lower fields and frequencies. In principle the measurement of the SLR rates as a function of the frequency provides a means to map the phonon density of states. Secondly, the high electron spin polarization at high fields has a strong influence on the spin fluctuations in relatively concentrated spin systems, and the contribution of the electron-electron dipolar interactions to the coherence rate can be partially quenched at low temperatures [1]. This not only allows the study of relatively concentrated spin systems by pulsed EPR (as for example magnetic nanoparticles and molecular magnets), it enables the separation of the contribution of the fluctuations of the electron spin system from other decoherence mechanisms. Besides choice of temperature and field, several strategies in sample design, pulse sequences, or clock transitions can be employed to extend the coherence time in nanomagnets. A review will be given of the decoherence mechanisms with an attempt at a quantitative comparison of experimental rates with theory. [1] Takahashi, S.; Hanson, R.; van Tol, J.; Sherwin, M.S. and Awschalom, D.D. *Phys. Rev. Lett.*, 101, 047601 (2008)

**12:27PM B21.00005 Evaluation of the exchange interaction and crystal fields in a prototype Dy<sub>2</sub> SMM**<sup>1</sup>, QING ZHANG, MYRIAM SARACHIK, City College of New York, CUNY, MICHAEL BAKER, Stanford University, YIZHANG CHEN, ANDREW KENT, New York University, EUFEMIO PINEDA, ERIC MCINNES, The University of Manchester — In order to gain an understanding of the INS and magnetization data obtained for Dy<sub>2</sub>, the simplest member of a newly synthesized family of dysprosium-based molecular magnets [1], we report on calculations of the magnetic behavior of a Dy<sub>2</sub> cluster with the formula [h<sub>2</sub>Q<sub>2</sub>][Dy<sub>2</sub>(h<sub>2</sub>)<sub>4</sub>(NO<sub>3</sub>)<sub>3</sub>]MeOH. The molecular complex contains one high symmetry Dy(III) ion and one low symmetry Dy(III) ion. Our calculations suggest that exchange coupling between the two ions controls the behavior of the magnetization at low temperature, while the crystal field of the low symmetry Dy(III) ion controls the behavior at higher temperature. A point charge electrostatic model, based on crystallographic coordinates, provides a starting point for the determination of the crystal field [2]. Parameters in these calculations are adjusted to provide best fits to inelastic neutron scattering data (INS) and low temperature magnetometry [3]: the INS measurements access crystal field energies and low temperature magnetization probes the Dy-Dy exchange interaction. [1] E. M. Pineda, et al. *Nat. Commun.* 5, 5243 (2014). [2] J.J. Baldov, et al *J. Comput. Chem.* 34 (22), 1961-1967, 2013. [3] N. F. Chilton, et al. *J. Comput. Chem.* 34, 1164-1175 (2013).

<sup>1</sup>Work supported by ARO W911NF-13-1-1025 (CCNY) and NSF-DMR- 1309202 (NYU).

**12:39PM B21.00006 The first single atom magnet**, FABIO DONATI, STEFANO RUSPONI, CHRISTIAN WÄCKERLIN, APARAJITA SINGHA, ROMANA BALTIC, KATHARINA DILLER, FRANÇOIS PATTHEY, EDGAR FERNANDES, HARALD BRUNE, Ecole Polytechnique Fédérale de Lausanne, JAN DREISER, Paul Scherrer Institute, ZELJKO SLJIVANCANIN, Vinča Institute of Nuclear Sciences, KURT KUMMER, European Synchrotron Radiation Facility, SEBASTIAN STEPANOW, LUCA PERSICHETTI, CORNELIU NISTOR, PIETRO GAMBARELLA, ETH Zürich — The prime feature of a magnet is to retain a significant fraction of its saturation magnetization in the absence of an external magnetic field. Realizing magnetic remanence in a single atom would allow storing and processing information in the smallest unit of matter. Here we show that individual rare-earth atoms on ultrathin insulating layers grown on non-magnetic metal substrates exhibit magnetic remanence and, therefore, are the first magnets formed by a single surface adsorbed atom. These magnets have a magnetic lifetime of 1500 s and a coercive field of 3.7 T at 10 K. In addition, their hysteresis loop remains open up to 30 K. This first example of a single atom magnet shows bistability at a temperature which is significantly higher than the best single molecule magnets reported so far. Its extraordinary stability is achieved by a suitable combination of magnetic ground state and adsorption site symmetry, and by decoupling the 4f spin from the underlying metal by a tunnel barrier.

**12:51PM B21.00007 Giant exchange interaction in mixed lanthanides**, NAOYA IWAHARA, VEACHESLAV VIERU, LIVIU UNGUR, LIVIU CHIBOTARU, Theory of Nanomaterials Group, Katholieke Universiteit Leuven — Combining strong magnetic anisotropy with strong exchange interaction is a long standing goal in the design of quantum magnets. The lanthanide complexes, while exhibiting a very strong ionic anisotropy, usually display a weak exchange coupling, amounting to only few wavenumbers. Recently, an isostructural series of mixed Ln-R-Ln complexes with R the N<sub>2</sub><sup>3-</sup> radical have been reported, in which the exchange splitting is estimated to reach hundreds wavenumbers [1,2]. Here we apply a new methodology allowing to establish on the basis of DFT and *ab initio* calculations the microscopic mechanism governing the unusual exchange interaction in these compounds [3]. We find it to be basically kinetic and highly complex, involving non-negligible contributions up to seventh power of total momentum  $\vec{J}$  of each Ln site. The performed analysis also elucidates the origin of magnetization blocking in these compounds. Contrary to general expectations the latter is not always favored by strong exchange interaction. [1] J. D. Rinehart, M. Fang, W. J. Evans, and J. R. Long, *Nat. Chem.* 3, 538 (2011). [2] J. D. Rinehart, M. Fang, W. J. Evans, and J. R. Long, *J. Am. Chem. Soc.* 133, 14236 (2011). [3] V. Vieru, N. Iwahara, L. Ungur, and L. F. Chibotaru, arXiv:1509.02206.

**1:03PM B21.00008 Visualizing Improved Spin Coupling in Large Magnetic Molecules**, JUDITH DONNER, Institute for Molecules and Materials, Radboud University Nijmegen, JAN-PHILIPP BROCHINSKI, BASTIAN FELDSCHE, THORSTEN GLASER, Faculty of Chemistry, University of Bielefeld, ALEXANDER AKO KHAJETOORIAN, DANIEL WEGNER, Institute for Molecules and Materials, Radboud University Nijmegen — In an attempt to combine a high spin ground state and a large magnetic anisotropy in one molecule, tripesalen-based complexes are promising building blocks for a new generation of single molecule magnets (SMMs). The spin coupling in these molecules is based on the spin polarization effect, which requires a delocalized aromatic  $\pi$ -system in the central carbon ring of the complex. Unfortunately, chemical analysis indicates that this ring can change its configuration to [6]radialene, therefore causing a loss of aromaticity and weakening the magnetic coupling. We have employed a combination of scanning tunneling microscopy (STM) and spectroscopy (STS) to investigate single Cu<sub>3</sub>-tripesalen and Cu<sub>3</sub>-tripesalen molecules, the latter being designed to show an enhanced intramolecular spin coupling. The large molecules were deposited in situ using the unconventional techniques pulse injection and rapid heating. A thorough structural and spectroscopic analysis allows us to discuss the electronic properties of the two complexes, with a special focus on the state of the central carbon ring. We find that even small changes in the ligand structure have a drastic influence on the intramolecular spin coupling, which opens the way for an improved rational design of future SMMs.

**1:15PM B21.00009 Exchange coupling and anisotropy effects on the low temperature magnetization dynamics in rare-earth dioxolene complexes**, ASMA AMJAD, GIORDANO PONETI, SILVIA SOTTINI, ANDREA DEI, LORENZO SORACE, INSTM, Università di Firenze — The prelude of relevant magnetic coupling in f-element based complexes is actively pursued to improve the single-molecule magnetic features. However, a quantitative analysis of magnetic properties of exchange-coupled anisotropic rare-earth based complexes is often hampered owing to the comparable magnitude of the crystal field with the magnetic coupling. In this study, we investigated the properties of complexes containing different ligands with comparable molecular structures and ligand field strengths. Comparative low-temperature magnetic and EPR study of homologous Ln<sup>III</sup>Semiquinonate (LnSQ) and Ln<sup>III</sup>Tropolonate (LnTrp) complexes, where Ln = Dy, Tb is investigated. Single-crystal EPR revealed that the direct exchange coupling in DySQ resulted in a highly anisotropic pseudo-triplet state. An out-of-phase susceptibility signal was observed for TbTrp only in the presence of an external magnetic field. Furthermore, the dynamics revealed slow relaxation of magnetization in the DySQ at low temperature which upon comparative study with the dynamics of the related DyTrp revealed a not so simple dependence on the crystal field effects of the coordination sphere of the lanthanide.

**1:27PM B21.00010 Anomalous power dependence in the zero-field resonance for the molecular nanomagnet  $\text{Cr}_7\text{Mn}$** <sup>1</sup>, C.A. COLLETT, Department of Physics, Amherst College, Amherst, MA, USA, G.A. TIMCO, R.E.P. WINPENNY, School of Chemistry, The University of Manchester, Manchester, UK, J.R. FRIEDMAN, Department of Physics, Amherst College, Amherst, MA, USA — We report electron-spin resonance studies of the paramagnetic ring  $[(\text{CH}_3)_2\text{NH}_2][\text{Cr}_7\text{MnF}_8((\text{CH}_3)_3\text{CCOO})_{16}]$  (" $\text{Cr}_7\text{Mn}$ "), a spin  $S=1$  molecular nanomagnet with a large zero-field ground-state tunnel splitting of  $\sim 4$  GHz. We perform parallel-mode electron-spin-resonance (ESR) spectroscopy with loop-gap resonators (LGRs) with resonance frequencies of 4-6 GHz. A crystal of  $\text{Cr}_7\text{Mn}$  is placed on the loop of the LGR with the sample's easy axis parallel to the field. We observe an ESR peak at zero dc field. With increasing radiation power, a pronounced dip develops in the center of the resonance peak, indicating a decoupling of the sample from the resonator with increased power. The onset of this decoupling depends on both the temperature and the applied power, with greater power required to observe the dip at higher temperatures. By pulsing the radiation, we can rule out that the dip is related to sample heating or saturation of the resonance. Power, temperature, and frequency dependence of the decoupling will be presented, and possible explanations will be discussed.

**1:39PM B21.00011 Time-resolved Measurements of Spontaneous Magnetic Deflagration of  $\text{Mn}_{12}\text{tBuAc}$** <sup>1</sup>, YIZHANG CHEN, A. D. KENT, New York Univ NYU, QING ZHANG, M. P. SARACHIK, City College of New York CUNY, M. L. BAKER, City College of New York CUNY and New York University NYU, D. A. GARANIN, Lehman College of CUNY, NAJAH MHESN, CHRISTOS LAMPROPOULOS, University of North Florida — Magnetic deflagration in molecular magnets has been triggered by heat pulses [1,2] and acoustic waves [3,4]. In this work we report spontaneous magnetic deflagration (i.e. deflagration that occurs without an external trigger) in the axially symmetric single molecule magnet  $\text{Mn}_{12}\text{tBuAc}$ . Magnetic hysteresis measurements show steps due to resonant quantum tunneling (RQT) below 1K, confirming the spin-Hamiltonian parameters for this material and previous results. Deflagration speeds measured with a newly constructed higher bandwidth (2MHz) setup will be presented as a function of transverse and longitudinal fields  $H_x \otimes H_z$  both on and off resonance. A large increase in front velocity near RQT steps is observed in experiments with swept transverse fields and will be discussed in light of models of deflagration. [1] S. McHugh *et al.* PRB **76**, 172410 (2007); [2] P. Subedi *et al.*, PRL **110**, 207203 (2013). [3] A. Hernández-Mínguez *et al.*, PRL **95**, 217205 (2005).

<sup>1</sup>Work supported by NSF-DMR-1309202 (NYU); ARO W911NF-13-1-0125 (CCNY); DMR-1161571(Lehman); Cottrell College Science Award (UNF).

**1:51PM B21.00012 ELECTRO-NUCLEAR CLOCK TRANSITIONS IN A  $\text{Ho(III)}$  MOLECULAR NANOMAGNET**<sup>1</sup>, DORSA KOMIJANI, M. SHIDDIQ, Department of Physics, Florida State University (NHMFL), FL, Y. DUAN, A. GAITA-ARINO, E. CORONADO, Instituto de Ciencia Molecular (ICMol), Universidad de Valencia, Spain, S. HILL, Department of Physics, Florida State University (NHMFL), FL — One of the challenges in the field of quantum information processing involves protecting qubits against decoherence. The primary source of decoherence in spin qubits at low temperatures is the dipolar interaction, which can be minimized using so-called clock transitions [1]. Here, we report pulsed EPR studies of the Holmium Polyoxometalate,  $[\text{Na}]_9[\text{Ho}_x\text{Y}_{1-x}(\text{W}_5\text{O}_{18})_2]$ , where we observe electro-nuclear clock transitions that involve coupled dynamics of the electron and nuclear spins ( $\Delta m_J = \pm 8$  and  $\Delta m_I = \pm 1$ ). These transitions are formally forbidden in EPR. However, the symmetry of this molecule generates admixtures of the ground doublet ( $m_J = \pm 4$ ) through second order perturbation, and application of a transverse magnetic field mixes  $m_I$  and  $m_I \pm 1$  states, allowing such transitions to occur in the vicinity of avoided level crossings. Pulsed EPR measurements on an  $x = 0.1$  sample, were carried out at a temperature of 5 K at X-band. These experiments suggest an enhancement in the coherence time at these electro-nuclear clock transitions which is significant for applications in hybrid magnetic qubits, where manipulation of the nuclear spin is controlled by EPR pulses. [1] G. Wolfowicz, *et al.*, Nature Nanotechnology **8**, 561 (2013).

<sup>1</sup>This work was supported by the NSF (DMR-1309463) and AFOSR.

**2:03PM B21.00013 A Crystal Field Approach to Orbitally Degenerate SMMs: Beyond the Spin-Only Hamiltonian**<sup>1</sup>, LAKSHMI BHASKARAN, Department of Physics and NHMFL, Florida State University, Tallahassee, USA, KATIE MARRIOTT, MARK MURRIE, WestCHEM, School of Chemistry, University of Glasgow, Glasgow, UK, STEPHEN HILL, Department of Physics and NHMFL, Florida State University, Tallahassee, USA — Single-Molecule Magnets (SMMs) with large magnetization reversal barriers are promising candidates for high-density information storage. Recently, a large uniaxial magnetic anisotropy was observed for a mononuclear trigonal bipyramidal (TBP)  $[\text{Ni}^{\text{II}}\text{Cl}_3(\text{Me-abco})_2]$  SMM [1]. High-field EPR studies analyzed on the basis of a spin-only Hamiltonian give  $D > 400 \text{ cm}^{-1}$ , which is close to the spin-orbit coupling parameter  $\lambda = 668 \text{ cm}^{-1}$  for  $\text{Ni}^{\text{II}}$ , suggesting an orbitally degenerate ground state. The spin-only description is ineffective in this limit, necessitating the development of a model that includes the orbital moment. Here we describe a phenomenological approach that takes into account a full description of crystal field, electron-electron repulsion and spin-orbit coupling effects on the ground state of a  $\text{Ni}^{\text{II}}$  ion in a TBP coordination geometry. The model is in good agreement with the high-field EPR experiments, validating its use for spectroscopic studies of orbitally degenerate molecular nanomagnets. [1] K. E. Marriott *et al.*, Chem Sci (published Online)

<sup>1</sup>This work was supported by the NSF (DMR-1309463)

**Monday, March 14, 2016 11:15AM - 2:15PM –**  
**Session B22 DCOMP: Theory and Simulation of Excited-State Phenomena in Semiconductors and Nanostructures I** 321 - Andre Schleife, University of Illinois at Urbana-Champaign

**11:15AM B22.00001 Hole localization, water dissociation mechanisms, and band alignment at aqueous-titania interfaces<sup>1</sup>**, JOHN L. LYONS, Brookhaven National Laboratory — Photocatalytic water splitting is a promising method for generating clean energy, but materials that can efficiently act as photocatalysts are scarce. This is in part due to the fact that exposure to water can strongly alter semiconductor surfaces and therefore photocatalyst performance. Many materials are not stable in aqueous environments; in other cases, local changes in structure may occur, affecting energy-level alignment. Even in the simplest case, dynamic fluctuations modify the organization of interface water. Accounting for such effects requires knowledge of the dominant local structural motifs and also accurate semiconductor band-edge positions, making quantitative prediction of energy-level alignments computationally challenging. Here we employ a combined theoretical approach to study the structure, energy alignment, and hole localization at aqueous-titania interfaces. We calculate the explicit aqueous-semiconductor interface using ab initio molecular dynamics, which provides the fluctuating atomic structure, the extent of water dissociation, and the resulting electrostatic potential. For both anatase and rutile TiO<sub>2</sub> we observe spontaneous water dissociation and re-association events that occur via distinct mechanisms. We also find a higher-density water layer occurring on anatase. In both cases, we find that the second monolayer of water plays a crucial role in controlling the extent of water dissociation. Using hybrid functional calculations, we then investigate the propensity for dissociated waters to stabilize photo-excited carriers, and compare the results of rutile and anatase aqueous interfaces. Finally, we use the GW approach from many-body perturbation theory to obtain the position of semiconductor band edges relative to the occupied 1b<sub>1</sub> level and thus the redox levels of water, and examine how local structural modifications affect these offsets.

<sup>1</sup>This work was performed in collaboration with N. Kharche, M. Z. Ertem, J. T. Muckerman, and M. S. Hybertsen. It made use of resources at the Center for Functional Nanomaterials, which is a U.S. DOE Office of Science Facility, at Brookhaven National Lab.

**11:51AM B22.00002 Role of excited states in Shockley-Read-Hall recombination in wide band-gap semiconductors**, AUDRIUS ALKAUSKAS, Center for Physical Sciences and Technology, Lithuania, CYRUS E. DREYER, JOHN L. LYONS, CHRIS G. VAN DE WALLE, University of California Santa Barbara — Defect-assisted recombination is an important limitation on efficiency of optoelectronic devices. However, since nonradiative capture rates decrease exponentially with energy of the transition, the mechanisms by which such recombination can take place in wide-band-gap materials are unclear. We investigate the role of electronic excited states in the recombination process, focusing on group-III nitrides, for which accumulating experimental evidence indicates that defect-assisted recombination is an important limiting factor in efficiency. Based on first-principles electronic structure calculations, we show that excited states of gallium vacancy complexes make these defects very efficient recombination centers. Our work provides new insights into the physics of nonradiative recombination. The mechanism discussed in this work is suggested to be very critical and ubiquitous in wide-band-gap semiconductors. This work was supported by DOE and the European Union.

**12:03PM B22.00003 Auger recombination in InN from first principles<sup>1</sup>**, ANDREW MCALLISTER, EMMANOUIL KIOUPAKIS, Univ of Michigan - Ann Arbor — Group-III Nitride materials are used in numerous electronic and optoelectronic devices including solid-state lighting, energy conversion, sensor technologies, and high-power electronics. Indium nitride in particular is interesting for fast electronics and optoelectronics in the infrared. Auger recombination is a non-radiative carrier recombination process that would limit the efficiency of these devices. The small band gap (0.7 eV) and the high intrinsic free-electron concentrations in InN possibly make Auger recombination particularly important in this material. We used first-principles computational methods to determine the Auger recombination rates in InN. Our results suggest that direct Auger recombination is dominant in this material and that phonon-assisted Auger processes are not as important as in wider-gap nitrides such as GaN.

<sup>1</sup>This research was supported by the National Science Foundation CAREER award through Grant No. DMR-1254314. Computational resources were provided by the DOE NERSC facility.

**12:15PM B22.00004 Electronic coherence and the kinetics of energy transfer in light-harvesting systems**, PENGFEI HUO, University of Rochester, DAVID COKER, Boston University, THOMAS MILLER, Caltech — Recent 2D-spectroscopy experiments have observed transient electronic coherence in natural and artificial light harvesting systems, which raises questions about the role of electronic coherence in facilitating excitation energy transfer (EET) processes. In this talk, we introduce the recently developed partial linearized path-integral (PLPI) method, which can accurately simulate exciton transfer dynamics across multiple reaction regimes, as well as reliably describe the electronic coherence among excitonic states. Further, we develop a strategy that enables the analysis of the relative impact of static and dynamic electronic coherence. With PLPI simulations, we find that energy transfer dynamics are almost entirely dominated by static coherence effects; dynamic coherence is found to cause only minor effects. These conclusions are consistent with the historical view that emphasizes the importance of energy-level alignment for efficient incoherent energy transfer, while suggesting a less important role for more exotic electronic coherence effects that have been recently emphasized.

**12:27PM B22.00005 The Optical Spectrum of LaAlO<sub>3</sub>: Quasiparticle Energies and the Effect of Lattice Screening**, XIAO ZHANG, ANDRE SCHLEIFE, University of Illinois, Urbana — Lanthanum aluminate (LaAlO<sub>3</sub>) is a commonly used high- $\kappa$  dielectric material but its exact optical properties are not well understood. By solving the Bethe-Salpeter Equation for the optical polarization function, which describes the interaction between electrons and holes, a precise prediction of the dielectric function can be obtained. However, for LaAlO<sub>3</sub>, there are two major problems limiting the computational study: The first problem is that due to the complicated conduction band structure, the quasiparticle effect needs to be taken into account, which makes the calculations costly. We resolved this problem by interpolating accurate eigenenergies computed using a hybrid exchange-correlation functional to a dense k-point grid. Another problem is that for such high- $\kappa$  materials, the lattice contribution to the dielectric screening may be important. We investigated this by computing the optical spectrum using electronic constant, static dielectric constant and the average of both and found that taking lattice contribution into account significantly reduces excitonic effects. All results are compared to available experiments.

**12:39PM B22.00006 Electronic and optical properties of Ga<sub>2</sub>O<sub>3</sub> from first principles**, KELSEY MENGLE, EMMANOUIL KIOUPAKIS, University of Michigan — Wide band-gap semiconductors such as Ga<sub>2</sub>O<sub>3</sub> are used in numerous applications including high voltage/temperature electronics, deep-UV emission, and transparent contacts. We have investigated the electronic and optical properties of Ga<sub>2</sub>O<sub>3</sub> with first-principles calculations based on density functional theory. The electronic and optical properties are calculated with many-body perturbation theory using the GW and Bethe-Salpeter equation methods. The semicore states of Ga are treated as valence electrons to accurately determine the band gap and band structure. We will present results for the structural, electronic, and optical properties of the various Ga<sub>2</sub>O<sub>3</sub> polymorphs, including  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>. This research was supported by the National Science Foundation through Grant No. DMR- 1534221. Computational resources were provided by the DOE NERSC facility.

**12:51PM B22.00007 Substrate Screening Induced Renormalization of Excited-States in 2D Materials**, NEERAV KHARCHI, VINCENT MEUNIER, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, NY 12180 — Two-dimensional (2D) materials offer an emerging platform for exploring novel electronic phenomena in reduced dimensionality systems. However, because of their atomic scale thickness, their excitation energy levels in 2D materials are strongly renormalized due to the screening by the surrounding environment. This effect is expected to have strong impact when the materials are integrated into functional devices. For example, the presently available GW calculations significantly overestimate the band gaps in graphene nanoribbons (GNRs) by as much as one eV compared to experiment. Here, we outline an integrated computational approach combining DFT, the GW approximation, and a classical image charge model to include substrate screening effects in a computationally tractable manner. We investigate the band gaps and defect charge transition levels (CTLs) in a prototypical 2D material, hexagonal boron nitride (hBN) and a prototypical 1D nanostructure, GNR. The band gaps and defect CTLs are strongly renormalized by several tenths of an eV in the substrate-supported versus the free-standing configurations. In the case of GNRs, the predicted band gaps are in an excellent agreement with recent STS experiments.

**1:03PM B22.00008 Electronic structure, transport properties, and excited states in CoTiSb, CoZrSb, and CoHfSb half-Heusler compounds**<sup>1</sup>, ANDERSON JANOTTI, ZHIGANG GUI, University of Delaware, Department of Materials Science and Engineering, JASON KAWASAKI, Kavli Institute at Cornell for Nanoscale Science, Cornell University, CHRIS PALMSTROM, Materials Department, University of California, Santa Barbara, BURAK HIMMETOGLU, Center for Scientific Computing, University of California, Santa Barbara — CoTiSb is a member of a large family of half-Heusler compounds with 18 valence electrons. CoTiSb is semiconductor material with a band gap a little over 1 eV, and it has been considered promising for thermoelectric applications. It can be grown on conventional III-V semiconductors, and could potentially be integrated in III-V devices. Here we present results of first-principles calculations of electronic structure, transport properties, and excited states in CoTiSb, as well as CoZrSb and CoHfSb. Electronic structures are studied using density functional theory within the local density approximation, hybrid functional and quasiparticle GW methods. Both room-temperature Seebeck coefficient and carrier mobility are calculated from first-principles. We also determine the band alignments to III-V semiconductors, and all the results are presented and discussed in the light of available experimental data.

<sup>1</sup>This work was supported by the DOE.

**1:15PM B22.00009 Ab Initio Calculations of Excited Carrier Dynamics in Gallium Nitride**, VATSAL JHALANI, MARCO BERNARDI, California Institute of Technology — Bulk wurtzite GaN is the primary material for blue light-emission technology. The radiative processes in GaN are regulated by the dynamics of excited (or so-called hot) carriers, through microscopic processes not yet completely understood. We present ab initio calculations of electron-phonon (e-ph) scattering rates for hot carriers in GaN. Our work combines density functional theory to compute the electronic states, and density functional perturbation theory to obtain the phonon dispersions and e-ph coupling matrix elements. These quantities are interpolated on fine Brillouin zone grids with maximally localized Wannier functions, to converge the e-ph scattering rates within 5 eV of the band edges. We resolve the contribution of the different phonon modes to the total scattering rate, and study the impact on the relaxation times of the long-range Fröhlich interaction due to the longitudinal-optical phonon modes.

**1:27PM B22.00010 Time Evolution of Charge Carriers & Phonons after Photo-Excitation by an Ultra-Short Light Pulse in Bulk Germanium**<sup>1</sup>, STEPHEN FAHY, University College Cork, FELIPE MURPHY-ARMANDO, Tyndall National Institute, Cork, Ireland, MARIANO TRIGO, Stanford Institute for Materials and Energy Science, SLAC National Accelerator Laboratory, IVANA SAVIC, EAMONN MURRAY, Tyndall National Institute, Cork, Ireland, DAVID REIS, Stanford Institute for Materials and Energy Science, SLAC National Accelerator Laboratory — We have calculated the time-evolution of carriers and generated phonons in Ge after ultrafast photo-excitation above the direct band-gap. The relevant electron-phonon and anharmonic phonon scattering rates are obtained from first-principles electronic structure calculations. Measurements of the x-ray diffuse scattering after excitation near the L point in the Brillouin zone find a relatively slow (5 ps, compared to the typical electron-phonon energy relaxation of the Gamma-L phonon) increase of the phonon population. We find this is due to emission caused by the scattering of electrons between the Delta and L valleys, after the initial depopulation of the Gamma valley. The relative slowness of this process is due to a combination of causes: (i) the finite time for the initial depopulation of the conduction Gamma valley; (ii) the associated electron-phonon coupling is relatively weaker (compared to Gamma-L, Gamma-Delta and Delta-Delta couplings); (iii) the TA associated phonon has a long lifetime and (iv) the depopulation of the Delta valley suppresses the phonon emission.

<sup>1</sup>supported by Science Foundation Ireland, Grant 12/1A/1601

**1:39PM B22.00011 Constrained Density Functional Theory by Imaginary Time-Step Method**, DANIEL KIDD, Vanderbilt University — Constrained Density Functional Theory (CDFT) has been a popular choice within the last decade for sidestepping the self interaction problem within long-range charge transfer calculations.<sup>1</sup> Typically an inner constraint loop is added within the self-consistent field iterations of DFT in order to enforce this charge transfer state by means of a Lagrange multiplier method.<sup>2</sup> In this work, an alternate implementation of CDFT is introduced, that of the imaginary time-step method, which lends itself more readily to real space calculations in the ability to solve numerically for 3D local external potentials which enforce arbitrary given densities. This method has been shown to reproduce the proper  $1/R$  dependence of charge transfer systems in real space calculations as well as the ability to generate useful constraint potentials. As an example application, this method is shown to be capable of describing defects within periodic systems using finite calculations by constraining the 3D density to that of the periodically calculated perfect system at the boundaries.

<sup>1</sup>Q. Wu and T. Voorhis, *J. Chem. Theory Comput.* 2, 765-774 (2006).

<sup>2</sup>Q. Wu and T. Voorhis, *Phys. Rev. A* 72, 024502 (2005).

**1:51PM B22.00012 Density functional study on a light-harvesting carotenoid-porphyrin-C<sub>60</sub> molecular triad in explicit solvent**, CARLOS DIAZ, TUNNA BARUAH, RAJENDRA ZOPE, University of Texas at El Paso — We investigate the effect of solvent on the electronic structure of a biomimetic molecular triad that shows photoinduced charge transfer in laboratory. The supramolecular triad contains three different units - C<sub>60</sub>, porphyrin, and beta-carotenoid. We have performed classical molecular dynamics simulation of the triad surrounded by 15000 water molecules using NAMD for 20 nanoseconds. Subsequently, we performed an all-electron density functional calculations (DFT) using large basis sets on the 50 snap-shots taken from the molecular dynamics simulation. The solvent effects in the DFT calculations are treated using both the explicit water molecules as well as using the point charge representation of water. The excitation energies and absorption spectra show that the polar solvent induces significant changes in the electronic structure of the triad.

**2:03PM B22.00013 Ab-Initio Computations of Electronic and Related Properties of cubic Lithium Selenide ( $\text{Li}_2\text{Se}$ )**, ABDOULAYE GOITA, Department of Electrical Engineering, Southern University and AM College, Baton Rouge, IFEANYI H. NWIGBOJI, Department of Computational Science, University of Texas at El Paso, El-Paso, TX 79968 USA, YURIY MALOZOVSKY, DIOLA BAGAYOKO, Department of Physics, Southern University and AM College, Baton Rouge, LA 70813, USA — We present theoretical predictions, from ab-initio, self-consistent calculations, of electronic and related properties of cubic lithium selenide ( $\text{Li}_2\text{Se}$ ). We employed a local density approximation (LDA) potential and the linear combination of atomic orbitals (LCAO). We performed the computations following the Bagayoko, Zhao, and Williams (BZW) method, as enhanced by Ekuma and Franklin (BZW-EF). Our results include electronic energies, total and partial densities of states, effective masses, and the bulk modulus. The theoretical equilibrium lattice constant is 5.882 Å. We found cubic  $\text{Li}_2\text{Se}$  to have a direct band gap of 4.363 eV (prediction), at  $\Gamma$ . This gap is 4.065 eV for a room temperature lattice constant of 6.017 Å. The calculated bulk modulus is 31.377 GPa. Acknowledgments: This work was funded in part by the National Science Foundation (NSF) and the Louisiana Board of Regents, through LASiGMA [Award Nos. EPS- 1003897, NSF (2010-15)-RII-SUBR] and NSF HRD-1002541, the US Department of Energy – National, Nuclear Security Administration (NNSA) (Award No. DE- NA0002630), LaSPACE, and LONI-SUBR.

**Monday, March 14, 2016 11:15AM - 2:03PM –**  
**Session B23 DMP DCOMP: Computational Materials Discovery and Design - Electronic Structure** 322 - Sahar Sharifzadeh, Boston University

**11:15AM B23.00001 Materials by design: methodological developments in the calculation of excited-state properties<sup>1</sup>**, MARCO GOVONI, Institute for Molecular Engineering, University of Chicago and Argonne National Laboratory — Density functional theory (DFT) is one of the main tools used in first principle simulations of materials; however several of the current approximations of exchange and correlation functionals do not provide the level of accuracy required for predictive calculations of excited state properties. The application to heterogeneous systems of more accurate post-DFT approaches such as Many-Body Perturbation Theory (MBPT) – for example to nanostructured, disordered, and defective materials – has been hindered by high computational costs. In this talk recent methodological developments in MBPT calculations will be discussed, as recently implemented in the open source code WEST [1], which efficiently exploits HPC architectures. Results using a formulation that does not require the explicit calculation of virtual states, nor the storage and inversion of large dielectric matrices will be presented; these results include quasi particle energies for systems with thousands of electrons and encompass the electronic structure of aqueous solutions, spin defects in insulators, and benchmarks for molecules and solids containing heavy elements. Simplifications of MBPT calculations based on the use of static response properties, such as dielectric-dependent hybrid functionals [2], will also be discussed.

[1] [www.west-code.org](http://www.west-code.org); M. Govoni, and G. Galli, J. Chem. Theory Comput. 11, 2680 (2015)

[2] J.H. Skone, M. Govoni, and G. Galli, Phys. Rev. B 89, 195112 (2014)

<sup>1</sup>Work done in collaboration with Hosung Seo, Peter Scherpelz, Ikutaro Hamada, Jonathan Skone, Alex Gaiduk, T. Anh Pham, and Giulia Galli. Supported by DOE-BES.

**11:51AM B23.00002 An Automated Ab Initio Approach for Identifying Small Band Gap Ferroelectric**, TESS SMIDT, SEBASTIAN REYES-LILLO, Physics Department, UC Berkeley; Molecular Foundry, Lawrence Berkeley National Lab, JEFFREY NEATON, Physics Department, UC Berkeley; Molecular Foundry, Lawrence Berkeley National Lab; Kavli Energy NanoSciences Institute at Berkeley — Small band gap ferroelectrics are scarce and yet hold promise for optoelectronics applications. In this work, we leverage the electronic and symmetry requirements that give rise to ferroelectricity to search for new small band gap ferroelectrics using the Materials Project and Inorganic Crystal Structure Database. We create an automated workflow that combines database queries, symmetry tools and high-throughput DFT to identify candidate classes of ferroelectrics. Using density functional theory and beyond, we reveal accurate band gap trends for new and previously synthesized compounds. The effect of chemical doping on the polarization and energy barrier is discussed for select cases.

**12:03PM B23.00003 Ab initio parametrization of bond-polarizability model for Raman spectroscopy of complex Si materials**, DAVID A. STRUBBE, JEFFREY C. GROSSMAN, Department of Materials Science and Engineering, Massachusetts Institute of Technology — Classical inter-atomic potentials can be successful at predicting the vibrations of materials at system sizes intractable by quantum methods. However, to predict Raman spectra, electrons must be re-introduced, for example via a bond-polarizability model which attributes the polarizability to cylindrically symmetrical inter-atomic bonds. Parameters in assumed functional forms are fit to experimental spectra, and then a Raman intensity can be computed for each mode. In the case of amorphous silicon, the existing models do not show satisfactory agreement with experimental spectra. To generate a more accurate and transferable bond-polarizability model, we have instead begun with ab initio calculated Raman tensors for a set of a-Si:H structures [DA Strubbe et al., arXiv:1511.01139]. This atomistic data set allows us to obtain parameters and functional forms for a general model, without confounding errors from the potentials. This Raman model can be used to study large structural models with relevance for photovoltaics, such as medium- and long-range order in a-Si:H, nanocrystalline Si, amorphous/crystalline interfaces, or a-Si:H nanowires, at sizes that would be inaccessible for ab initio calculations. We analyze the applicability of this approach to other materials systems.

**12:15PM B23.00004 Self-consistent perturbation theory for two dimensional twisted bilayers**, SHARMILA N. SHIRODKAR, GEORGIOS A. TRITSARIS, EFTHIMIOS KAXIRAS<sup>1</sup>, John A. Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts 02138, USA — Theoretical modeling and ab-initio simulations of two dimensional heterostructures with arbitrary angles of rotation between layers involve unrealistically large and expensive calculations. To overcome this shortcoming, we develop a methodology for weakly interacting heterostructures that treats the effect of one layer on the other as perturbation, and restricts the calculations to their primitive cells<sup>2</sup>. Thus, avoiding computationally expensive supercells. We start by approximating the interaction potential between the twisted bilayers to that of a hypothetical configuration (viz. ideally stacked untwisted layers), which produces band structures in reasonable agreement with full-scale ab-initio calculations for commensurate and twisted bilayers of graphene (Gr) and Gr/hexagonal boron nitride (h-BN) heterostructures. We then self-consistently calculate the charge density and hence, interaction potential of the heterostructures. In this work, we test our model for bilayers of various combinations of Gr, h-BN and transition metal dichalcogenides, and discuss the advantages and shortcomings of the self-consistently calculated interaction potential.

<sup>1</sup>Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA.

<sup>2</sup>Georgios A. Tritsaritis *et. al.*, Perturbation theory for weakly coupled two-dimensional layers, **under review**.

**12:27PM B23.00005 Simplified Quantum Transport Theory for Finite Bias and Temperature<sup>1</sup>**, XIAOQUANG ZHANG, YUNING WU, Univ of Florida - Gainesville, SOKRATES PANTELIDES, Vanderbilt University — We reformulate the Landauer-Buttiker formula for quantum transport by explicitly accounting for the energy and bias voltage dependence of the transmission probability. Under the assumption of a constant electric field, a simple formula for the differential conductance under a finite bias and at a finite temperature is derived that does not require a nonequilibrium self-consistent calculation. Calculation for the tunneling current through Au-Benzendithiol-Au molecular junction shows excellent agreement with the nonequilibrium Green's function (NEGF) method at zero temperature. Temperature dependent I-V curves for a number of devices are demonstrated.

<sup>1</sup>Supported by NSF grant 1508898

**12:39PM B23.00006 High-throughput determination of Hubbard U for cubic perovskites using the ACBN0 functional.**, LAALITHA LIYANAGE, University of North Texas, ANDREW SUPKA, PRIYA GOPAL, Central Michigan University, LUIS AGAPITO, University of North Texas, GUS HART, Brigham Young University, MARCO FORNARI, Central Michigan University, STEFANO CURTAROLO, Duke University, MARCO BUONGIORNO NARDELLI, University of North Texas — High-throughput (HT) density functional theory (DFT) computations are the method of choice for rapid screening of materials properties and materials development. However, traditional DFT is not adequate for the investigation of all systems. For materials containing transition metal elements, methods such as DFT+U or hybrid functionals are needed for an accurate prediction of the electronic structure. As an efficient and accurate alternative we have recently introduced the ACBN0 functional for DFT as a new pseudo-hybrid Hubbard density functional that is a parameter-free extension of traditional DFT+U that has been proved to correct both the band gap and the relative position of the different bands in transition metal compounds. We implemented ACBN0 in a Medium-Throughput Framework (MTFrame) designed to automate DFT calculations for systems that share a single reference crystal structure. Using the MTFrame, we have determined the effective U values for 3969 cubic perovskites (ABO<sub>3</sub>) built by permutating 63 different elements in the A and B sites. Analysis of resulting data reveals the effects of Hubbard U on the electronic properties and crystal structure. Finally, machine learning algorithms are used to find correlations in the extracted data and the U values.

**12:51PM B23.00007 A tool for accelerating material calculations through the generation of highly efficient *k*-point grids**, TIM MUELLER, PANDU WISESA, Johns Hopkins University — The calculation of many material properties requires the evaluation of an integral over the Brillouin zone, which is commonly approximated by sampling a regular grid of points, known as *k*-points, in reciprocal space. We have developed an automated tool for generating *k*-point grids that significantly accelerates the calculation of material properties compared to commonly used methods. Our tool, which is being made freely available to the public, is capable of generating highly efficient *k*-point grids in a fraction of a second for any crystalline material. We present an overview of our method, benchmark results, and a discussion of how it can be integrated into a high-throughput computing environment.

**1:03PM B23.00008 Advancing Efficient All-Electron Electronic Structure Methods Based on Numeric Atom-Centered Orbitals for Energy Related Materials<sup>1</sup>**, VOLKER BLUM, MEMS Department, Duke University, Durham, NC 27708 — This talk describes recent advances of a general, efficient, accurate all-electron electronic theory approach based on numeric atom-centered orbitals; emphasis is placed on developments related to materials for energy conversion and their discovery. For total energies and electron band structures, we show that the overall accuracy is on par with the best benchmark quality codes for materials, but scalable to large system sizes (1,000s of atoms) and amenable to both periodic and non-periodic simulations. A recent localized resolution-of-identity approach for the Coulomb operator enables  $O(N)$  hybrid functional based descriptions of the electronic structure of non-periodic and periodic systems, shown for supercell sizes up to 1,000 atoms; the same approach yields accurate results for many-body perturbation theory as well. For molecular systems, we also show how many-body perturbation theory for charged and neutral quasiparticle excitation energies can be efficiently yet accurately applied using basis sets of computationally manageable size. Finally, the talk highlights applications to the electronic structure of hybrid organic-inorganic perovskite materials, as well as to graphene-based substrates for possible future transition metal compound based electrocatalyst materials.

<sup>1</sup>All methods described here are part of the FHI-aims code. VB gratefully acknowledges contributions by numerous collaborators at Duke University, Fritz Haber Institute Berlin, TU Munich, USTC Hefei, Aalto University, and many others around the globe.

**1:39PM B23.00009 Simple Rules for Solid-state Design: From Bulk to Interface**, KEITH BUTLER, ARON WALSH, ADAM JACKSON, DAN DAVIES, University of Bath, FUMIYASU OBA, YU KUMAGAI, Tokyo Institute of Technology, WALSH MATERIALS DESIGN TEAM, JSPS COLLABORATION — High-throughput screening enterprises such as Materials Project and the QCMD are well suited to the application of density functional theory for assessing the merits of known bulk materials. The blind exploration of the new combinations and permutations of the periodic table is a daunting task, to paraphrase Samuel Beckett we feel *lost before the confusion of innumerable prospects*. Centuries of research have provided us with myriad rules for assessing the feasibility of a given stoichiometry and the likelihood of particular crystal arrangements. We explore the ways in which chemical knowledge and state-of-the-art computational physics can be combined to accelerate materials design. We present the SMOCT (Semiconducting Materials by Analogy and Chemical Theory) package, which combines these rules with searching of chemical space to predict plausible and heretofore unknown compounds. I will then provide some illustrative examples of materials' design focusing on several important issues: (i) designing new photovoltaic materials [1], (ii) the role of surfaces and polymorphism in controlling electronic properties [2,3], and (iii) the design of porous materials [4]. [1] K. T. Butler et al., *Energy Environ. Sci.*, **2015**, 8, 838 [2] K. T. Butler et al., *Phys. Rev. B*, **2014**, 89, 115320 [3] J. Buckeridge, et al., *Chem. Mater.*, **2015**, 27, 3844 [4] K. T. Butler, et al., *J. Am. Chem. Soc.*, **2014**, 136, 2703

**1:51PM B23.00010 ACBN0-tool for accelerated materials discovery.**, PRIYA GOPAL, Central Michigan University, LAALITHA LIYANAGE, LUIS AGAPITO, University of North Texas, SEUNGHUN LEE, ICHIRO TAKEUCHI, University of Maryland, GUS HART, Brigham Young University, STEFANO CURTAROLO, Duke University, MARCO FORNARI, Central Michigan University, MARCO BUONGIORNO NARDELLI, University of North Texas — High-Throughput QM computation of material properties by abinitio methods has become the foundation of an effective approach to materials design. One of the major challenges in mapping the materials genome is in developing efficient computational tools that are cost-effective and accurate at the same time. In this talk, we discuss the newly developed ACBN0 pseudo-hybrid Hubbard density functional where the Hubbard energy within the DFT + U formulation is calculated self consistently. The U depends on the electron density and depends both on the geometry and chemical environment of the system. We show that ACBN0 improves the description of both the structural and electronic properties in a range of complex materials from Zn/Cd based chalcogenides to the TMOs. The magnetic properties are better described compared to the LDA/GGA functionals. We will also discuss the application of the ACBN0 approach to surfaces, doped and multi-valent systems where it is possible to evaluate U for different sites and chemical bonding. For all the complex materials studied here, we find that the electronic properties are significantly improved over the DFT values and the accuracy is at par with the HSE values at a fraction of the computational cost.

**Monday, March 14, 2016 11:15AM - 2:03PM —**  
**Session B24 DMP: Optical Effects Near Metallic Nanostructures** 323 - Latha Venkataraman, Columbia University

**11:15AM B24.00001 Optical functionality of plasmon-exciton nanomaterials in the strong coupling regime**, MAXIM SUKHAREV, Arizona State University — Understanding optical plasmon-exciton interaction in hybrid plasmonic nanostructures is important for tuning the optical response, e.g. for applications in nonlinear optics, organic solar cells, or organic light-emitting diodes. In developing such nanostructures, the strong coupling phenomena play crucial role allowing to efficiently transfer energy between plasmons and molecular excitons on a femtosecond time scale. In this talk I will discuss modeling aspects of various optical phenomena at plasmonic interfaces using Maxwell-Bloch equations in three dimensions. Various plasmonic systems including periodic V-grooves, bowtie antennas, nanowires, periodic hole arrays, and others will be considered. In particular, I will demonstrate that one can design hybrid nanomaterials with highly pronounced Fano resonances using femtosecond lasers. I will show that it is possible to use ultra-short laser pulses to materials with desired properties and functionality. Electromagnetic energy transport in systems composed of closely spaced nanowires in a presence of molecular excitons will also be discussed.

**11:51AM B24.00002 Surface Enhance Infrared Absorption in nanogap structures**, YAJING LI, PAVLO ZOLOTAVIN, DOUGLAS NATELSON, Rice University — Understanding the energy dissipation at the interface of molecules and metal nanostructures is of interest. We fabricate self-aligned gold nanostructures with nanometer-scale interelectrode spacing. Those gold nanostructures support highly hybridized plasmon modes with great enhanced local electric field. Previous studies have proven those structures to be suitable substrates for surface-enhanced Raman spectroscopy with single-molecule sensitivity, which enables the study of molecular vibrational and electronic physics. We propose those structures as possible probes of the energy dissipation at the nanometer gap. By measuring the absorption spectrum of molecules assembled in the junction, we can estimate the local field intensity at the gap and discuss the plasmonic responses of these self-aligned structures under infrared excitation.

**12:03PM B24.00003 Optically induced changes to the tunneling properties of molecular junctions.**<sup>1</sup>, PAVLO ZOLOTAVIN, CHARLOTTE EVANS, DOUGLAS NATELSON, Department of Physics & Astronomy, Rice University — We report increased conductance under laser illumination in plasmonically active atomic scale gold junction in a cryogenic environment (substrate temperatures down to 4 K). Additionally, we observe changes in the bias dependence of differential conductance, which we attribute to local heating due to the illumination. We differentiate between plasmon and direct gold absorption by investigating the polarization dependence of the observed temperature change. The effect is quantified by measuring optically induced changes in the resistance of the metal nanowire and by the change in the magnitude of simultaneously measured Johnson-Nyquist noise. A combination of these techniques provides independent measurements of effective lattice and electronic temperatures. Unlike previous experiments at room temperature and 80 K, we report a substantially larger light-driven temperature increase of 80-120K for devices fabricated on SiO<sub>2</sub>/Si substrates held at substrate temperatures as low as 4 K. The implications of the observed behavior for electronic transport in single molecular junctions with plasmonically active nanowire leads will be discussed.

<sup>1</sup>ARO award W911 NF-13-1-0476

**12:15PM B24.00004 Propagating plasmon excitation of molecular junctions for spectroscopy**<sup>1</sup>, CHARLOTTE EVANS, PAVLO ZOLOTAVIN, DOUGLAS NATELSON, Rice University Department of Physics and Astronomy — Electronic transport and simultaneous optical measurements on molecule-containing junctions can provide critical information about the dissipation of energy through inelastic processes. Gold bowtie nanostructures have been used for electronic transport and as plasmonically active substrates for surface-enhanced Raman scattering (SERS), conventionally with exciting light incident directly on the molecular junction. Electromigrating these devices created interelectrode nanogaps with single-molecule sensitivity in which the Raman scattering rate is dominated by plasmonically enhanced electromagnetic fields due to the presence of the metal nanojunction near the molecules of interest. Direct optical excitation of the junction region, however, can cause heating of the metal, molecular instability via conformational and chemical changes, and breakdown over time. Adding metallic gratings to the electrode design enables the excitation of propagating plasmon modes that can couple into the junction region without direct excitation by far-field radiation. We will present preliminary data on how the addition of these gratings affects single-molecule SERS and the electrical properties of the molecules in these junctions.

<sup>1</sup>This research was funded by NSF Graduate Research Fellowships Program DGE-1450681 and ARO award W911 NF-13-1-0476.

**12:27PM B24.00005 Enhancement of Resonant Energy Transfer Due to Evanescent-wave from the Metal**, AMRIT POUDEL, Northwestern University, XIN CHEN, Xi'an Jiaotong University, MARK RATNER, Northwestern University — The high density of evanescent modes in the vicinity of a metal leads to enhancement of the near-field Forster resonant energy transfer (FRET) rate. We present a mathematical formulation based on classical electromagnetic theory using the dyadic Greens function and investigate the effect of metallic environment using material permittivity in local and nonlocal limits, which provides better estimates of the transfer rate at small separations from the metal. Furthermore, we present a general formula of FRET rate for multiple donors and acceptors in the presence of arbitrary dielectric environment and discuss the path interference effect on FRET rate.

**12:39PM B24.00006 Two-photon up-conversion affected by inter-molecule correlations near metallic nanostructure**<sup>1</sup>, YOSHIKI OSAKA, NOBUHIKO YOKOSHI, HAJIME ISHIHARA, Osaka Prefecture University — Optical antennas, which consist of metallic nanostructures, concentrate free-propagating light into localized surface plasmons (LSP). Such a localized field enables effective interactions between light and molecules nearby the metal surfaces. However, as the light intensity decreases to single-photon level, large dissipation in the metals always inhibits the effective photon-molecule interaction via LSP. We have theoretically elucidated that controlling quantum interference in an antenna-molecule coupled system strongly suppresses the photon-dissipations, and leads to efficient two-photon processes in the molecule. However, it is difficult to prepare only one molecule nearby the metal. Therefore, as a beachhead into a multi-molecule system, we will consider the case that two photons couple with two molecules under one LSP. In rapid intuition, the appearance of the second molecule seemingly damages the up-conversion process. In the presentation, we reveal that controlling the inter-molecule interaction could resolve the difficulty, and lead to the efficient up-conversion through the quantum interference among three-bodies, i.e., LSP and two molecules.

<sup>1</sup>Supported by a Grant-in-Aid for JSPS Fellows No. 13J09308

## **12:51PM B24.00007 Finite-Difference Time-Domain (FDTD) Modeling of Gold Core-Shell Structures with Different Shell Morphology for Surface-Enhanced Raman Spectroscopy (SERS)<sup>1</sup>**

, ZOHRE GORUNMEZ, DEBRINA JANA, JIE HE, LAURA SAGLE, THOMAS BECK, University of Cincinnati — Core-shell (CS) nanostructures have received attention in recent years due to their usefulness in applications ranging from catalysis to cancer treatment. SERS has been shown to be one of the most sensitive techniques for molecular detection, achieving single molecule detection. It has been established that the electromagnetic mechanism (EM) provides the main contribution to SERS enhancement due to the normal Raman spectroscopy arising from coupling of both the incident and re-emitted fields. The FDTD technique has been developed to provide numerical solutions to Maxwell's time-dependent curl equations in order to promise modeling capabilities for EM enhancement of SERS. Herein, we apply this method to the study of three morphologically different gold core-shell nanoparticles to investigate their contributions to SERS. In these structures, the dye/probe molecule resides in between the shell and the core and only the shell morphology is altered. The data shows that the surface plasmon resonances (PRs) influencing the SERS of the probe molecules, due to the coupling of the core and shell, are tunable by changing the shell morphologies and CS structures with sharp features on their surfaces highlight larger enhancements due to stronger localized surface PRs.

<sup>1</sup>University of Cincinnati start-up funds, NSF, Ohio Supercomputer Center, and the Ministry of National Education of the Republic of Turkey.

## **1:03PM B24.00008 Block copolymer based design of highly sensitive substrates for detecting single molecules by surface enhanced Raman scattering**

, ATIKUR RAHMAN, CHARLES BLACK, Brookhaven National Lab — Surface enhanced Raman spectroscopy (SERS) relies on substrates with nanometer-scale curvature in order to concentrate and amplify the incident electromagnetic field to increase the spectroscopic signature of Raman scattering. The localization and amplification of incident light is maximum between two plasmonic nanostructures called as "hot spot". Here, we report a new, scalable method for fabricating high-performance SERS substrates based on self-assembly of nanostructured block copolymer thin films. Due to the high spatial density and extremely high field strengths of substrate hot spots, these substrate are capable of enhancing Raman scattering signals from target molecules by more than 10 billion times. We will describe the process of fabricating these remarkable diagnostic tools, which are  $\sim \text{cm}^2$  area substrates composed of an extremely high density ( $\sim 10^{11} / \text{cm}^2$ ) of hexagonally-arranged Au or Ag nanoparticles positioned atop  $\sim 70\text{nm}$  tall silicon nanopillars. Key to the substrate performance is the sub-5 nm separation between particles, which we control with nm level precision. By systematically varying the gap between nanoparticles, we demonstrate that both the high hotspot density and sub 5nm hot spot gap are necessary to achieve the highest degree of enhancement of the Raman signal. The enormous enhancements provided by these substrates make possible the detection of single molecules.

## **1:15PM B24.00009 Single-step, high yield synthesis of gold nanoworms and their surface enhanced Raman scattering properties**

, WAQQAR AHMED, COMSATS Institute of Information Technology, JAN M. VAN RUITENBEEK, Kamerlingh Onnes Laboratory, Niels Bohrweg 2, Leiden University — Rod-shaped gold nanoparticles have attracted enormous attention owing to their interesting optical properties arising from the surface plasmon resonances. Slight deviation from the rod morphology can markedly change the optical properties. For example, worm-shaped gold nanoparticles can have more than two plasmon peaks. Furthermore, they show much higher local field enhancements as compared to their rod-shaped counterparts. We have devised a simple seedless, high-yield protocol for the synthesis of gold nanoworms (NWs). NWs were grown simply by reducing  $\text{HAuCl}_4$  with ascorbic acid in a high pH reaction medium, and in the presence of growth directional agents, cetyltrimethylammonium bromide and  $\text{AgNO}_3$ . In contrast to the seed-mediated growth of gold nanorods where a seed grows into a rod, NWs grow by oriental attachment of nanoparticles. By varying different reaction parameters we were able to control the length of NWs from a few nanometers to micrometers. Furthermore, the aspect ratio can also be tuned over a wide range. Gold NWs show excellent surface enhanced Raman scattering (SERS) properties. Ultra-low concentrations of various target molecules were detected using NWs based SERS substrates.

## **1:27PM B24.00010 A condensed matter field theory for quantum plasmonics**

, FOUAD BALLOUT, ORTWIN HESS, Imperial College London — In recent years plasmonics has advanced to ever decreasing length scales reaching dimensions comparable to the de Broglie wavelength of an electron, which has a manifest influence on the plasmon dispersion relation. The associated phenomenology lies beyond the reach of the classical drude free electron theory or its nonlocal extension and adequate models are needed to address the quantum matter aspects of light-matter interaction that are responsible for plasmonic quantum size effects. We present on the basis of the jellium model a quantum field theory of surface-plasmon polaritons in which they emerge as extended objects as a result of an inhomogeneous condensation of bosons around a topological singularity describing the surface. The benefit of this approach lies in relating the electromagnetic fields belonging to such a macroscopic quantum state with the surface topology and nonlocal response function (expressed in terms of the retarded photon self-energy) of the delimited electron gas sustaining that state.

## **1:39PM B24.00011 Combining magneto-optics with plasmonics in gold-nickel nanoparticle arrays**

, MIKKO KATAJA, SARA POURJAMAL, NanoSpin, Aalto University, NICOLÓ MACCAFERRI, PAOLO VAVASSORI, CIC NanoGUNE, TOMMI HAKALA, MIKKO HUTTUNEN, PÄIVI TÖRMÄ, COMP, Aalto University, SEBASTIAAN VAN DIJKEN, NanoSpin, Aalto University — Periodic arrays of metallic nanoantennas support intense surface lattice resonances (SLRs) with very narrow linewidths that arise from radiative coupling between the surface plasmon polaritons of the individual nanoparticles. Combining plasmonic systems with active components such as magneto-optical materials opens up new possibilities for active optical devices. Here, we present a new versatile method of integrating ferromagnetic and noble metal plasmonic nanostructures leading to strong magneto-optical responses in conjunction with drastically enhanced optical reflectivity. The structures under study consist of nickel and gold nanoparticles that are ordered into periodic checkerboard arrays. The gold constituent of these hybrid arrays guarantees intense optical reflectivity. Yet, compared to pure nickel arrays, the magneto-optical signal is practically retained. Local analyses of the radiation fields indicate that the nickel and gold nanoparticles both actively contribute to the magneto-optical activity of the hybrid lattice via radiative coupling. The results also demonstrate that the size of the noble metal nanoparticles can be used to tailor magneto-optical spectra, providing a new tool for designer magneto-optical materials.

## **1:51PM B24.00012 Surface lattice resonances and magneto-optical response in magnetic nanoparticle arrays**

, TOMMI HAKALA, MIKKO KATAJA, ALEKSI JULKU, MIKKO HUTTUNEN, SEBASTIAAN VAN DIJKEN, PÄIVI TORMA, Aalto University — We show that periodic rectangular arrays of magnetic nanoparticles display collective surface plasmon modes which are coupled by the radiation fields from each particle. The two directions of the lattice are coupled by the magnetic-field-controllable spin-orbit coupling in the nanoparticles. When breaking the symmetry of the lattice, we find that the optical response shows Fano-type surface lattice resonances whose frequency is determined by the periodicity orthogonal to the polarization of the incident field. In striking contrast, the magneto-optical Kerr response is controlled by the period in the parallel direction. The spectral separation of the response for longitudinal and orthogonal excitations provides versatile tuning of narrow and intense magneto-optical resonances.

**Monday, March 14, 2016 11:15AM - 2:03PM —**

**Session B25 DCMF: Superconducting Materials: Growth, Structure, and Properties** 324 - Joseph Prestigiacomo, Naval Research Laboratory

**11:15AM B25.00001 Superconductivity Study of  $\text{LaO}_{0.5}\text{F}_{0.5}\text{BiS}_2$  using Nuclear Magnetic Resonance**<sup>1</sup>, SHRISHTI YADAV, OSCAR BERNAL, California State University, Los Angeles, LEI SHU, JIAN ZHANG, Fudan University, Shanghai, DUYGU YAZICI, KEVIN HUANG, M. B. MAPLE, University of California, San Diego, La Jolla, CA, CALIFORNIA STATE UNIVERSITY TEAM, FUDAN UNIVERSITY TEAM —  $\text{LaO}_{0.5}\text{F}_{0.5}\text{BiS}_2$  is a member of the recently discovered class of  $\text{BiS}_2$ -layered superconductors. It has a superconducting temperature  $T_c$  close to 3 K when prepared under normal conditions. Pressure makes  $T_c$  as high as 10 K.  $T_c$  is also close to 10 K at ambient pressure for samples synthesized under pressure (2 GPa). We are conducting a  $^{19}\text{F}$ -NMR study in a polycrystalline powder of  $\text{LaO}_{0.5}\text{F}_{0.5}\text{BiS}_2$  ( $T_c \sim 3$  K). We report static and dynamic NMR parameters as functions of temperature, between 1.8 and 300 K. Our data show changes of sample behavior on cooling below both 10 and 3 K, and a modulation on the spin-echo-amplitude decay, which we discuss in some detail.

<sup>1</sup>NSF/DMR-1105380 (Cal State LA) and the NSF of China, grant 1147060 (Fudan U)

**11:27AM B25.00002 Ferrodistoritive lattice modes and polytypism in  $\text{LaO}_{1-x}\text{F}_x\text{BiS}_2$  superconductor**, ANUSHIKA ATHAUDA, DESPINA LOUCA, Univ of Virginia, CHRISTINA HOFFMAN, Oak Ridge National Laboratory, YANG REN, Argonne National Laboratory, XIANGDE ZHU, SAICHARAN ASWARTHAM, JASMINKA TERZIC, GANG CAO, Univ of Kentucky —  $\text{LaO}_{1-x}\text{F}_x\text{BiS}_2$  is a disordered, non-magnetic superconductor with a transition temperature of 10.8 K at  $x = 0.5$ . The crystal structure of  $\text{LaO}_{1-x}\text{F}_x\text{BiS}_2$  is investigated using synchrotron X-ray and neutron diffraction experiments. The Bragg pattern obtained in  $hk0$  plane could not be reproduced by either the long-presumed nominal symmetry  $P4/nmm$  or other theoretically suggested symmetries and indicated the possibility that the symmetry is lower than expected. The Bragg structure can be reproduced by a model involving coordinated ferrodistoritive in-plane displacements of sulfur. Several possibilities of sulfur displacement arrangements can reproduce the data equally well leading to the possibility of domains. When several domains are averaged together the fitting results improve. Therefore, the structure most likely consists of polytypes stacked along the  $c$ -axis. In the superconducting planes, the structure needs to be uniform, otherwise domain walls are created due to antiferrodistoritive arrangements, giving rise to additional peaks not present in the data.

**11:39AM B25.00003 Rattling induced superconductivity in  $\text{RV}_2\text{Al}_{20}$  (R = Sc, Lu, Y) aluminides — an experimental and theoretical study**<sup>1</sup>, MICHAL WINIARSKI, Gdansk University of Technology, BARTLOMIEJ WIENDLOCHA, AGH University of Science and Technology, MALGORZATA STERNIK, Institute of Nuclear Physics, Polish Academy of Sciences, PIOTR WISNIEWSKI, DARIUSZ KACZOROWSKI, Institute for Low Temperatures and Structure Research, Polish Academy of Sciences, TOMASZ KLIMCZUK, Gdansk University of Technology — Polycrystalline samples of four ternary intermetallics  $\text{RV}_2\text{Al}_{20}$  (R = Sc, Y, La, and Lu) were synthesized. Structural studies carried out using powder x-ray diffraction and Rietveld analysis show that all compounds crystallize in  $\text{CeCr}_2\text{Al}_{20}$ -type structure composed of icosahedral Al-R cages. Results of physical properties measurements reveal that  $\text{ScV}_2\text{Al}_{20}$ ,  $\text{YV}_2\text{Al}_{20}$ , and  $\text{LuV}_2\text{Al}_{20}$  are weakly-coupled BCS superconductors with critical temperatures  $T_c = 1.0, 0.57$ , and  $0.60$  K, respectively. Electronic and phonon structure calculations reveal the key role of low-frequency anharmonic vibrations of R atoms (rattling effect) for the appearance of superconductivity. A correlation between phonon and crystal structures was observed, allowing to search for new  $\text{RV}_2\text{Al}_{20}$  superconductors.

<sup>1</sup>Project was financially supported by the National Science Centre (Poland) grant (DEC-2012/07/E/ST3/00584).

**11:51AM B25.00004 Influence of ZnO and  $\text{Dy}_2\text{O}_3$  on  $\text{MgB}_2$  Bulks Fabricated by High Temperature and Pressure Reaction**, MIKE SUMPTION, YUAN YANG, MSE, The Ohio State University — ZnO and  $\text{Dy}_2\text{O}_3$  have been considered as dopants for the improvement of superconducting properties in  $\text{MgB}_2$  bulks. However, the effect of these dopants is still unclear: some studies reported these metal oxides worked as new pinning centers and others was attributed the effects to Mg site substitution. In addition, low temperature reactions may explore limited solubility regimes for these dopants. In order to study the intrinsic effect of ZnO and  $\text{Dy}_2\text{O}_3$  in  $\text{MgB}_2$ , a high temperature solid state sintering method has been used to fabricate dense and homogeneous  $\text{MgB}_2$  bulks. Even higher temperature excursions above the peritectic allow us to explore the solubility limits. To do this we used an induction furnace built inside of a high pressure vessel which allowed us to reach  $1700^\circ\text{C}$  and 1500 Psi. A slow cooling rate ( $2^\circ\text{C}/\text{min}$ ) was used in an attempt to obtain a homogeneous nucleation and phase distribution. A series of  $\text{MgB}_2$  bulk samples with ZnO and  $\text{Dy}_2\text{O}_3$  additives were synthesized through this high pressure and temperature procedures. The resulting microstructures of these bulk samples were revealed by SEM and TEM. Atomic substitution were evaluated by high resolution XRD. The upper critical field  $B_{c2}$ , irreversible field  $B_{irr}$ , and  $T_c$  were obtained from both magnetic and resistivity measurements. The roles of substitution vs precipitate induced strain on  $B_{c2}$  enhancements with adding ZnO and  $\text{Dy}_2\text{O}_3$  were discussed.

**12:03PM B25.00005  $\text{Mo}_5\text{PB}_2$ : a new superconductor in the  $\text{Cr}_5\text{B}_3$  structure type with  $T_c = 9.2$  K**<sup>1</sup>, MICHAEL MCGUIRE, DAVID PARKER, Oak Ridge National Laboratory — Superconductivity has been reported recently in several ternary silicide-borides adopting the tetragonal  $\text{Cr}_5\text{B}_3$  structure type, including  $\text{Nb}_5\text{Si}_{3-x}\text{B}_x$ ,  $\text{Mo}_5\text{SiB}_2$ , and  $\text{W}_5\text{SiB}_2$ , with critical temperatures ranging from 5.8-7.8 K. Here we report superconductivity with  $T_c$  exceeding 9 K in the phosphorus-containing analogue  $\text{Mo}_5\text{PB}_2$ . We have synthesized polycrystalline samples of the compound, made measurements of electrical resistivity, magnetic susceptibility, and heat capacity, and performed first principles electronic structure calculations. The highest  $T_c$  values occur in slightly phosphorus rich samples, with composition near  $\text{Mo}_5\text{P}_{1.1}\text{B}_{1.9}$ . Together with the measured properties, the calculations suggest the superconductivity in these materials may be multi-band.

<sup>1</sup>Research sponsored by the US Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

**12:15PM B25.00006 Superconductivity and ferromagnetism in Pd doped  $\text{Y}_9\text{Co}_7$** <sup>1</sup>, TOMASZ KLIMCZUK, JUDYTA STRYCHALSKA, Gdansk University of Technology, JOE THOMPSON, Los Alamos National Laboratory, ROBERT CAVA, Princeton University — The ferromagnetic superconductor  $\text{Y}_9\text{Co}_7$  was chemically doped with Pd in an attempt to form  $\text{Y}_9\text{Co}_{7-x}\text{Pd}_x$  for  $0 < x < 0.4$ . The lattice parameter  $a$  does not depend on  $x$ ; whereas,  $c$  increases with increasing Pd content up to  $x = 0.2$ , which turned out to be the palladium solubility limit. Superconductivity ( $T_{sc} = 2.4$  K) and ferromagnetism ( $T_C = 4.5$  K) were observed only for the parent  $\text{Y}_9\text{Co}_7$  compound. For the lowest tested Pd doping level ( $x=0.05$ ), strong enhancement of ferromagnetism is observed ( $T_C = 9.35$  K), but superconductivity is not seen above 1.8K. The Curie temperature rapidly increases from 4.5 K to about 10 K for a Pd concentration  $x=0.1$  and remains almost unchanged for  $\text{Y}_9\text{Co}_{6.8}\text{Pd}_{0.2}$ .

<sup>1</sup>Project was financially supported by the National Science Centre (Poland) grant (DEC-2012/07/E/ST3/00584).

**12:27PM B25.00007 Quench-condensing superconducting thin films using the Fab on a Chip approach<sup>1</sup>**, HAN HAN, Boston Univ, MATTHIAS IMBODEN, cole Polytechnique Fdrale de Lausanne, PABLO DEL CORRO, Bajas Temperaturas, Instituto Balseiro, THOMAS STARK, RICHARD LALLY, Boston Univ, FLAVIO PARDO, CRISTIAN BOLLE, SLIM Line, Bell Labs, Alcatel-Lucent, DAVID BISHOP, Boston Univ — Micro-electromechanical systems (MEMS) being manufactured in a macroscopic fab inspires the idea of getting the process further down to fabricate even smaller structures, namely nano-structures, using MEMS. The Fab on a Chip concept was proposed based on such ideas. By implementing the final-step, additive fabrication approach, manufacturing, characterization and experiments of nano-structures are integrated *in-situ*. Due to the miniature size of MEMS, the thickness precision is significantly improved while the power consumption is significantly depressed, making the quench-condensation of very thin films well controlled and easily achievable. Among various types of nano-structures, quench-condensed superconducting thin films are of great interest for physicists. Here we present such experiments done on superconducting thin films quench-condensed using the Fab on a Chip. We show that we are able to fabricate very thin films with its thickness precisely controlled, and the base temperature kept under ~3K during the process. The resistivity data demonstrates the high purity and uniformity of the film, as well as the annealing effect when cycling to higher temperatures. Based on the tremendous results obtained from the superconducting thin films, more complex nano-circuits can be fabricated and investigated using the Fab on a Chip, enabling a new approach for novel condensed matter physics experiments. This research is funded by the NSF through their CMMI division.

<sup>1</sup>This research is funded by the NSF through their CMMI division.

**12:39PM B25.00008 Application of metamaterial nanoengineering to triple the superconducting critical temperature of bulk aluminum<sup>1</sup>**, VERA SMOLYANINOVA, KATHRYN ZANDER, THOMAS GRESOCK, CHRISTOPHER JENSEN, WILLIAM ZIMMERMAN, Towson University, JOSEPH PRESTIGIACOMO, MICHAEL OSOFSKY, Naval Research Laboratory, ZHEN XING, MUMTAZ QAZILBASH, College of William and Mary, IGOR SMOLYANINOV, University of Maryland — Recent experiments have shown the viability of the metamaterial approach to dielectric response engineering for enhancing the transition temperature,  $T_c$ , of a superconductor [1]. In this report, we demonstrate the use of Al<sub>2</sub>O<sub>3</sub>-coated aluminium nanoparticles to form the recently proposed epsilon near zero (ENZ) core-shell metamaterial superconductor [2] with a  $T_c$  that is three times that of pure aluminium [3]. IR reflectivity measurements confirm the predicted metamaterial modification of the dielectric function thus demonstrating the efficacy of the ENZ metamaterial approach to  $T_c$  engineering. The developed approach advances potentials for efficient nanofabrication of bulk aluminium-based metamaterial superconductors. These results open up numerous new possibilities of considerable  $T_c$  increase in other simple superconductors. [1]. V. N. Smolyaninova et al., Scientific Reports 4, 7321 (2014) [2] I. I. Smolyaninov and V. N. Smolyaninova, Phys. Rev. B 91, 094501 (2015). [3] V. N. Smolyaninova et al., Scientific Reports 5, 15777 (2015)

<sup>1</sup>This work was supported in part by NSF grant DMR-1104676.

**12:51PM B25.00009 ABSTRACT WITHDRAWN —**

**1:03PM B25.00010 Interplay of superconductivity and magnetism in oxy-chalcogen cuprates YBaSrCu<sub>3</sub>O<sub>x</sub>Se<sub>y</sub><sup>1</sup>**, ARMEN GULIAN, VAHAN NIKOGHOSYAN<sup>2</sup>, Chapman University, VADIM GRINENKO, Leibniz-Institute IFW-Dresden, PF 270116, Dresden D-01171, Germany — In YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> superconductors we substituted one atom of Sr for Ba, and simultaneously doped the composition by Se. The resulting substance demonstrates two superconducting transitions: at 34K and 12K. Moreover, at 18K it reveals the Wohleben effect, jumping from a diamagnetic to paramagnetic response, while keeping the resistance zero. At about 4K, a ferromagnetic state sets up yielding a re-entrance effect, noticeable as an upturn in magnetic susceptibility and, in some samples, in resistivity. This substance behaves very differently from the reported YBaSrCu<sub>3</sub>O<sub>7</sub> or YBa<sub>2</sub>Cu<sub>3</sub>O<sub>x</sub>Se<sub>y</sub>: simultaneous presence of Se- and Sr-ions yields magnetic moments in the lattice. We present data on DC and AC magnetization, on heat capacity and resistivity in magnetic fields, on crystalline phases, as well as on composition. We also discuss possible mechanisms responsible for the observed effects.

<sup>1</sup>This work is supported in part by the ONR Grant N00014-15-12095

<sup>2</sup>Also: Physics Research Institute, National Academy of Sciences, Ashtarak, 0203, Armenia

**1:15PM B25.00011 Novel Superoxygenated Phases in Superconducting Cuprate Thin Films<sup>1</sup>**, C. ZHANG, H. ZHANG, University of Toronto, N. GAUQUELIN, G. A. BOTTON, Canadian Centre for Electron Microscopy & Brockhouse Institute for Materials Research, C. MCMAHON, D. G. HAWTHORN, University of Waterloo, J. Y. T. WEI, University of Toronto & Canadian Institute for Advanced Research — The superconducting critical temperature ( $T_c$ ) of hole-doped cuprates tends to increase with their lattice complexity, which is generally correlated with higher states of oxidation. For YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7- $\delta$</sub>  (YBCO-123), it is known that solid-state reaction in high-pressure oxygen can induce the formation of more complex and oxidized phases such as Y<sub>2</sub>Ba<sub>4</sub>Cu<sub>7</sub>O<sub>15- $\delta$</sub>  (YBCO-247) and Y<sub>2</sub>Ba<sub>4</sub>Cu<sub>8</sub>O<sub>16</sub> (YBCO-248). In this work, we apply this superoxygenation concept of material synthesis to nanoscale thin films which, owing to their large surface-to-volume ratio, are more thermodynamically reactive than bulk samples. Epitaxial thin films of YBCO-123 were grown by pulsed laser deposition on (La,Sr)(Al,Ta)O<sub>3</sub> substrates, and post-annealed in up to 500 atm of oxygen at 800C. Our post-annealed films show robust superconducting transitions with  $T_c$  ranging from 80 to 93K. Transmission electron microscopy and X-ray absorption spectroscopy were used to probe the lattice structure and oxygen stoichiometry. Our measurements show clear evidence of conversion to YBCO-247 and YBCO-248 in the superoxygenated films, as well as YBCO-125, a novel YBCO phase that has three CuO chains per unit cell and potentially higher  $T_c$ .

<sup>1</sup>Work supported by NSERC, CFI/OIT, and CIFAR.

**1:27PM B25.00012 Quasi-One Dimensional Analogues of BiS<sub>2</sub>-Based Superconductors<sup>1</sup>**, JESSICA PANELLA, JUAN CHAMORRO, TYREL MCQUEEN, Johns Hopkins Univ — Many recently-reported superconductors have layered structures consisting of superconducting planes separated by insulating charge reservoir layers. Studies linking the width of the blocking layer to the critical temperature of the superconductivity onset draw a direct connection from the superconducting properties to the structure. We report three new compounds (Sr<sub>2</sub>O<sub>2</sub>Bi<sub>2</sub>Se<sub>3</sub>, Ba<sub>2</sub>O<sub>2</sub>Bi<sub>2</sub>Se<sub>3</sub>, and Sr<sub>2</sub>O<sub>2</sub>Sb<sub>2</sub>Se<sub>3</sub>) which are quasi-one dimensional analogues of the bismuth sulfide and bismuth selenide superconductors, providing a unique opportunity to study the role of dimensionality on superconductivity. The physical properties of the compounds were studied via magnetic susceptibility, thermal transport, resistivity, and heat capacity.

<sup>1</sup>This work is supported by a Cottrell Research Scholar Fellowship.

## **1:39PM B25.00013 Vertical Magnetic Levitation Force Measurement on Single Crystal YBaCuO Bulk at Different Temperatures**

, SUKRU CELIK, Department of Energy Systems Engineering, Faculty of Engineering and Architecture, Sinop University, 57000, Sinop, TURKEY, SAIT BARIS GUNER, Department of Physics, Faculty of Arts and Sciences, Recep Tayyip Erdogan University, 53100 Rize, TURKEY, KEMAL OZTURK, Department of Physics, Faculty of Arts and Sciences, Karadeniz Technical University, 61100 Trabzon, TURKEY, OZGUR OZTURK, Department of Physics, Faculty of Arts and Sciences, Kastamonu University, 37100 Kastamonu, TURKEY — Magnetic levitation force measurements of HTS samples are performed with the use of liquid nitrogen. It is both convenient and cheap. However, the temperature of the sample cannot be changed (77 K) and there is problem of frost. So, it is necessary to build another type of system to measure the levitation force high  $T_c$  superconductor at different temperatures. In this study, we fabricated YBaCuO superconducting by top-seeding-melting-growth (TSMG) technique and measured vertical forces of them at FC (Field Cooling) and ZFC (Zero Field Cooling) regimes by using our new designed magnetic levitation force measurement system. It was used to investigate the three-dimensional levitation force and lateral force in the levitation system consisting of a cylindrical magnet and a permanent cylindrical superconductor at different temperatures (37, 47, 57, 67 and 77 K).

## **1:51PM B25.00014 Low Temperature Properties and Quantum Criticality of CrAs<sub>1-x</sub>P<sub>x</sub> single crystal.**

, JIANLIN LUO, Institute of Physics, Chinese Academy of Sciences, INSTITUTE OF PHYSICS, CHINESE ACADEMY OF SCIENCES TEAM — We report a systematically study of resistivity and specific heat on phosphorus doped CrAs<sub>1-x</sub>P<sub>x</sub> single crystals with  $x=0$  to 0.2. With the increasing of phosphorus doping concentration  $x$ , the magnetic and structural transition temperature  $T_N$  is suppressed. Non-fermi liquid behavior and quantum criticality phenomenon are observed from low temperature resistivity around critical doping with  $x_c \sim 0.05$  where the long-range antiferromagnetic ordering is completely suppressed. The low temperature specific heat of CrAs<sub>1-x</sub>P<sub>x</sub> is contributed by the thermal excitation of phonons and electrons. The electronic specific heat coefficient  $\gamma$ , which reflects the effective mass of quasi-particles, shows maximum around  $x_c \sim 0.05$ , also indicating the existence of quantum critical phenomenon around the critical doping. The value of Kadowaki-Woods ratio of CrAs<sub>1-x</sub>P<sub>x</sub> shows no significant different from that of CrAs. Work is done in collaboration with Fukun Lin, Wei Wu, Ping Zheng, Guozhi Fan, Jinguang Cheng.

## **Monday, March 14, 2016 11:15AM - 2:15PM –**

**Session B26 DMP: Graphene and Graphene/hexagonal Boron Nitride Superlattices** 325 - Jianhao Chen, ICQM, Peking University

## **11:15AM B26.00001 High-frequency current oscillations in graphene-boron nitride resonant tunnel diodes<sup>1</sup>**

, MARK GREENAWAY, JENN GASKELL, LAURENCE EAVES, University of Nottingham, KOSTYA NOVOSELOV, ARTEM MISHCHENKO, ANDRE GEIM, University of Manchester, MARK FROMHOLD, University of Nottingham — The successful realisation of multilayer graphene-hBN-graphene resonant tunnelling diodes (graphene-RTDs) with negative differential conductance (NDC) and MHz current oscillations offers the exciting possibility of exploiting them as high-frequency oscillators and mixers [1, 2]. In this paper, we examine their potential for generating higher frequencies by simulating the oscillations in the tunnel current and charge that arise when the device is biased in the NDC region and placed in a resonant circuit. Using the Bardeen transfer Hamiltonian method, we examine the effect on the device characteristics of the twist angle,  $\theta$ , between the two graphene electrodes, the hBN barrier thickness and of the carrier density in the graphene electrodes, which can be adjusted by chemical doping or by an applied bias voltage. The simulations accurately reproduce our recently-reported measurements on these RTDs (Fig. 4, [2]). The results of simulations show that frequencies of tens of GHz are achievable by optimising the device parameters [3]. References: [1] L. Britnell et al., Nature Communications 4, 1794 (2013). [2] A. Mishchenko et al., Nature Nanotechnology 9, 808 (2014). [3] J. Gaskell et al., Applied Physics Letters 107, 103105 (2015)

<sup>1</sup>Leverhulme Trust, UK

## **11:27AM B26.00002 Band structure engineering of graphene by a local gate defined periodic potential**

, CARLOS FORSYTHE, PATRICK MAHER, DIEGO SCARABELLI, CORY DEAN, Columbia University, PHILIP KIM, Harvard University — Recent improvements in 2-dimensional (2D) material layering have resulted in enhanced device quality and created pathways for new device architectures. We fabricate periodic arrays from a patterned local back gate and a uniform top gate on hBN encapsulated graphene channels. The symmetry and lattice size of the periodic potential can be determined by state-of-art electron beam lithography and etching, achieving a lattice constant of 35 nm. The strength of the electric potential modulation can be controlled through applied voltage on the patterned gate. We observe signatures of superlattice modulation near the main Dirac peak in the density dependent resistance measurement at zero magnetic field. Current studies focus on the exploration of Hofstadter fractal band structures under magnetic fields. Our nano-patterned engineered superlattices on graphene hold great promise for wider applications.

## **11:39AM B26.00003 Layer resolved capacitive probing of graphene bilayers**

, ALEXANDER ZIBROV, Department of Physics, UC Santa Barbara, Santa Barbara, CA 93106, USA, FRANOIS PARMENTIER, Service de Physique de l'Etat Condense, DSM/IRAMIS/SPEC, CNRS UMR 3680, CEA Saclay, 91191 Gif sur Yvette cedex, France, JIA LI, Department of Physics, Columbia University, New York, NY 10027, USA, LEI WANG, Department of Electrical Engineering, Columbia University, New York, NY 10027, USA, BENJAMIN HUNT, Physics Department, Carnegie Mellon University, Pittsburgh, PA 15213, CORY DEAN, Department of Physics, Columbia University, New York, NY 10027, USA, JAMES HONE, Department of Mechanical Engineering, Columbia University, New York, NY 10027, USA, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, 1-1 Namiki, Tsukuba, Japan, ANDREA YOUNG, Department of Physics, UC Santa Barbara, Santa Barbara, CA 93106, USA — Compared to single layer graphene, graphene bilayers have an additional which-layer degree of freedom that can be controlled by an external electric field in a dual-gated device geometry. We describe capacitance measurements capable of directly probing this degree of freedom. By performing top gate, bottom gate, and penetration field capacitance measurements, we directly extract layer polarization of both Bernal and twisted bilayers. We will present measurements of hBN encapsulated bilayers at both zero and high magnetic field, focusing on the physics of the highly degenerate zero-energy Landau level in the high magnetic field limit where spin, valley, and layer degeneracy are all lifted by electronic interactions.

## **11:51AM B26.00004 Topologically-driven valley polarization in twisted graphene/hexagonal boron nitride heterostructures**

, LEONARDO BASILE, Escuela Politécnica Nacional, JUAN CARLOS IDROBO, Oak Ridge National Laboratory — Valley polarization, that is, selective electronic localization in a momentum valley, has been proposed on materials presenting either a strong spin-orbit coupling (SOC) or with a weak SOC but in the presence of electric and magnetic fields. In this talk, we identify a non-centro symmetric system which can also present valley polarization purely by topological means without the necessity of SOC. We find that twisted bilayers of graphene/hexagonal boron nitride heterostructures have different absorption for right- and left- circular polarized light, indicating valley polarization. This induced polarization occurs due to band folding of the electronic bands, i.e., it has a topological origin.

**12:03PM B26.00005 Bandgap opening in bilayer graphene at metal contacts** , RYO NOUCHI, Osaka Prefecture University — A bandgap is opened in bilayer graphene (BLG) by introducing a potential difference between the two graphene layers, raising expectations for its application to a transistor channel. The potential difference can be introduced, for example by charge transfer from surface adsorbates. Thus, a finite bandgap is expected to be opened also at a metal contact, an inevitable component of transistors, where interfacial charge transfer occurs to align the Fermi levels of the metallic electrode and the underlying BLG. The bandgap at the metal-BLG interface can be detected by the superlinear current-voltage characteristics in back-gate field-effect transistors, caused by carriers propagating through the bandgap, i.e., by the band-to-band transport [1]. The superlinearity was higher in the positively-gated region, attributed to hole doping from the Cr/Au electrodes. The control experiments using single-layer graphene (SLG) did not have a superlinearity, which is consistent with the fact that a sizeable bandgap is not expected at the metal-SLG interface. The current transport through the bandgap should be an additional source of electrode-contact resistance. [1] R. Nouchi, Appl. Phys. Lett. 105, 223106 (2014).

**12:15PM B26.00006 Anomalous conductivity noise in gapped bilayer graphene heterostructure** , MOHAMMED ALI AAMIR, PARITOSH KARNATAK, T. PHANINDRA SAI, ARINDAM GHOSH, Department of Physics, Indian Institute of Science, Bangalore - 560012, India — Bilayer graphene has unique electronic properties it has a tunable band gap and also, valley symmetry and pseudospin degree of freedom like its single layer counterpart. In this work, we present a study of conductance fluctuations in dual gated bilayer graphene heterostructures by varying the Fermi energy and the band gap independently. At a fixed band gap, we find that the conductance fluctuations obtained by Fermi energy ensemble sampling increase rapidly as the Fermi energy is tuned to charge neutrality point (CNP) whereas the time-dependent conductance fluctuations diminish rapidly. This discrepancy is completely absent at higher number densities, where the transport is expected to be through the 2D bulk of the bilayer system. This observation indicates that near the CNP, electrical transport is highly sensitive to Fermi energy, but becomes progressively immune to time-varying disorder. A possible explanation may involve transport via edge states which becomes the dominant conduction mechanism when the bilayer graphene is gapped and Fermi energy is situated close to the CNP, thereby causing a dimensional crossover from 2D to 1D transport. Our experiment outlines a possible experimental protocol to probe intrinsic topological states in gapped bilayer graphene.

**12:27PM B26.00007 Tuning the Band Gap of Bilayer Graphene by Sandwich-Like Stacking<sup>1</sup>** , ZHENPENG HU, Nankai University — As far as we know, graphene has been taken as a potential host material for next-generation electric devices. However, this attractive prospect has been blocked by the metallic character of graphene. Although many methods have been proposed to get a moderate energy gap, such as hydrogenated graphene (graphane), but all the intrinsic advantages (carrier's mobility, etc...) of graphene have been destroyed. Here, we report that a large energy gap of graphene bilayer can be opened without breaking its natural characters by sandwiching it between functionalized BN substrates. Also, we show that the band gap of graphene bilayer can be tuned from 0.35 eV to 0.50 eV, depending on the substrates. The gap value is much larger than any other methods, and the structure of graphene bilayer is perfectly kept. And the energy gap is robust, namely, once the sandwiched substrates are selected, the relative position of substrates and graphene bilayer hardly changes the energy gap. Since the proposed way is easy to be realized in experiments, our results will hopefully accelerate the application of graphene in semiconductor devices and promote the development of the graphene technology.

<sup>1</sup>This work is supported by NSFC 21203099

**12:39PM B26.00008 Anomalous Coulomb drag in bilayer graphene double layers** , XIAOMENG LIU, Harvard University, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Material Science, PHILIP KIM, Harvard University — Bilayer graphene double-layer structure consists of two layers of bilayer graphene separated by atomically thin hexagonal boron nitride (hBN). With a perfect Fermi surface nesting and strong electron-electron interaction ( $E_{Coulomb} > E_{kinetic}$ ), such systems offer exciting platforms to study interaction driven phenomena, such as Coulomb drag and exciton condensation. We fabricate ultra-clean encapsulated bilayer graphene double layers with dry pick-up method. Room temperature drag measurement on our devices shows the sign of drag agree with the typical Fermi liquid behavior. However, at lower temperatures, the sign of drag reversed, indicating a new drag mechanism emerges and dominates. We measure this with different geometry, temperature, bias and gating to investigate the origin of such effect and discuss the implication of the drag sign changes.

**12:51PM B26.00009 Coulomb Drag Measurements in Bilayer-Bilayer Graphene Device** , JIA LI, CORY DEAN, Columbia University — We report Coulomb drag measurements on bilayer-bilayer graphene devices assembled using the Van De Waals transfer technique. The two bilayer graphene flakes are encapsulated and separated by hBN. High temperature measurements reveal positive drag response when the carrier types are different in two graphene layers, and negative when carrier types are the same, a result that is similar to previous measurements reported in monolayer graphene devices. However, upon cooling to low temperature, novel drag response is observed in the low density region. We also report a new device set-up which improves measurement quality for Coulomb drag measurements at low temperature.

**1:03PM B26.00010 Planar Tunneling Spectroscopy of Graphene Nanodevices** , JOEL I-JAN WANG, LANDRY BRETHERAU, Massachusetts Institute of Technology, USA, RICCARDO PISONI, Massachusetts Institute of Technology, USA/Politecnico di Milano, Italy, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science (NIMS), Japan, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology, USA — 2-D Van-der-Waals mesoscopic physics have seen a rapid development in the last 10 years, with new materials each year added to the toolbox. Stacking them like Lego enables the combination of their individual electronic properties. In particular, hexagonal boron nitride, which is an insulator, gives the possibility to perform planar (2-D to 2-D) tunneling spectroscopy within this type of heterostructures. Unlike standard transport measurements, tunneling spectroscopy enables to probe the electronic properties in the energy domain. Moreover, since planar tunneling probes a large area of the system, global quantum features such as quantum Hall effect, superconducting proximity effect or quantum confinement can be investigated. In this talk, we will present implementation of heterostructures consisting of graphene, hexagonal boron nitride, and graphite, fabricated for planar tunneling spectroscopy. In order to reveal the intrinsic properties of materials, the fabrication scheme aims at preserving the pristine nature of the 2-DEGS as well as minimizing the doping introduced by external probes. As a demonstration, measurements of these devices in normal states, high magnetic field environment, and induced superconducting state will be presented.

**1:15PM B26.00011 Observation of Large Intrinsic Gap in Rhombohedral-Stacked Tetralayer Graphene** , KEVIN MYHRO, SHI CHE, YANMENG SHI, YONGJIN LEE, KEVIN THILAHAR, University of California, Riverside, DMITRY SMIRNOV, National High Magnetic Field Laboratory, Tallahassee, FL, CHUN NING LAU, University of California, Riverside — Few-layer graphene has attracted attention in the scientific community as a novel 2D material due to its observed quantum hall effect, high electronic mobility, high transparency and tensile strength, among other properties. In rhombohedral-stacked few-layer graphene, the very flat band near the charge neutrality point is unstable to electronic interactions, and gives rise to states with spontaneous broken symmetries. Intrinsic gaps of ~2 meV and 40 meV are observed in bilayer and trilayer graphene, respectively. Here, we report the observation of an even larger gap in suspended rhombohedral-stacked tetralayer graphene (r-4LG) samples. We will present the latest data of the evolution of the gapped state with temperature and external fields, and compare with theoretical models.

**1:27PM B26.00012 Observation of Hysteresis in Rhombohedral-Stacked Trilayer Graphene**, SHI CHE, YONGJIN LEE, YANMENG SHI, KEVIN MYHRO, TIMOTHY ESPIRITU, DAVID TRAN, JAIRO VELASCO, YAFIS BARLAS, CHUN NING (JEANIE) LAU, University of California, Riverside — Few-layer graphene is an attractive platform for exploration of physical processes confined to two dimensions. Diverging density of states in rhombohedral-stacked trilayer graphene (r-TLG) leads to strong electronic correlation. Recently an intrinsic insulating phase with 40 meV gap has been observed at charge neutrality point (CNP) in r-TLG, which is consistent with an layer antiferromagnetic state. By using dual-gated suspended r-TLG device, we observe hysteresis loops in conductance in the vicinity of CNP, which suggests the possible evidence of spontaneous spin polarization or presence of domains with different anomalous Hall conductivities.

**1:39PM B26.00013 Experimental realization of gate controlled topological conducting channels in bilayer graphene**, J. LI, K. J. MCFAY, Z. ZERN, J. ZHU, Department of Physics, Penn State University, University Park, USA, K. WANG, Y. F. REN, Z. H. QIAO, ICQD, USTC, Hefei, China, K. WATANABE, T. TANIGUCHI, National Institute for Material Science, 1-1 Namiki, Tsukuba, Japan — Manipulating the valley degree of freedom in two-dimensional honeycomb lattices can potentially lead to a new type of electronics called valleytronics. In electrically gapped bilayer graphene, the broken inversion symmetry leads to non-zero and asymmetric Berry curvature  $\Omega$  in the K and K' valleys of the Brillouin zone. Reversing the sign of  $\Omega$  at the internal line junction of two oppositely gated bilayer graphene is predicted to yield counter-propagating edge modes, the so-called kink states, with quantized conductance of  $4e^2/h$  in the absence of valley mixing. We have overcome fabrication challenges to implement high-quality hBN encapsulated, dual-split-gates structures necessary to observe the kink states. Here I present experimental evidences of the kink states. In the absence of a magnetic field, the kink states have a mean free path of a few hundred nm. Ballistic conductance of  $4e^2/h$  is achieved in a perpendicular magnetic field. We discuss the potential valley-mixing mechanisms and the role of the magnetic field. Experimental results are supported by numerical studies. We will also discuss ongoing efforts in realizing valley-controlled transmission and guiding of the kink states, which is a significant step towards the development of valleytronics.

**1:51PM B26.00014 Topological valley transport at bilayer graphene domain walls**, LONG JU, ZHIWEN SHI, NITYAN NAIR, YINCHUAN LV, CHENHAO JIN, JAIRO VELASCO JR., CLAUDIA OJEDA-ARISTIZABAL, Univ of California - Berkeley, HANS BECHTEL, MICHAEL MARTIN, Lawrence Berkeley National Lab, ALEX ZETTL, JAMES ANALYTIS, Univ of California - Berkeley, PAUL MCEUEN, Cornell University, FENG WANG, Univ of California - Berkeley — Electron valley, a degree of freedom that is analogous to spin, can lead to novel topological phases in bilayer graphene. An external electric field can induce a tunable bandgap in bilayer graphene, and domain walls between AB- and BA-stacked bilayer graphene can support protected chiral edge states of quantum valley Hall insulators. In this talk, I will present our efforts on revealing the topologically protected edge states at AB-BA domain walls by combining near field infrared nanoscopy with electrical transport measurement. These one-dimensional valley-polarized conducting channels feature a ballistic length of about 400 nanometres at 4 kelvin.

**2:03PM B26.00015 Electronic excitation spectrum of ABC-stacked multilayer graphene**, Y. HENNI, K. NOGAJEWSKI, Laboratoire National des Champs Magnétiques Intenses, CNRS, H. P. OJEDA COLLADO, G. USAJ, C. A. BALSEIRO, Centro Atómico Bariloche and Instituto Balseiro, Comisión Nacional de Energía Atómica, M. POTESKI, C. FAUGERAS, Laboratoire National des Champs Magnétiques Intenses, CNRS — The electronic properties of ABC graphene trilayers has attracted lot of attention recently due to their potential applications in engineering carbon-based devices with gate tunable electrical conductivity. Moreover, ABC-stacked thin layers of graphite are predicted to host peculiar surface electronic states, with a flat dispersion over most of the Brillouin zone. The associated high density of states is likely to favour the emergence of exotic electronic phases, such as charge density waves or even superconductivity. We present a micro-magneto-Raman scattering study of a thin graphite flake produced by exfoliation of natural graphite, composed of  $\sim 15$  graphene layers, and including a large ABC-stacked domain. Exploring the low temperature Raman scattering spectrum of this domain up to  $B=29T$ , we identify inter Landau level electronic excitations within the surface flat bands, together with electronic excitations involving the gapped states in the bulk. This interband electronic excitation at  $B=0T$  can be observed, up to room temperature, directly in the Raman scattering spectrum as a broad ( $\sim 180\text{cm}^{-1}$ ) feature. Because the energy gap strongly depends on the number of layers, this electronic excitation can be used to identify and characterize ABC-stacked graphite thin layers.

**Monday, March 14, 2016 11:15AM - 2:15PM –**

**Session B27 DCMP: Strongly Correlated Physics in d-electron Systems** 326 - Christianne Beekman, Florida State University

**11:15AM B27.00001  $\mu$ SR study of the stoichiometric  $\text{NbFe}_2$** , DANIEL MARGINEDA, SEAN GIBLIN, School of Physics and Astronomy Cardiff University, UK, ROSS STEWART, ISIS Facility, Rutherford Appleton Laboratory, UK, JON DUFFY, Department of Physics, University of Warwick, UK, STEPHEN DUGDALE, HH Wills Physics Laboratory, Department of Physics, Bristol, UK, JON TAYLOR, European Spallation Source ERIC, Lund, Sweden — Quantum critical points (QCP) are important as understanding how fluctuating ground states can be lifted by novel correlated electron states such as unconventional superconductivity is not clear.  $\text{Nb}_{1-y}\text{Fe}_{2+y}$  is a good candidate to investigate such criticality as it displays a rich magnetic phase diagram and quantum criticality in a d-band metal. We investigate the magnetic ground state of stoichiometric  $\text{NbFe}_2$  by bulk magnetisation and muon spin relaxation. Local magnetism clearly emerges below the critical temperature  $T_N = 10.3K$  and is dominated by quasi-static moments with an even distribution of magnetic fields  $\Delta_{eff}$  ranging from 0 to  $\sim 140G$ . A small moment of  $M \sim 0.02\mu_B/Fe$  is estimated, which is small because of the delocalised electronic distribution. In this work a stronger Curie-Weiss enhancement and an increased critical field suggests sample sensitivity to site mixing effects during the sample growth. Similar results are explained by a Spin Density Wave (SDW) with a large correlation length but the absence of oscillations cannot confirm this scenario: magnetic phase controlled by short-range interactions driven by Nb/Fe site mixing or an incommensurate helical SDW phase could both explain the field random orientation.

<sup>1</sup>Supported by EPSRC of UK

**11:27AM B27.00002 The Possibility of a Structural Quantum Critical Point in  $\text{LaCu}_{6-x}\text{Au}_x$** , L. POUDEL, Univ of Tennessee, Knoxville and Oak Ridge National Laboratory, A. F. MAY, Oak Ridge National Laboratory, M. KOEHLER, Univ of Tennessee, Knoxville, C. DE LA CRUZ, M. A. MCGUIRE, S. CALDER, Oak Ridge National Laboratory, V. KEPPENS, Univ of Tennessee, Knoxville, D. MANDRUS, A. D. CHRISTIANSON, Univ of Tennessee, Knoxville and Oak Ridge National Laboratory — Understanding the critical phenomena near a quantum critical point (QCP) has attracted a substantial interest from the condensed matter physics community. Despite this interest, QCPs involving the zero temperature termination of a continuous structural phase transition remain largely unexplored. Here, we study the structural properties of the  $\text{LaCu}_{6-x}\text{Au}_x$  series, which appears to be an ideal candidate to exhibit a SQCP. The orthorhombic-monoclinic transition temperatures in  $\text{LaCu}_{6-x}\text{Au}_x$  decrease with Au-composition until a complete suppression of the monoclinic phase occurs at the SQCP,  $x = 0.3$ . The lattice component of the low-temperature heat capacity exhibits a maximum at the critical concentration, providing a further indication of the presence of a SQCP in the  $\text{LaCu}_{6-x}\text{Au}_x$  series.

**11:39AM B27.00003 Evolution of Quantum Critical Behavior In A Concentrated Ternary Solid Solution: NiCoCr<sub>x</sub>**, BRIAN SALES, KE JIN, HONGBIN BEI, MALCOLM STOCKS, GERMAN SAMOLYUK, ANDREW MAY, MICHAEL MCGUIRE, Oak Ridge National Laboratory — The face centered cubic (fcc) alloy NiCoCr<sub>x</sub> with x near 1 is found to be close to the Cr concentration where the ferromagnetic transition temperature, T<sub>c</sub> goes to 0. Near this composition these alloys exhibit a resistivity linear in temperature to 2 K, a perfectly linear magnetoresistance, and an excess -TlnT contribution to the low temperature heat capacity. As the Cr concentration is decreased from 1, the Curie temperature and the saturation magnetization, M<sub>0</sub>, both increase exponentially with x. For x = 0.5, T<sub>c</sub> ≈ 217 K, but M<sub>0</sub> is only 0.26 Bohr magnetons/atom, indicating highly itinerant ferromagnets for 0.5 < x < 0.8. All of the low temperature electrical, magnetic and thermodynamic properties of the alloys with compositions near x=1 are not typical of a Fermi liquid and suggest strong magnetic fluctuations associated with a quantum critical region. This new class of concentrated solid solution fcc alloys are ideal model systems to study the effects of chemical disorder on emergent properties near a quantum critical point. Research supported by the DOE Office of Science, Materials Science and Engineering Division, and the Energy Dissipation to Defect Evolution EFRC.

**11:51AM B27.00004 Finite mass enhancement across bandwidth controlled Mott transition in NiS<sub>2-x</sub>Se<sub>x</sub><sup>1</sup>**, GARAM HAN, Center for Correlated Electron Systems, Institute for Basic Science (IBS), Seoul 151-742, Korea, W. S. KYUNG, Institute of Physics and Applied Physics, Yonsei University, Seoul 120-749, Korea, Y. K. KIM, Center for Correlated Electron Systems, Institute for Basic Science (IBS), Seoul 151-742, Korea, C. M. CHENG, K. D. TSUEI, National Synchrotron Radiation Research Center, Hsinchu 30076, Taiwan, K. D. LEE, N. HUR, Department of Physics, Inha University, Incheon 402-751, Korea, H.-D. KIM, C. KIM, Center for Correlated Electron Systems, Institute for Basic Science (IBS), Seoul 151-742, Korea — One of the most important and still debated issues in the strongly correlated electron systems is on the metal insulator transition (MIT) mechanism. In the bandwidth controlled Mott transition (BCMT) scenario, which Mott originally proposed, MIT occurs through a mass divergence in which the effective mass of the quasi-particle (QP) diverges approaching the MIT. The interpretation is supported by dynamic mean field theory (DMFT) model calculations. However, few direct observations have been made yet due to various experimental restrictions. In this talk, I present systematic angle resolved photoemission studies on the MIT in NiS<sub>2-x</sub>Se<sub>x</sub>, which is a well-known BCMT material. We observed not only the bandwidth shrinkage but also the coherent quasi-particle peak (QP) which is not of the surface origin. In addition, we experimentally showed the mass of the QP remains finite approaching the MIT.

<sup>1</sup>This work was supported by IBS-R009-D1

**12:03PM B27.00005 Revealing the electronic ground state of ReNiO<sub>3</sub> combining Ni-L<sub>3</sub> x-ray absorption and resonant inelastic x-ray scattering**, VALENTINA BISOGNI, Brookhaven National Laboratory, New York, SARA CATALANO, University of Geneva, Switzerland, ROBERT GREEN, University of British Columbia, Canada, MARTA GIBERT, RAOUL SCHERWITZL, University of Geneva, Switzerland, YAOBO HUANG, Paul Scherrer Institute, Switzerland, SHADI BALANDESH, University of British Columbia, Canada, VLADIMIR N. STROCOV, Paul Scherrer Institute, Switzerland, PAVLO ZUBKO, University of Geneva, Switzerland, GEORGE SAWATZKY, University of British Columbia, Canada, JEAN-MARC TRISONE, University of Geneva, Switzerland, THORSTEN SCHMITT, Paul Scherrer Institute, Switzerland — Rare-earth nickelates ReNiO<sub>3</sub> attract a lot of interest thanks to their intriguing physical properties like sharp metal to insulator transition, unusual magnetic order and expected superconductivity in nickelate-based heterostructures. Full understanding of these materials, however, is hampered by the difficulties in describing their electronic ground state (GS). Taking a NdNiO<sub>3</sub> thin film as a representative example, we reveal with x-ray absorption and resonant inelastic x-ray scattering unusual coexistence of bound and continuum excitations, providing strong evidence for abundant O 2p holes in the GS of these materials. Using an Anderson impurity model interpretation, we show that these distinct spectral signatures arise from a Ni 3d<sup>8</sup> configuration along with holes in the O 2p valence band, confirming suggestions that these materials exhibit a negative charge-transfer energy, with O 2p states extending across the Fermi level.

**12:15PM B27.00006 Polyanion Driven Antiferromagnetic and Insulating Ground State of Olivine Phosphates: LiMPO<sub>4</sub><sup>1</sup>**, AJIT KUMAR JENA, B. R. K. NANDA, Indian Inst of Tech-Madras, CONDENSED MATTER THEORY & COMPUTATION TEAM — Through density functional calculations we have investigated the electronic and magnetic properties of LiMPO<sub>4</sub>, where M is a 3d transition metal element. We find that contrary to many transition metal oxides, in these Olivine phosphates the band gap is originated due to crystal field anisotropy as well as weak O-p – M-d covalent interaction. Both of them are attributed to the presence of PO<sub>4</sub><sup>3-</sup> polyanion. The anisotropic crystal field, in the absence of covalent interactions, creates atomically localized non-degenerate M-d states and therefore the gap is a natural outcome. Onsite repulsion, due to strong correlation effect, further enhances the gap. These localized d states favor high-spin configuration which leads to antiferromagnetic ordering due to Hund's coupling. Experimentally observed low Neel temperature of this family of compounds is explained from the DFT obtained spin exchange interaction parameters.

<sup>1</sup>Work supported by Nissan Research Program.

**12:27PM B27.00007 *Ab initio* quantum Monte Carlo calculations of ground-state properties of manganese's oxides<sup>1</sup>**, VINIT SHARMA, JARON T. KROGEL, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, P.R.C. KENT, Center for Nanophase Materials Sciences and Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, FERNANDO A. REBOREDO, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA — One of the critical scientific challenges of contemporary research is to obtain an accurate theoretical description of the electronic properties of strongly correlated systems such as transition metal oxides and rare-earth compounds, since state-of-art ab-initio methods based on approximate density functionals are not always sufficiently accurate. Quantum Monte Carlo (QMC) methods, which use statistical sampling to evaluate many-body wave functions, have the potential to answer this challenge. Owing to the few fundamental approximations made and the direct treatment of electron correlation, QMC methods are among the most accurate electronic structure methods available to date. We assess the accuracy of the diffusion Monte Carlo method in the case of rocksalt manganese oxide (MnO). We study the electronic properties of this strongly-correlated oxide, which has been identified as a suitable candidate for many applications ranging from catalysts to electronic devices. "This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division."

<sup>1</sup>Ab initio quantum Monte Carlo calculations of ground-state properties of manganese oxides

**12:39PM B27.00008 Angle resolved photoemission spectroscopy and X-ray diffraction study on IrTe<sub>1.6</sub>Se<sub>0.4</sub>**, D.-H. KIM, K.-T. KO, KYOO KIM, J.-H. PARK, Pohang Univ of Sci & Tech, B.-G. PARK, T.-Y. KOO, Pohang Accelerator Laboratory, J.-J. YANG, S.-W. CHEONG, Dept. Physics and Astronomy, Rutgers University, USA — IrTe<sub>2</sub> shows an interesting phase transition accompanying q = (1/5, 0, 1/5) lattice distortion, Ir valence fluctuation, and J<sub>eff</sub> = 1/2 dimer formation. In order to study the role of anion doping, we investigated IrTe<sub>1.6</sub>Se<sub>0.4</sub> which is known to exhibit q = (1/6, 0, 1/6) lattice distortion and higher transition temperature, about 370 K. The electronic structure of IrTe<sub>1.6</sub>Se<sub>0.4</sub> single crystal was investigated by using angle resolved photoemission spectroscopy before and after the dimerization transition, which displays abrupt changes. Ir valence, investigated by corelevel X-ray photoemission, varies continuously from a pure Ir<sup>3+</sup> state to Ir<sup>4+</sup>:Ir<sup>3+</sup> ≈ 1 : 1 state, while x-ray diffraction measurement reveals a first order structure transition. In this talk, we will discuss an implication of our observations.

**12:51PM B27.00009 Consequences of breaking time reversal symmetry in LaSb: a resistivity plateau and extreme magnetoresistance**, FAZEL TAFTI, QUINN GIBSON, SATYA KUSHWAHA, NEEL HALDOLAARACHCHIGE, ROBERT CAVA, Princeton University, CAVA LAB TEAM — Time reversal symmetry protects the metallic surface modes of topological insulators (TIs). The transport signature of robust metallic surface modes of TIs is a plateau that arrests the exponential divergence of the insulating bulk with decreasing temperature. This universal behavior is observed in all TI candidates ranging from  $\text{Bi}_2\text{Te}_2\text{Se}$  to  $\text{SmB}_6$ . Recently, several topological semimetals (TSMs) have been found that exhibit extreme magnetoresistance (XMR) and TI universal resistivity behavior revealed only when breaking TRS, a regime where TIs theoretically cease to exist. Amongst these new materials, TaAs and NbP are nominated for Weyl semimetal due to their lack of inversion symmetry,  $\text{Cd}_3\text{As}_2$  is nominated for Dirac semimetal due to linear band crossing, and  $\text{WTe}_2$  is nominated for resonant compensated semimetal due to perfect electron-hole symmetry. Here we introduce LaSb, a simple rock-salt structure material without broken inversion symmetry, without perfect linear band crossing, and without perfect electron-hole symmetry. Yet LaSb portrays all the exotic field induced behaviors of the aforementioned semimetals. It shows the universal TI resistivity with a plateau at 15 K, revealed by a magnetic field, ultrahigh mobility of carriers, quantum oscillations with 2D Fermi surface, and XMR of about one million percent. Due to its dramatic simplicity, LaSb is the ideal model system to formulate a theoretical understanding of the exotic consequences of breaking TRS in TSMs.

**1:03PM B27.00010 Low-energy Electrodynamics of non-Drude Transport in the Strongly Correlated Ferromagnetic Metal  $\text{SrRuO}_3$** , YOUNG WANG, G. BOSSE, Y. LUBASHEVSKY, J. P. SHECKELTON, The Institute for Quantum Matter, Johns Hopkins Univ., D. E. SHAI, Laboratory of Atomic and Solid State Physics, Dept. of Physics, Cornell Univ., C. ADAMO, Dept. of Materials Science and Engineering, Cornell Univ., D.G. SCHLÖM, Dept. of Materials Science and Engineering, Kavli Institute at Cornell for Nanoscale Science, Cornell Univ., K. M. SHEN, Laboratory of Atomic and Solid State Physics, Dept. of Physics, Kavli Institute at Cornell for Nanoscale Science, Cornell Univ., N. P. ARMITAGE, The Institute for Quantum Matter, Johns Hopkins Univ. — While the highly correlated complex oxide perovskite ferromagnet  $\text{SrRuO}_3$  has been studied for decades, interest remains in its unusual transport properties. Here we report time-domain THz conductivity measurements taken from room temperature down to 1.5 K on a low disorder film of  $\text{SrRuO}_3$ . Previous optical measurements have shown a deviation from Drude-like transport in this material. We investigate these deviations using an extended Drude model analysis and find evidence for an effective non-Fermi liquid-like behavior in the frequency dependence of the scattering rate. The high quality of our film, reflected in its large residual resistivity ratio, allows us to better isolate the inelastic scattering channels. We have also extended these experiments down to the microwave regime and in this context investigate possible origins of this non-Drude transport, including the possibility of very low frequency interband transitions that are caused by small octahedral rotations and tilting that are inherent in the class of materials.

**1:15PM B27.00011 Surface Broken Symmetry on Orthorhombic Double-layer  $\text{Sr}_3(\text{Ru}_{1-x}\text{Mn}_x)_2\text{O}_{7-1}$** , CHEN CHEN, Louisiana State University, V. B. NASCIMENTO, Departamento de Física, ICEX-UFMG, ZHENYU DIAO, JIANDI ZHANG, RONGYING JIN, E. W. PLUMMER, Louisiana State University — The surface of double-layered ruthenate  $\text{Sr}_3\text{Ru}_2\text{O}_7$  exhibits octahedra tilt distortion and an enhanced rotational distortion caused by the broken symmetry. Previous LEED IV calculation reveals that the tilt angle is  $(2.51.7)^\circ$  at 80 K (B. Hu *et al.*, Physical Review B 81, 184104 (2010)). A glide symmetry and a mirror symmetry along this direction are both broken. Results from LEED IV simulations show that both broken symmetries originate from the emergence of surface tilt. The degree of broken symmetry is more sensitive to the tilt angle, thus producing a smaller error than from conventional LEED IV calculation. When Mn doping is induced into the compound, the tilt is removed and the symmetry of the LEED pattern returns to what is expected for rotation, two glide planes and four-fold symmetry.

<sup>1</sup>Supported by NSF DMR-1002622

**1:27PM B27.00012 Band dependent magneto thermoelectric measurements on  $\text{Ca}_3\text{Ru}_2\text{O}_7$** , HUI XING, Shanghai Jiao Tong University, CHENYI SHEN, Zhejiang University, LIBIN WEN, JIAMING HE, SHUN WANG, Shanghai Jiao Tong University, JIN PENG, JIANJIAN GE, Tulane University, YOUNG ZOU, MINGLIANG TIAN, High Magnetic Field Laboratory, Chinese Academy of Sciences, ZHUAN XU, Zhejiang University, ZHIQIANG MAO, Tulane University, YING LIU, Pennsylvania State University, Shanghai Jiao Tong University —  $\text{Ca}_3\text{Ru}_2\text{O}_7$  features a Neel transition at 56 K followed by a structure and metal-insulator transition at 48 K as the temperature is lowered, suggesting a complex structure-property relationship driven by electron correlated effects. However, the electronic states of  $\text{Ca}_3\text{Ru}_2\text{O}_7$  are not understood. ARPES measurements revealed the presence of an electron Fermi arc, while the expected hole Fermi arc is missing. Quantum oscillations showed the existence of a small Fermi surface, but the details of the Fermi surface, including whether the hole Fermi arc is present, are not determined. We performed band-dependent thermoelectric measurement with the temperature gradient directed to a specific crystalline axis. Magneto thermopower along crystalline a and b axes,  $S_a$  and  $S_b$ , both of which are negative in sign and nearly identical at high temperatures, were found to behave markedly differently below the metal-insulator transition, with  $S_b$  changing its sign from being negative to positive. Our analysis suggests that  $S_a$  and  $S_b$  in  $\text{Ca}_3\text{Ru}_2\text{O}_7$  are dominated by the electron and hole Fermi arcs, respectively. The implications of our data on the physics of  $\text{Ca}_3\text{Ru}_2\text{O}_7$  will be discussed.

**1:39PM B27.00013 Quasi-continuum excitation in Co-doped  $\text{CaRuO}_3$** <sup>1</sup>, JAGATH GUNASEKERA, ASHUTOSH DAHAL, Univ of Missouri - Columbia, JOSE RODRIGUEZ, LELAND HARRIGER, NIST Center for Neutron Research, TOM HEITMANN, Missouri University Research Reactor, DEEPAK SINGH, Univ of Missouri - Columbia — Spin-1/2 systems provide a unique platform to study the interplay between magnetism and quantum mechanics that often depict novel properties, such as quantum spin liquid or singlet-to-triplet transition. In this presentation, we report an interesting observation of singlet-to-triplet transition in Co-doped  $\text{CaRuO}_3$ , even though none of the magnetic atoms (Co or Ru) exhibit spin-1/2 properties. What we have found that as Co atom gradually replaces Ru in  $\text{CaRuO}_3$ , the system tends to develop a localized excitation around  $Q=1 \text{ \AA}^{-1}$  at 5.9 meV at low temperature. At roughly 20% doping percentage of Co, the inelastic excitation is well described by singlet-to-triplet transition of  $S=1/2$ . As the measurement temperature increases, the localized excitation fades into a sort of Q-independent background that becomes stronger as a function of temperature. This behavior is also well manifested by ac susceptibility measurements where the dynamic susceptibility tends to get stronger as the temperature increases. Our analysis suggests that Co-doping in  $\text{CaRuO}_3$  locally creates  $3d^7$  electronic configuration, which can be described by  $S=1/2$  in this disordered system.

<sup>1</sup>U.S. Department of Energy, Office of Basic Energy Sciences under Grant No. DE-SC0014461

**1:51PM B27.00014 Electronic correlation effects in  $\text{SrRuO}_3$  ultra-thin films**, LIANG SI, Institute of Solid State Physics, Vienna University of Technology, ZHICHENG ZHONG, Max Planck Institute for Solid State Research, OLEG JANSON, GANG LI, JAN TOMCZAK, KARSTEN HELD, Institute of Solid State Physics, Vienna University of Technology, COMPUTATIONAL MATERIALS SCIENCE TEAM, ELECTRONIC STRUCTURE OF CORRELATED MATERIALS TEAM —  $\text{SrRuO}_3$  (SRO) is a ferromagnetic metal with an appreciably high Curie-temperature of 160 K and a ferromagnetic moment of 0.8-1.6  $\mu_B/\text{Ru}$ . Recent experimental studies on SRO thin films show that both electronic and magnetic ground states drastically depend on the nature of the surface. Ultra-thin (001)-oriented films are insulating and lack ferromagnetism, while in (111)-oriented films ferromagnetic moments and  $T_c$  are enhanced compared with bulk. Here we investigate SRO films by density functional theory (DFT)+U and DFT+dynamical mean-field theory (DMFT). In agreement with the experiments, we find that metallic ferromagnetism in SRO (001)-oriented films vanishes below a certain critical layer thickness. We propose a new route for tuning the properties of these thin films and show that room temperature ferromagnetism can be attained by electron doping. For the SRO (111)-oriented thin films, we find that the enhanced  $T_c$  is facilitated by electronic correlation effects and the geometric confinement. The experimentally observed enhancement of ferromagnetic moments in SRO(111)-oriented thin films is addressed by considering the stability of the high-spin Ru state in the presence of oxygen vacancies. Finally, the topological properties of SRO (111)-oriented bilayers will be discussed.

**2:03PM B27.00015 Ambipolar transport in the field-suppressed superconducting state of quasi-one-dimensional  $\text{Li}_{0.9}\text{Mo}_6\text{O}_{17}$** <sup>1</sup>, JOSHUA L. COHN, University of Miami, CARLOS A. M. DOS SANTOS, Escola de Engenharia de Lorena - USP, Brazil, JOHN J. NEUMEIER, Montana State University — We present resistivity, Hall, Seebeck, and Nernst coefficient measurements in the range  $0.4\text{ K} \leq T \leq 20\text{ K}$  on single crystals of the quasi-one-dimensional (Q1D) metal,  $\text{Li}_{0.9}\text{Mo}_6\text{O}_{17}$  with current along the Q1D metallic chains. At temperatures below the nominal superconducting transition temperature ( $T_c = 2\text{ K}$ ), a transition from hole-like ( $\mu_0 H < 1\text{ T}$ ) to electron-like ( $\mu_0 H \geq 2\text{ T}$ ) behavior is evidenced in the magnetotransport coefficients. Possible insights from these results into the nature of the mysterious density-wave order<sup>a,b</sup> responsible for the upturn in resistivity below  $\sim 25\text{ K}$  will be discussed.

<sup>a</sup> C. A. M. dos Santos *et al.*, Phys. Rev. Lett. **98**, 266405 (2007).

<sup>b</sup> X. Xu *et al.*, Phys. Rev. Lett. **102**, 206602 (2009).

<sup>1</sup>Work supported by the U.S. Department of Energy, Office of Basic Energy Sciences (DE-FG02-12ER46888, Univ. Miami), the National Science Foundation (DMR-0907036, Mont. St. Univ.), and in Lorena by the CNPq (308162/2013-7) and FAPESP (2009/54001-2).

## Monday, March 14, 2016 11:15AM - 2:03PM —

Session B28 DMP: Topological Kondo Insulators 327 - Natalia Drichko, The Johns Hopkins University

**11:15AM B28.00001 Surface conductance and one-dimensional edge state transport in topological Kondo insulator  $\text{SmB}_6$** <sup>1</sup>, JOHNPIERRE PAGLIONE, University of Maryland — The Kondo insulator compound  $\text{SmB}_6$ , with hybridization between itinerant conduction electrons and localized *f*-electrons driving an insulating gap and metallic surface states at low temperatures, is an ideal candidate for realizing the topological Kondo insulator state. By exploiting the presence of a time reversal symmetry breaking surface ferromagnetic state, we investigate the topological nature of metallic surface states, finding evidence of one-dimensional surface transport with conductance values approaching the quantized value of  $e^2/h$  and originating from the chiral edge channels of ferromagnetic domain walls. We will review our milliKelvin magnetotransport measurements of the edge state transport phenomenon in  $\text{SmB}_6$ , as well as thickness and surface gating studies that conclusively prove the surface nature of low temperature conductance.

<sup>1</sup>This research was supported by AFOSR (FA9550-14-1-0332) and NSF (DMR-0952716).

**11:51AM B28.00002 Effect of Sm valence variation on hybridization gap and in-gap excitons in  $\text{SmB}_6$  studied by Raman spectroscopy**<sup>1</sup>, MICHAEL VALENTINE, SEYED KOOPAYEH, WILLIAM A. PHELAN, TYREL MCQUEEN, NATALIA DRICHKO, Institute for Quantum Matter, Johns Hopkins University, PRISCILA ROSA, ZACHARY FISK, University of California, Irvine —  $\text{SmB}_6$  is a proposed topological Kondo insulator where the presence of topological nontriviality can be tuned by variations in the Sm valence. A range of samples where Sm valence was varied by increasing numbers of Sm vacancies was investigated using Raman spectroscopy over a temperature range of 10 to 300 K. We show a possibility to characterize the presence of Sm vacancies on the order of 1

<sup>1</sup>The work at IQM was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Material Sciences and Engineering, under Grant No. DEFG02-08ER46544

**12:03PM B28.00003 Origin of bulk quantum oscillations in the bulk Kondo insulating ground state of  $\text{SmB}_6$** , SUCHITRA SEBASTIAN, B. S. TAN, Y.-T. HSU, University of Cambridge, B. ZENG, NHMFL, M. CIOMAGA HATNEAN, University of Warwick, N. HARRISON, Z. ZHU, LANL, M. HARTSTEIN, M. KIOURLAPPOU, M. SRIVASTAVA, University of Cambridge, M. D. JOHANNES, Naval Research Laboratory, T. P. MURPHY, J.-H. PARK, L. BALICAS, NHMFL, N. SHITSEVALOVA, National Academy of Sciences of Ukraine, G. G. LONZARICH, University of Cambridge, G. BALAKRISHNAN, University of Warwick — I will discuss our recent observation of quantum oscillations corresponding to a bulk Fermi surface in the Kondo insulator  $\text{SmB}_6$ , and consider their possible origin. New complementary experimental results will be presented which raise the interesting question of whether the underlying ground state corresponds to a novel Kondo regime in which the spin channel is gapless while the charge channel is gapped.

**12:15PM B28.00004 Angular Dependence of Quantum Oscillations in  $\text{SmB}_6$** , M. HARTSTEIN, B. S. TAN, Y.-T. HSU, University of Cambridge, B. ZENG, NHMFL, M. CIOMAGA HATNEAN, University of Warwick, N. HARRISON, Z. ZHU, LANL, M. KIOURLAPPOU, A. SRIVASTAVA, University of Cambridge, M. D. JOHANNES, Naval Research Laboratory, T. P. MURPHY, J.-H. PARK, L. BALICAS, NHMFL, N. SHITSEVALOVA, National Academy of Sciences of Ukraine, G. G. LONZARICH, University of Cambridge, G. BALAKRISHNAN, University of Warwick, S. E. SEBASTIAN, University of Cambridge — Recent proposals of low-dimensional electronic states in the Kondo insulator,  $\text{SmB}_6$  have lead to renewed interest in the material. In this study we present quantum oscillation measurements of high quality single-crystals of  $\text{SmB}_6$ . Magnetic torque was measured in magnetic fields up to 40 T, allowing the observation of quantum oscillation frequencies ranging from 50 T to 15,000 T in multiple samples prepared by different groups. The size and the angular dependence of the oscillations indicate the striking concurrence of an electronically insulating bulk and a large, bulk Fermi surface. Comparison of the measured oscillations with similar measurements of metallic rare-earth hexaborides supports such a Fermi surface. Our model, previously employed for the metallic hexaborides, describes large ellipsoidally distorted spheres centred at X-points of the Brillouin zone, and smaller ellipsoids positioned at neck points, and gives a good account of the observed frequencies.

**12:27PM B28.00005 Effect of Gap on Quantum Oscillations**, HRIDIS PAL, FRDRIK PICHON, Laboratoire de Physique des Solides, Universit Paris-Sud, JEAN-NOL FUCHS, Laboratoire de Physique Thorique de la Matire Condense, Universit Pierre et Marie Curie, Paris, MARK GOERBIG, GILLES MONTAMBAUX, Laboratoire de Physique des Solides, Universit Paris-Sud — One of the manifestations of the quantization of energy levels in a magnetic field is quantum oscillations. In a metal, oscillations in several physical observables occur each time a Landau level crosses the Fermi level, and is, therefore, a Fermi surface property. In a gapped system, since there is no Fermi surface, such oscillations are not expected. One can ask, what happens to these oscillations as a metal is slowly turned into an insulator by introducing a gap at the Fermi level. To address this, we consider a simple model of two overlapping bands that hybridize to open a gap, and investigate how the oscillations change as the gap is slowly increased, both at zero and non-zero temperature. We show that the oscillations in such gapped systems show marked deviation from the canonical Lifshitz-Kosevich results routinely used to study quantum oscillations in metals.

**12:39PM B28.00006 Quantum oscillation in narrow-gap topological insulators<sup>1</sup>**, LONG ZHANG, XUE-YANG SONG, FA WANG, Peking University — The canonical understanding of quantum oscillation in metals is challenged by the observation of de Haas-van Alphen effect in an insulator,  $\text{SmB}_6$  [Tan *et al.*, Science **349**, 287 (2015)]. Based on a two-band model with inverted band structure, we show that the periodically narrowing hybridization gap in magnetic fields can induce the oscillation of low-energy density of states in the bulk, which is observable provided that the activation energy is small and comparable to the Landau level spacing. Its temperature dependence strongly deviates from the Lifshitz-Kosevich theory. The nontrivial band topology manifests itself as a nonzero Berry phase in the oscillation pattern, which crosses over to a trivial Berry phase by increasing the temperature or the magnetic field. Further predictions to experiments are also proposed.

<sup>1</sup>This work was supported by the National Key Basic Research Program of China (Grant No. 2014CB920902) and the National Science Foundation of China (Grant No. 11374018).

**12:51PM B28.00007 Reduction of the low-temperature bulk gap in the topological Kondo insulator samarium hexaboride under high magnetic fields<sup>1</sup>**, STEVEN WOLGAST, YUN SUK EO, KAI SUN, CAGLIYAN KURDAK, University of Michigan, Department of Physics, DAE-JEONG KIM, ZACHARY FISK, University of California at Irvine, Department of Physics and Astronomy — The mixed-valent insulator samarium hexaboride exhibits a narrow bandgap at low temperatures, formed by strong-correlation interactions between itinerant  $d$  electrons and  $f$  states localized to the Sm ions, and surface states accessible to transport below about 2 K. Spectroscopic measurements of the bandgap suggest a gap size of 15-20 meV, but transport measurements of thermally-activated carriers suggest the Fermi energy is about 3 meV below the conduction band edge. Here, we study the activated transport gap in pulsed magnetic fields up to 60 T between 1.5 K and 4 K. The magnetoresistance of the surface states, which has only very weak temperature dependence, is distinct from that of the bulk states, which exhibit thermally-activated behavior. The activation energy shrinks by 50% at fields up to 60 T. Data up to 93 T suggest that the transport gap continues to close, but is only fully-closed at even higher fields. We compare the measured reduction to theoretically-expected behavior due to Zeeman shifts of the Sm ion  $f$ -state transition energies. Meanwhile, the surface state shows no hints of Shubnikov-de Haas oscillations, which places constraints on any 2D surface carrier's mobility.

<sup>1</sup>Performed in part at the NHMFL (NSF CA DMR-1157490 and the State of Florida), and the LNF (NNIN, supported by NSF). Supported by NSF grant Nos. DMR-1006500, DMR-1441965, and DMR-0801253.

**1:03PM B28.00008 Magnetotransport Measurements on  $\text{SmB}_6$  - Cornering the Parameter Space for Carrier Density and Mobility<sup>1</sup>**, YUN SUK EO, STEVEN WOLGAST, CAGLIYAN KURDAK, KAI SUN, Dept. of Physics, University of Michigan, DAE-JEONG KIM, ZACHARY FISK, Dept. of Physics and Astronomy, University of California, Irvine, MONICA CIOMAGA HATNEAN, GEETHA BALAKRISHNAN, Dept. of Physics, University of Warwick — There is growing interest in studying the conducting surface of  $\text{SmB}_6$ , which is believed to originate from its nontrivial band topology. Up to date, different measurement techniques, including ARPES, dHvA, and Hall bar transport still disagree on important parameters such as the carrier density. In order to find the carrier density ( $n$ ) and mobility ( $\mu$ ) for the Dirac pockets participating in transport, we measure magnetotransport on Corbino devices fabricated on (100), (110), and (111) surfaces grown by floating zone and flux methods. Our samples do not exhibit Shubnikov-de Haas oscillations at high field pulsed measurements up to 90 Tesla, which provides an upper bound of  $\mu$  of each channels. Also, angle-dependent magnetotransport up to 35 T allows us to extract an effective  $n$  and  $\mu$  of the combined channels. Together, a parameter space that confines the possible  $n$  and  $\mu$  of each channel is constructed, and appears to be in agreement with ARPES reports. Additionally, the effective  $n$  and  $\mu$  change up to 20 percent when applying magnetic field up to 35 T. We will discuss how the Landau fan diagram can be nonlinear by this effect.

<sup>1</sup>This project was funded by NSF grant DMR-1006500. This project was performed at the National High Magnetic Field Laboratory, and in the Lurie Nanofabrication Facility.

**1:15PM B28.00009 Kondo Interactions from Band Reconstruction in  $\text{YbInCu}_4$** , JASON HANCOCK, University of Connecticut, IGNACE JARRIGE, Brookhaven National Laboratory, AKIO KOTANI, Photon Factory, H. YAMAOKA, RIKEN, N. TSUIJII, K. ISHII, JAEA, M. UPTON, D. CASA, J. KIM, T. GOG, Argonne — We combine resonant inelastic x-ray scattering and model calculations in the Kondo lattice compound  $\text{YbInCu}_4$ , a system characterized by a dramatic increase in Kondo temperature and associated valence fluctuations below a first-order valence transition at  $T \simeq 42$  K. The bulk-sensitive, element-specific, and valence-projected charge excitation spectra reveal an unusual quasigap in the Yb-derived state density which drives an instability of the electronic structure and renormalizes the low-energy effective Hamiltonian at the transition. Our results provide long-sought experimental evidence for a link between temperature-driven changes in the low-energy Kondo scale and the higher-energy electronic structure of this system.

**1:27PM B28.00010 Temperature-dependent Helicity of In-gap states of  $\text{SmB}_6$ <sup>1</sup>**, SOOYOUNG JANG, Lawrence Berkeley Natl Lab, POSTECH, J.D. DENLINGER, Lawrence Berkeley Natl Lab, C.-H. MIN, F. REINERT, U. Würzburg, BOYOUN KANG, B.-K. CHO, GIST, D.J. KIM, Z. FISK, UC Irvine, KEUN SU KIM, POSTECH, J. W. ALLEN, U. of Michigan — Mixed-valent  $\text{SmB}_6$  with a temperature (T) dependent bulk gap is the first candidate example of a new class of strongly correlated topological insulators with  $f$ - $d$  band inversion. Previous angle-resolved photoemission (ARPES) on cleaved  $\langle 100 \rangle$  surfaces of  $\text{SmB}_6$  have quantified the T-evolution of (i) the Sm  $4f$  state coherence, (ii) the X-point  $f$ -conduction band energy and many-body gap destabilization, and (iii) the intimately connected fate of in-gap states. In this work we additionally characterize the T-evolution of the in-gap state orbital angular momentum helicity using circular dichroism. We show that the onset of dichroism, above 100K, coincides with the dimensional crossover from high T 3D non-helical bulk  $d$ -band states crossing  $E_F$  to low T 2D in-gap surface states where the dichroic asymmetry reaches 100%. With the assumption of topological surface state anti-parallel spin-momentum locking, this result can be viewed as supporting previous spin-resolved ARPES measurements of in-gap state helical spin structure.

<sup>1</sup>Supported by U.S. DOE at the Advanced Light Source (DE-AC02-05CH11231).

**1:39PM B28.00011 In-gap states on the non-polar (110) surface of  $\text{SmB}_6$ <sup>1</sup>**, J.D. DENLINGER, SOOYOUNG JANG, Lawrence Berkeley Nat'l Lab, C.-H. MIN, F. REINERT, U. Würzburg, BOYOUN KANG, B.-K. CHO, GIST, D.J. KIM, Z. FISK, U.C. Irvine, J.W. ALLEN, U. of Michigan — Mixed-valent  $\text{SmB}_6$  with a temperature-dependent bulk gap is the first candidate example of a new class of strongly correlated topological insulators with  $f$ - $d$  band inversion. The topological origin of in-gap states on cleaved (001) surfaces as measured by angle-resolved photoemission (ARPES) is not without controversy, since the  $\bar{X}$  states span the full  $\sim 20$  meV hybridization gap at low temperature without exhibiting any clear Dirac point. Furthermore, reports exist of band-bending due to the polarity of the (001) surface and depth-dependent deviations from bulk stoichiometry or Sm valency. In this work we explore ARPES of the non-polar (110) surface of  $\text{SmB}_6$  prepared by polishing and high-temperature annealing. We find in-gap states at  $\bar{X}$  and  $\bar{Y}$  points with very similar properties as the (001)  $\bar{X}$  states. We discuss the relevance of these findings to the TI and other proposed models, and to the recent discrepancy between 2D [1] and 3D [2] interpretations of dHvA Fermi surface orbits.

[1] G. Li, *et al.*, Science **346**, 1208 (2014).

[2] B.S. Tan, *et al.*, Science **349**, 287 (2015).

<sup>1</sup>Supported by U.S. DOE at the Advanced Light Source (DE-AC02-05CH11231).

**1:51PM B28.00012 Effect of Magnetic Substitution on Topological Kondo Insulator SmB<sub>6</sub>**, TRISTIN METZ, YASUYUKI NAKAJIMA, XIANGFENG WANG, JOHNPIERRE PAGLIONE, University of Maryland, College Park — The Kondo topological insulator SmB<sub>6</sub> is an ideal candidate to realize protected metallic surface states driven by strong electron correlations. Recent experiments [1] provide evidence for one-dimensional electron transport on the surface of SmB<sub>6</sub>, associated with the existence of topologically nontrivial chiral edge states at the boundaries of intrinsic surface ferromagnetic domains. If these surface states are indeed topologically nontrivial they will be destroyed by the introduction of time reversal symmetry breaking magnetic impurities. We investigate the effect of magnetic impurities on SmB<sub>6</sub> through transport measurements in Fe and Ni substituted SmB<sub>6</sub> at very low temperatures. [1] Nakajima et. al., arXiv:1312.6132

**Monday, March 14, 2016 11:15AM - 2:15PM –**

**Session B29 DCMP: Quantum Spin Hall Effect** 328 - Dong-Ling Deng, University of Maryland

**11:15AM B29.00001 Quantum spin Hall effect in two-dimensional transition-metal dichalcogenide Haeckelites<sup>1</sup>**, SI-MIN NIE, ZHIDA SONG, HONGMING WENG, ZHONG FANG, Chinese Academy of Sci (CAS), T03 TEAM — The Quantum Spin Hall (QSH) effect, discovered nearly ten years ago, is such a promising option, because it can be viewed as the time-reversal-invariant version of the QH effect, which does NOT need any external magnetic field and can be in principle realized at room temperature. So far, QSH effect has only been observed in HgTe/CdTe and InAs/GaSb quantum wells. Both of them require precisely controlled MBE growth and ultralow temperature. The study of 2D TI has been seriously hampered due to lack of proper materials with large band gap, stable structure, and easy fabrication. In this report, I will introduce a family of the single layer 2D transition metal dichalcogenide (TMD) Haeckelites MX<sub>2</sub> (M=W or Mo, X=S, Se or Te), which can host QSH effect. The phonon spectra indicate that these Haeckelites are dynamically stable. Further, a simple tight-binding model based on square-like lattice has been established to uncover the underlying mechanism. This will extend further studies from graphene-based hexagonal lattice to square-like lattice and broad the range for searching topological materials largely.

<sup>1</sup>National Natural Science Foundation of China, the 973 program of China

**11:27AM B29.00002 Quantum Spin Hall Effect in thin films of topological crystalline insulators.**, RYSZARD BUCZKO, SHIVA SAFAEI, MARTA GALICKA, PERLA KACMAN, Institute of Physics Polish Academy of Sciences, Warsaw, Poland — The quantum spin Hall effect (QSHE) is predicted to exist in topological crystalline insulator materials [1]. Using a tight-binding approach we demonstrate that in (111)-oriented thin films of SnSe and SnTe the energy gaps depend in an oscillatory fashion on the layer thickness. The calculated topological invariant indexes and edge state spin polarizations show that in the negative energy gaps regions (~20–40 monolayers) a 2D topological insulator phase appears. In this range of thicknesses in both SnSe and SnTe, edge states are obtained with Dirac cones having opposite spin polarization in their two branches. While in SnTe layers a single Dirac cone appears at the projection of  $\Gamma$  point of the 2D Brillouin zone, in SnSe layers three Dirac cones at  $M$  points projections are obtained. Unfortunately, in SnSe films an overlapping of bands at  $\Gamma$  and  $M$  diminishes the final band gap in the vicinity of all  $M$  points and the edge states appear either against the background of the bands or within a very small energy gap. We show that this problem can be removed by applying to the layers a biaxial strain [2]. This should enable observation of the QSHE also in SnSe layers. 1. S. Safaei, et al., New J. Phys. 17, 063041 (2015). 2. S. Safaei et al, arXiv: 1508.01364 [cond-mat.mtrl-sci].

**11:39AM B29.00003 Transport in quantum spin Hall systems in parallel magnetic fields**, MICHAEL WIMMER, RAFAL SKOLASINSKI, TU Delft, Netherlands, DMITRY PIKULIN, University of British Columbia, Canada, JASON ALICEA, Caltech, US — Edge states in quantum spin Hall (QSH) systems are protected by time-reversal symmetry, resulting in a quantized conductance. A magnetic field breaks that protection, and should lead to a deviation from perfect quantization. We will discuss generic features of semiconductor-based QSH systems (such as HgTe/CdTe and InAs/GaSb) that affect the magnetic field dependence of edge state conductance, focusing on the effect of an in-plane field.

**11:51AM B29.00004 Giant Rashba spin splitting with unconventional spin texture in a quantum spin Hall insulator<sup>1</sup>**, CARLOS MERA ACOSTA, OSCAR BABILONIA, University of Sao Paulo, CP 66318, 05315-970, Sao Paulo, SP, Brazil, LEONARDO ABDALLA, University of Colorado, Boulder, Colorado 80309, USA, ADALBERTO FAZZIO, University of Sao Paulo, CP 66318, 05315-970, Sao Paulo, SP, Brazil — We propose a non-centrosymmetric honeycomb-lattice quantum spin Hall effect family formed by atoms of the groups IV, V and VII of the periodic table. We make a structural analysis, a  $Z_2$  characterization. According to our ab-initio phonon calculations, the system formed by Bi, Pb and I atoms is only mechanically stable system. This material presents a Rashba-type spin-splitting and a hexagonal warping effect, which lead to an unusual spin texture. Due to this spin texture, the backscattering is forbidden for both edge conductivity channels and bulk conductivity channels. This suggests that, contrary to what happens in most systems with nontrivial topological phases, the bulk states would not pose a problem for spintronic devices. The value of the spin-splitting due to the Rashba effect is about 60 meV, which is huge compared with the values found in 2D systems and surprisingly is on the order of the highest found in 3D systems.

<sup>1</sup>We would like to thank the financial support by the Sao Paulo research fundation (FAPESP).

**12:03PM B29.00005 Large band gap quantum spin hall insulators of fluorinated Pb-X (X= C, Si, Ge, Sn)**, JOSE EDUARDO PADILHA, Universidade Federal do Parana - Jandaia do Sul, RENATO BORGES PONTES, Universidade Federal de Goias, TOME MAURO SCHMIDT, ROBERTO HIROKI MIWA, Universidade Federal de Uberlandia, ADALBERTO FAZZIO, Universidade de Sao Paulo — The Quantum Spin Hall Insulating (QSHI) phase was first observed in the HgTe/CdTe quantum well structure. However, the observed band gap of 5 meV is too small for practical applications. Other materials have also been proposed for the observation of the QSHI phase, such as silicene, germanene, stanene, and its halogenated phases. The spin-orbit interaction is a key feature in topological insulators, raising the interest in heavy elements, such as Bismuth. In fact, Bi is responsible for the high spin-orbit coupling that drives the band inversion in Bi<sub>2</sub>Se<sub>3</sub> and Bi<sub>2</sub>Te<sub>3</sub>. Another element that also has a large spin-orbit interaction is Lead (Pb). Here we present a set of 2D QSH insulators with a very large band gap based on fluorinated Pb-X (X= C, Si, Ge, Sn). First-principles phonon dispersion calculations indicate that these systems are structurally and mechanically stable. By performing DFT-based electronic structure calculations we show that 2D Pb-X functionalized with fluorine are topological insulators with very large band gaps (over 0.7 eV). Additional calculations, for nanoribbons structures, show the presence of a Dirac cone at the center of the Brillouin zone. These results can establish a new route to the observation of QSHI phase at room temperature.

**12:15PM B29.00006 Fully and partially iodinated germanane as a platform for the observation of the quantum spin Hall effect.** , JOSE EDUARDO PADILHA, Universidade Federal do Parana, ADALBERTO FAZZIO, LEONARDO ABDALLA, ANTONIO JOSE ROQUE DA SILVA, Universidade de Sao Paulo — The Quantum Spin Hall Effect (QSHE) proposed in 2005 by Kane and Mele for graphene and by S.-C. Zhang et al. in 2006 for the HgTe/CdTe, became a very exciting area of condensed matter physics. Several materials have been proposed to overcome the issue of the small SOC band gap presented by the graphene and HgTe/CdTe structures, such the elemental materials germanene, stanene and others binary compounds with band gaps that goes to several meV to few eV. Motivated by the recent isolation of the trivial insulator germanane, a fully hydrogenated germanene, we show that a partially substitution of the hydrogen atoms in only one side of the material by iodine, creates a two dimensional topological insulator with a large band gap of 0.49 eV. This functionalization opens up new routes for the observation of the quantum spin Hall effect in a fully two-dimensional material. We also show that creating nanoroads or nanoribbons with the pattern functionalization of germanane by iodine in a ordered or disordered way, topologically protected interfaces states arises at the boundary of germanane/iodinated germanane.

**12:27PM B29.00007 Spin Hall Conductivity and Spin Chern Number for Dirac Systems** , ELIF YUNT, OMER FARUK DAYI, Istanbul Tech Univ — A semiclassical differential form formalism of the spin Hall effect for Dirac systems is presented. In this formalism, space coordinates and momenta are usual dynamical variables, whereas spin is not a dynamical degree of freedom. Spin depicts itself in the matrix-valuedness of equations of motion. We demonstrate that the main contribution to the spin Hall conductivity is given by the spin Chern number whether the spin is conserved or not at the quantum level. We illustrated the formulation within the Kane-Mele model of graphene in the absence and in the presence of the Rashba spin-orbit coupling term. Kane-Mele Model of graphene, which incorporates intrinsic spin-orbit interaction, constitutes the first example of a two dimensional topological insulator. We established the anomalous Hall conductivity as well as the spin Hall conductivity from the term linear in the electric field and the Berry curvature in the the anomalous velocity term. In a basis where the component of spin under consideration is diagonal this term is diagonal. We argue that this semiclassical procedure of calculating the spin Hall conductivity can be generalized to any dimension.

**12:39PM B29.00008 Room Temperature Quantum Spin Hall Insulators with a Buckled Square Lattice** , WEI LUO, HONGJUN XIANG, None — Two-dimensional (2D) topological insulators (TIs), are excellent candidates for coherent spin transport related applications. Currently, most known 2D TIs are based on a hexagonal lattice. Here, we propose that there exists the quantum spin Hall effect (QSHE) in a new tight-binding (TB) model for a two-orbital system with the buckled square lattices. We show that the band inversion is due to the hybridization between the  $p_x$  and  $p_y$  orbitals, while the spin-orbit coupling (SOC) induced nearest-neighbor effective hopping is responsible for a band gap opening at the Dirac cone. Through performing global structure optimization, we predict a new three-layer quasi-2D (Q2D) structure which has the lowest energy among all structures with the thickness less than 6.0 Å for the BiF system. It is identified to be a Q2D TI with a large band gap (0.69 eV). The electronic states of the Q2D BiF system near the Fermi level are mainly contributed by the middle Bi square lattice, which are sandwiched by two inert BiF<sub>2</sub> layers. This is beneficial since the interaction between a substrate and the Q2D material may not change the topological properties of the system, as we demonstrate in the case of the NaF substrate. Our analysis shows that the low-energy physics of the Q2D BiF system can be qualitatively described by our newly proposed two-orbital TB model. Our study not only predicts a Q2D QSH insulator for realistic room temperature (RT) applications, but also provides a new lattice system for engineering topological states such as quantum anomalous Hall effect.

**12:51PM B29.00009 Superconducting quantum spin-Hall systems with giant orbital g-factors<sup>1</sup>** , EWELINA HANKIEWICZ, ROLF REINTHALER, GRIGORY TKACHOV, Wurzburg University, Germany — Topological aspects of superconductivity in quantum spin-Hall systems (QSHSs) such as thin layers of three-dimensional topological insulators (3D TIs) or two-dimensional TIs are in the focus of current research. Here, we describe a novel superconducting quantum spin-Hall effect (quantum spin Hall system in the proximity to the s-wave superconductor and in the orbital in-plane magnetic field), which is protected against elastic backscattering by combined time-reversal and particle-hole symmetry [1]. This effect is characterized by spin-polarized edge states, which can be manipulated in weak magnetic fields due to a giant effective orbital g-factor, allowing the generation of spin currents. The phenomenon provides a novel solution to the outstanding challenge of detecting the spin-polarization of the edge states. Here we propose the detection of the edge polarization in the three-terminal junction using unusual transport properties of superconducting quantum Hall-effect: a non-monotonic excess current and a zero-bias conductance splitting. [1] R. W. Reintaler, G. Tkachov, and E. M. Hankiewicz Phys. Rev. B 92, 161303(R) (2015)

<sup>1</sup>We thank for the financial support the German Science Foundation (DFG), grants No HA 5893/4-1 within SPP 1666, HA5893/5-2 within FOR1162 and TK60/1-1 (G.T.), as well the ENB graduate school "Topological insulators".

**1:03PM B29.00010 Effective spin dephasing mechanism in confined two-dimension topological insulators** , JUNJIE QI, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, HAIWEN LIU, International Center for Quantum Materials and School of Physics, Peking University, Beijing 100871, China, HUA JIANG, College of Physics, Optoelectronics and Energy, Soochow University, Suzhou 215006, China, X.C. XIE, International Center for Quantum Materials and School of Physics, Peking University, Beijing 100871, China, XIE'S GROUP TEAM — A Kramers pair of helical edge states in quantum spin Hall effect (QSHE) is robust against normal dephasing but not robust to spin dephasing. In our work, we provide an effective spin dephasing mechanism in the puddles of two-dimension QSHE, which is simulated as quantum dots modeled by 2D massive Dirac Hamiltonian. We demonstrate that the spin dephasing effect can originate from the combination of the Rashba spin-orbit coupling and electron-phonon interaction, which gives rise to inelastic backscattering in edge states within the topological insulator quantum dots, although the time-reversal symmetry is preserved throughout. Finally, we discuss the tunneling between extended helical edge states and local edge states in the QSH quantum dots, which leads to backscattering in the extended edge states. These results can explain the more robust edge transport in InAs/GaSb/AlSb QSH systems.

**1:15PM B29.00011 Effects of magnetic impurities on transport in 2D topological insulators** , XIAOQIAN DANG, J.D. BURTON, EVGENY TSYMBAL, University of Nebraska-Lincoln — Understanding the transport properties of topological insulators could bring such materials from fundamental research to potential applications. Here we report on the theoretical investigations of the effects of magnetic impurities on transport properties of model two-dimensional (2D) topological insulators (TIs). We utilize the tight-binding form of the Bernevig-Hughes-Zhang model and investigate the transport properties by employing the Landauer-Büttiker formalism. We explore the current distribution in 2D TIs resulting from scattering by a magnetic impurity which breaks time-reversal symmetry. We find that a magnetic impurity could drive anti-resonant behavior of the conductance, as revealed from full backscattering of the electron current flowing at one of the edges of the TI. This phenomenon occurs due to spin-flip scattering when the Fermi energy matches the impurity state and the magnetic moment of the impurity is aligned along the TI edge. Additionally, we explore the effect of an external magnetic gate attached to the system and show that changing the magnetization orientation within the gate allows the control of conductance. This geometric setup could be realized experimentally providing the opportunity to tune transport properties of 2D TIs by a magnetic gate.

**1:27PM B29.00012 One-dimensional edge states in Bi(111) bilayer grown on Sb<sub>2</sub>Te<sub>3</sub>**<sup>1</sup>, YAOYI LI, SHIVANI RAJPUT, DUSHYANT TOMER, LIAN LI, Univ of Wisconsin, Milwaukee — Well-ordered Bi bilayer islands with zigzag edges are grown epitaxially on Sb<sub>2</sub>Te<sub>3</sub>(111) film by molecular beam epitaxy. Scanning tunneling microscopy imaging shows that the Bi film assumes the lattice of the Sb<sub>2</sub>Te<sub>3</sub>, thus is coherently strained. Tunneling spectroscopy further reveals robust edge states, confirming it as a two-dimensional topological insulator. This is consistent with first-principles calculations that indicate the preservation of the topological nature of the Bi bilayer and edge states with only an energy shift even in the presence of strong interaction between Bi and Sb<sub>2</sub>Te<sub>3</sub>. These findings suggest that the interface between 2D and 3D TIs can be a promising platform to synthesize new topological matter.

<sup>1</sup>This research was supported by NSF DMR-1335215.

**1:39PM B29.00013 Controlling the Flow of Spin and Charge in Nanoscopic Topological Insulators**<sup>1</sup>, DIRK MORR, JOHN VAN DYKE, University of Illinois at Chicago — Rapid advances in quantum computation and spin electronics, heralded by the discovery of topological insulators, have been hampered by the inability to control the flow of spin and charge currents at the nanoscale. In this talk, I will demonstrate that such control can be established in nanoscopic two-dimensional topological insulators (TIs) by breaking their time reversal symmetry via magnetic defects. This allows for the emergence of two novel phenomena: the creation of nearly 100

<sup>1</sup> This work was supported by the U. S. Department of Energy, Office of Science, Basic Energy Sciences, under Award No. DE-FG02-05ER46225.

weiku@bnl.gov

**1:51PM B29.00014 Hunting down magnetic monopoles in 2D topological insulators**, HE, Stony Brook University and BNL, CMPMSD AT BNL TEAM — Contrary to the existence of electric charge, magnetic monopoles have never been observed. It is thus extraordinary to find that magnetic monopoles can be pictured conceptually in topological insulators. For 2D topological insulators, the topological invariant corresponds to the total flux of an effective magnetic field (the Berry curvature) over the reciprocal space. Upon compactifying the Brillouin zone to a compact manifold as a torus, the non-zero total flux can be considered to originate from magnetic monopoles with quantized charge. The intrinsic difficulty via extending a 2D problem to a 3D reciprocal space, and then demonstrate that analytical continuation offers a natural solution in which 1) the magnetic monopoles emerge naturally in pairs each forming a string above and below the Brillouin zone, and 2) the total charge below the real axis gives exactly the topological invariant. In essence, the robustness of the topological invariant is protected by the total charge in the lower complex plane, a mapping intriguing even mathematically. Finally, we will illustrate the physical transition, providing a natural description of the metallic nature in the phase boundary, and offering a clear explanation of the induced via a local change in reciprocal space.

Stony Brook University & BNL

<sup>1</sup>Work supported by US DOE BES DE-AC02-98CH10886

**2:03PM B29.00015 Circle of crossings and Berry curvatures in 2D topological insulators**<sup>1</sup>, MARIUS RADU, YULI LYANDA-GELLER, Department of Physics and Astronomy, Purdue University — HgTe forms a two-dimensional topological insulator when sandwiched between CdTe barriers for a HgTe layer wider than the critical thickness. We derive single-particle and two-particle interaction Hamiltonians describing physics of these compounds by using  $\mathbf{k} \cdot \mathbf{p}$  theory and extended Kane model. We include contributions from upper conduction bands with orbital states of p-symmetry that bring about the terms describing lack of inversion symmetry in host semiconductors. A crucial ingredient is hetero-interface contribution to intrinsic spin-orbit interactions that drives significant anticrossing gaps in spectra at zero wavevector, but results in a circle of spectral crossings at finite wavevectors. Single-particle Hamiltonian and two-particle Hamiltonian contain important spin-dependent terms. The spin-dependent interaction couples orbital motion of one particle with evolution of spin of the other particle. Such particle-particle interactions do not conserve spin and lower the symmetry of exchange interactions, leading, e.g., to Dzyaloshinskii-Moriya exchange term. We study the effects of new interactions on Berry curvature and spin-Hall conductance.

<sup>1</sup>This research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-SC0010544

**Monday, March 14, 2016 11:15AM - 2:03PM —**

**Session B30 DMP: Ferroelectric Walls, Heterostructures and Superlattices** 329 - Rossitza Pentcheva, University of Duisburg-Essen

**11:15AM B30.00001 Two-dimensional electron gases at head-to-head and tail-to-tail domain walls in ferroelectric thin films.**<sup>1</sup>, PABLO GARCÍA-FERNÁNDEZ, Universidad de Cantabria, JORGE ÍÑIGUEZ, Luxembourg Institute of Science and Technology, JAVIER JUNQUERA, Universidad de Cantabria — Symmetry breaking at ferroelectric domain walls gives rise to new physical properties, offering the opportunity to use the domain walls themselves as a functional separate object in a device. One example is the appearance of an enhanced conductivity at the boundaries between ferroelectric domains in oxides. A realistic first-principles simulation of the domain walls is limited to highly-symmetric cleanly-cut walls in order to keep the number of atoms in the simulation box small. Here we use a recently developed second-principles method that treats all the lattice degrees of freedom and the relevant electronic ones on the same foot with high accuracy at a modest computational cost. We apply it to the demanding physical problem of head-to-head (HH) and tail-to-tail (TT) domain walls in ferroelectric PbTiO<sub>3</sub> thin films. These interfaces present a large and unfavourable electrostatic energy due to the polarization-induced bound charge at the domain wall. An accurate simulation should capture eventual charge transfers between the walls, and the concomitant electron-lattice coupling. We show how the polarization discontinuity in HH and TT domain walls in PbTiO<sub>3</sub> thin films can be effectively screened by the formation of two-dimensional electron gases of electrons and holes.

<sup>1</sup>Financial support from MINECO Grant No. FIS2012-37549-C05-04

**11:27AM B30.00002 First-principles prediction of a native ferroelectric metal<sup>1</sup>**, JORGE INIGUEZ, Luxembourg Institute of Standards and Technology, ALESSIO FILIPPETTI, CNR-IOM SLACS Cagliari, VINCENZO FIORENTINI, Universit di Cagliari and CNR-IOM SLACS Cagliari, FRANCESCO RICCI, Universit di Cagliari, PIETRO DELUGAS, Istituto Italiano di Tecnologia IIT — The possibility that metals may support ferroelectricity is an intriguing open issue. Over the years, various compounds have been referred to as ferroelectric metals, including non-centrosymmetric metals as well as ferroelectrics whose polar distortion survives moderate metallicity induced by doping or proximity. Yet, we think none of these systems embodies a truly ferroelectric metal with native switchable polarization and native metallicity coexisting in a single phase. Here we report a first-principles prediction of such a material. We show that the layered perovskite Bi<sub>5</sub>Ti<sub>5</sub>O<sub>17</sub> has a non-zero density of states at the Fermi level and metal-like conductivity, as well as a spontaneous polarization in zero field. Further, we predict that the polarization of Bi<sub>5</sub>Ti<sub>5</sub>O<sub>17</sub> is switchable both in principle (the material complies with the sufficient symmetry requirements) and in practice (in spite of being a metal, Bi<sub>5</sub>Ti<sub>5</sub>O<sub>17</sub> can sustain a sizable potential drop along the polar direction, as needed to revert its polarization by application of an electric bias). Our results also reveal striking behaviors – such as the self screening mechanism at work in thin Bi<sub>5</sub>Ti<sub>5</sub>O<sub>17</sub> layers – emerging from the intimate interplay between polar distortions and free carriers in such an exotic material.

<sup>1</sup>Supported by MIUR-PRIN, Fondazione Banco di Sardegna, FNR Luxembourg, MINECO-Spain, CINECA-ISCRA and CESGA.

**11:39AM B30.00003 Polarization in asymmetrical intermixed interfaces in SrTiO<sub>3</sub>/PbTiO<sub>3</sub> superlattices**, SIMON DIVILOV, MARIVI FERNANDEZ-SERRA, GREG HSING, MATTHEW DAWBER, State Univ of NY- Stony Brook — We used first principles density functional theory to study the effects on polarization of asymmetrical intermixing. In our systems, one interface has intermixed A-cations and the other one is pure. We analyze both monodomain and polydomain SrTiO<sub>3</sub>/PbTiO<sub>3</sub> (STO/PTO) superlattices with varying periods. We report how the difference in energy and spontaneous polarization, between the two stable polarization states, scales with period, domain size, thickness of the intermixed layer and oxygen vacancies. Our results are used to explain the origin of the intrinsic polarization asymmetry observed in experimental measurements of ferroelectric hysteresis loops.

**11:51AM B30.00004 Domain Structure and Properties in Inhomogeneously-Strained Ferroelectric Thin Films**, LANE MARTIN, University of California, Berkeley — Epitaxial thin-film growth and the ability to deterministically apply lattice mismatch strain has enabled dramatic control over the structure and properties of a range of ferroelectric materials. Modern ferroelectric films, including bilayer and superlattice heterostructures, have also provided access to exotic structures and properties not available in the bulk. In this work, we focus on recent advances in our understanding of how strain can be manipulated and controlled to elicit new types of responses and new understandings about response in ferroelectric materials. In particular, we will explore new modalities of strain control of ferroelectric materials that go beyond traditional lattice mismatch effects and how this can be used to enhance performance, independently tune susceptibilities, and provide new insights into the nature of these complex materials. In particular, we will focus on the deterministic production of large strain gradients (on the order of  $>10^{-5} \text{ m}^{-1}$ ) via purposeful compositional gradients. We will highlight work on compositionally-graded versions of PbZr<sub>1-x</sub>Ti<sub>x</sub>O<sub>3</sub> and Ba<sub>1-x</sub>Sr<sub>x</sub>TiO<sub>3</sub> where careful control of lattice mismatch and chemistry combine to produce large strain gradients, exotic properties, and new approaches to independently control traditionally coupled properties. As part of this discussion, we will explore the evolution of the crystal and domain structure as a function of the end-members of the compositional gradient, thickness of the film, and substrate. Advanced band-excitation piezoresponse force microscopy, switching spectroscopy, and non-linearity studies have been applied. These studies reveal both unexpected crystal and domain structures can be stabilized in these heterostructures and exotic low- and high-field responses can be obtained. Of particular interest will be the results of temperature-dependent probes of susceptibility which reveal large, nearly temperature-independent properties from 25-500C and the observation of highly-mobile ferroelastic domain wall structures which can give rise to local enhancement of susceptibilities. These observations could represent a ground-breaking advance in the performance of these materials.

**12:27PM B30.00005 Epitaxial strain effects on layered polar oxides from first-principles**, XUEZENG LU, JAMES RONDINELLI, Department of Materials Science and Engineering, Northwestern University, MATERIALS THEORY AND DESIGN GROUP TEAM — Epitaxial strain is a powerful tool to generate ferroelectric phases in thin films owing to polarization-strain coupling. The coupling of the oxygen rotations to strain can also be exploited to realize oxygen rotation-sensitive properties such as metal-insulator transitions and magnetic reconstructions. Here, we use electronic structure calculations to investigate the effects of biaxial strain on (001) thin films of the hybrid-improper ferroelectric Ca<sub>3</sub>Ti<sub>2</sub>O<sub>7</sub>. Besides the bulk *Cmc*<sub>21</sub> phase, we also find a new phase emerges under both experimentally accessible biaxial compressive and tensile strains. Furthermore, a large change in the dielectric anisotropy of the film is found at the tensile phase boundary, which we propose could be electric field tunable. Our results may offer a route to search for new functionalities in layered-perovskite oxides.

**12:39PM B30.00006 First-principles study of charge-order-driven ferroelectricity in LaVO<sub>3</sub>/SrVO<sub>3</sub> superlattices<sup>1</sup>**, SE YOUNG PARK, Rutgers University, ANIL KUMAR, Los Alamos National Laboratory, KARIN RABE, Rutgers University — We investigate the structure and electronic properties of the 1:1 superlattice composed of LaVO<sub>3</sub> and SrVO<sub>3</sub> using the density functional theory plus U (DFT+U) method. We find two low-energy antiferromagnetic Mott-insulating phases with distinct charge ordering patterns. In one of these phases, spontaneous polarization normal to the interface is nonzero due to a layered charge-ordering. The polarization calculated by the Berry phase method is 32  $\mu\text{C}/\text{cm}^2$ ; we have identified a possible switching path on which the system remains insulating. When fully relaxed, the energy per 5-atom-unit-cell of the polar state is only 3 meV higher than the non-polar state and we find that the energy difference can be reduced to zero by tensile strain. This suggests that the polar state could be induced by applied electric field, and, depending on the switching process, a ferroelectric hysteresis loop could be observed.

<sup>1</sup>Support: ONR N00014-11-0666

**12:51PM B30.00007 Microwave conductance of ferroelectric domain walls in lead titanate**, ALEXANDER TSELEV, YE CAO, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831, PU YU, Department of Physics and Collaborative Innovation Center for Quantum Matter, Tsinghua University, Beijing 100084, China, SERGEI V. KALININ, PETRO MAKSYMOVYCH, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831 — Numerous theoretical works predicted electronically conducting domain walls in otherwise insulating ferroelectric crystals. A number of recent experiments reported conducting walls, although conductivity itself and a conclusive proof of conductance mechanism remain elusive, largely due to the electrical contact problem. The latter can be overcome using high-frequency AC voltage. Here we will present our successful measurements of microwave conductance at 180° domain walls in lead titanate using microwave microscopy. AC conducting domain walls can be repeatably reconfigured and have extraordinary stability in time and temperature. AC conductivity is detected even when DC is not. Quantitative modeling reveals that the conductance of domain walls is comparable to doped silicon. We will also present a new and robust mechanism to create charged domain walls in any ferroelectric lattice. Overall, this sets the stage for a new generation of local experiments on conducting domain walls, and furthers the prospects of their application in fast electronic devices. AT, YC, SVK, PM supported by Division of Materials Sciences and Engineering, Office of Science, Basic Energy Sciences, U. S. DOE. PY supported by the National Basic Research Program of China (2015CB921700).

**1:03PM B30.00008 Metastable antiparallel polarization configurations in BaTiO<sub>3</sub>/PbZr<sub>0.2</sub>Ti<sub>0.8</sub>O<sub>3</sub> epitaxial bilayer**, PAVEL SALEV, ALEXEI GRIGORIEV, The University of Tulsa — A combination of LGD and semiconductor theories predicts the electrostatic screening of a large polarization mismatch between BaTiO<sub>3</sub> (BTO) and Pb(Zr,Ti)O<sub>3</sub> (PZT) ferroelectric layers. The source of this screening is in an increased concentration of interfacial free charge carriers due to the strong bending of electronic bands inside the layers. The enhanced concentration of free charges at the interface can allow for independent polarization reversal in each ferroelectric layer suggesting possible antiparallel polarization configurations in BTO/PZT bilayer. We confirmed these theoretical predictions of layer-by-layer switching by demonstrating double polarization switching in epitaxial BTO/PZT thin films. The layer-by-layer switching leads to formation of head-to-head (H-H) and tail-to-tail (T-T) polarization configurations, which have an enhanced dielectric permittivity when compared to parallel polarization domain configurations. While both H-H and T-T states are unstable at a zero electric field, we found that antiparallel polarization configurations can be stabilized by applying a small bias. Our findings provide a pathway to engineer new multilayer systems with switchable multistate polarizations and dielectric responses.

**1:15PM B30.00009 Thickness dependence of ferroelectric stability in SrRuO<sub>3</sub>/BaTiO<sub>3</sub>/La<sub>0.7</sub>Sr<sub>0.3</sub>MnO<sub>3</sub> ferroelectric tunnel junctions**, J. D. BURTON, EVGENY TSYMBAL, University of Nebraska - Lincoln — Ferroelectric tunnel junctions (FTJs) must meet key requirements in order to become viable device structures. One factor which can limit functionality is the thickness of the ferroelectric layer. The ferroelectric must be thin enough that a detectable tunnel current can flow through it, but if it is too thin, screening of the depolarization field by the electrodes will be insufficient for polarization stability. One mechanism to produce a large change in the tunneling resistance, i.e. a large tunneling electro resistance (TER), is to use asymmetric electrodes. This is disadvantageous from the point of view of switchability, however: the electric field due to the mismatch between metal work functions leads to a preference for one polarization state over the other and, in thinner FTJs, may render one of the polarization states unstable. To explore this effect we perform first-principles density functional calculations on SrRuO<sub>3</sub>/BaTiO<sub>3</sub>/La<sub>0.7</sub>Sr<sub>0.3</sub>MnO<sub>3</sub> (SRO/BTO/LSMO) FTJs with varying BTO thicknesses. We find an energetic preference for polarization to point away from the LSMO electrode. FTJs with BTO thicknesses at or below 4 unit-cells polarization pointing toward LSMO is unstable, and therefore are unswitchable. Analysis reveals that, in addition to the work function mismatch, the difference in screening lengths and the intrinsic layer-by-layer polar nature of LSMO play a significant role in this instability. We will also present an analysis of these effects on the tunneling barrier profile as well as on the TER effect.

**1:27PM B30.00010 Ferroelectric switching in epitaxial PbZr<sub>0.2</sub>Ti<sub>0.8</sub>O<sub>3</sub>/ZnO/GaN heterostructures**, JUAN WANG, PAVEL SALEV, ALEXEI GRIGORIEV, The University of Tulsa — As a wide-bandgap semiconductor, ZnO has gained substantial interest due to its favorable properties including high electron mobility, strong room-temperature luminescence, etc. The main obstacle of its application is the lack of reproducible and low-resistivity p-type ZnO. P-type doping of ZnO through the interface charge injection, which can be achieved by the polarization switching of ferroelectric films, is a tempting solution. We explored ferroelectric switching behavior of PbZr<sub>0.2</sub>Ti<sub>0.8</sub>O<sub>3</sub>/ZnO/GaN heterostructures epitaxially grown on Sapphire substrates by RF sputtering. The electrical measurements of Pt/PbZr<sub>0.2</sub>Ti<sub>0.8</sub>O<sub>3</sub>/ZnO/GaN ferroelectric-semiconductor capacitors revealed unusual behavior that is a combination of polarization switching and a diode I-V characteristics.

**1:39PM B30.00011 Room-temperature Ferroelectricity in Uniaxially Strained Single-crystalline SrTiO<sub>3</sub> Freestanding Films**, DI LU, GLAM, Dept. of Phys., Stanford Univ., SAM CROSSLEY, HYEOK YOON, GLAM, Dept. of Appl. Phys., Stanford Univ., YASUYUKI HIKITA, SIMES, SLAC, HAROLD HWANG, GLAM, Dept. of Appl. Phys., Stanford Univ.; SIMES, SLAC — Single crystal pure bulk SrTiO<sub>3</sub> (STO) is an incipient ferroelectric whose dielectric permittivity rises to high values as temperature is reduced, but remains paraelectric to the lowest observable temperatures. Ferroelectric phases of STO may be stabilized via doping and strain, whose common effect is to split the spatial free energy well of ionic displacements. With epitaxial strain of the order of a few percent, Curie temperatures  $T_C \sim 293$  K have been observed. By exploiting a highly novel process to exfoliate epitaxial oxide films deposited by pulsed laser deposition, we have isolated sub-100 nm-thick freestanding films of STO which are readily manipulated and mechanically strained to high levels. Measurements of the in-plane dielectric properties for various applied strains reveal a continuously tunable ferroelectric  $T_C$ . A two-order-of-magnitude enhanced dielectric response is displayed by a 1.2%-strained sample at  $T_C \sim 290$  K, as compared with the same sample unstrained at the same temperature. This is consistent with a phenomenological Ginzburg-Landau model, and previous studies on anchored films. The functional properties of strained STO have generated intense interest and debate, and have been suggested for device applications due to e.g. high voltage-tunable dielectric properties. Our work exhibits strain as a continuously variable experimental degree of freedom, which can induce numerous functional effects.

**1:51PM B30.00012 Manipulation of Carrier Density near Ferroelectric/Semiconductor Interfaces**, MEHMET KESIM, University of Connecticut, I. BURC MISIRLIOGLU, Sabanci University, JOSEPH MANTESE, United Technologies Research Center, S. PAMIR ALPAY, University of Connecticut — Switchable polarization of a ferroelectric (FE) opens up the opportunity to control the charge density and transport characteristics at the FE/metal and FE/semiconductor (SC) heterointerfaces. Carrier manipulation near such regions can be used in high density non-volatile memories, switchable diodes, and photovoltaic devices. FEs can be utilized as gate oxides in a metal oxide field-effect transistor configuration for non-volatile memory applications with lower gate voltages compared to that of transistors with linear dielectrics. The channel conductance can be modulated reversibly, for instance, by tuning the magnitude and spatial distribution of polarization in the FE. In this study, we show that FE heterostructures can be used to manipulate the conductivity of a FE/SC interface. We employ a non-linear thermodynamic model based on Landau-Ginzburg-Devonshire (LGD) theory to obtain the equilibrium polarization of heterostructures. The carriers along the heterostructures are mapped through coupling the LGD equation with the Maxwell equations and Fermi – Dirac distribution of charged carriers/ionized dopants in the FE and SC. We consider various configurations including FE/SC/paraelectric and FE/SC/FE stacks to investigate the carrier distribution and band bending near such interfaces. The resulting properties are explained through the phase transition characteristics and domain structure of the stacks.

**Monday, March 14, 2016 11:15AM - 2:15PM –**

**Session B31 DCP: Advances in Density Functional Theory II** 331 - John Perdew, Temple University

### 11:15AM B31.00001 Self-Interaction Corrected Density Functional Approximations with Unitary Invariance: Applications to Molecules

, MARK PEDERSON, Department of Chemistry, Johns Hopkins University — For a system of  $2N$  electrons, the Fermi-hole may be interpreted as the square of a normalized "Fermi orbital",  $F(\mathbf{a}) \equiv \rho_{\sigma}(\mathbf{a}, \mathbf{r}) / \sqrt{\rho_{\sigma}(\mathbf{a})}$ . This normalized orbital captures all of the spin density at its position of definition, or descriptor,  $(\mathbf{a})$ . Given a set of  $N$  quasi-classical electronic positions  $(\mathbf{a}_i)$  and a spin density-matrix composed of  $N$  Kohn-Sham orbitals, the resulting set of Fermi orbitals may then be used to construct a set of localized Loewdin-orthonormalized orbitals[1]. These orbitals are explicitly a functional of the spin density and are related to the Kohn-Sham orbitals by a unitary transformation that is parametrically dependent on the set quasi-classical electronic descriptors. The construction of such localized orbitals allows for the restoration of unitary invariance into the original Perdew-Zunger self-interaction correction[2,3] and provides a possible simplification compared to the localization-equation based solution of self-interaction corrected functionals[4]. This talk will discuss the construction of this Fermi-orbital-based self-interaction corrected method and the minimization algorithm that relies upon analytical derivatives[3] of the self-interaction energy with respect to the Fermi-orbital descriptors. Recent applications to a large set of molecules including aromatic molecules, molecules with open transition-metal centers, and molecules with frustrated Kekule' structures will be discussed. Initial applications indicate improvements in atomization energies of pi-bonded systems and demonstrate the desired downward shift of orbital energies relative to their Kohn-Sham counterparts. [1]W.L.Luken and D.N. Beratan, *Theo. Chim. Acta* **61**, 265-281 (1982). [2]M.R. Pederson, A. Ruzsinszky and J. P. Perdew, *J. Chem. Phys.* **140**, 121103 (2014). [3]M.R. Pederson and T. Baruah, *Advance in Atomic, Molecular and Optical Physics* **64**, 153-180 (2015). [4]M. R. Pederson, R. A. Heaton, and C. C. Lin, *J. Chem. Phys.* **80**, 1972 (1984).

### 11:51AM B31.00002 Fermi-orbitals for improved electronic structure calculations on coordination complexes.<sup>1</sup>

, DER-YOU KAO, Department of Mechanical and Aerospace Engineering, The George Washington University, MARK R. PEDERSON, Department of Chemistry, Johns Hopkins University, JAMES D. LEE, Department of Mechanical and Aerospace Engineering, The George Washington University — An improved density-functional formalism[1,2] proceeds by adopting the Perdew-Zunger expression for a self-interaction-corrected (SIC) density-functional energy but evaluates the total energy based on Fermi Orbitals (FOs). Each localized electron is represented by an FO, determined from the occupied Kohn-Sham orbitals and a semi-classical FO descriptor. The SIC energy is then minimized through the gradients of the energy with respect to these descriptors. In addition to providing a review of the methodology, work here identifies the need for an algorithm which thoroughly searches over initial configurations. The strategy for sampling and prioritizing initial configurations is described. Applications on coordination complexes are presented. The FO descriptors and FOs for semi-classical and quantum-mechanical understanding of bonding is discussed. Cohesive energies are improved and the eigenvalues are shifted downward relative to the standard DFT results. Spin-dependent vibrational spectra, as a possible means for spectroscopic determination of the transition-metal moment, are also presented. [1]Pederson et al, *JCP*, **140**, 121103 (2014). [2]Baruah & Pederson, *AAMOPS*, **64**, 153-180 (2015).

<sup>1</sup>DK acknowledges her fellowship from The George Washington University Institute of Nanotechnology.

### 12:03PM B31.00003 Fermi orbital self-interaction corrected electronic structure of molecules beyond local density approximation<sup>1</sup>

, TORSTEN HAHN, SIMON LIEBING, JENS KORTUS, Institute for Theoretical Physics, TU Freiberg, Germany, MARK PEDERSON, Department of Chemistry, Johns Hopkins University, Baltimore, Maryland 21218, USA — The correction of the self-interaction error that is inherent to all standard density functional theory (DFT) calculations is an object of increasing interest. We present our results on the application of the recently developed Fermi-orbital based approach for the self-interaction correction (FO-SIC) to a set of different molecular systems [1,2]. Our study covers systems ranging from simple diatomic to large organic molecules. Our focus lies on the direct estimation of the ionization potential from orbital eigenvalues and on the ordering of electronic levels in metal-organic molecules. Further, we show that the Fermi orbital positions in structurally similar molecules appear to be transferable. [1] M. R. Pederson, A. Ruzsinszky, and J. P. Perdew, *J. Chem. Phys.* **140**, 121103 (2014). [2] M. R. Pederson, *J. Chem. Phys.* **142**, 064112 (2015).

<sup>1</sup>Support by DFG FOR1154 is greatly acknowledged.

### 12:15PM B31.00004 Magnetic Exchange Couplings in Transition Metal Complexes from DFT<sup>1</sup>

, JUAN PERALTA, Dept of Physics and Sci of Adv. Mat. Program, Central Michigan Univ — In this talk I will review our current efforts for the evaluation of magnetic exchange couplings in transition metal complexes from density functional theory. I will focus on the performance of different DFT approximations, including a variety of hybrid density functionals, and show that hybrid density functionals containing approximately 30% Hartree-Fock type exchange are in general among the best choice in terms of accuracy. I will also describe a novel computational method to evaluate exchange coupling parameters using analytic self-consistent linear response theory. This method avoids the explicit evaluation of energy differences, which can become impractical for large systems. Our approach is based on the evaluation of the transversal magnetic torque between two magnetic centers for a given spin configuration using explicit constraints of the local magnetization direction *via* Lagrange multipliers. This method is applicable in combination with any modern density functional with a noncollinear spin generalization and can be utilized as a "black-box". I will show proof-of-concept calculations in frustrated  $\text{Fe}_7^{\text{III}}$  disk-shaped clusters, and dinuclear  $\text{Cu}^{\text{II}}$ ,  $\text{Fe}^{\text{III}}$ , and heteronuclear complexes.

<sup>1</sup>NSF DMR-1206920

### 12:27PM B31.00005 Local spin analyses using density functional theory

, BAYILEYEGN ABATE, JUAN PERALTA, Central Michigan University — Local spin analysis is a valuable technique in computational investigations magnetic interactions on mono- and polynuclear transition metal complexes, which play vital roles in catalysis, molecular magnetism, artificial photosynthesis, and several other commercially important materials. The relative size and complex electronic structure of transition metal complexes often prohibits the use of multi-determinant approaches, and hence, practical calculations are often limited to single-determinant methods. Density functional theory (DFT) has become one of the most successful and widely used computational tools for the electronic structure study of complex chemical systems; transition metal complexes in particular. Within the DFT formalism, a more flexible and complete theoretical modeling of transition metal complexes can be achieved by considering noncollinear spins, in which the spin density is 'allowed to' adopt noncollinear structures in stead of being constrained to align parallel/antiparallel to a universal axis of magnetization. In this meeting, I will present local spin analyses results obtained using different DFT functionals. Local projection operators are used to decompose the expectation value  $\langle S^2 \rangle$  of the total spin operator; first introduced by Clark and Davidson.

### 12:39PM B31.00006 The Lieb-Oxford bound and the exchange-correlation kernel from the strictly-correlated electrons functional<sup>1</sup>

, PAOLA GORI-GIORGI, VU University Amsterdam — I will present some recent results based on the strictly-correlated electrons (SCE) functional: 1) a rigorous method to set lower bounds to the optimal particle-number dependent constant appearing in the Lieb-Oxford bound, and 2) an investigation of exact properties in the time domain, including an analytical expression for the kernel in one-dimension, with an analysis of its behavior for the case of bond-breaking excitations.

<sup>1</sup>ERC Consolidator Grant 648932

**1:15PM B31.00007 Exchange-correlation functionals from a local interpolation along the adiabatic connection**, STEFAN VUCKOVIC, VU University Amsterdam, TOM IRONS, ANDREW TEALE, Nottingham University, ANDREAS SAVIN, UPMC Paris, PAOLA GORI-GIORGI, VU University Amsterdam — We use the adiabatic connection formalism to construct a density functional by doing an interpolation between the weak and the strong coupling regime. Combining the information from the two limits, we are able to construct an exchange-correlation (xc) density functional free of the bias towards weakly correlated system, which is present in the majority of approximate xc functionals. Previous attempts in doing the interpolation between the two regimes, such as the interaction strength interpolation (ISI), had a fundamental flaw: the lack of size-consistency, as the corresponding functional depends non-linearly on the global (integrated over all space) ingredients. To recover size-consistency in such a framework, we move from the global to local quantities. We use the energy densities as local quantities in the gauge of the electrostatic potential of the xc hole. We use the “strictly-correlated electrons” (SCE) approach to compute the energy densities in the strong-coupling limit and the Lieb maximization algorithm to extract the energy densities from the low-coupling regime. We then test the accuracy of the local interpolation schemes by using the nearly exact local energy densities. In this talk I am going to present our results with the emphasis on strongly correlated systems.

**1:27PM B31.00008 The exact density functional for two electrons in one dimension**, ARON COHEN, University of Cambridge, PAULA MORI-SANCHEZ, Universidad Autonoma de Madrid — The exact universal density functional  $F[\rho]$  is calculated for real space two-electron densities in one dimension  $\rho(x)$  with a soft-Coulomb interaction. It is calculated by the Levy constrained search  $F[\rho] = \min_{\Psi \rightarrow \rho} \langle \Psi | \hat{T} + \hat{V}_{ee} | \Psi \rangle$  over wavefunctions of a two-dimensional Hilbert space  $\Psi(x_1, x_2) \rightarrow \rho(x_1)$  and can be directly visualized. We do an approximate constrained search via density matrices and a direct approximation to natural orbitals. This allows us to make an accurate approximation to the exact functional that is calculated using a search over potentials. We investigate the exact functional and the performance of many approximations on some of the most challenging electronic structure in two-electron systems, from strongly-correlated electron transfer to the description of a localized-delocalized transition. The exact Kohn-Sham potential,  $v_s(x)$ , and exact Kohn-Sham eigenvalues,  $\epsilon_i$ , are calculated and this allows us to discuss the band-gap problem versus the perspective of the exact density functional  $F[\rho]$  for all numbers of electrons. We calculate the derivative discontinuity of the exact functional in an example of a Mott-Insulator, one-dimensional stretched  $H_2$ .

**1:39PM B31.00009 Landscape of the exact energy functional for a simplified universe**, PAULA MORI-SANCHEZ, Universidad Autonoma de Madrid, ARON COHEN, University of Cambridge — One of the great challenges of electronic structure theory is the quest for the exact functional of density functional theory (DFT). Its existence is proven, but it is a complicated multivariable functional that is almost impossible to conceptualize. In this talk we study the asymmetric two-site Hubbard model because it has only a two-dimensional universe of density matrices, hence the exact functional becomes a simple function of two variables whose three dimensional energy landscape can be visualized and explored. A walk on this unique landscape, tilted to an angle defined by the one-electron Hamiltonian, gives a valley whose minimum is the exact total energy. This is contrasted with the landscape of some approximate functionals, explaining their failure for electron transfer in the strongly correlated limit. We show concrete examples of pure-state density matrices that are not  $v$ -representable due to the underlying non-convex nature of the energy landscape. The exact functional is calculated for all numbers of electrons, including fractional, allowing the derivative discontinuity to be visualized and understood. The fundamental gap for all possible systems is obtained solely from the derivatives of the exact functional.

**1:51PM B31.00010 Spontaneous charge carrier localization in extended one-dimensional systems**, VOJTĚCH VLČEK<sup>1</sup>, HELEN EISENBERG, Hebrew University of Jerusalem, Israel, GERD STEINLE-NEUMANN, Bayerisches Geoinstitut, Universität Bayreuth, Germany, ROI BAER, Hebrew University of Jerusalem, Israel — Charge carrier localization in extended atomic systems can be driven by disorder, point defects or distortions of the ionic lattice. Herein we give first-principles theoretical computational evidence that it can also appear as a purely electronic effect in otherwise perfectly ordered periodic structures and we show that electronic eigenstates can spontaneously localize upon excitation. Optimally-tuned range separated density functional calculations reveal that in trans-polyacetylene and polythiophene the hole density localizes on a length scale of several nanometers. This is due to exchange induced translational symmetry breaking of the charge density. Ionization potentials, optical absorption peaks, excitonic binding energies and the optimally-tuned range parameter itself all become independent of polymer length when it exceeds the critical localization length scale. These first-principles findings show, for the first time, that charge localization is not caused by lattice distortion but rather it is their cause, changing the physical models of polaron formation and dynamics, helping to explain experimental findings that polarons in conjugated polymers form instantaneously after exposure to ultrafast light pulses.

<sup>1</sup>secondary affiliation: Bayerisches Geoinstitut, Universität Bayreuth, Germany

**2:03PM B31.00011 Self-consistent calculation of Hubbard U parameters within linear-scaling DFT**, GLENN MOYNIHAN, School of Physics, CRANN and AMBER, Trinity College Dublin, GILBERTO TEOBALDI, Stephenson Institute, University of Liverpool, DAVID D. O'REGAN, School of Physics, CRANN and AMBER, Trinity College Dublin — DFT+U has proven to be a computationally efficient method for correcting for the underestimation of electron localization effects, or for the absent derivative discontinuity, inherent in conventional density functionals. Invoking an approximate interpretation of DFT+U as a corrective penalty functional for the spurious curvature of the total-energy with respect to subspace occupancy, the Hubbard U parameter may be calculated [1,2], in which case DFT+U may be considered to be fully first-principles approach. We describe our approach for computing the Hubbard U and Hund's J parameters within ONETEP, a linear-scaling DFT code which comprises a complete DFT+U+J [3] implementation including ionic forces and a flexible choice of population analyses [4,5]. We discuss issues of charge preservation and self-consistency, and we demonstrate the capability of our method by means of numerical tests on the ground-state properties of selected molecules that present challenges for approximate DFT. [1] W. E. Pickett, et al., Phys. Rev. B, 58, 1201 (1998). [2] H. J. Kulik, et al., Phys. Rev. Lett. 97, 103001 (2006). [3] B. Himmetoglu, et al., Phys. Rev. B 84, 115108 (2011). [4] D. D. O'Regan, et al., Phys. Rev. B 85, 085107 (2012). [5] D. D. O'Regan, et al., Phys. Rev. B 83, 245124 (2011).

**Monday, March 14, 2016 11:15AM - 2:15PM—**

**Session B32 DCP: Emerging Nanomaterials for Solar Energy Conversion I** 332 - Gordana Dukovic, University of Colorado

**11:15AM B32.00001 TBA**, MICHAEL GRAETZEL, Ecole Polytechnique Federale de Lausann, EPFL — No abstract available.

**11:51AM B32.00002 First-principles determination of the structural, vibrational, and thermodynamic properties of Methylammonium Lead Iodide Perovskite**, WISSAM SAIDI, University of Pittsburgh, WISSAM SAIDI TEAM — Intrinsic energy-loss processes in solar cells ultimately increase the operational temperature, which can have profound effect on the power conversion efficiency of solar cells. Here I report investigations on the temperature effects on structural and mechanical properties of  $CH_3NH_3PbI_3$  using well-converged first-principles calculations with van der Waals dispersion corrections. The computed lattice parameters for cubic and tetragonal phases at finite temperature are found within 1% of experimentally measured values. Furthermore, the finite-temperature potential energy surface shows how the mechanical properties of the cubic and tetragonal phases of  $CH_3NH_3PbI_3$  evolve with temperature. Finally, I discuss the implications of these calculations on the nature of the tetragonal-to-cubic phase transition, and show that the underpinnings of this transition can be largely attributed to the phonons associated with methylammonium cations.

**12:03PM B32.00003 Rashba Spin-Orbit Coupling Enhanced Carrier Lifetime in  $\text{CH}_3\text{NH}_3\text{PbI}_3$** <sup>1</sup>, FAN ZHENG, LIANG Z. TAN, University of Pennsylvania, SHI LIU, Carnegie Institution for Science, ANDREW M. RAPPE, University of Pennsylvania — Organometal halide perovskites are promising solar-cell materials for next-generation photovoltaic applications, in particular these materials have long carrier lifetime and diffusion length. Recently, the strong spin-orbit coupling of organometal halide perovskites have attracted the great attention, the consequences of the Rashba effect, driven by this strong spin-orbit coupling, on the photovoltaic properties of these materials are largely unexplored. In this work, taking the electronic structure of methylammonium lead iodide as an example, we propose an intrinsic mechanism for enhanced carrier lifetime in 3D Rashba materials. Based on first-principles calculations and a Rashba spin-orbit model, we demonstrate that the recombination rate is reduced due to the spin-forbidden transition. These results are important for understanding the fundamental physics of organometal halide perovskites and for optimizing and designing the materials with better performance. The proposed mechanism including spin degrees of freedom offers a new paradigm of using 3D Rashba materials for photovoltaic applications.

<sup>1</sup>This work was supported by Department of Energy, Office of Naval Research, National Science Foundation. Computational support was from the HPCMO of the DOD and the NERSC center of the DOE.

**12:15PM B32.00004 Rotational Dynamics of Organic Cations in  $\text{CH}_3\text{NH}_3\text{PbI}_3$  Perovskite**, TIANRAN CHEN, BENJAMIN FOLEY, Univ of Virginia, BAHAR IPEK, Univ of Delaware, MADHUSUDAN TYAGI, JOHN COPLEY, CRAIG BROWN, NCNR, JOSHUA CHOI, SEUNG-HUN LEE, Univ of Virginia — Methylammonium lead iodide ( $\text{CH}_3\text{NH}_3\text{PbI}_3$ ) based solar cells have shown impressive power conversion efficiencies of above 20%. However, the microscopic mechanism of the high photovoltaic performance is yet to be fully understood. Particularly, the dynamics of  $\text{CH}_3\text{NH}_3^+$  cations and their impact on relevant processes are still poorly understood. Using elastic and quasi-elastic neutron scattering techniques and group theoretical analysis, we studied rotational modes of the  $\text{CH}_3\text{NH}_3^+$  cation in  $\text{CH}_3\text{NH}_3\text{PbI}_3$ .<sup>[1]</sup> Our results show that, in the cubic and tetragonal phases, the  $\text{CH}_3\text{NH}_3^+$  ions exhibit four-fold rotational symmetry of the C-N axis ( $C_4$ ) along with three-fold rotation around the C-N axis ( $C_3$ ), while in orthorhombic phase only  $C_3$  rotation is present. Around room temperature, the characteristic relaxation time for the  $C_4$  rotation is found to be 5ps while for the  $C_3$  rotation is 1ps. The T-dependent rotational relaxation times were fitted with Arrhenius equations to obtain activation energies. Our data show a close correlation between the  $C_4$  rotational mode and the temperature dependent dielectric permittivity. Our findings on the rotational dynamics of  $\text{CH}_3\text{NH}_3^+$  and the associated dipole have important implications on understanding the low exciton binding energy and slow charge recombination rate in  $\text{CH}_3\text{NH}_3\text{PbI}_3$  which are directly relevant for the high solar cell performance. [1] T. Chen et al., Phys. Chem. Chem. Phys., 2015, DOI: 10.1039/C5CP05348J.

**12:27PM B32.00005 Imaging the long diffusion lengths of photo-generated carriers in mixed halide perovskite films**<sup>1</sup>, SHUHAO LIU, Department of Physics, Case Western Reserve University, LILI WANG, CLEMENS BURDA, Department of Chemistry, Case Western Reserve University, XUAN GAO, Department of Physics, Case Western Reserve University — Organometal halide perovskite has emerged as a promising photovoltaic material due to its low-cost synthesis process and outstanding performance. Though long diffusion length of photo-generated carriers plays a very important role in its success, a direct measurement of carrier diffusion lengths is still lacking. We fabricated highly crystalline  $\text{CH}_3\text{NH}_3\text{PbI}_{3-x}\text{Cl}_x$  thin film devices on  $\text{SiO}_2/\text{Si}$  substrate with either nickel or gold as contact electrodes and parylene as encapsulation layer. By performing spatially scanned photocurrent imaging measurement with a local illumination spot, we show that photo-generated carriers in the prepared perovskite have very long diffusion lengths, with hole diffusion length  $L_h = 22 \pm 7 \mu\text{m}$  and electron diffusion length  $L_e = 8 \pm 4 \mu\text{m}$ . Our work provides scanning photocurrent microscopy as a powerful tool to directly extract hole and electron diffusion lengths at the same time, and may be further used to elucidate the vastly different carrier diffusion lengths (on order of 100nm to 100 $\mu\text{m}$ ) in organometal halide perovskites prepared by different methods.

<sup>1</sup>X.G. and S.L. thank NSF (grant DMR-1151534) and AFOSR (grant FA9550-12-1-0441) for funding support.

**12:39PM B32.00006 Characterizing structural overpotentials for bubble evolution on nanostructured semiconductor-electrocatalyst interfaces**, ROBERT H. CORIDAN, Department of Chemistry and Biochemistry, University of Arkansas — Nanostructured electrocatalysts can improve the kinetics of solar-driven photocatalysis at a semiconductor-liquid junction while minimizing the effect on the energetics of that junction. A relevant example is Pt-decorated Si electrodes for hydrogen evolution from water splitting. Nanostructuring can also impair the reaction kinetics by introducing mass transport overpotentials. For reactions that evolve gas, the active surface area can be blocked by bubbles on discrete catalytic sites, possibly halting the reaction entirely. Here, we explore these issues by measuring the high-frequency dynamics of bubbles evolved from nanostructured electrocatalysts at a semiconductor-electrolyte interface. Using transmission x-ray phase contrast microscopy, we can image gas-evolving reactions as a way to directly measure the effects of adhesion, catalyst structure, and buoyancy on the reaction kinetics. From these measurements, we develop a model for electrolytic bubble evolution and transport that considers coalescence on neighboring sites, surface interactions, and the non-equilibrium shape dynamics of bubbles. This model can be used to identify favorable catalyst motifs that promote bubble clearance and mitigate their influence on reaction kinetics for water splitting applications.

**12:51PM B32.00007 TBA**, GORDANA DUKOVIC, University of Colorado — No abstract available.

**1:27PM B32.00008 Highly stable bimetallic AuIr/TiO<sub>2</sub> catalyst: physical origin of the intrinsic stability against sintering.**, ERNESTO MARINERO, CHAN WAN HAN, School of Materials Engineering, Purdue University, PAULAMI MAJUNDAR, School of Chemical Engineering, Purdue University, ANTONIO AGUILAR-TAPIA, RODOLFO ZANELLA, CCADET, Universidad Nacional Autonoma de Mexico, JEFFREY GREELEY, School of Chemical Engineering, Purdue University, VOLKAN OTARLAN, School of Materials Engineering, Purdue University — It has been a long-lived research topic in the field of heterogeneous catalysis to find a way to stabilizing supported Au catalysts against sintering. Herein, we report highly stable AuIr bimetallic nanoparticles on TiO<sub>2</sub> synthesized by sequential deposition-precipitation. To understand the physical origin of the high stability AuIr/TiO<sub>2</sub> system, we have used scanning transmission electron microscopy (STEM), STEM-tomography and density functional theory (DFT) calculations. 3D structures of AuIr/TiO<sub>2</sub> obtained by STEM-tomography indicate that AuIr nanoparticles on TiO<sub>2</sub> have intrinsically lower free energy and less driving force for sintering than Au nanoparticles. DFT calculations on segregation behavior of AuIr slabs on TiO<sub>2</sub> showed that the presence of Ir near the TiO<sub>2</sub> surface increases the adhesion energy of the bimetallic slabs to the TiO<sub>2</sub> and the attractive interactions between Ir and TiO<sub>2</sub> lead to higher stability of the AuIr nanoparticles compared to Au nanoparticles.

**1:39PM B32.00009 Surface Proton Hopping and Coupling Pathway of Water Oxidation on Cobalt Oxide Catalyst.**, HIEU PHAM, Lawrence Berkeley National Laboratory, MU-JENG CHENG, University of California, Berkeley, HEINZ FREI, LIN-WANG WANG, Lawrence Berkeley National Laboratory — We propose an oxidation pathway of water splitting on cobalt oxide surface with clear thermodynamic and kinetic details. The density-functional theory studies suggest that the coupled proton-electron transfer is not necessarily sequential and implicit in every elementary step of this mechanistic cycle. Instead, the initial O-O bond could be formed by the landing of water molecule on the surface oxos, which is then followed by the dispatch of protons through the hopping manner and subsequent release of di-oxygen. Our theoretical investigations of intermediates and transition states indicate that all chemical conversions in this pathway, including the proton transfers, are possible with low activation barriers, in addition to their favorable thermodynamics. Our hypothesis is supported by recent experimental observations of surface superoxide that is stabilized by hydrogen bonding to adjacent hydroxyl group, as an intermediate on fast-kinetics catalytic site.

**1:51PM B32.00010 The Dye Sensitized Photoelectrosynthesis Cell (DSPEC) for Solar Water Splitting and CO<sub>2</sub> Reduction<sup>1</sup>** , THOMAS MEYER, LEILA ALIBABAEI, BENJAMIN SHERMAN, MATTHEW SHERIDAN, University of North Carolina at Chapel Hill, DENNIS ASHFORD, Eastman Chemical, ALEX LAPIDES, KYLE BRENNAMAN, ANIMESH NAYAK, SUBHANGI ROY, KYUNG-RYANG WEE, MELISSA GISH, JERRY MEYER, JOHN PAPANIKOLAS, University of North Carolina at Chapel Hill — The dye-sensitized photoelectrosynthesis cell (DSPEC) integrates molecular level light absorption and catalysis with the bandgap properties of stable oxide materials such as TiO<sub>2</sub> and NiO. Excitation of surface-bound chromophores leads to excited state formation and rapid electron or hole injection into the conduction or valence bands of n or p-type oxides. Addition of thin layers of TiO<sub>2</sub> or NiO on the surfaces of mesoscopic, nanoparticle films of semiconductor or transparent conducting oxides to give core/shell structures provides a basis for accumulating multiple redox equivalents at catalysts for water oxidation or CO<sub>2</sub> reduction.

<sup>1</sup>UNC EFRC Center for Solar Fuels, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001011

**2:03PM B32.00011 The Interface Between Chemical and Oxide Materials in the DSPEC.<sup>1</sup>** , THOMAS MEYER, LEILA ALIBABAEI, BENJAMIN SHERMAN, MATTHEW SHERIDAN, University of North Carolina at Chapel Hill, DENNIS ASHFORD, Eastman Chemical, ALEX LAPIDES, KYLE BRENNAMAN, ANIMESH NAYAK, SUBHANGI ROY, University of North Carolina at Chapel Hill — Significant challenges exist for both chemical and oxide materials in the Dye Sensitized Photoelectrosynthesis Cell (DSPEC) for water oxidation or CO<sub>2</sub> reduction. They arise from light absorption, the energetics of electron or hole injection, the accumulation of multiple redox equivalents at catalysts for water oxidation or water/CO<sub>2</sub> reduction in competition with back electron transfer, and sustained, long term performance. These challenges are being met by the use of a variety of chromophores (metal complexes, organic dyes, porphyrins), broad application of nanoparticle mesoscopic oxide films, atomic layer deposition (ALD) to prepare core/shell and stabilizing overlayer structures, and recent advances in the molecular catalysis of water oxidation and CO<sub>2</sub> reduction.

<sup>1</sup>UNC EFRC Center for Solar Fuels, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001011

## **Monday, March 14, 2016 11:15AM - 2:15PM – Session B33 DPOLY: Polymers in Batteries 336 - Brad Frieberg, NIST**

**11:15AM B33.00001 Correlating morphology to dc conductivity in polymerized ionic liquids<sup>1</sup>** , CIPRIAN IACOB, Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA 16802 USA, ATSUSHI MATSUMOTO, TADASHI INOUE, Department of Macromolecular Science, Osaka University, Toyonaka, Osaka 560-0043 Japan, JAMES RUNT, Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA 16802 USA — Polymerized ionic liquids (PILs) combine the attractive mechanical characteristics of polymers and unique physico-chemical properties of low molecular weight ionic liquids in the same material. PILs have shown remarkable advantages when employed in electrochemical devices such as dye-sensitized solar cells and lithium batteries, among others. Understanding their ionic transport mechanism is the key for designing highly conductive PILs. In the current study, the correlation between morphology and charge transport in two homologous series of PILs with systematic variation of the alkyl chain length and anions is investigated using broadband dielectric spectroscopy, rheology, differential scanning calorimetry and X-ray scattering. As the alkyl chain length increases, the backbone-to-backbone separation increases, and dc-conductivity consequently decreases. The cations dominate structural dynamics since they are attached to the polymer chains, while the anions are smaller and more mobile ionic species thereby controlling the ionic conductivity. Further interpretation of decoupling of dc conductivity from the segmental relaxation enabled the correlation between polymer morphology and dc conductivity.

<sup>1</sup>Supported by the National Science Foundation, Polymers Program

**11:27AM B33.00002 Formation and growth of lithium metal dendrites through solid block copolymer membranes** , KATHERINE HARRY, UC Berkeley, KENNETH HIGA, Lawrence Berkeley National Laboratory, NITASH BALSARA, UC Berkeley — Dendrite growth from lithium metal in electrochemical systems is the primary problem that precludes the wide use of lithium metal as an anode material. While polystyrene-block-poly(ethylene oxide) copolymer electrolytes extend cell life by suppressing dendrite growth, dendrites eventually do grow and the batteries fail by a short-circuit. *In situ* hard X-ray microtomography experiments coupled with stress simulations shed light on the formation and growth of dendritic structures through stiff solid polymer electrolyte membranes.

**11:39AM B33.00003 All Solid-State Lithium Metal Batteries Using Cross-linked Polymer Electrolytes** , QIWEI PAN, CHRISTOPHER LI, Drexel University, SOFT MATERIALS TEAM — Nowadays, to prepare all solid-state lithium metal batteries with high rate capability and stability using solid polymer electrolytes (SPEs) is still a grand challenge because of the interfaces between the SPE and the electrodes. In this presentation, we report a series of hybrid SPEs with controlled network structures by using POSS as cross-linker. These hybrid network SPEs show promising ionic conductivity, mechanical properties, and lithium dendrite growth resistance. All solid-state LiFePO<sub>4</sub>/Li batteries were also prepared using these SPEs as the electrolytes to study the effect of conductivity and mechanical properties of the SPEs on the performance of the batteries. At 90 °C, the prepared cells show high rate capability and stability. Capacity up to 160 mAh/g can be obtained at a C/2 rate during the galvanostatic cycling. Capacity retention of the cells is higher than 80% after 250 cycles. Battery performance at 60 °C and decay mechanism of the batteries will also be discussed.

## 11:51AM B33.00004 NMR Investigations of Structure and Dynamics in Polymers for Energy Storage Applications<sup>1</sup>

, STEVEN GREENBAUM, Hunter College of the City University of New York — Materials innovation is needed to realize major progress in energy storage capacity for lithium batteries and capacitors. Polymers hold considerable promise as ion conducting media in batteries and electrochemical capacitors and as dielectrics in thin film capacitors. Structural studies of materials utilized in lithium battery technology are hampered by the lack of long-range order found in well-defined crystalline phases. Powder x-ray diffraction yields structural parameters that have been averaged over hundreds of lattice sites, and is unable to provide structural information about amorphous phases. Our laboratory uses solid state nuclear magnetic resonance (NMR) methods to investigate structural and chemical aspects of lithium ion cathodes, anodes, electrolytes, interfaces and interphases. NMR is element- (nuclear-) specific and sensitive to small variations in the immediate environment of the ions being probed, for example  $\text{Li}^+$ , and in most cases is a reliably quantitative spectroscopy in that the integrated intensity of a particular spectral component is directly proportional to the number of nuclei in the corresponding material phase. NMR is also a powerful tool for probing ionic and molecular motion in lithium battery electrolytes with a dynamic range spanning some ten orders of magnitude through spin-lattice relaxation and self-diffusion measurements. Broadband relaxometry based on Fast Field Cycling NMR (FFCNMR) methods can span three to four of these orders of magnitude in a single set of measurements. Results of several recent NMR investigations performed on our lab will be presented. We explore the ion transport mechanism in polyether-based and lithium polymer electrolytes and those based on other base polymers, in particular, the extent to which ionic motion is coupled to polymer segmental motion. Polycarbonates are being considered as a possible replacement for polypropylene in high power thin film capacitors due to their favorable dielectric properties. We investigate the effects of incorporation of two types of additives in the polymer film on the ring-flip motions corresponding to the  $\gamma$  relaxation: (i) high dielectric constant ceramic particles; (ii) polar organic diluent molecules. The low frequency realm of broadband relaxometry allows meaningful comparison with dielectric relaxation studies of these samples performed by collaborators.

<sup>1</sup>Work Supported in part by the U.S. Office of Naval Research

## 12:27PM B33.00005 Li conductivity in siloxane-based polymer electrolytes

, ERIC STACY, Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, United States, FEI FAN, HONGBO FENG, CATALIN GAINARU, JIMMY MAYS<sup>1</sup>, ALEXEI SOKOLOV<sup>2</sup>, Department of Chemistry, University of Tennessee, Knoxville, Tennessee 37996, United States — Polymer electrolytes containing lithium ions are ideal candidates for electrochemical devices and energy storage applications. Understanding their ionic transport mechanism is the key for rational designing of highly conductive polymer matrices. Complementing dielectric spectroscopy investigations by results from rheology and differential scanning calorimetry we focused on the interplay between dynamics of lithium ions and the polymer matrix based on polysiloxane backbone. Our results demonstrate that the conductivity and the degree of decoupling between ion dynamics and structural relaxation depend strongly not only on the ions concentration, but also on the polarity and size of the polymeric side-groups.

<sup>1</sup>Chemical Science Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, United States

<sup>2</sup>Chemical Science Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, United States

## 12:39PM B33.00006 Systematic Experimental and Computational Investigation of Ion Transport in Novel Polyether Electrolytes

, DANIELLE PESKO, University of California, Berkeley, MICHAEL WEBB, California Institute of Technology, YUKYUNG JUNG, QI ZHENG, Cornell University, THOMAS MILLER III, California Institute of Technology, GEOFFREY COATES, Cornell University, NITASH BALSARA, University of California, Berkeley — Polyethers, such as poly(ethylene oxide) (PEO), are considered to be the most promising polymer electrolyte materials due to their high ionic conductivity and electrochemical stability, both essential for battery applications. To gain a fundamental understanding of the transport properties of polyether systems, we design a systematic set of linear PEO-like polymers to explore the effect of adding carbon spacers to the backbone of the chain. Ac impedance spectroscopy is employed to measure the ionic conductivity of polyether/lithium salt electrolytes; the results elucidate tradeoffs between lowering the glass transition temperature and diluting the polar groups on the polymer chain. Molecular-level insight is provided by molecular dynamics simulations of the polyether electrolytes. We define the useful and intuitive metric of “connectivity”, a parameter calculated from simulations which describes the physical arrangements of solvation sites in a polymer melt. Direct comparison of experiment and theory allows us to determine the relationship between connectivity and conductivity. The comparison provides insight regarding the factors that control conductivity, and highlights considerations that must be taken when designing new ion-conducting polymers.

## 12:51PM B33.00007 Highly Flexible Self-Assembled $\text{V}_2\text{O}_5$ Cathodes Enabled by Conducting Diblock Copolymers

, HYOSUNG AN, JARED MIKE, Texas AM University, KENDALL SMITH, LISA SWANK, YEN-HAO LIN, STACY PESEK, RAFAEL VERDUZCO, Rice University, JODIE LUTKENHAUS, Texas AM University — Structural energy storage materials combining load-bearing mechanical properties and high energy storage performance are desired for applications in wearable devices or flexible displays. Vanadium pentoxide ( $\text{V}_2\text{O}_5$ ) is a promising cathode material for possible use in flexible battery electrodes, but it remains limited by low  $\text{Li}^+$  diffusion coefficient and electronic conductivity, severe volumetric changes upon cycling, and limited mechanical flexibility. Here, we demonstrate a route to address these challenges by blending a diblock copolymer bearing electron- and ion-conducting blocks, poly(3-hexylthiophene)-*block*-poly(ethyleneoxide) (P3HT-*b*-PEO), with  $\text{V}_2\text{O}_5$  to form a mechanically flexible, electro-mechanically stable hybrid electrode.  $\text{V}_2\text{O}_5$  layers were arranged parallel in brick-and-mortar-like fashion held together by the P3HT-*b*-PEO binder. This unique structure significantly enhances mechanical flexibility, toughness and cyclability without sacrificing capacity. Electrodes comprised of 10 wt% polymer have unusually high toughness ( $293 \text{ kJ/m}^3$ ) and specific energy ( $530 \text{ Wh/kg}$ ), both higher than reduced graphene oxide paper electrodes.

## 1:03PM B33.00008 Effects of plasticization on ionic conductivity enhancement of crosslinked polymer electrolyte membrane

, RUIXUAN HE, THEIN KYU, University of Akron, DR. KYU'S TEAM — Glass transition temperatures ( $T_g$ ) of solid polymer electrolyte membranes (PEM), comprised of polyethylene glycol diacrylate (PEGDA) prepolymer, lithium bis(trifluoromethanesulfonyl) imide (LiTFSI) salt, and succinonitrile (SCN) plasticizer, were systematically examined before and after crosslinking in the isotropic region guided by their ternary phase diagram. With increasing LiTFSI concentration, the  $T_g$  of uncured binary PEGDA/LiTFSI mixture increases drastically due to molecular complexation between lithium cation and ether oxygen, but ionic conductivity is very low ( $<10^{-6} \text{ S cm}^{-1}$ ). Upon curing, this  $T_g$  increases and further reduces ionic conductivity. Upon adding SCN plasticizer, the  $T_g$  of PEM has significantly decreased to  $-60^\circ\text{C}$  and ionic conductivity also increased to the superionic conductor level of  $10^{-3} \text{ S cm}^{-1}$ . The analysis of ionic conductivity vs.  $T_g$  behavior by Vogel-Tamman-Fulcher(VTF) equation revealed that this ionic conductivity enhancement is due to SCN plasticization resulting in lowering the network  $T_g$  as well as lowering the activation energy. Supported by NSF-DMR 1161070.

## 1:15PM B33.00009 Atomistic Simulations of Ternary Polymer Electrolytes Containing Ionic Liquids: Ion Transport and Viscoelastic Behavior

, SANTOSH MOGURAMPELLY, VENKAT GANESAN, Univ of Texas, Austin — Influence of the BMIMPF<sub>6</sub> ionic liquid on ion transport and viscoelastic properties of ternary polymer electrolytes containing polyethylene oxide solvated with LiPF<sub>6</sub> salt and the underlying mechanisms are investigated. By employing atomistic molecular dynamics and trajectory extended kinetic Monte Carlo simulation techniques, we observe enhanced ionic mobilities and conductivities of the PEO/LiPF<sub>6</sub>-BMIMPF<sub>6</sub> ternary electrolytes upon the addition ionic liquid into the PEO/LiPF<sub>6</sub> binary electrolyte. The dispersion of the BMIMPF<sub>6</sub> ionic liquid into the PEO/LiPF<sub>6</sub> electrolyte is found to (a) promote dissociation of existing LiPF<sub>6</sub> ion-pairs and (b) slightly accelerate the polymer segmental dynamics. Together, these effects are observed to collectively give rise to an increase in ionic mobilities and conductivities of the ternary polymer electrolyte. On the other hand, Rouse analysis reveals that the storage and loss modulus of the ternary polymer electrolytes are coupled to their ion conducting properties.

**1:27PM B33.00010 Effects of cation and anion solvation on ion transport in functionalized perfluoropolyethers electrolytes**, KSENIA TIMACHOVA, MAHATI CHINTAPALLI, Univ of California - Berkeley, KEVIN OLSEN, JOSEPH DESIMONE, University of North Carolina - Chapel Hill, NITASH BALSARA, Univ of California - Berkeley — Advances in polymer electrolytes for use in lithium batteries have been limited by the incorporation of selective lithium binding groups that provide necessary solvation for the lithium but ultimately restrict the mobility of the lithium ions relative to anions. Perfluoropolyether electrolytes (PFPE) are a new class of nonflammable liquid polymer electrolytes that have been functionalized with solvating groups for both lithium ions and fluorinated anions. PFPEs with different endgroups mixed with  $\text{LiN}(\text{SO}_2\text{CF}_3)_2$  salt have shown substantial differences in conductivity and allows us to investigate the effects of varying solvating environments on ion transport. To study the independent motion of cations and anions in these systems, the individual diffusion coefficients of the  $\text{Li}^+$  and  $(\text{SO}_2\text{CF}_3)_2^-$  ions were measured using pulsed-field gradient nuclear magnetic resonance (PFG-NMR). Comparing conductivity calculated using these diffusion coefficients with electrochemical measurements yields an estimation for the number of charge carrier in the system. The amount of salt dissociation, not the mobility of the salt, is the primary driver of differences in electrochemical conductivities between PFPEs with different solvating groups.

**1:39PM B33.00011 Aggregate-mediated charge transport in ionomeric electrolytes**, KERAN LU, JANNA MARANAS, SCOTT MILNER, Pennsylvania State University — Polymers such PEO can conduct ions, and have been studied as possible replacements for organic liquid electrolytes in rechargeable metal-ion batteries. More generally, fast room-temperature ionic conduction has been reported for a variety of materials, from liquids to crystalline solids. Unfortunately, polymer electrolytes generally have limited conductivity; these polymers are too viscous to have fast ion diffusion like liquids, and too unstructured to promote cooperative transport like crystalline solids. Ionomers are polymer electrolytes in which ionic groups are covalently bound to the polymer backbone, neutralized by free counterions. These materials also conduct ions, and can exhibit strong ionic aggregation. Using coarse-grained molecular dynamics, we explore the forces driving ionic aggregation, and describe the role ion aggregates have in mediating charge transport. The aggregates are string-like such that ions typically have two neighbors. We find ion aggregates self-assemble like worm-like micelles. Excess charge, or free ions, occasionally coordinate with aggregates and are transported along the chain in a Grotthuss-like mechanism. We propose that controlling ionomer aggregate structure through materials design can enhance cooperative ion transport.

**1:51PM B33.00012 Versatile cation transport in imidazolium based polymerized ionic liquids**, CHRISTOPHER EVANS, UCSB, RACHEL SEGALMAN, University of California, Santa Barbara — Polymerized ionic liquids (PIL) with tethered imidazolium groups are able to conduct a diverse array of cations relevant for energy applications. The well-known complexation of imidazolium with transition metals is exploited to bind ions such as  $\text{H}^+$ ,  $\text{Li}^+$ ,  $\text{Cu}^{2+}$ , and  $\text{Ni}^{2+}$  by doping the neutral PIL with the appropriate Cation-TFSI $^-$  salt. Conductivities were first determined via AC impedance indicating that  $\text{H}^+$  salts lead to the highest conductivity (due to low ion mass and potential Grotthuss mechanism) followed by  $\text{Cu}^{2+}$ ,  $\text{Li}^+$ ,  $\text{Ag}^+$ , and  $\text{Ni}^{2+}$ . The equilibrium constant for imidazolium complexation is larger for  $\text{Cu}^{2+}$  relative to  $\text{Li}^+$ ,  $\text{Ag}^+$ , and  $\text{Ni}^{2+}$  imidazolium complexes leading to greater salt dissociation and higher conductivities. For LiTFSI and CuTFSI $_2$  salts, metallic lithium or copper electrodes were employed in battery cells to pass a steady DC current and confirm that the cations are in fact carrying current. Interestingly, the divalent  $\text{Cu}^{2+}$  also ionically crosslinks the polymer leading to a plateau in the viscosity. Thus, divalent ions provide a unique route to high conductivity, high modulus polymeric electrolytes. Future studies involving ZnTFSI $_2$  and MgTFSI $_2$  for battery applications are proposed to examine how versatile the PIL platform is for cation transport.

**2:03PM B33.00013 Ion conduction in high ion content PEO-based ionomers.**, DAVID CALDWELL II, JANNA MARANAS, Pennsylvania State University — Solid Polymer Electrolytes (SPEs) can enable the design of batteries that are safer and have higher capacity than batteries with traditional volatile organic electrolytes. The current limitation for SPEs is their low conductivity, resulting from a conduction mechanism strongly coupled to the dynamics of the polymer host matrix. Our previous work indicated the possibility of a conduction mechanism through the use of ion aggregates. In order to investigate this mechanism, we performed a series of molecular dynamics simulations of PEO-based ionomers at high ion content. Our results indicate that conduction through ion aggregates are partially decoupled from polymer dynamics and could enable the development of higher conductive SPEs.

**Monday, March 14, 2016 11:15AM - 2:03PM –**  
**Session B34 DPOLY DCOMP FIAP: Where Simulation, Theory, and Experiment Meet Across Length Scales I** 337 - Robert Riggelman, University of Pennsylvania

**11:15AM B34.00001 Theory of Chirality Transfer in Block Copolymer Melts**, ISHAN PRASAD, GREGORY GRASON, Univ of Mass - Amherst — Block copolymers assemble into a rich spectrum of ordered phases, with complexity driven by asymmetry in copolymer architecture. Despite decades of study, influence of intrinsic chirality on equilibrium mesophase assembly of block copolymers is not well understood and largely unexplored. Self-consistent field theory has been largely instrumental in prediction of physical properties of polymeric systems. Recently, a polar orientational self-consistent field (oSCF) theory was adopted to model chiral block copolymers having a thermodynamic preference for cholesteric ordering in chiral segments, and which confirmed the equilibrium stability of a helical cylinder morphology observed for chiral diblocks. Here, I describe a newly developed oSCF theory for chiral nematic copolymers, where segment orientations are characterized by quadrupolar interactions, and focus our study on intra-domain nematic ordering in flexible block copolymer assemblies, and in particular, mechanisms of transfer of segment chirality to mesochiral symmetries of self-assembled bicontinuous network morphologies.

**11:27AM B34.00002 Relationship of Structural and Stress Relaxation in Disordered Diblock Copolymer Melts**, TAHER GHASIMAKBARI, DAVID MORSE, University of Minnesota — We use molecular dynamics simulations to study the relationship between the relaxation of composition fluctuations and the relaxation of stress and birefringence in simple models of disordered block copolymer melts. Simulations of different simulation models of in corresponding thermodynamic states of unentangled melts are shown to exhibit equivalent dynamical behavior, thus confirming dynamic universality for unentangled systems. Structural relaxation is characterized by measuring the van Hove dynamic structure function  $S(q^*, t)$  at the critical wavenumber  $q^*$  at which the static structure function is maximum, and measuring how the associated relaxation time depends on distance from the order-disorder transition. The behavior of this quantity is compared to that of the dynamic viscoelastic modulus  $G(t)$ , which is obtained by computing autocorrelations of stress fluctuations. Relationship to relevant experiments is also briefly discussed.

**11:39AM B34.00003 Equilibrium and Kinetics of Block Copolymers Micelles**, JOSHUA MYSONA, DAVID MORSE, University of Minnesota — Both equilibrium properties of micelles, such as the critical micelle concentration (CMC), and dynamical properties such as the micelle lifetime are difficult to study in simulations because of the slow dynamics of the processes by which micelles are created and destroyed. We first discuss a method of precisely identifying the CMC in a simple model of block copolymer micelles in a homopolymer matrix, which makes use of thermodynamic integration to compute the free energy of formation. We then examine the free energy barriers to competing mechanisms for creating and destroying micelles, which could occur predominantly either by a step-wise process involving insertion and extraction of single molecules or by fission and fusion of entire micelles.

**11:51AM B34.00004 Connecting Molecular Dynamics Simulations and Fluids Density Functional Theory of Block Copolymers<sup>1</sup>**, LISA HALL, The Ohio State University — Increased understanding and precise control over the nanoscale structure and dynamics of microphase separated block copolymers would advance development of mechanically robust but conductive materials for battery electrolytes, among other applications. Both coarse-grained molecular dynamics (MD) simulations and fluids (classical) density functional theory (fDFT) can capture the microphase separation of block copolymers, using similar monomer-based chain models and including local packing effects. Equilibrium free energies of various microphases are readily accessible from fDFT, which allows us to efficiently determine the equilibrium nanostructure over a large parameter space. Meanwhile, MD allows us to visualize specific polymer conformations in 3D over time and to calculate dynamic properties. The fDFT density profiles are used to initialize the MD simulations; this ensures the MD proceeds in the appropriate microphase separated state rather than in a metastable structure (useful especially for nonlamellar structures). The simulations equilibrate more quickly than simulations initialized with a random state, which is significant especially for long chains. We apply these methods to study the interfacial behavior and microphase separated structure of diblock and tapered block copolymers. Tapered copolymers consist of pure A and B monomer blocks on the ends separated by a tapered region that smoothly varies from A to B (or from B to A for an inverse taper). Intuitively, tapering increases the segregation strength required for the material to microphase separate and increases the width of the interfacial region. Increasing normal taper length yields a lower domain spacing and increased polymer mobility, while larger inverse tapers correspond to even lower domain spacing but decreased mobility. Thus the changes in dynamics with tapering cannot be explained by mapping to a diblock system at an adjusted effective segregation strength.

<sup>1</sup>This material is based upon work supported by the National Science Foundation under Grant 1454343 and the Department of Energy under Grant DE-SC0014209.

**12:27PM B34.00005 Multi-fluid models of polymeric liquids**, DOUGLAS TREE, GLENN FREDRICKSON, Univ of California - Santa Barbara — Industrial processes for producing polymer-based materials often operate away from equilibrium, making the final microstructure – and thus the properties of the material – dependent on processing history. Current simulation methods struggle to accurately describe such processes. Traditional fluid dynamics is able to capture transport behavior, but lacks the complex phase behavior characteristic of many polymeric liquids. Coarse-grained particle models can handle the complexity, but are constrained by time and length scales. Consequently, we explore an alternative field-theoretic framework based on the “two-fluid” model originally proposed by Brochard and de Gennes. To demonstrate feasibility, we derive a model and develop an efficient numerical method for a ternary polymer solution. Subsequently, we use this model and method to examine the physics of the immersion precipitation process, used industrially to produce polymer membranes.

**12:39PM B34.00006 Using Self Consistent Field Theory on Polymeric Mixtures**, KIER VON KONIGSLOW, CHUL PARK, RUSSELL THOMPSON, University of Waterloo — The ability to predict the solubility of a particular solvent in a polymer fluid is essential to the production of polymer foams. For the past 40 years, the primary model employed to this end has been an expansion of Flory-Huggins lattice fluid theory developed by Sanchez and Lacombe (S-L theory). S-L theory, while useful in the uniform limit, is limited to homogeneous systems. Self-Consistent Field Theory (SCFT), which has long been in use in polymer physics, is a mean-field theory capable of modeling the equilibrium behaviour of both homogeneous and inhomogeneous systems. We are investigating whether SCFT, applied to polymer-solvent mixtures, is in agreement with SL-theory in the homogeneous limit. Should this prove successful, we hope to use SCFT to model more general mixtures, including inhomogeneous nanocellular polymer foam systems.

**12:51PM B34.00007 The Effects of Branching and Deuterium Labeling on Polymer Blend Miscibility<sup>1</sup>**, JEFFREY DEFELICE, Dartmouth College, JULIA HIGGINS, Imperial College, JANE LIPSON, Dartmouth College — Local structural or chemical changes made to one component of a polymer blend can have a significant impact on miscibility. In this talk we will focus on several blends involving linear and 4-arm star polystyrene (PS), both hydrogenous and deuterated, and poly(vinylmethylether) (PVME). We consider the effect of the structural change on the miscibility of PS/PVME, then turn to the added effect of deuterium labeling, both on this blend and for isotopic PS mixtures. Using our Locally Correlated Lattice (LCL) model we are able to identify trends in the physical properties of pure components, such as: free volume, thermal expansion coefficient, and cohesive energy density. We find that branching and labeling, both independently and cumulatively, affect pure component properties. Our ability to correlate structural and chemical changes with trends in physical properties leads to predictions about the compatibility of pure components, and thus their blend miscibility.

<sup>1</sup>The authors gratefully acknowledge support from NSF DMR-1403757 and GAANN

**1:03PM B34.00008 Monte Carlo field-theoretic simulations of a homopolymer blend<sup>1</sup>**, RUSSELL SPENCER, MARK MATSEN, University of Waterloo — Fluctuation corrections to the macrophase segregation transition (MST) in a symmetric homopolymer blend are examined using Monte Carlo field-theoretic simulations (MC-FTS). This technique involves treating interactions between unlike monomers using standard Monte-Carlo techniques, while enforcing incompressibility as is done in mean-field theory. When using MC-FTS, we need to account for a UV divergence. This is done by renormalizing the Flory-Huggins interaction parameter to incorporate the divergent part of the Hamiltonian. We compare different ways of calculating this effective interaction parameter. Near the MST, the length scale of compositional fluctuations becomes large, however, the high computational requirements of MC-FTS restrict us to small system sizes. We account for these finite size effects using the method of Binder cumulants, allowing us to locate the MST with high precision. We examine fluctuation corrections to the mean field MST,  $\chi N = 2$ , as they vary with the invariant degree of polymerization,  $\bar{N} = \rho^2 a^6 N$ . These results are compared with particle-based simulations as well as analytical calculations using the renormalized one loop theory.

<sup>1</sup>This research was funded by the Center for Sustainable Polymers.

**1:15PM B34.00009 Development of Simulation Methods in the Gibbs Ensemble to Predict Polymer-Solvent Phase Equilibria**, THOMAS GARTNER, University of Delaware, Dept. of Chemical and Biomolecular Engineering, THOMAS EPPS, ARTHI JAYARAMAN, University of Delaware, Dept. of Chemical and Biomolecular Engineering, Dept. of Materials Science and Engineering — Solvent vapor annealing (SVA) of polymer thin films is a promising method for post-deposition polymer film morphology control. The large number of important parameters relevant to SVA (polymer, solvent, and substrate chemistries, incoming film condition, annealing and solvent evaporation conditions) makes systematic experimental study of SVA a time-consuming endeavor, motivating the application of simulation and theory to the SVA system to provide both mechanistic insight and scans of this wide parameter space. However, to rigorously treat the phase equilibrium between polymer film and solvent vapor while still probing the dynamics of SVA, new simulation methods must be developed. In this presentation, we compare two methods to study polymer-solvent phase equilibrium—Gibbs Ensemble Molecular Dynamics (GEMD) and Hybrid Monte Carlo/Molecular Dynamics (Hybrid MC/MD). Liquid-vapor equilibrium results are presented for the Lennard Jones fluid and for coarse-grained polymer-solvent systems relevant to SVA. We found that the Hybrid MC/MD method is more stable and consistent than GEMD, but GEMD has significant advantages in computational efficiency. We propose that Hybrid MC/MD simulations be used for unfamiliar systems in certain choice conditions, followed by much faster GEMD simulations to map out the remainder of the phase window.

### **1:27PM B34.00010 Effect of Composition and Chain Length on $\chi$ Parameter of Polyolefin Blends: A Molecular Dynamics Study**, RAJESH KHARE, ASHWIN RAVICHANDRAN, CHAU-CHYUN CHEN, Texas Tech Univ —

Polymer blends exhibit complex phase behavior which is governed by several factors including temperature, composition and molecular weight of components. The thermodynamics of polymer blends is commonly described using the  $\chi$  parameter. While variety of experimental studies exist on identifying the factors affecting the  $\chi$  parameter, a detailed molecular scale understanding of these is a topic of current research. We have studied the effect of blend composition and chain length on  $\chi$  parameter values for two model polyolefin blends. The blends studied are: polyisobutylene (PIB)/polybutadiene (PBD) and polyethylene (PE)/atactic polypropylene (aPP). Molecular dynamics simulations in combination with the integral equation theory formalism proposed by Schweizer and Curro [Journal of Chemical Physics, 91, 5059 (1989)] are used to determine the  $\chi$  parameter for these systems and thereby study the effect of blend composition and chain length. The resulting  $\chi$  parameter values are explained in terms of the molecular structure of these polymeric systems.

**1:39PM B34.00011 Molecular Simulation of Olefin Oligomer Blend Phase Behavior**, QILE CHEN, TIMOTHY LODGE, ILJA SIEPMANN, University of Minnesota, MRSEC COLLABORATION — Material properties (e.g. toughness) of polyolefin mixtures are closely tied to their phase behavior that often cannot be accurately predicted by the widely used Flory-Huggins (FH) theory. In this work, configurational-bias Monte Carlo (CBMC) simulations in the Gibbs ensemble were used to compute the phase behavior of oligomeric olefins. The cohesive energy density of pure melts and the free energy of mixing were obtained from these simulations, and the discrepancy between the binary interaction  $\chi$  parameter from simulation and from the FH theory was quantified. Structural analysis and the calculated excess mixing properties provided some rationale into the interpretation of these results.

### **1:51PM B34.00012 A Semi-Empirical Multi-Scale Dynamic Monte Carlo Model of Organic Photovoltaic Performance in RIR-MAPLE Bulk Heterojunction Films**, ADRIENNE STIFF-ROBERTS, AYOMIDE ATEWOLOGUN, Duke University (RT-MRSEC) —

A semi-empirical method for investigating the performance of OPVs in resonant infrared, matrix-assisted pulsed laser evaporation (RIR-MAPLE) films is explored. Emulsion-based RIR-MAPLE offers a unique experimental backdrop for investigating trends through simulation and gaining a better understanding of how different thin film characteristics impact OPV device performance. A novel multi-scale formulation of the Dynamic Monte Carlo (DMC) model is developed based on observable morphology features. Specifically, using confocal microscopy, we observe the presence of micro-scale regimes of pure materials and nano-scale regions of the composite blend. This enables us to assign weighted percentages to DMC implementations on two different scales: the microscale and nanoscale regions. In addition to this, we use input simulation parameters acquired by characterization of as-deposited films. The semi-empirical multi-scale model presented serves as a unique simulation opportunity for exploring different properties of RIR-MAPLE deposited OPVs, their effects on OPV performance and potential design routes for improving device efficiencies. This work was supported, in part, by the Office of Naval Research under Grant N00014-10-1-0481 and the NSF Triangle MRSEC on Soft Matter.

## **Monday, March 14, 2016 11:15AM - 2:15PM —**

**Session B35 DBIO: The Physics of Cellular Organization** 338 - Michael Gramlich, Ali Tabei, Washington University, University of Northern Iowa

### **11:15AM B35.00001 Liquid-like bundles of crosslinked actin filaments contract without motors**

, KIMBERLY WEIRICH, University of Chicago — The actin cytoskeleton is a dynamic, structural material that drives cellular-scale deformations during processes such as cell migration and division. Motor proteins are responsible for actively driving many deformations by buckling and translocating actin filaments. However, there is evidence that deformations, such as the constriction of the actin bundle that drives the separation of cells during division, can occur without motors, mediated instead by crosslinker proteins. How might crosslinkers, independent of motors, drive contraction of a bundle? Using a model system of purified proteins, we show that crosslinkers, analogous to molecular cohesion, create an effective surface tension that induces bundle contraction. Crosslinked short actin filaments form micron-sized spindle-shaped bundles. Similar to tactoid granules found at the isotropic-nematic phase transition in liquid crystals, these bundles coarsen and coalesce like liquid droplets. In contrast, crosslinked long filaments coarsen into a steady state of bundles that are frozen in a solid-like network. Near the liquid-solid boundary, filaments of intermediate length initially form bundles that spontaneously contract into tactoid droplets. Our results, that crosslinked actin bundles are liquid-like with an effective surface tension, provide evidence for a mechanism of motor-independent contractility in biological materials.

### **11:51AM B35.00002 F-actin Severing Facilitates Distinct Mechanisms of Stress Relaxation in the Actin Cytoskeleton<sup>1</sup>**, TAEYOON KIM, Weldon School of Biomedical Engineering, Purdue University, WONYEONG JUNG, School of Mechanical Engineering, Purdue University, MICHAEL MURRELL, Systems Biology Institute and Department of Biomedical Engineering —

Rheological behaviors of actin cytoskeleton play an important role in physiological processes including cell migration and division. The actin cytoskeleton shows a wide variety of viscoelastic responses to external mechanical cues, such as strain-stiffening and stress relaxation. It has been hypothesized that the stress relaxation originates mainly from transient nature of cross-linkers that connect pairs of F-actins. By contrast, potential impacts of rich F-actin dynamics to the stress relaxation have been neglected in most previous studies. Here, using a computational model, we demonstrated that severing of F-actins induced by buckling during strain-stiffening can facilitate a very distinct mode of stress relaxation in the actin cytoskeleton from that induced by the transient cross-linkers. We also explored conditions where the severing-induced stress relaxation becomes prominent. This finding provides a more complete understanding of rheological behaviors of the actin cytoskeleton.

<sup>1</sup>We gratefully acknowledge the support of the National Science Foundation (1434013-CMMI and 1434095-CMMI).

### **12:03PM B35.00003 A cycling state that can lead to glassy dynamics in intracellular transport**

, MONIKA SCHOLZ, Univ of Chicago, STANISLAV BUROV, Bar-Ilan University, KIMBERLY L. WEIRICH, BJORN J. SCHOLZ, Univ of Chicago, S.M ALI TABELI, University of Northern Iowa Cedar Falls, MARGARET L. GARDEL, AARON DINNER, Univ of Chicago — Power-law dwell times have been observed for molecular motors in living cells, but the origins of these trapped states are not known. We introduce a minimal model of motors moving on a two-dimensional network of filaments, and simulations of its dynamics exhibit statistics comparable to those observed experimentally. Analysis of the model trajectories, as well as experimental particle tracking data, reveals a state in which motors cycle unproductively at junctions of three or more filaments. We formulate a master equation for these junction dynamics and show that the time required to escape from this vortex-like state can account for the power-law dwell times. We identify trends in the dynamics with the motor valency for further experimental validation. We demonstrate that these trends exist in individual trajectories of myosin II on an actin network. We discuss how cells could regulate intracellular transport and, in turn, biological function, by controlling their cytoskeletal network structures locally.

**12:15PM B35.00004 Stochastic Molecular Transport on Microtubule Bundles with Structural Defects**, M.W. GRAMLICH, Washington University School of Medicine in St. Louis, S.M. ALI TABEL, University of Northern Iowa — Intracellular transport involves complex coordination of multiple components such as: the cytoskeletal network and molecular motors. Perturbations in this process can amplify over time and space, thereby affecting transport. One little studied component of transport are structural defects in the cytoskeletal network. In this talk we will present a stochastic model of the interaction of the molecular motor, kinesin-1, and a bundled cytoskeletal network of microtubules, and explicitly explore the role of microtubule ends (a type of defect) on long-range transport. We will show how different types of end distributions can ultimately result in the same observed transport behavior for bundles. We compare transport on completely uniform bundles, found in the axon, to completely random bundles, found in dendrites. Because of the un-biased random bundle nature, defects affect transport on dendrite bundles more than on uniform bundles in the axon. Further, defects act as large spatial-scale traps that result in random wait-times which have been assumed in previous models.

**12:27PM B35.00005 Size scaling of microtubule asters in confinement<sup>1</sup>**, JAMES PELLETIER, Dept., of Physics, Massachusetts Institute of Technology, Dept., of Systems Biology, Harvard Medical School, CHRISTINE FIELD, Dept., of Systems Biology, Harvard Medical School, KASPARS KRUTKRAMELIS, Dep., of Chemical Engineering, University of Wyoming, NIKTA FAKHRI, Dept., of Physics, Massachusetts Institute of Technology, JOHN OAKEY, Dept., of Chemical Engineering, University of Wyoming, JAY GATLIN, Dept., of Molecular Biology, University of Wyoming, TIMOTHY MITCHISON, Dept., of Systems Biology, Harvard Medical School — Microtubule asters are radial arrays of microtubules (MTs) nucleated around organizing centers (MTOCs). Across a wide range of cell types and sizes, aster positioning influences cellular organization. To investigate aster size and positioning, we reconstituted dynamic asters in *Xenopus* cytoplasmic extract, confined in fluorinated oil microfluidic emulsions. In large droplets, we observed centering of MTOCs. In small droplets, we observed a breakdown in natural positioning, with MTOCs at the droplet edge and buckled or bundled MTs along the interface. In different systems, asters are positioned by different forces, such as pushing due to MT polymerization, or pulling due to bulk or cortical dynein. To estimate different contributions to aster positioning, we biochemically perturbed dynactin function, or MT or actin polymerization. We used carbon nanotubes to measure molecular motions and forces in asters. These experimental results inform quantitative biophysical models of aster size and positioning in confinement.

<sup>1</sup>JFP was supported by a Fannie and John Hertz Graduate Fellowship.

**12:39PM B35.00006 The role of catch-bonds in acto-myosin mechanics and cell mechanosensitivity**, UMUT AKALP, FRANCK J. VERNEREY, Univ of Colorado - Boulder — Contraction and spreading of adherent cells are important phenomena in range of cellular processes such as differentiation, morphogenesis, and healing. In this presentation, we propose a novel mechanism of adherent cell mechanosensing, based on the idea that the contractile acto-myosin machinery behaves as a catch-bond. For this, we construct a simplified model of the acto-myosin structure that constitute the building block of stress fibers and express the stability of cross-bridges in terms of the force-dependent bonding energy of the acto-myosin bond. Consistent with experimental measurements, we then consider that the energy barrier of the acto-myosin bond increases for tension and show that this response is enough to explain the force-induced stabilization of an SF. The resulting model eventually takes the form of a force-sensitive, active visco-elastic material, powered by ATP hydrolysis. The model is used to investigate the organization and contraction of the actin cytoskeleton of cells laying on arrays of microposts. Upon comparison with experimental observations and measurements, simulations show that the catch-bond hypothesis is satisfactory to predict the sensitivity of adherent cells to substrate stiffness as well as the complex organization of the actin cytoskeleton.

**12:51PM B35.00007 Feedback Interactions of Polymerized Actin with the Cell Membrane: Waves, Pulses, and Oscillations<sup>1</sup>**, ANDERS CARLSSON, Washington University in St Louis — Polymerized filaments of the protein actin have crucial functions in cell migration, and in bending the cell membrane to drive endocytosis or the formation of protrusions. The nucleation and polymerization of actin filaments are controlled by upstream agents in the cell membrane, including nucleation-promoting factors (NPFs) that activate the Arp2/3 complex to form new branches on pre-existing filaments. But polymerized actin (F-actin) also feeds back on the assembly of NPFs. We explore the effects of the resulting feedback loop of F-actin and NPFs on two phenomena: actin pulses that drive endocytosis in yeast, and actin waves traveling along the membrane of several cell types. In our model of endocytosis in yeast, the actin network is grown explicitly in three dimensions, exerts a negative feedback interaction on localized patch of NPFs in the membrane, and bends the membrane by exerting a distribution of forces. This model explains observed actin and NPF pulse dynamics, and the effects of several interventions including i) NPF mutations, ii) inhibition of actin polymerization, and iii) deletion of a protein that allows F-actin to bend the cell membrane. The model predicts that mutation of the active region of an NPF will enhance the accumulation of that NPF, and we confirm this prediction by quantitative fluorescence microscopy. For actin waves, we treat a similar model, with NPFs distributed over a larger region of the cell membrane. This model naturally generates actin waves, and predicts a transition from wave behavior to spatially localized oscillations when NPFs are confined to a small region. We also predict a transition from waves to static polarization as the negative-feedback coupling between F-actin and the NPFs is reduced.

<sup>1</sup>Supported by NIGMS Grant R01 GM107667

**1:27PM B35.00008 Whole Cell Model of Actin Diffusion and Reaction based on Single Molecule Speckle Microscopy Measurements**, LAURA MCMILLEN, DIMITRIOS VAVYLONIS, Lehigh University, VAVYLONIS GROUP TEAM — It is debated whether transport of actin across the cell by diffusion alone is sufficiently fast to account for the rapid reorganization of actin filaments at the leading edge of motile cells. In order to investigate this question, we created a 3D model of the whole cell that includes reaction and diffusion of actin using a particle Monte Carlo method. For the lamellipodium of the simulated cell we use the model by Smith et al. Biophys. J 104:247 (2013), which includes two diffuse pools of actin, one which is slowly diffusing and the other which diffuses more quickly, as well as a pool of filamentous actin undergoing retrograde flow towards the cell center. We adjusted this model to fit a circular geometry around the whole cell. We also consider actin in the cell center which is either diffusing or in stationary filamentous form, representing cortical actin or actin in stress fibers. The local rates of polymerization and the lifetime distributions of polymerized actin were estimated from single molecule speckle microscopy experiments by the group of N. Watanabe. With this model we are able to simulate prior experiments that monitored the redistribution of actin after photoactivation or fluorescence recovery after photobleaching in various parts of the cell. We find that transport by diffusion is sufficient to fit these data, without the need for an active transport mechanism, however significant concentration gradients may develop at steady state.

**1:39PM B35.00009 Chemotaxis to Excitable Waves in Dictyostelium Discoideum<sup>1</sup>**, ARPAN BHOWMIK, Rice Univ, WOUTER-JAN RAPPEL, University of California, San Diego, HERBERT LEVINE, Rice Univ — In recent years, there have been significant advances in our understanding of the mechanisms underlying chemically directed motility by eukaryotic cells such as Dictyostelium. In particular, the LEGI model has proven capable of providing a framework for quantitatively explaining many experiments that present Dictyostelium cells with tailored chemical stimuli and monitor their subsequent polarization. Here, we couple the LEGI approach to an excitable medium model of the cAMP wave-field that is self-generated by the cells and investigate the extent to which this class of models enables accurate chemotaxis to the cAMP waveforms expected in vivo. Our results indicate that the ultra-sensitive version of the model does an excellent job in providing natural wave rectification, thereby providing a compelling solution to the “back-of-the-wave paradox” during cellular aggregation.

<sup>1</sup>This work was supported by National Institutes of Health Grant P01 GM078586

**1:51PM B35.00010 Mechanical feedback stabilizes budding yeast morphogenesis**, SAMHITA BANAVAR, MICHAEL TROGDON, LINDA PETZOLD, OTGER CAMPAS, Univ of California - Santa Barbara — Walled cells have the ability to remodel their shape while sustaining an internal turgor pressure that can reach values up to 10 atmospheres. This requires a tight and simultaneous regulation of cell wall assembly and mechanochemistry, but the underlying mechanisms by which this is achieved remain unclear. Using the growth of mating projections in budding yeast (*S. cerevisiae*) as a motivating example, we have developed a theoretical description that couples the mechanics of cell wall expansion and assembly via a mechanical feedback. In the absence of a mechanical feedback, cell morphogenesis is inherently unstable. The presence of a mechanical feedback stabilizes changes in cell shape and growth, and provides a mechanism to prevent cell lysis in a wide range of conditions. We solve for the dynamics of the system and obtain the different dynamical regimes. In particular, we show that several parameters affect the stability of growth, including the strength of mechanical feedback in the system. Finally, we compare our results to existing experimental data.

**2:03PM B35.00011 Mechanical Trade-offs in Experimentally Evolved Multicellular Yeast**, SHANE JACOBSEN, JENNIFER PENTZ, WILLIAM RATCLIFF, PETER YUNKER, Georgia Tech — The evolution of multicellularity as much about physics as it is about biology, as selection acts on the physical properties of multicellular bodies. Nascent multicellular organisms are confronted by internal and external forces that act on large length scales and are capable of fracturing intercellular bonds. We study the evolution of the mechanical properties of multicellular 'snowflake' yeast that were selected for increased size over ~1,500 generations<sup>1,2</sup>. While these snowflakes evolve to be larger by mitigating internal forces, they also become more susceptible to fracturing when faced with external compressive forces. Using confocal microscopy and direct mechanical measurements, we investigate the physical underpinnings and consequences of this strength-toughness trade-off. **References:** <sup>1</sup>W. Ratcliff *et al.* 2012. PNAS. 109:1959–1600. <sup>2</sup>W. Ratcliff *et al.* 2015. Nature Communications. 6:6102.

## Monday, March 14, 2016 11:15AM - 2:15PM –

Session B36 GSOF DBIO GSNP/DFD: Active Matter II 339 - Robin Selinger, Kent University

**11:15AM B36.00001 Material Flows in an Active Nematic Liquid Crystal**, STEPHEN DECAMP, GABRIEL REDNER, APARNA BASKARAN, MICHAEL HAGAN, ZVONIMIR DOGIC, Brandeis University — Active matter systems are composed of energy consuming constituent components which drive far-from-equilibrium dynamics. As such, active materials exhibit energetic states which would be unfavorable in passive, equilibrium materials. We study one such material; an active nematic liquid crystal which exists in a dynamical steady state where  $\pm 1/2$  defects are continuously generated and annihilated at a constant rate. The active nematic is composed of micron-sized microtubule filaments which are highly concentrated into a quasi-2D film that resides on an oil-water interface. Kinesin motor proteins drive inter-filament sliding which results in net extensile motion of the microtubule film. Notably, we find a mesophase in which motile  $\pm 1/2$  defects, acquire system-spanning orientational order. Currently, we are tracking material flows generated by the active stresses in the system to measure length scales at which energy is dissipated, and to measure the relation between internally generated flows and bend in the nematic field.

**11:27AM B36.00002 Antipolar ordering of topological charges in active liquid crystals**, JORN DUNKEL, MIT, ANAND OZA, Courant Institute — Recent experiments demonstrated that ATP-driven microtubule-kinesin bundles can self-assemble into two-dimensional active liquid crystals that exhibit a rich creation and annihilation dynamics of topological defects, reminiscent of particle-pair production processes in quantum systems. This remarkable discovery has sparked considerable theoretical and experimental interest. Here, we present and validate a minimal continuum theory for this new class of active matter systems by merging universality ideas with the classical Landau-de Gennes theory. The resulting model agrees quantitatively with recently published data and, in particular, predicts a previously unexplained regime of antipolar order. Our analysis implies that active liquid crystals are governed by the same generic ordering principles that determine the non-equilibrium dynamics of dense bacterial suspensions and elastic bilayer materials. Moreover, the theory manifests a profound energetic analogy with strongly interacting quantum gases. Generally, our results suggest that complex nonequilibrium pattern-formation phenomena might be predictable from a few fundamental symmetric-breaking and scale-selection principles.

**11:39AM B36.00003 Points or vectors? The polar structure of disclinations in active and passive nematics**, LUCA GIOMI, ARTHUR VROMANS, Leiden University — Topological defects play a pivotal role in the physics of liquid crystals and represent one of the most prominent and well studied aspects of mesophases. While in two-dimensional nematics, disclinations are traditionally treated as point-like objects, recent experimental studies on active nematics have suggested that half-strength disclinations might in fact possess a polar structure. In this talk I will provide a precise definition of polarity for half-strength nematic disclinations, introduce a simple and robust method to calculate this quantity from experimental and numerical data and investigate how the orientational properties of active and passive half-strength disclinations affect their dynamics.

**11:51AM B36.00004 Theory and Experiments of Topologically Driven Flows in Nematic Suspensions**, CHRISTOPHER CONKLIN, JORGE VINALS, University of Minnesota, CHENHUI PENG, YUBING GUO, SERGIJ SHIVANOVSKII, QI-HUO WEI, OLEG LAVRENTOVICH, Kent State University — We present theory, numerical solutions, and experiments of electric field driven flows in nematic liquid crystals (LC) in which a patterned molecular orientation acts as an electrolytic active medium. Surface patterning by photoalignment in a thin cell is used to create various alignments of a nematic liquid crystal film, that may include topological defects. The active patterned LC electrolyte converts electric field energy into LC flows and transport of embedded particles of any type (fluid, solid, gaseous) along predefined trajectories, and without limitation on the electric nature (charge, polarizability) of these particles and interfaces. Flow is quadratic in the electric field which leads, even for an imposed AC field, to systematic flow velocities, including persistent vortices of controllable rotation speed and direction. The latter are essential for micro- and nanoscale mixing applications.

**12:03PM B36.00005 Controlling Defects and Flow in Active Nematic Suspensions<sup>1</sup>**, SURAJ SHANKAR, Department of Physics, Syracuse University, PAU GUILLAMAT BASSEDAS, JORDI IGNÉS-MULLOL, FRANCESC SAGUÉS, Department of Physical Chemistry and IN2UB, Universitat de Barcelona, M. CRISTINA MARCHETTI, Department of Physics, Syracuse University — Experiments on active nematics composed of cytoskeletal biopolymers activated by molecular motors have shown that in these systems topological defects drive self-sustained flows and the transition to spatio-temporal chaos. In active nematics, defects become dynamical entities and behave like self-propelled particles. In a freely suspended nematic layer the defect speed is controlled by the activity and the viscosity of the active fluid that is so far unknown. Experiments, however, are carried out on very thin nematic layers at an oil-water interface. Our collaborators in Barcelona have shown that increasing the viscosity of the oil can substantially slow down the defects and increase their number. Considering a model of an active nematic at an oil-water interface, we have calculated the defect speed as a function of oil viscosity and find that theory and experiments agree well when the oil viscosity is changed over four orders of magnitude. Importantly, by combining theory and experiments these results provide a parameter-free estimate for the interfacial viscosity of the active nematic layer, which has never been measured before.

<sup>1</sup>This research was supported by the grants NSF-DMR-1305184 and MINECO FIS 2013-41144P

**12:15PM B36.00006 Active nematics on the surface of a torus<sup>1</sup>**, PERRY ELLIS, YA-WEN CHANG, ALBERTO FERNANDEZ-NIEVES, Georgia Institute of Technology — Nematic materials on the surface of a sphere must have a net topological charge of  $s = +2$ . In equilibrium nematics experiments have shown that this net topological charge can be realized with four  $s = +1/2$  defects, which also corresponds to the theoretically expected ground state configuration. Surprisingly, even though active nematics are continuously driven out of equilibrium by the internal energy of the nematogens, when confined to the surface of a sphere these materials can also realize this net topological charge with four  $s = +1/2$  defects. In contrast to the spherical confinement case, the situation for toroidal confinement has not been experimentally explored despite the existence of theory and simulation work examining the structure of ordered materials on the surface of a torus. Here, we experimentally realize an extensile active nematic confined to a toroidal surface and explore how the interplay between topology, activity, and nematic elasticity affect the structure and dynamics of the material.

<sup>1</sup>PWE is supported by FLAMEL under grant NSF 1258425

**12:27PM B36.00007 Dynamics and Instabilities of an overdamped active nematic liquid crystal<sup>1</sup>**, ELIAS PUTZIG, APARNA BASKARAN, Brandeis University — Active nematics have been studied extensively in the context of suspensions of active particles, with a Stokes equation describing the flow of the surrounding fluid. Here we will present a continuum model of an overdamped (often termed 'dry') active nematic, where activity enters through self-induced flows. These flows represent the ability of the internal forces to convect, shear, or rotate the nematic order. The self-induced shear gives rise to an instability in the homogeneous ordered state which is analogous to that seen in active suspensions. The self-induced rotation gives rise to a new instability. A phase diagram from this model will be presented, and the phenomenology will be compared with what is seen in experimental and simulated active systems.

<sup>1</sup>We would like to acknowledge grant support through NSF (NSF-DMR-1149266), (DMR-0820492), (NIH-5T32EB009419) and IGERT (DGE-1068620).

**12:39PM B36.00008 Viscoelastic and elastomeric active matter: linear instability and nonlinear dynamics**, EWAN J. HEMINGWAY, Durham University, M. E. CATES, University of Cambridge, M. C. MARCHETTI, Syracuse University, S. M. FIELDING, Durham University — We consider a continuum model of active viscoelastic matter, whereby a model of an active nematic liquid-crystal is coupled to a minimal model of polymer dynamics with a viscoelastic relaxation time  $\tau_c$ . To explore the resulting interplay between active and polymeric dynamics, we first generalise a linear stability analysis (from earlier studies without polymer) to derive criteria for the onset of spontaneous flow. Perhaps surprisingly, our results show that the spontaneous flow instability persists even for divergent polymer relaxation times. We explore the novel dynamical states to which these instabilities lead by means of nonlinear numerical simulations. This reveals oscillatory shear-banded states in 1D, and activity-driven turbulence in 2D, even in the limit  $\tau_c \rightarrow \infty$ . Adding polymer can also have calming effects, increasing the net throughput of spontaneous flow along a channel in a new type of "drag-reduction", an effect that may have implications for cytoplasmic streaming processes within the cell.

**12:51PM B36.00009 A Kinetic Model of Active Extensile Bundles**, DANIEL GOLDSTEIN, BULBUL CHAKRABORTY, APARNA BASKARAN, Brandeis Univ — Recent experiments in active filament networks reveal interesting rheological properties (Dan Chen: APS March Meeting 2015 D49.00001). This system consumes ATP to produce an extensile motion in bundles of microtubules. This extension then leads to self generated stresses and spontaneous flows. We propose a minimal model where the activity is modeled by self-extending bundles that are part of a cross linked network. This network can reorganize itself through buckling of extending filaments and merging events that alter the topology of the network. We numerically simulate this minimal kinetic model and examine the emergent rheological properties and determine how stresses are generated by the extensile activity. We will present results that focus on the effects of confinement and network connectivity of the bundles on stress fluctuations and response of an active gel.

**1:03PM B36.00010 Shortening actin filaments cause force generation in actomyosin network to change from contractile to extensile**, NITIN KUMAR, MARGARET GARDEL, James Franck Institute, University of Chicago — Motor proteins in conjunction with filamentous proteins convert biochemical energy into mechanical energy which serves a number of cellular processes including cell motility, force generation and intracellular cargo transport. In-vitro experiments suggest that the forces generated by kinesin motors on microtubule bundles are extensile in nature whereas myosin motors on actin filaments are contractile. It is not clear how qualitatively similar systems can show completely different behaviors in terms of the nature of force generation. In order to answer this question, we carry out in vitro experiments where we form quasi 2D filamentous actomyosin networks and vary the length of actin filaments by adding capping protein. We show that when filaments are much shorter than their typical persistence length (approximately 10 microns), the forces generated are extensile and we see active nematic defect propagation, as seen in the microtubule-kinesin system. Based on this observation, we claim that the rigidity of rods plays an important role in dictating the nature of force generation in such systems. In order to understand this transition, we selectively label individual filaments and find that longer filaments show considerable bending and buckling, making them difficult to slide and extend along their length.

**1:15PM B36.00011 Dynamics of Actively Driven Crosslinked Microtubule Networks**, VIKRANT YADAV, KASIMIRA STANHOPE, University of Massachusetts, Amherst, ARTHUR A. EVANS, University of Wisconsin, Madison, JENNIFER L. ROSS, University of Massachusetts, Amherst — We have designed a model experiment to explore dynamics of crosslinked active microtubule clusters crosslinked with MAP65. Microtubule clusters are allowed to settle on a slide coated with kinesin-1 molecular motors, which move microtubules. We systematically tune either concentration of cross linkers bound to microtubule ( $\rho_c$ ) or the global concentration of microtubules ( $\rho_{MT}$ ). We quantified the shape of the cluster by measuring the standard deviation ( $\sigma$ ) of the cluster outline. At low  $\rho_{MT}$  or  $\rho_c$  the network is in an expanding state. At higher  $\rho_{MT}$  or  $\rho_c$  expansion slows down, reaches zero at a critical density, and become negative indicating contraction. Further increase of  $\rho_{MT}$  or  $\rho_c$  halts any kind of dynamics. The  $\rho_{MT}$ - $\rho_c$  phase space shows distinct regions of extensile, contractile and static regimes. We model these results using active hydrodynamic theory. Microtubules are modeled as active rods whereas effect of crosslinkers is modeled using a collision term that prefers anti-parallel alignment of microtubules. A linearized analysis of hydrodynamic equation predicts existence of density driven expanding, contracting, and static phases for microtubule clusters.

**1:27PM B36.00012 Competing dynamic phases of active polymer networks<sup>1</sup>**, SIMON FREEDMAN, Univ of Chicago, SHILADITYA BANERJEE, AARON R. DINNER, James Franck Institute, Univ of Chicago — Recent experiments on in-vitro reconstituted assemblies of F-actin, myosin-II motors, and cross-linking proteins show that tuning local network properties can changes the fundamental biomechanical behavior of the system. For example, by varying cross-linker density and actin bundle rigidity, one can switch between contractile networks useful for reshaping cells, polarity sorted networks ideal for directed molecular transport, and frustrated networks with robust structural properties. To efficiently investigate the dynamic phases of actomyosin networks, we developed a coarse grained non-equilibrium molecular dynamics simulation of model semiflexible filaments, molecular motors, and cross-linkers with phenomenologically defined interactions. The simulation's accuracy was verified by benchmarking the mechanical properties of its individual components and collective behavior against experimental results at the molecular and network scales. By adjusting the model's parameters, we can reproduce the qualitative phases observed in experiment and predict the protein characteristics where phase crossovers could occur in collective network dynamics. Our model provides a framework for understanding cells' multiple uses of actomyosin networks and their applicability in materials research.

<sup>1</sup>Supported by the Department of Defense (DoD) through the National Defense Science & Engineering Graduate Fellowship (NDSEG) Program.

**1:39PM B36.00013 Rapid non-equilibrium turnover fluidizes entangled F-actin solutions**, PATRICK M. MCCALL, Dept of Physics, Univ of Chicago, DAVID R. KOVAR, Depts of MGCB and BMB, Univ of Chicago, MARGARET L. GARDEL, Dept of Physics, Univ of Chicago — The actin cytoskeleton of living cells is a semiflexible polymer network which regulates cell division, motility, and morphogenesis by controlling cell shape. These complex shape-changing processes require both mechanical deformation and remodeling of the actin cytoskeleton. Molecular motors generate internal forces to drive deformation, while cytoskeletal remodeling is regulated by non-equilibrium polymer turnover. Although the mechanical properties of equilibrium actin filament (F-actin) networks are well-described by theories of semiflexible polymers, these theories do not incorporate the effects of non-equilibrium turnover. To address this experimentally, we developed a model system in which both the turnover rate and the length distribution of purified F-actin can be tuned independently at steady-state through the combined action of actin regulatory proteins. Specifically we tune the concentrations of cofilin, profilin, and formin to regulate F-actin severing, recycling, and nucleation, respectively. We find that the actin turnover rate can be tuned by cofilin up to 25-fold ( $31 \pm 2$  subunits/sec/filament). Surprisingly, changes in turnover rate have no effect on the steady-state F-actin length distribution, which is instead set by formin concentration. Passive microrheology measurements show that increased turnover leads to striking fluidization in both entangled and crosslinked networks. Non-equilibrium turnover thus enables modulation of network mechanics, which impacts force transmission and material deformation.

**1:51PM B36.00014 Critical forces for actin filament buckling and force transmission influence transport in actomyosin networks**, SAMANTHA STAM, Univ of Chicago, MARGARET GARDEL, Dept. of Physics, Univ of Chicago — Viscoelastic networks of biopolymers coordinate the motion of intracellular objects during transport. These networks have nonlinear mechanical properties due to events such as filament buckling or breaking of cross-links. The influence of such nonlinear properties on the time and length scales of transport is not understood. Here, we use in vitro networks of actin and the motor protein myosin II to clarify how intracellular forces regulate active diffusion. We observe two transitions in the mean-squared displacement of cross-linked actin with increasing motor concentration. The first is a sharp transition from initially subdiffusive to diffusive-like motion that requires filament buckling but does not cause net contraction of the network. Further increase of the motor density produces a second transition to network rupture and ballistic actin transport. This corresponds with an increase in the correlation of motion and thus may be caused when forces propagate far enough for global motion. We conclude that filament buckling and overall network contraction require different amounts of force and produce distinct transport properties. These nonlinear transitions may act as mechanical switches that can be turned on to produce observed motion within cells.

**2:03PM B36.00015 Detection of Non-Equilibrium Fluctuations in Active Gels<sup>1</sup>**, ALEXANDRU BACANU, Massachusetts Institute of Technology, USA, CHASE BROEDERSZ, Ludwig-Maximilians-University of Munich, Germany, JANNES GLADROW, Georg-August University of Goettingen, Germany, FRED MACKINTOSH, Vrije Universiteit, Netherlands, CHRISTOPH SCHMIDT, Georg-August University of Goettingen, Germany, NIKTA FAKHRI, Massachusetts Institute of Technology, USA — Active force generation at the molecular scale in cells can result in stochastic non-equilibrium dynamics on mesoscopic scales. Molecular motors such as myosin can drive steady-state stress fluctuations in cytoskeletal networks. Here, we present a non-invasive technique to probe non-equilibrium fluctuations in an active gel using single-walled carbon nanotubes (SWNTs). SWNTs are semiflexible polymers with intrinsic fluorescence in the near infrared. Both thermal and active motor-induced forces in the network induce transverse fluctuations of SWNTs. We demonstrate that active driven shape fluctuations of the SWNTs exhibit dynamics that reflect the non-equilibrium activity, in particular the emergence of correlations between the bending modes. We discuss the observation of breaking of detailed balance in this configurational space of the SWNT probes.

<sup>1</sup>Supported by National Defense Science and Engineering Graduate Student Fellowship (NDSEG)

## Monday, March 14, 2016 11:15AM - 2:15PM —

### Session B37 GSOF DBIO: Phase Transitions and Self-Assembly in Biological Systems II 340

— Michael Hagan, Brandeis University

**11:15AM B37.00001 Imaging the Dynamics of Individual Viruses in Solution<sup>1</sup>**, AARON GOLDFAIN, REES GARMANN, YOAV LAHINI, Harvard University, John A. Paulson School of Engineering and Applied Sciences, VINOTHAN MANOHARAN, Harvard University, John A. Paulson School of Engineering and Applied Sciences and the Department of Physics — We have developed optical microscopy techniques that can detect and track individual, unlabeled viruses at thousands of frames per second. We use these techniques to study fast, dynamic processes in the life cycles of bacteriophages (viruses that infect bacteria). I will describe experiments that capture the ejection of double stranded DNA from bacteriophage  $\lambda$ . During the 1-2 second ejection, the DNA genome transitions from a compact, highly ordered spool within the capsid into an extended random coil in solution. By quantifying the amount of light scattered from a single  $\lambda$  phage as its DNA ejects, we measure the amount of DNA remaining in the virus capsid as a function of time. Measuring small fluctuations in the rate of ejection may uncover clues about the complex conformational rearrangements that the DNA undergoes while escaping the capsid.

<sup>1</sup>Funded in part by the NSF GRFP

**11:27AM B37.00002 Chirality of Viral Capsids**, SANJAY DHARMAVARAM, Dept. of Mechanical and Aerospace Engineering, UCLA, FANGMING XIE, University of Science and Technology, China, ROBIJN BRUINSMA, Dept. of Physics and Astronomy, UCLA, WILLIAM KLUG, Dept. of Mechanical and Aerospace Engineering, UCLA, JOSEPH RUDNICK, Dept. of Physics and Astronomy, UCLA — Most icosahedral viruses are classified by their T-number which identifies their capsid in terms of the number of capsomers and their relative arrangement. Certain T-numbers ( $T = 7$  for instance) are inherently chiral (with no reflection planes) while others (e.g.  $T = 1$ ) are achiral. We present a Landau-Brazovskii (LB) theory for weak crystallization in which a scalar order parameter that measures density of capsid proteins successfully predicts the various observed T-numbers and their respective chiralities. We find that chiral capsids gain stability by spontaneously breaking symmetry from an unstable chiral state. The inherently achiral LB-free energy does not preferentially select a particular chiral state from its mirror reflection. Based on the physical observation that proteins are inherently chiral molecules with directional interactions, we propose a new chiral term to the LB energy as a possible selection mechanism for chirality.

**11:39AM B37.00003 A Simple Model for Immature Retrovirus Capsid Assembly<sup>1</sup>**, STEFAN PAQUAY, PAUL VAN DER SCHOOT, Eindhoven University of Technology, The Netherlands, BOGDAN DRAGNEA, Indiana University, Bloomington, Indiana — In this talk I will present simulations of a simple model for capsomeres in immature virus capsids, consisting of only point particles with a tunable range of attraction constrained to a spherical surface. We find that, at sufficiently low density, a short interaction range is sufficient for the suppression of five-fold defects in the packing and causes instead larger tears and scars in the capsid. These findings agree both qualitatively and quantitatively with experiments on immature retrovirus capsids, implying that the structure of the retroviral protein lattice can, for a large part, be explained simply by the effective interaction between the capsomeres.

<sup>1</sup>We thank the HFSP for funding under grant RGP0017/2012.

**11:51AM B37.00004 Autophagy selectivity through receptor clustering** , ANDREW RUTENBERG, AIDAN BROWN<sup>1</sup>, Dalhousie University — Substrate selectivity in autophagy requires an all-or-none cellular response. We focus on peroxisomes, for which autophagy receptor proteins NBR1 and p62 are well characterized. Using computational models, we explore the hypothesis that physical clustering of autophagy receptor proteins on the peroxisome surface provides an appropriate all-or-none response. We find that larger peroxisomes nucleate NBR1 clusters first, and lose them due to competitive coarsening last, resulting in significant size-selectivity. We then consider a secondary hypothesis that p62 inhibits NBR1 cluster formation. We find that p62 inhibition enhances size-selectivity enough that, even if there is no change of the peroxophagy rate, the volume of remaining peroxisomes can significantly decrease. We find that enhanced ubiquitin levels suppress size-selectivity, and that this effect is more pronounced for individual peroxisomes. Sufficient ubiquitin allows receptor clusters to form on even the smallest peroxisomes. We conclude that NBR1 cluster formation provides a viable physical mechanism for all-or-none substrate selectivity in peroxophagy. We predict that cluster formation is associated with significant size-selectivity.

<sup>1</sup>now at Simon Fraser University

**12:03PM B37.00005 Statistical Mechanics and Thermodynamics of Viral Evolution** , BARBARA JONES, JAMES KAUFMAN, IBM Research – Almaden — Using methods drawn from physics we study the life cycle of viruses. We analyze a model of viral infection and evolution using the “grand canonical ensemble” and formalisms from statistical mechanics and thermodynamics. Using this approach we determine possible genetic states of a model virus and host as a function of two independent pressures—immune response and system temperature. We show the system has a real thermodynamic temperature, and discover a new phase transition between a positive temperature regime of normal replication and a negative temperature “disordered” phase of the virus. We distinguish this from previous observations of a phase transition that arises as a function of mutation rate. From an evolutionary biology point of view, at steady state the viruses naturally evolve to distinct quasispecies. The approach used here could be refined to apply to real biological systems, perhaps providing insight into immune escape, the emergence of novel pathogens and other results of viral evolution.

**12:15PM B37.00006 Metastable Amyloid Phases and their Conversion to Mature Fibrils** , MARTIN MUSCHOL, TATIANA MITI, MENTOR MULAJ, Dept. of Physics, University of South Florida, Tampa FL 33620, JEREMY SCHMIT, Dept. of Physics, Kansas State University, Manhattan, KS 66506 — Self-assembly of proteins into amyloid fibrils plays a key role in both functional biological responses and pathogenic disorders which include Alzheimer's disease and type II diabetes. Amyloid fibril assembly frequently generates compact oligomeric and curvilinear polymeric intermediates which are implicated to be toxic to cells. Yet, the relation between these early-stage oligomeric aggregates and late-stage rigid fibrils, which are the hallmark structure of amyloid plaques, has remained unclear. Our measurements indicate that lysozyme amyloid oligomers and their curvilinear fibrils only form after crossing a salt and protein concentration dependent threshold. These oligomeric aggregates are structurally distinct from rigid fibrils and are metastable against nucleation and growth of rigid fibrils. Our experimental transition boundaries match well with colloidal model predictions accounting for salt-modulated charge repulsion. We also report our preliminary findings on the mechanism by which these metastable oligomeric phases are converted into stable amyloid fibrils.

**12:27PM B37.00007 Patterns for Fluid Management: The Mechanical Origins of Microarchitectures** , ASJA RADJA, MAXIM LAVRETOVICH , ERIC HORSLEY, RANDALL KAMIEN, ALISON SWEENEY, University of Pennsylvania — Pollen grains are the vehicles for the male germ line in land plants and are famous for the intricate microarchitectures of their protective coverings. It is not known whether these sub-micron-scale patterns have a functional role. A given microarchitectural pattern is maintained over geological time within a single species, yet, despite similar mechanisms of pollen development in all species, different species have extremely variable patterns. Until recently, many proposed mechanisms of pollen pattern formation were attributed to top-down assembly processes directed by the pollen cytoskeleton. We propose a novel view in which bottom-up mechanical processes akin to thermodynamic phase transitions may cause the final pollen structure. Here, we present a temporal view of pattern formation using several microscopy techniques. Our data show a rapid appearance of surface microstructures. We test the hypothesis of bottom-up pattern formation by physically manipulating the pattern formation process with mechanical forces and chemical solvents. Our data are consistent with bottom-up formation of these patterns; we discuss a hypothesis of pattern formation in this system involving Brazovskii phase transitions templated on a spherical geometry.

**12:39PM B37.00008 Pollen Patterning as a Brazovskii Phase Transition on a Sphere** , MAXIM LAVRETOVICH, ERIC HORSLEY, ASJA RADJA, ALISON SWEENEY, RANDALL KAMIEN, University of Pennsylvania — Pollen grains acquire intricate, varied surface patterns during development. The patterns are reproducible within a single plant species, and yet exhibit a wide variation among species, despite having similar developmental steps. We model this pattern formation on spherical grains as a phase transition to a spatially modulated phase, characterized by an unstable wavelength  $\lambda_0$ . On the infinite, flat plane, the patterned phase consists of uniform stripes, as shown by Brazovskii. We find that, by contrast, the patterns may be much more varied on a spherical surface because the topological defects which must be present in the pattern may be accommodated in a variety of ways. This variation may explain the wide range of observed pollen patterns. We also argue that the first-order character of the transition may be responsible for the robust reproducibility of the patterns in a single plant species. Finally, we compute the free energy difference between the unpatterned, smooth phase and robust patterned phases on the sphere. These calculations point toward possible future experimental tests of our model.

**12:51PM B37.00009 Non-deterministic self-assembly of two tile types on a lattice** , SALVATORE TESORO, University of Cambridge — I will present a complex behaviour that is both interesting from a statistical and complex systems point of view and from a more abstract point of view on complexity and evolutionary theory. I will introduce simple a theoretical framework to predict and describe all possible growth behaviours that self-assembly of two tile types can produce on a 2D lattice, given binary interaction rules between the faces of the tiles in the system. Such simple set up can give rise to critical transitions between bound and unbound growth regimes and other non-critical behaviours. I will illustrate how this work completes efforts conducted by Ahnert et Al. in the field of Complexity and Evolution, whereby deterministic self-assembly pathways have been exploited as a useful tool in addressing questions on complexity and modularity in nature. I will further show how this theoretical framework can be experimentally verified using DNA-tiles as a building material and providing experimental validation of the theoretical predictions made.

**1:03PM B37.00010 Generic Phase Diagram of Binary Superlattices<sup>1</sup>** , ALEXEI TKACHENKO, Brookhaven National Laboratory — Emergence of a large variety of self-assembled superlattices is a dramatic recent trend in the fields of nanoparticle and colloidal sciences. Motivated by this development, we propose a model that combines simplicity with a remarkably rich phase behavior, applicable to a wide range of such self-assembled systems. Those include nanoparticle and colloidal assemblies driven by DNA-mediated interactions, electrostatics, and possibly, by controlled drying. In our model, a binary system of Large and Small hard sphere (L and S) interact via selective short-range (“sticky”) attraction. In its simplest version, this Binary Sticky Sphere model features attraction only between ‘S’ and ‘L’ particles, respectively. We demonstrate that in the limit when this attraction is sufficiently strong compared to  $kT$ , the problem becomes purely geometrical: the thermodynamically preferred state should maximize the number of S-L contacts. A general procedure for constructing the phase diagram as a function of system composition  $f$ , and particle size ratio  $r$ , is outlined. In this way, the global phase behavior can be calculated very efficiently, for a given set of plausible candidate phases. Furthermore, the geometric nature of the problem enables us to generate those candidate phases through a well defined and intuitive construction. We calculate the phase diagrams both for 2D and 3D systems, and compare the results with existing experiments. Most of the 3D superlattices observed to date are featured in our phase diagram, while several more are yet to be discovered.

<sup>1</sup>The research was carried out at the CFN, DOE Office of Science Facility, at BNL, under Contract No. DE-SC0012704

### 1:15PM B37.00011 Geometric and Topological Transitions of Small Clusters of Liquid Particles

JAMES GIAMMONA, OTGER CAMPAS, Univ of California - Santa Barbara — The geometry and topology of small particle clusters has been studied in several disciplines due to the fundamental nature of the problem and its relevance to applications. Recent theoretical work can predict observed packings for small numbers of hard, spherical particles, but little is known about how using deformable particles changes the geometry and topology of these clusters. To study this problem, we simulate small clusters of liquid particles using a Langevin approach and obtain the geometrical and topological transitions for clusters of  $N$  particles (up to  $N=7$ ) as the particles interfacial tension and adhesion energy are varied. As particles become more adhesive and increase their contact angle, we observe well-defined packing transitions in the clusters. For  $N=5$ , a topological transition occurs at a critical value of the contact angle. For  $N=6$ , we obtain two stable cluster geometries for a given value of the contact angle, namely an 8-faced deltahedron and an octahedron. For  $N=7$ , there appears to be a complex landscape of cluster geometries and topologies, with transitions occurring at well-defined values of the contact angle. Our findings can help in the controlled assembly of particular arrangements of small clusters of bubbles or adherent droplets.

### 1:27PM B37.00012 Helices Of Helices

MAHSA SIAVASHPOURI, MARK ZAKHARY, Brandeis Univ, CHRISTIAN WACHAUF, HENDRIK DIETZ, Technische Universität München, ZVONIMIR DOGIC, Brandeis University — Twisted ribbons are characteristic structural motifs that are prevalent in nature. However correlation between the macroscopic properties of the final self-assemblies and the microscopic features of the constituent molecules remain unknown. We describe a new class of supramolecular 1D assemblages with tunable mechanical properties. Using DNA origami technique, we design and structure rod-like colloidal particles that have excluded volume interactions and self-assemble into twisted ribbons in presence of attractive interactions mediated by non-absorbing polymers. By comparing behavior of DNA origami filaments and rodlike viruses we demonstrate that self-assembly into 1D twisted ribbons is universal and independent of the system materials. Tuning the molecular properties of the DNA origami particles, determines the physical properties of the entire self-assembled structures. Furthermore, to understand the connection between the chirality at the molecular scale and the macroscopic chiral structures, we measured twist periodicity (pitch) of cholesteric phase associated to various DNA origami designs which can develop a new framework in understanding microscopic origin of chirality in liquid crystals.

### 1:39PM B37.00013 Theory of Microphase separation in bidisperse Chiral membranes

RAUNAK SAKHARDANDE, STEFAN STANOJEVIEA, ARVIND BASKARAN, MICHAEL HAGAN, APARNA BASKARAN, BULBUL CHAKRABORTY, Brandeis University — We discuss the phase behavior of bidisperse chiral colloidal membranes, which are monolayers of rodlike molecules containing two species of rods, each with opposite handedness. Using a Ginzburg Landau theory, we show that the system exists in three stable states, separated by first-order phase transitions: a compositionally homogeneous state, macrophase separation between the two rod species, and a micro-phase separated state in which the minority rod species forms circular domains with a well-defined, narrow size distribution. We find that the phase behavior can be controlled by tuning two parameters, one associated with the driving force for membrane assembly, and the other related to the difference in chirality between the two rod species. We discuss implications of the calculated phase diagram for a recently developed experimental system in which bidisperse colloidal membranes comprised of two species of rodlike viruses exhibit micro-phase separation.

### 1:51PM B37.00014 Measuring the equation of state for a 2D colloidal membrane: A microfluidic approach to buffer exchange

ANDREW BALCHUNAS, RAFAEL CABANAS, SETH FRADEN, ZVONIMIR DOGIC, Brandeis University — Previous work has shown that monodisperse rod-like colloidal particles, such as a filamentous bacteriophage, self assemble into a 2D monolayer smectic in the presence of a non-adsorbing depleting polymer. These structures have the same functional form of bending rigidity and lateral compressibility as conventional lipid bi-layers, so we name the monolayer smectic a colloidal membrane. We have developed a microfluidic device such that the osmotic pressure acting on a colloidal membrane may be controlled via a full in situ buffer exchange. Rod density within individual colloidal membranes was measured as a function of osmotic pressure and a first order phase transition, from 2D fluid to 2D solid, was observed.  $k_{on}$  and  $k_{off}$  rates of rod to membrane binding were measured by lowering the osmotic pressure until membrane evaporation occurred.

### 2:03PM B37.00015 Tuning Raft Interactions in Colloidal Membranes using Component Chirality

JOIA MILLER, Brandeis University, PRERNA SHARMA, Indian Institute of Science, ZVONIMIR DOGIC, Brandeis University — Two-dimensional colloidal membranes composed of rods of different lengths display rich phase behavior. In particular, the chirality of constituent rods stabilizes assembly of colloidal rafts, micron-sized droplets enriched in one type of rod floating in a membrane background with a different rod composition. Raft interactions are mediated by local rod twisting due to their rods' inherent chirality, leading to long-range repulsive interactions. We explore the behavior of rafts while reducing the net chirality of the membrane background. Even in the achiral limit, stable or metastable rafts form. However, in the achiral case the long-range interactions between rafts are attractive but not pairwise additive, resulting in the assembly of clusters of individual rafts. The membrane background has large-scale density fluctuations which we correlate to the raft interactions. Our work demonstrates a new method for assembly of well-defined clusters, one that does not rely on complex colloidal synthesis, but rather on the unique anisotropic environment of the colloidal membranes.

## Monday, March 14, 2016 11:15AM - 2:03PM —

Session B38 DPOLY FIAP: Nanocomposites from Nano to Meso 341 - Jian Yang, Dow Chemical Company

### 11:15AM B38.00001 Nanoparticle Ordering in Semicrystalline Polymers

VIANNEY GIMENEZ-PINTO, DAN ZHAO, SANAT KUMAR, Columbia University — One way to engineer the macroscopic properties of a crystalline polymer matrix is to place nanoparticles into them, but in an organized manner. We have recently found that NP organization can be controlled by varying the crystal growth rate. We develop a coarse-grained model to study this situation. In particular, we focus on the out-of-equilibrium dynamics of nanoparticles being pushed/engulfed by a solidification front depending on crystallization velocity  $v_s$ . Particle engulfment occurs when  $v_s$  is higher than a critical velocity  $v_c$ . When  $v_s$  is smaller than  $v_c$ , particles are pushed by the crystallization front and organize in a 2-D plane. Even though most models for particle engulfment consider dynamic force equilibrium at  $v_c$ , we show the system is not in equilibrium in this regime. Thus, we consider conditions for engulfment based on particle velocity with respect to crystal growth rate. Our results agree with experimental observations on anisotropic organization of nanoparticles in semicrystalline polymers driven by crystallization speed.

### 11:27AM B38.00002 Dispersion of Mixed Brush Gold Nanorods in Polymer Matrices

ROBERT FERRIER, JASON KOSKI, ROBERT RIGGLEMAN, RUSSELL COMPOSTO, University of Pennsylvania — In this work we investigate, both experimentally and through hybrid particle/self-consistent field theoretic (hSCFT) calculations, the dispersion state of gold nanorods (AuNRs) grafted with homopolymer, bidispersed, or mixed polymer brushes. AuNRs are grafted with 11.5 kg/mol PS (HNRs), 11.5 kg/mol PS and 5.3 kg/mol PS (BNRs), or 11.5 kg/mol PS and 5 kg/mol poly(methyl methacrylate) (PMMA) (MBNRs) and cast in PS or PMMA films consisting of short to very long chains compared to the grafted brush. We further investigated the MBNR systems by varying the length of the PS brush. Overall, we find that the MBNRs dispersed markedly better than the other brush types (HNRs or BNRs) in PS matrices. We utilize hSCFT calculations, in particular potential of mean force (PMF) and brush profile calculations, to elucidate the thermodynamics of these systems. The PMFs and brush profiles exhibit similar trends for the BNRs and MBNRs where the short grafted chain forces the longer grafted chain away from the AuNR surface and promotes wetting by the matrix chains. The hSCFT calculations demonstrated qualitative trends consistent with the aggregation observed for AuNRs in PMMA matrices. Therefore, we have demonstrated that MBNR dispersion in polymer matrices is enhanced compared to the HNR and BNR cases, which extends the dispersion window for new combinations of nanorods and polymers.

**11:39AM B38.00003 Examination of nanoparticle dispersion using a novel GPU based radial distribution function code** , THOMAS ROSCH, National Institute of Standards and Technology, MATTHEW WADE, Case Western Reserve University, FREDERICK PHELAN, National Institute of Standards and Technology — We have developed a novel GPU-based code that rapidly calculates radial distribution function (RDF) for an entire system, with no cutoff, ensuring accuracy. Built on top of this code, we have developed tools to calculate the second virial coefficient ( $B_2$ ) and the structure factor from the RDF, two properties that are directly related to the dispersion of nanoparticles in nanocomposite systems. We validate the RDF calculations by comparison with previously published results, and also show how our code, which takes into account bonding in polymeric systems, enables more accurate predictions of  $g(r)$  than current state of the art GPU-based RDF codes currently available for these systems. In addition, our code reduces the computational time by approximately an order of magnitude compared to CPU-based calculations. We demonstrate the application of our toolset by the examination of a coarse-grained nanocomposite system and show how different surface energies between particle and polymer lead to different dispersion states, and effect properties such as viscosity, yield strength, elasticity, and thermal conductivity.

**11:51AM B38.00004 Analysis of the kinetics of filler segregation in granular block copolymer microstructure** , BONGJOON LEE, Carnegie Mellon University, MARKUS BLEUEL, NIST Center for Neutron Research, DAVID OTT, MICHAEL BOCKSTALLER, Carnegie Mellon University, CARNEGIE MELLON UNIVERSITY TEAM — To realize the application of block copolymers in areas ranging from dynamically tunable photonic crystals to solid-state electrolytes, it is important to understand the role of additives in the evolution of microstructure (i.e. grain size and shape as well as distribution) during thermal processing. Previous studies have revealed the interaction of filler species (such as homopolymers or particle additives) to drive the segregation of filler into grain boundary regions, thereby stabilizing grain boundary and arresting grain growth. In this contribution we present a novel approach based on combined Ultra-Small Angle Neutron Scattering (USANS) and electron microscopy analysis (involving large area image reconstruction) to quantitatively determine the kinetics of filler segregation and its affect on grain size evolution in block copolymer blends. Calculation of the scattering length density of the grain boundary network is shown to provide detailed information about the rate and time dependence of filler segregation. For the particular case of a poly(styrene-*b*-isoprene)/*d*-polystyrene blends system it is found that 2 vol% of filler segregation during the early stage of thermal annealing is sufficient to arrest grain growth.

**12:03PM B38.00005 Localization of Individual Nanoparticle in the Perforated Lamellar Phase of Self-assembled Block Copolymer Driven by Entropy Minimization** , TAE WON NAM, Korea Adv Inst of Sci & Tech — Although precisely controlled microdomains of block copolymers (BCP) provide an excellent guiding matrix for multiple nanoparticles (NPs) to be controllably segregated into a desired polymer block, localization and positioning of individual NPs have not been demonstrated. Here, we report a unique one-to-one positioning phenomenon of guest Au NPs in the host BCP microdomains; each of polystyrene-functionalized Au NPs is embedded within the perforation domain of hexagonally perforated lamellar (HPL) morphology of poly(dimethylsiloxane-*b*-styrene) BCP. The local minimization of free energy achieved by the placement of Au NPs into the center of the perforation domain is theoretically supported by the self-consistent field theory (SCFT) simulation. We propose a novel design principle for more precisely controllable nanocomposites by developing a new route of NP arrangement within a polymer matrix.

**12:15PM B38.00006 Predicting the dynamics and thermodynamics of nanoparticles in block copolymers** , ROBERT RIGGLEMAN, University of Pennsylvania — In applications involving polymer nanocomposites, controlling the dispersion of the nanoparticles is one of the most critical aspects of their design. For example, optimal mechanical properties are typically found when particles are maximally dispersed, while varying the interparticle spacing on the nm length scale can tune the optical properties of a composite. In all of these cases, the distribution of nanoparticles is a complex interplay of entropic and energetic interactions between the matrix polymers, nanoparticles, particle surface-grafted polymers, and even the processing conditions. Recently, my group has been extending the polymer field theory framework to enable the study of inhomogeneous polymer nanocomposites. The framework has the advantage of being computationally efficient and able to treat anisotropic particles (nanorods) and explicit surface chemistry, such as grafted nanoparticles. In this talk, I will describe some of our recent results with the method studying the distribution and interactions between nanoparticles in block copolymer matrices. First, I will show how we have quantified the interactions between nanoparticles and block copolymer grain boundaries. Second, I will describe our more recent efforts using non-equilibrium methods to study the role of processing, such as solvent annealing, on the distribution of nanoparticles in block copolymer thin films.

**12:51PM B38.00007 A Novel Method to Characterize Nanorod Orientation and Aggregation in Polymer Nanocomposites**<sup>1</sup> , ETHAN GLOR, ROBERT FERRIER, RUSSELL COMPOSTO, ZAHRA FAKHRAAI, Univ of Pennsylvania — Gold nanorods provide an ideal system for the systematic change of optical properties through changes in the rod aspect ratio. Furthermore, the dispersity and orientation of the nanorods within a polymer matrix greatly affects the optical properties of the composites. Here, we use spectroscopic ellipsometry to characterize the properties of nanocomposite thin films. The optical properties of the nanorod are modeled as an effective index of refraction for a disordered meta-material. This effective medium index is then related to the longitudinal surface plasmon resonance (LSPR) of the nanorods. The degree of birefringence in the LSPR frequency, as determined by variable angle ellipsometry measurements, can help determine the average orientation of the rods in the thin film as well as the degree of aggregation. With this method, one can quickly and accurately define the average orientation and average aggregation of nanorods within a nanocomposite with a single measurement. Ellipsometry also allows us to perform *in-situ* variable temperature measurements to monitor properties such as nanoparticle shape and the glass transition temperature of the matrix.

<sup>1</sup> Acknowledgement: NSF-PIRE-1545884, MRSEC (NSF-DMR-11- 20901)

**1:03PM B38.00008 Microstructure of 3D-Printed Polymer Composites Investigated by Small-Angle Neutron Scattering**<sup>1</sup> , TAE HUI KANG, Oak Ridge National Lab, BRETT G. COMPTON, University of Tennessee, WILLIAM T. HELLER, VOKER S. URBAN, CHAD E. DUTY, CHANGWOO DO, Oak Ridge National Lab — Polymer composites printed from the large scale printer at Manufacturing Demonstration Facility at Oak Ridge National Laboratory have been investigated by small-angle neutron scattering (SANS). For the Acrylonitrile Butadiene Styrene (ABS)/Carbon Fiber (CF) composites, the microstructure of polymer domains and the alignment of CF have been characterized across the layer from the printed piece. CF shows strong anisotropic alignment along the printing direction due to the flow of polymer melt at the nozzle. Order parameter of the anisotropy which ranges from -0.11 to -0.06 exhibits strong correlation with the position within the layer: stronger alignment near the layer interface. It is also confirmed that the existence of CF reduces the polymer domain correlation length significantly and reinforces the mechanical strength of the polymer composites. For the Epoxy/nano-clay platelet composites, the effect of processing condition, nozzle size, and the addition of the another filler, Silicon Carbide (SC), have been investigated by SANS. Nano-clay platelet shows strong anisotropic alignment along the printing direction as well. Order parameter of the anisotropy varies according to nozzle size and presence of the SC, and difference disappears at high Q region.

<sup>1</sup> Scientific User Facilities Division and Materials Sciences and Energy Division, Office of Basic Energy Sciences, U.S. Department of Energy.

**1:15PM B38.00009 Large Volume Self-Organization of Polymer/Nanoparticle Hybrids with Millimeter Scale Grain Sizes using Brush Block Copolymers**, DONGPO SONG, JAMES WATKINS, Department of Polymer Science and Engineering, University of Massachusetts Amherst — The lack of sufficient long-range order in self-assembled nanostructures is a bottleneck for many nanotechnology applications. In this work, we report that exceptionally large volume of highly ordered arrays (single grains) on the order of millimeters in scale can be rapidly created through a unique innate guiding mechanism of brush block copolymers (BBCPs). The grain volume is over 1 billion times larger relative to that of typical self-assembled linear BCPs (LBCPs). The use of strong interactions between nanoparticles (NPs) and BBCPs enables the high loadings of functional materials, up to 76 wt% (46 vol%) in the target domain, while maintaining excellent long-range order. Overall this work provides a simple route to precisely control the spatial orientation of functionalities at nanometer length scales over macroscopic volumes, thereby enabling the production of hybrid materials for many important applications.

**1:27PM B38.00010 Tuning the interactions between nanoparticles in block copolymer domains**, BEN LINDSAY, University of Pennsylvania, JEFFREY METH, DuPont, RUSSELL COMPOSTO, ROBERT RIGGLEMAN, University of Pennsylvania — Block copolymer nanocomposites have the potential to become a platform for new materials with improved thermal, electrical, or optical properties compared to neat polymers. However, it is critical to control the dispersion of the nanoparticles in the block copolymer matrix, and thus it is important to understand how nanoparticles interact with each other within block copolymer domains. In this work, we use a polymer nanocomposite field theory (PNC-FT) that was recently developed in our group to study the interactions of nanoparticles within both cylindrical and lamellar block copolymer structures. We find that the nanoparticles induce a curvature in the A-B interface in the block copolymer, which plays a significant role in the interparticle interactions, leading to a non-monotonic potential of mean force between the particles. This effect becomes more pronounced as the nanoparticle size increases. Finally, we will also present results showing the effect of nanoparticle surface functionality (polymer grafting) on the interparticle interactions.

**1:39PM B38.00011 Novel Polymer Nanocomposites Resulted from Melt Processing of Polystyrene-Based Substrates Coated with Layer-by-Layer Assemblies**, IMAN SOLTANI, RICHARD J. SPONTAK, North Carolina State Univ — The novel polymer nanocomposites (PNCs) prepared through two steps of coating polystyrene-based substrates with layer-by-layer (LBL) deposition of montmorillonite and alternative polyelectrolyte layers of polyethyleneimine and polyethylene terephthalate ionomer, followed by their cyclic melt pressing, demonstrated particular morphologies. Transmission electron microscopy images at high magnification scales showed the occurrence of swollen intercalation and flocculated exfoliations of clay platelets, down to a few nanometer thickness, inside and sometimes out of LBL assemblies crushed portions. In fact, intercalation and exfoliation of clay platelets, established in LBL assemblies, increased by shear applied through their repetitive melt pressing. Additionally, x-ray diffractometry traces confirmed the aforementioned increase in clay intercalation. These high aspect ratio LBL assemblies portions formed highly tortuous labyrinths, which may work as scavenging centers to promote barrier properties of the PNCs against transport of gases like oxygen and carbon dioxide. It is despite spontaneously low interaction between hydrophobic styrenic groups and almost hydrophilic natural clay and moderate efficiency of cyclic pressing for providing intensive shear stress on samples.

**1:51PM B38.00012 Stabilization of PS/PLA cocontinuous blends by interfacial graphene<sup>1</sup>**, LIAN BAI, Department of Chemical Engineering and Materials Science, University of Minnesota, SIYAO HE, Department of Chemistry, University of Minnesota, JOHN FRUEHWIRTH, Department of Chemical Engineering and Materials Science, University of Minnesota, ANDREAS STEIN, Department of Chemistry, University of Minnesota, XIANG CHENG, CHRISTOPHER MACOSKO, Department of Chemical Engineering and Materials Science, University of Minnesota — Reduced graphene oxide (r-GO) is known to be effective in increasing the conductivity of cocontinuous polymer blends with a lower electrical percolation threshold. However, little is known regarding the localization and dynamics of r-GO along with morphology change during annealing. In this study, we develop a facile method to stabilize the polystyrene (PS)/polylactic acid (PLA) cocontinuous blends with r-GO jammed at interface. In this method, the non-functionalized GO is premixed with PLA via solvent method, and then reduced in-situ at 210°C to obtain a PLA/r-GO polymer composite. This composite is further mixed with PS via batch melt compounding. We observe the migration of r-GO from the PLA phase to the interface during annealing. The interfacial r-GO suppresses the coarsening of cocontinuous morphology and increases the conductivity of the filled polymer blend. Moreover, we systematically investigate the relationship between r-GO localization, rheological and conductivity change during annealing of r-GO filled PLA/PS blends.

<sup>1</sup>University of Minnesota Industrial Partnership for Research in Interfacial and Materials Engineering (IPRIME)

**Monday, March 14, 2016 11:15AM - 2:15PM —**

**Session B39 DBIO GSOFT: Physics of Cancer and Development I** 342 - Arpita Upadhyaya, University of Maryland

**11:15AM B39.00001 Real-time Visualization of Tissue Dynamics during Embryonic Development and Malignant Transformation**, KENNETH YAMADA, National Institutes of Health, National Institute of Dental and Craniofacial Research — Tissues undergo dramatic changes in organization during embryonic development, as well as during cancer progression and invasion. Recent advances in microscopy now allow us to visualize and track directly the dynamic movements of tissues, their constituent cells, and cellular substructures. This behavior can now be visualized not only in regular tissue culture on flat surfaces ('2D' environments), but also in a variety of 3D environments that may provide physiological cues relevant to understanding dynamics within living organisms. Acquisition of imaging data using various microscopy modalities will provide rich opportunities for determining the roles of physical factors and for computational modeling of complex processes in living tissues. Direct visualization of real-time motility is providing insight into biology spanning multiple spatio-temporal scales. Many cells in our body are known to be in contact with connective tissue and other forms of extracellular matrix. They do so through microscopic cellular adhesions that bind to matrix proteins. In particular, fluorescence microscopy has revealed that cells dynamically probe and bend the matrix at the sites of cell adhesions, and that 3D matrix architecture, stiffness, and elasticity can each regulate migration of the cells. Conversely, cells remodel their local matrix as organs form or tumors invade. Cancer cells can invade tissues using microscopic protrusions that degrade the surrounding matrix; in this case, the local matrix protein concentration is more important for inducing the micro-invasive protrusions than stiffness. On the length scales of tissues, transiently high rates of individual cell movement appear to help establish organ architecture. In fact, isolated cells can self-organize to form tissue structures. In all of these cases, in-depth real-time visualization will ultimately provide the extensive data needed for computer modeling and for testing hypotheses in which physical forces interact closely with cell signaling to form organs or promote tumor invasion.

**11:51AM B39.00002 Emergence of tissue mechanics from cellular processes: shaping a fly wing**, MATTHIAS MERKEL, Max Planck Institute for the Physics of Complex Systems, Dresden (MPI-PKS), RAPHAEL ETOURNAY, Max Planck Institute of Molecular Biology and Genetics, Dresden (MPI-CBG), MARKO POPOVIC, AMITABHA NANDI, MPI-PKS, HOLGER BRANDL, MPI-CBG, GUILLAUME SALBREUX, Crick Institute, London, SUZANNE EATON, MPI-CBG, FRANK JLICHER, MPI-PKS — Nowadays, biologists are able to image biological tissues with up to 10,000 cells in vivo where the behavior of each individual cell can be followed in detail. However, how precisely large-scale tissue deformation and stresses emerge from cellular behavior remains elusive. Here, we study this question in the developing wing of the fruit fly. To this end, we first establish a geometrical framework that exactly decomposes tissue deformation into contributions by different kinds of cellular processes. These processes comprise cell shape changes, cell neighbor exchanges, cell divisions, and cell extrusions. As the key idea, we introduce a tiling of the cellular network into triangles. This approach also reveals that tissue deformation can also be created by correlated cellular motion. Based on quantifications using these concepts, we developed a novel continuum mechanical model for the fly wing. In particular, our model includes active anisotropic stresses and a delay in the response of cell rearrangements to material stresses. A different approach to study the emergence of tissue mechanics from cellular behavior are cell-based models. We characterize the properties of a cell-based model for 3D tissues that is a hybrid between single particle models and the so-called vertex models.

**12:03PM B39.00003 Quantifying the mechanics of embryonic tissues in vivo and in situ**, OTGER CAMPAS, University of California, Santa Barbara — The sculpting of tissues and organs involves a tight spatiotemporal regulation of several physical fields, including active mechanical stresses and the local material properties. Despite the relevance of mechanics in embryonic morphogenesis, very little is known about the mechanisms by which tissue mechanics affects/controls developmental processes, mainly because it has not been possible to quantify mechanics within developing tissues in vivo and in situ. I will present two new techniques that permit direct quantification of (1) mechanical stresses at both tissue and cellular scales and (2) the material properties of the cellular microenvironment, in situ within living tissues and developing organs. Using these novel techniques, we characterize the mechanics of cell aggregates (in vitro), living mouse mandibles (ex vivo) and live zebrafish embryonic tissues (in vivo).

**12:15PM B39.00004 Cancer cell elasticity response to the mechanics of microenvironment**, JINGQIANG LI, RAYMOND FANG, KEVIN JIANG, Rice University, IAN LIAN, Lamar University, CHING-HWA KIANG, Rice University, RICE UNIVERSITY TEAM, LAMAR UNIVERSITY TEAM — Cells can sense and respond to the mechanical properties of their microenvironment. In particular, the rigidity of the cell's microenvironment is regarded as a physical parameter of interest given its regulation of various cellular processes, including proliferation, differentiation and migration. Currently, in vitro cancer studies primarily performed by monolayer culture grown on the rigid polystyrene surfaces, but in vivo cancer cells interact with much softer tissue. Here, we utilize a new soft substrate cell culture platform to mimic tissues with various stiffness within the physiological range (0.2–100 kPa). We apply atomic force microscopy (AFM) to probe the elastic behaviors of three different cancer cell lines so as to emulate the essential features in the in vivo microenvironment. We observed that the substrate stiffness has a significant effect on the cell morphology and elasticity. The results of our study could have important implications regarding to the physics of cancer metastasis.

**12:27PM B39.00005 Cell Membrane Softening in Cancer Cells**, SEBASTIAN SCHMIDT, CHRIS HNDEL, JOSEF KS, Leipzig University — Biomechanical properties are useful characteristics and regulators of the cell's state. Current research connects mechanical properties of the cytoskeleton to many cellular processes but does not investigate the biomechanics of the plasma membrane. We evaluated thermal fluctuations of giant plasma membrane vesicles, directly derived from the plasma membranes of primary breast and cervical cells and observed a lowered rigidity in the plasma membrane of malignant cells compared to non-malignant cells. To investigate the specific role of membrane rigidity changes, we treated two cell lines with the Acetyl-CoA carboxylase inhibitor Sorafenib. It changed the lipidome of cells and drastically increased membrane stiffness by up-regulating short chained membrane lipids. These altered cells had a decreased motility in Boyden chamber assays. Our results indicate that the thermal fluctuations of the membrane, which are much smaller than the fluctuations driven by the cytoskeleton, can be modulated by the cell and have an impact on adhesion and motility.

**12:39PM B39.00006 Network motifs that stabilize the hybrid epithelial/mesenchymal phenotype<sup>1</sup>**, MOHIT KUMAR JOLLY, DONGYI JIA, Rice Univ, SATYENDRA TRIPATHI, SAMIR HANASH, SENDURAI MANI, MD Anderson Cancer Center, ESHEL BEN-JACOB, HERBERT LEVINE, Rice Univ — Epithelial to Mesenchymal Transition (EMT) and its reverse – MET – are hallmarks of cancer metastasis. While transitioning between E and M phenotypes, cells can also attain a hybrid epithelial/mesenchymal (E/M) phenotype that enables collective cell migration as a cluster of Circulating Tumor Cells (CTCs). These clusters can form 50-times more tumors than individually migrating CTCs, underlining their importance in metastasis. However, this hybrid E/M phenotype has been hypothesized to be only a transient one that is attained en route EMT. Here, via mathematical modeling, we identify certain 'phenotypic stability factors' that couple with the core three-way decision-making circuit (miR-200/ZEB) and can maintain or stabilize the hybrid E/M phenotype. Further, we show experimentally that this phenotype can be maintained stably at a single-cell level, and knockdown of these factors impairs collective cell migration. We also show that these factors enable the association of hybrid E/M with high stemness or tumor-initiating potential. Finally, based on these factors, we deduce specific network motifs that can maintain the E/M phenotype. Our framework can be used to elucidate the effect of other players in regulating cellular plasticity during metastasis.

<sup>1</sup>This work was supported by NSF PHY-1427654 (Center for Theoretical Biological Physics) and the CPRIT Scholar in Cancer Research of the State of Texas at Rice University

**12:51PM B39.00007 Combinatorial Interventions Inhibit the Epithelial-to-Mesenchymal Transition and Support Hybrid Cellular Phenotypes<sup>1</sup>**, JORGE G. T. ZANUDO, S.N. STEINWAY, The Pennsylvania State University, P.J. MICHEL, D.J. FEITH, T.P. LOUGHRAN JR., University of Virginia School of Medicine, REKA ALBERT, The Pennsylvania State University — Epithelial-to-mesenchymal transition (EMT) is a developmental process hijacked by cancer cells to leave the primary tumor site and spread to other parts of the body. The molecular network regulating EMT involves the cooperation and cross-talk between multiple signaling pathways and key transcription factors, which we incorporated into systems-level logical network model for EMT. Using the EMT network model, we investigate potential EMT-suppressing interventions by identifying which individual and combinatorial perturbations suppress the induction of EMT by TGF $\beta$ , an important signal driving EMT in liver cancer. We find that all non-trivial interventions are combinatorial and involve the inhibition of the SMAD complex together with other targets, several of which we experimentally tested and validated using liver cancer cell lines. We compare the combinatorial interventions with the results from a network control method we recently developed, which allowed us to determine the specific feedback regulatory motifs through which the interventions suppress EMT. Our results also reveal that blocking certain network components gives rise to steady states that are intermediate to the epithelial and mesenchymal states, supporting the existence of hybrid epithelial-mesenchymal states.

<sup>1</sup>Supported by NSF grants PHY 1205840 and IIS 1161001, and NIH grant F30DK093234.

**1:03PM B39.00008 Testing the differential adhesion hypothesis across the epithelial-mesenchymal transition**, STEVE PAWLIZAK, ANATOL FRITSCH, STEFFEN GROSSER, LINDA OSWALD, Leipzig University, LISA MANNING, Syracuse University, JOSEF KAS, Leipzig University — We analyze the properties of three epithelial/mesenchymal cell lines that exhibit a shift in cadherin levels characteristic of an epithelial-mesenchymal transition (EMT) associated with processes such as metastasis, to quantify the role of cell cohesion in cell sorting and compartmentalization. We develop a unique set of methods to measure cell-cell adhesiveness, cell stiffness and cell shapes, and compare the results to predictions from cell sorting in mixtures of cell populations. We find that the final sorted state is extremely robust among all three cell lines independent of epithelial or mesenchymal state, suggesting that cell sorting may play an important role in organization and boundary formation in tumours. We find that surface densities of adhesive molecules do not correlate with measured cell-cell adhesion, but do correlate with cell shapes, cell stiffness and the rate at which cells sort, in accordance with an extended differential adhesion hypothesis (DAH). Surprisingly, the DAH does not correctly predict the final sorted state. This suggests that these tissues are not behaving as immiscible fluids, and that dynamical effects such as directional motility, friction and jamming may play an important role in tissue compartmentalization across the EMT.

**1:15PM B39.00009 Polymeric Nanocomposite that Mimics in vivo ECM Topography in Tissue using Magnetic Field-induced Particle Self-assembly.**, JIYUN KIM, JACK STAUNTON, KANDICE TANNER, National Institutes of Health — 3D biomaterials that mimic a certain physical or chemical aspect of cellular environment have been used to recreate the diversity of the tissue microenvironment. Especially, physical characteristics of these materials such as topography, dimension and stiffness, have known to have crucial effects on cell fate and cell malignancy. Here, we propose a technique that is able to create diverse topographies in 3D polymeric scaffold for the purpose of mimicking the structural aspect of tissue microenvironment. To achieve this, we exploit the magnetic field-directed assembly of super paramagnetic particles to fabricate chain-distributed architecture such that we can study the effects of extracellular matrix (ECM) topography on cell behavior. First, we chemically cross-link proteins including fibronectin, laminin and bovine albumin serum on the surface of magnetic particles to make the building blocks for artificial topography. Then, we assemble these particles by applying the parallel magnetic field in a surrogate polymeric matrix and solidify the matrix to maintain the assembled topography. Using this simple technique, we patterned diverse topographies in 3D including globular, fibril or interfaced architectures without chafing other material characteristics of the scaffold matrix, such as stiffness and molecular diffusion. We demonstrated that the fibril architecture guides the dendritic extension of fibroblasts and neuron-like cells, compared to the cells grown in the globular architecture lacking anisotropic guidance cues.

**1:27PM B39.00010 Interplay of differential cell mechanical properties, motility, and proliferation in emergent collective behavior of cell co-cultures<sup>1</sup>**, LEO SUTTER, DAN KOLBMAN, Rochester Institute of Technology, MINGMING WU, MINGLIN MA, Cornell University, MOUMITA DAS, Rochester Institute of Technology — The biophysics of cell co-cultures, i.e. binary systems of cell populations, is of great interest in many biological processes including formation of embryos, and tumor progression. During these processes, different types of cells with different physical properties are mixed with each other, with important consequences for cell-cell interaction, aggregation, and migration. The role of the differences in their physical properties in their collective behavior remains poorly understood. Furthermore, until recently most theoretical studies of collective cell migration have focused on two dimensional systems. Under physiological conditions, however, cells often have to navigate three dimensional and confined micro-environments. We study a confined, three-dimensional binary system of interacting, active, and deformable particles with different physical properties such as deformability, motility, adhesion, and division rates using Langevin Dynamics simulations. Our findings may provide insights into how the differences in and interplay between cell mechanical properties, division, and motility influence emergent collective behavior such as cell aggregation and segregation experimentally observed in co-cultures of breast cancer cells and healthy breast epithelial cells.

<sup>1</sup>This work was partially supported by a Cottrell College Science Award

**1:39PM B39.00011 How do heterogeneities in single cell rigidity influence the mechanical behavior at the tissue level?**, DAPENG BI, Rockefeller University, FRANZISKA WETZEL, ANATOL FRITSCH, University of Leipzig, M. CRISTINA MARCHETTI, M. LISA MANNING, Syracuse University, JOSEF KAES, University of Leipzig — It has been long recognized that solid tumor tissues are mechanically more rigid than surrounding healthy tissues. However recent experiments have shown that in primary tumor samples from patients with mammary and cervix carcinomas, cells exhibit a broad distribution of rigidities, with a higher fraction of softer and more contractile cells compared to normal tissues. This gives rise to a paradox: does softness emerge from adaptation to mechanical and chemical cues in the external microenvironment, or are soft cells already present inside a primary solid tumor? Motivated by these observations, we study a model of dense tissues that incorporates the experimental data for cell stiffness variations to reveal that, surprisingly, tumors with a significant fraction of very soft cells can still remain rigid. Moreover, in tissues with the observed distributions of cell stiffnesses, softer cells spontaneously self-organize into lines or streams, possibly facilitating cancer metastasis.

**1:51PM B39.00012 Modeling the Spatiotemporal Evolution of the Melanoma Tumor Microenvironment**, ALEXANDRA SIGNORIELLO, MARCUS BOSENBERG, Yale University, MARK SHATTUCK, City College of New York, COREY O'HERN, Yale University — The tumor microenvironment, which includes tumor cells, tumor-associated macrophages (TAM), cancer-associated fibroblasts, and endothelial cells, drives the formation and progression of melanoma tumors. Using quantitative analysis of in vivo confocal images of melanoma tumors in three spatial dimensions, we examine the physical properties of the melanoma tumor microenvironment, including the numbers of different cell types, cell size, and morphology. We also compute the nearest neighbor statistics and measure intermediate range spatial correlations between different cell types. We also calculate the step size distribution, mean-square displacement, and non-Gaussian parameter from the spatial trajectories of different cell types in the tumor microenvironment.

**2:03PM B39.00013 Stochastic modeling and experimental analysis of phenotypic switching and survival of cancer cells under stress**, SEYED ALIREZA ZAMANI DAHAJ, NIRAJ KUMAR, BALA SUNDARAM, JONATHAN CELLI, RAHUL KULKARNI, Department of Physics, University of Massachusetts Boston — The phenotypic heterogeneity of cancer cells is critical to their survival under stress. A significant contribution to heterogeneity of cancer cells derives from the epithelial-mesenchymal transition (EMT), a conserved cellular program that is crucial for embryonic development. Several studies have investigated the role of EMT in growth of early stage tumors into invasive malignancies. Also, EMT has been closely associated with the acquisition of chemoresistance properties in cancer cells. Motivated by these studies, we analyze multi-phenotype stochastic models of the evolution of cancer cell populations under stress. We derive analytical results for time-dependent probability distributions that provide insights into the competing rates underlying phenotypic switching (e.g. during EMT) and the corresponding survival of cancer cells. Experimentally, we evaluate these model-based predictions by imaging human pancreatic cancer cell lines grown with and without cytotoxic agents and measure growth kinetics, survival, morphological changes and (terminal evaluation of) biomarkers with associated epithelial and mesenchymal phenotypes. The results derived suggest approaches for distinguishing between adaptation and selection scenarios for survival in the presence of external stresses.

**Monday, March 14, 2016 11:15AM - 2:15PM —**

**Session B40 GSNP DFD: Fluids and Elasticity 343 - Doug Holmes, Boston University**

**11:15AM B40.00001 Direct measurement of surface stress of stretched soft solids.** , QIN XU, ERIC DUFRESNE, Mechanical Engineering and Materials Science, Yale University — The wetting profile of liquid droplets on soft solids is determined by the competition between elasticity and solid surface stress. Near the contact point, the bulk elasticity becomes negligible such that Neumann's classic analysis nicely captures the wetting geometry and provides us an effective approach to directly measure the solid surface stress. Here, we report our experiments using confocal microscopy in studying the wetting of liquids on soft PDMS gels. While the droplets are sitting on the top, the substrates are biaxially strained. We observe that the wetting profiles and the three-phase contact angles are changing dramatically as the substrate is stretched. With Neumann's principle, we obtain the quantitative relation between surface stress of the PDMS and the applied strain. These results suggest a significant strain-dependence of surface energy and surface stress for our PDMS.

**11:27AM B40.00002 A numerical modeling capability for the interplay between surface energy and elasticity in soft materials** , DAVID HENANN, YUHAO WANG, Brown University — Surface energy is an important factor in the deformation of fluids but is typically a minimal or negligible effect in solids. However, when a solid is soft and its characteristic dimension is small, forces due to surface energy can become important and induce significant elastic deformation. The interplay between surface energy and elasticity can lead to interesting elasto-capillary phenomena. We have developed a finite-element formulation for problems involving these effects in both 2D and 3D settings and will demonstrate the simulation capability by examining two elasto-capillary problems. (1) The Rayleigh-Plateau instability in an elastic material — In a fluid, this instability causes fluid jets to break up into droplets; however, as shown in recent experiments (Mora et al., PRL, 2010), break-up is prohibited in an elastic material, resulting in a stable undulatory configuration. (2) The effect of fluid-filled droplet inclusions on a soft solid — When the matrix material is stiff, the presence of fluid-filled inclusions leads to a more compliant composite material; however, recent experiments (Style, et al., Nature Physics, 2014) have shown that when the matrix material is more compliant, the presence of droplets leads to stiffening. In this talk, we will show that our simulation capability predicts all experimentally observed phenomena and provides a straightforward route for describing nonlinear aspects of elasto-capillarity, which are difficult to address via analytics.

**11:39AM B40.00003 Elastocapillary Deformations and Fracture of Soft Gels** , KAREN DANIELS, NC State University, MARION GRZELKA, ENS-Cachan, JOSHUA BOSTWICK, Clemson University — When a droplet is placed on the surface of a soft gel, the surface deforms by an amount proportional to the elastocapillary length calculated from the ratio of surface tension and elastic modulus. For sufficiently large deformations, the gel can fracture due to the forces generated under the liquid-gel contact line. We observe that a starburst of channel fractures forms at the surface of the gel, driven by fluid propagating away from the central droplet. To understand the initiation of these cracks, we model the substrate as an incompressible, linear-elastic solid and quantify the elastic response. This provides quantitative agreement with experimental measurements of the number of fracture arms as a function of material properties and geometric parameters. In addition, we find that the initiation process is thermally-activated, with delay time that decreases as a function of the elastocapillary length.

**11:51AM B40.00004 Surface tension and deformation in soft adhesion** , KATHARINE JENSEN, Yale University — Modern contact mechanics was originally developed to account for the competition between adhesion and elasticity for relatively stiff deformable materials like rubber, but much softer sticky materials are ubiquitous in biology, engineering, and everyday consumer products. In such soft materials, the solid surface tension can also play an important role in resisting shape change, and significantly modify the physics of contact with soft matter. We report indentation and pull-off experiments that bring small, rigid spheres into adhesive contact with compliant silicone gel substrates, varying both the surface functionalization of the spheres and the bulk elastic properties of the gels. We map the resulting deformation profiles using optical microscopy and image analysis. We examine the substrate geometry in light of capillary and elastic theories in order to explore the interplay of surface tension and bulk elasticity in governing soft adhesion.

**12:27PM B40.00005 Elastocapillary Swelling: When coalesced structures curl apart** , DOUGLAS HOLMES, Boston University, PIERRE-THOMAS BRUN, MIT, ANUPAM PANDEY, University of Twente, SUZIE PROTIERE, Institut Jean Le Rond d'Alembert — We consider the elastocapillary rise between swellable structures using a favorable solvent. We study the elastocapillary rise and subsequent swelling-induced bending, and characterize the dynamic deformations and resulting equilibrium configurations for various beam geometries. Our analysis highlights the importance of two characteristic length scales, and uses these lengths to predict both the elastocapillary rise and the critical curvature for peeling. We predict the transition between coalescence dominated beams and bending dominated beams using a balance of bending, stretching, and surface energies, and use a relaxed constraint on Euler's elastica to describe the fluid ratcheting.

**12:39PM B40.00006 Effects of elasto-capillarity on periodic films folding and unfolding** , OSAMA BILAL, ANDRE FOEHR, JINWOONG CHA , CHIARA DARAI, Department of Mechanical and Process Engineering, ETH-Zurich — Thin films interact with liquid surfaces through elastocapillary forces. These forces can control structural deformations of wetted thin films. Deformations arise from the interplay between the elastic strain energy in the bulk of the films, and the energy on the surface. In this work, we study the interplay between the surface tension of water and periodic patterns on different thin films. Our analysis explores the utilization of these periodically patterned films for the deployability of micro and nano-systems. The main attention is paid to the experimental results of this phenomenon and the results are supported by numerical analysis.

**12:51PM B40.00007 Wrinkles and folds in a compressed granular raft** , ETIENNE JAMBON-PUILLET, CHRISTOPHE JOSSERAND, SUZIE PROTIERE, Institut Jean le Rond d'Alembert, Univ Paris 6 UPMC, CNRS UMR 7190, France — Wrinkles and folds occur in a wide variety of situations, we find them in Nature but also in man-made products. They typically appear when a thin sheet bound to a foundation is compressed. Here we demonstrate that particle laden interfaces, despite being made of discrete very hard particles, can form wrinkles and folds like a soft elastic solid. We call granular raft a close packed monolayer of heavy, athermal particles at the interface between two fluids. We use beads of different materials with diameters ranging from 30  $\mu\text{m}$  to 0.8  $\text{mm}$  dispersed at a planar oil/water interface. Upon uniaxial compression the raft buckles out of plane like a soft elastic solid and forms a periodic wrinkling pattern, then the deformation localizes in a large unique fold/crease. This behavior is reminiscent of a compressed elastic sheet floating on water. We will highlight similarities and differences between the mechanical properties of our discrete heavy granular raft and a continuous elastic floating film. Finally we will show how elasticity and gravity contribute to rationalize the original shape of the fold we observe.

**1:03PM B40.00008 Wrapping with a splash** , DEEPAK KUMAR, University of Massachusetts Amherst, JOSEPH PAULSEN, Syracuse University, THOMAS RUSSELL, NARAYANAN MENON, University of Massachusetts Amherst — Ultrathin sheets have been used to encapsulate drops of one fluid in another. When the sheet is thin enough that bending energies are much smaller than interfacial energies, experiment and theory show that optimal wrappings are achieved without any special sheet design [1]. Here we study wrappings generated by the impact of an oil droplet onto an ultrathin (30-200 nm) polystyrene film floating on water. Depending on the energy of impact, a large deformation of the air-water interface is followed by formation of an oil phase wrapped around by the polymer film, submerged in the water. Even though the energetic cost of bending of the polymer film is very small, we find that successful wrapping requires an impact energy much larger than the energy difference between the initial and final configurations. We explore the dynamics of the fluid and the sheet in this process with a view to devising an efficient method to create optimal wrappings. [1] J.D. Paulsen, V. Dmery, C.D. Santangelo, T.P. Russell, B. Davidovitch, and N. Menon, doi:10.1038/nmat4397 (2015).

**1:15PM B40.00009 Deformation of flexible micro helices under flow**, MARINE DAIEFF, ANKE LINDNER, OLIVIA DU ROURE, PMMH-ESPCI, Paris, France, ALEXANDER MOROZOV, University of Edinburgh, United Kingdom, JONATHAN PHAM, ALFRED CROSBY, University of Massachusetts, Amherst, USA — The interaction of small helices with fluids is important because of its relevance to both fundamental science and technological applications, such as swimming microrobots or microflow sensors. Helically shaped flagella are also exploited by swimming microorganisms to move through their surrounding fluids. Here we study experimentally the deformation of flexible helical ribbons under flow in a microfluidic channel. The size of the helix is typically microscale for the diameter and nanoscale for the thickness. We focus on two different aspects: the overall shape of the helix and the viscous frictional properties. The frictional coefficients determined by our experiments are consistent with calculated values in the context of resistive force theory. Deformation of helices by viscous flow is well-described by non-linear finite extensibility. Due to the non-uniform distribution of the pitch under distributed loading, we identify both linear and nonlinear behavior along the contour length of a single helix. Utilizing our system, we explore the impact of non-Newtonian fluid properties on the mechanics of helix-fluid interactions.

**1:27PM B40.00010 Dynamics and propulsion of a rotating flexible helical rod near a no-slip rigid boundary**, MOHAMMAD JAWED, HUSSAIN KARIMI, PEDRO REIS, Massachusetts Institute of Technology — We study the effect of a no-slip rigid boundary on the locomotion of uni-flagellar bacteria in a viscous fluid at low Reynolds number conditions, through a combination of computer simulations and experiments. In our analogue model experiments, we exploit the prominence of geometry in this class of problems to rescale the original micron-scale system onto the desktop-scale. We manufacture elastomeric filaments with fully customizable geometric and material properties, and rotate them in a glycerin bath at a finite distance away from a rigid boundary. The experimental results are compared against numerical simulations that combine the Discrete Elastic Rods method in conjunction with Lighthill Slender Body Theory. The no-slip boundary condition on the wall is implemented by the method of images. We first show that the filament buckles above a critical rotation frequency due to fluid loading, and then quantify the dependence of this critical threshold on the distance from the boundary. Excellent agreement is found between experiments and simulations, with no fitting parameters. Moreover, we find that the generated propulsion force is strongly affected by the presence of a nearby boundary.

**1:39PM B40.00011 Fluid-structure interaction of reticulated porous wings**, ELIZABETH STRONG, MOHAMMAD JAWED, PEDRO REIS, MIT — Insects of the orders *Neuroptera* and *Hymenoptera* locomote via flapping flight with reticulated wings that have porous structures that confers them with remarkable lightweight characteristics. Yet these porous wings still perform as contiguous plates to provide the necessary aerodynamic lift and drag required for flight. Even though the fluid flow past the bulk of these insects may be in high Reynolds conditions, viscosity can dominate over inertia in the flow through the porous sub-features. Further considering the flexibility of these reticulated wings yields a highly nonlinear fluid-structure interaction problem. We perform a series of dynamically-scaled precision model experiments to gain physical insight into this system. Our experiments are complemented with computer simulations that combine the Discrete Elastic Rods method and a model for the fluid loading that takes into account the 'leakiness' through the porous structure. Our results are anticipated to find applications in micro-air vehicle aerodynamics.

**1:51PM B40.00012 Switchable and Tunable Aerodynamic Drag on Cylinders**, MARK GUTTAG, FRANCISCO LOPZ JIMNEZ, MIT, PRIYANK UPADHYAYA, SHANMUGAM KUMAR, Masdar Institute, PEDRO REIS, MIT — We report results on the performance of Smart Morphable Surfaces (Smporhs) that can be mounted onto cylindrical structures to actively reduce their aerodynamic drag. Our system comprises of an elastomeric thin shell with a series of carefully designed subsurface cavities that, once depressurized, lead to a dramatic deformation of the surface topography, on demand. Our design is inspired by the morphology of the giant cactus (*Carnegiea gigantea*) which possesses an array of axial grooves, thought to help reduce aerodynamic drag, thereby enhancing the structural robustness of the plant under wind loading. We perform systematic wind tunnel tests on cylinders covered with our Smorhs and characterize their aerodynamic performance. The switchable and tunable nature of our system offers substantial advantages for aerodynamic performance when compared to static topographies, due to their operation over a wider range of flow conditions.

**2:03PM B40.00013 Fanning the Optimal Breeze with an Abanico**, GRACE GOON, JOEL MARTHELOT, PEDRO REIS, MIT, MIT EGS LAB TEAM — Flexible hand-held fans, or abanicos, are universally employed as cooling devices that are both portable and sustainable. Their to and fro axial motion about one's hand generates an airflow that increases the evaporation rate near the skin and refreshes. We study this problem in the context of fluid-structure interaction, through precision model experiments. We first characterize the elastic properties of a semi-circular thin plates with various thickness and evaluate their aerodynamic performance in a custom built apparatus. The air velocity profile that results from the flapping motion of the fan is characterized for different driving conditions. A systematic variation of the geometric and elastic parameters, along with an exploration of the parameter space of the periodic driving motion (amplitude and frequency), allows us to establish optimal design and operational conditions for maximal output of the generated airflow, while minimizing the input power.

**Monday, March 14, 2016 11:15AM - 2:15PM –**

**Session B42 DPOLY: Physics of Copolymers** | 345 - Chaitanya Ullal, Rensselaer Polytechnic Institute

**11:15AM B42.00001 Block Copolymer Bottlebrushes: New Routes to Ever Smaller Microdomain Sizes**, MAHESH MAHANTHAPPA, Univ of Minn - Minneapolis, FRANK SPEETJENS, Univ of Wisconsin - Madison — Block copolymer self-assembly presents exciting opportunities for the development of nanotemplates for advanced lithography applications, wherein the microdomain sizes (~10–100 nm) are governed by the total copolymer degree of polymerization,  $N$ . However, this methodology is limited in its smallest achievable length scale, since AB diblock copolymers self-assemble only above a critical  $N$  that depends on the magnitude of the effective segmental interaction parameter  $\chi_{AB}$ . Numerous recent reports have focused on developing “high  $\chi_{AB}$ ” AB diblocks that self-assemble at low values of  $N$ . In this talk we explore the ability of non-linear polymer architectures to induce block copolymer ordering at reduced length scales. Thus, we describe the melt and thin-film self-assembly behavior of block copolymer bottlebrushes derived from linking the block junctions of low molecular weight AB diblocks. We quantitatively demonstrate that increasing the bottlebrush backbone degree of polymerization ( $N_{\text{backbone}}$ ) results in a larger reduction in the critical copolymer arm degree of polymerization ( $N_{\text{arm}}$ ) required for self-assembly, thus reducing the length scales at which these materials self-assemble.

**Monday, March 14, 2016 11:15AM - 2:15PM –**

**Session B41 DBIO: Systems Biology** | 344 - Josh Shaevitz, Princeton University

**11:15AM B41.00001 Whole-brain calcium imaging with cellular resolution in freely behaving *Caenorhabditis elegans***, JEFFREY NGUYEN, FREDERICK SHIPLEY, ASHLEY LINDER, GEORGE PLUMMER, MOCHI LIU, SAGAR SETRU, JOSHUA SHAEVITZ, ANDREW LEIFER, Princeton University — The ability to acquire large-scale recordings of neuronal activity in awake and unrestrained animals is needed to provide new insights into how populations of neurons generate animal behavior. Acquiring this data, however, is challenging because it is difficult to track and image individual neurons as an animal deforms its posture and moves many body lengths. Here, we present an instrument capable of recording intracellular calcium transients from the majority of neurons in the head of a freely behaving *Caenorhabditis elegans* with cellular resolution while simultaneously recording the animals position, posture, and locomotion. 3D volumetric fluorescent images of neurons expressing the calcium indicator GCaMP6s are recorded at 6 head-volumes/s using spinning disk confocal microscopy. At the same time, we record low magnification images of the animal to measure the animals behavior and track its head as it moves. We develop a time independent neuronal matching algorithm that uses non-rigid point set registration and machine learning to correctly match neurons across time. Using this method, we are able to observe calcium transients from up to 90 neurons for over 4 min and correlate the neural activity with the animals behavior.

**11:27AM B41.00002 Dynamics of adaptive immunity against phage in bacterial populations**, SERENA BRADDE, CUNY, MARIJA VUCELJA, University of Virginia, TIBERIU TESILEANU, CUNY, VIJAY BALASUBRAMANIAN, University of Pennsylvania — The CRISPR (clustered regularly interspaced short palindromic repeats) mechanism allows bacteria to adaptively defend against phages by acquiring short genomic sequences (spacers) that target specific sequences in the viral genome. We propose a population dynamical model where immunity can be both acquired and lost. The model predicts regimes where bacterial and phage populations can co-exist, others where the populations oscillate, and still others where one population is driven to extinction. Our model considers two key parameters: (1) ease of acquisition and (2) spacer effectiveness in conferring immunity. Analytical calculations and numerical simulations show that if spacers differ mainly in ease of acquisition, or if the probability of acquiring them is sufficiently high, bacteria develop a diverse population of spacers. On the other hand, if spacers differ mainly in their effectiveness, their final distribution will be highly peaked, akin to a “winner-take-all” scenario, leading to a specialized spacer distribution. Bacteria can interpolate between these limiting behaviors by actively tuning their overall acquisition rate.

**Monday, March 14, 2016 11:15AM - 2:15PM —**

**Session B42 DPOLY: Physics of Copolymers I** 345 - Chaitanya Ullal, Rensselaer Polytechnic Institute

**11:27AM B42.00002 Rich Phase Behavior of Sphere-Forming Asymmetric ABA'C Block Copolymer Melts<sup>1</sup>**, SID CHANPURIYA, AKASH ARORA, KYUNGTAEE KIM, KEVIN DORFMAN, FRANK BATES, Univ of Minnesota - Twin Cities — Motivated by self-consistent field theory simulations, the effect of ABA' corona block length asymmetry on the phase behavior of ABA'C-type tetrablock terpolymers has been examined. The chosen model system, poly(styrene)-*b*-poly(isoprene)-*b*-poly(styrene)-*b*-poly(ethylene oxide) (SIS'O), has been characterized using a combination of small-angle X-ray scattering, transmission electron microscopy, and dynamic mechanical spectroscopy. Asymmetric SIS'O tetrablocks reveal a rich variety of sphere-forming phases over compositions and molecular weights where symmetric SISO polymers formed only hexagonally oriented cylinders. These include FCC, HCP, and complex symmetries such as the Frank-Kasper  $\sigma$  and A15 phases.

<sup>1</sup>NSF Award 1333669

**11:39AM B42.00003 Formation of Frank-Kasper  $\sigma$ -phase from polydisperse diblock copolymers**, MEIJIAO LIU, WEIHUA LI, Fudan University, AN-CHANG SHI, McMaster University — Recent experimental and theoretical studies have revealed a number of complex spherical phases including the complex Frank-Kasper  $\sigma$ -phase, which consists of 30 spheres in a unit cell. It is desirable to understand the mechanisms for the formation of the complex spherical phases such as the A15-phase and the Frank-Kasper  $\sigma$ -phase in block copolymers. Based on the observation that the A15-phase and the Frank-Kasper  $\sigma$ -phase are composed of spherical domains with different sizes, we hypothesize that polydispersity of the block copolymers could be used to obtain these complex phases. We tested this hypothesis by carrying out self-consistent field theory for polydisperse AB diblock copolymers. Specially we studied the relative stability of various spherical phases, including the fcc, bcc, A15 and Frank-Kasper  $\sigma$ -phase, in binary blends composed of AB block copolymers different lengths of the A-blocks. Our results revealed that the Frank-Kasper  $\sigma$ -phase could be stabilized by tailoring the length ratio as well as the compositions of the two diblock copolymers. The distribution of the diblocks in the system indicates that copolymer segregation is the origin of the formation of spherical domains with different sizes.

**Monday, March 14, 2016 11:15AM - 2:15PM —**

**Session B41 DBIO: Systems Biology** 344 - Josh Shaeviz, Princeton University

**11:39AM B41.00003 Distinguishing Feedback Mechanisms in Clock Models<sup>1</sup>**, ALEXANDER GOLDEN, DAVID LUBENSKY, University of Michigan, Ann Arbor — Biological oscillators are very diverse but can be classified based on dynamical motifs such as type of feedback. The *S. Elongatus* circadian oscillator is a novel circadian oscillator that can operate at constant protein number by modifying covalent states. It can be reproduced in vitro with only 3 different purified proteins: KaiA, KaiB, and KaiC. We use computational and analytic techniques to compare models of the *S. Elongatus* post-translational oscillator that rely on positive feedback with models that rely on negative feedback. We show that introducing a protein that binds competitively with KaiA to the KaiB-KaiC complex can distinguish between positive and negative feedback as the primary driver of the rhythm, which has so far been difficult to address experimentally.

<sup>1</sup>NSF Grant DMR-1056456

**11:51AM B41.00004 Starvation-induced dormancy in *E. coli***, EMRAH SIMSEK, MINSU KIM, Emory Univ — Isogenic bacterial populations can exhibit phenotypic heterogeneity. Phenotypic heterogeneity is often viewed as a bet-hedging strategy to cope with environmental fluctuations, and believed to be under genetic control. The experimental evidence of this view, however, is limited. Here, we report experimental evidence that prompts reconsideration of this view. Observing how starved *E. coli* cells resume growth upon nutrient upshift at the single-cell level in real time, we revealed that physiological and metabolic state of starved cells, as well as growth resumption kinetics, vary from cell to cell. Upon nutrient upshift, a majority of cells resume growth instantly, but a small fraction maintain a non-growth state for several hours or days (i.e., long lag time). Hence they are dormant cells. The fraction strongly depends on the duration of starvation. The dormancy does not confer resistance to starvation. Oxidative damage accumulated during starvation leads to the appearance of dormant cells. Taken together, our data suggests that a dormant subpopulation appears as an inevitable consequence of starvation, rather than cellular decision to cope with starvation. Hence, the existence of a genetic program and adaptive value as a bet-hedging strategy to cope with starvation stress may not be needed to explain the emergence of bacterial dormancy.

**Monday, March 14, 2016 11:15AM - 2:15PM –**

**Session B42 DPOLY: Physics of Copolymers | 345 - Chaitanya Ullal, Rensselaer Polytechnic Institute**

**11:51AM B42.00004 Phase Behavior of SIS'O Tetrablock Terpolymers: A Self-consistent Field Theory Study**

, AKASH ARORA, DAVID C. MORSE, FRANK S. BATES, KEVIN D. DORFMAN, Univ of Minn - Minneapolis — Block copolymers with three or more blocks show richer phase behavior than diblock copolymers. In this work, we use self-consistent field theory (SCFT) to study the phase behavior of *ABA'C* type tetrablock terpolymers. In particular, we are motivated by experimental studies on poly(styrene-*b*-isoprene-*b*-styrene-*b*-ethylene oxide) (SIS'O) that report interesting phases such as core-shell spheres and cylinders, the Frank-Kasper  $\sigma$  phase, and the dodecagonal quasicrystalline morphology. We compare SCFT predictions to experimental results for SIS'O copolymers using values of the Flory-Huggins interaction parameters that are estimated from analysis of literature data on related systems.

**12:03PM B42.00005 Preparation and Morphology of AB<sub>n</sub> Mictoarm Block Copolymers.**

, ATSUSHI TAKANO, MOMOKA WATANABE, YUSUKE ASAI, Department of applied chemistry, Graduate School of Engineering, Nagoya University, JIRO SUZUKI, High Energy Accelerator Research Organization (KEK), YUSHU MATSUSHITA, Department of applied chemistry, Graduate School of Engineering, Nagoya University — A series of AB<sub>n</sub> mictoarm block copolymers (bottle brush copolymers) consisting of polystyrene (S) as a backbone and polyisoprenes (I) as grafts were precisely synthesized by an anionic polymerization, and their microphase-separated structures were investigated by transmission electron microscopy (TEM) and small-angle X-ray scattering (SAXS). A copolymer with composition of  $\phi_S=0.57$  and number of grafts(*n*) of 10 shows characteristic cylindrical structure, where microdomains of S reveals hexagonal cross section with non-constant mean curvature interface. While a sample with composition of  $\phi_S=0.37$  and number of grafts(*n*) of 40 shows spherical structure with rather large S isolated domains and characteristic domain packing manner was found. Furthermore composition dependence of microphase-separated structures for SIn mictoarm block copolymers were investigated and compared to SI diblock copolymer system.

**Monday, March 14, 2016 11:15AM - 2:15PM –**

**Session B41 DBIO: Systems Biology | 344 - Josh Shaevitz, Princeton University**

**12:03PM B41.00005 Queueing-Based Synchronization and Entrainment for Synthetic Gene Oscillators<sup>1</sup>**

, WILLIAM MATHER, NICHOLAS BUTZIN, PHILIP HOCHENDONER, CURTIS OGLE, Dept. of Physics, Virginia Polytechnic Inst. and State University — Synthetic gene oscillators have been a major focus of synthetic biology research since the beginning of the field 15 years ago. They have proven to be useful both for biotechnological applications as well as a testing ground to significantly develop our understanding of the design principles behind synthetic and native gene oscillators. In particular, the principles governing synchronization and entrainment of biological oscillators have been explored using a synthetic biology approach. Our work combines experimental and theoretical approaches to specifically investigate how a bottleneck for protein degradation, which is present in most if not all existing synthetic oscillators, can be leveraged to robustly synchronize and entrain biological oscillators. We use both the terminology and mathematical tools of queueing theory to intuitively explain the role of this bottleneck in both synchronization and entrainment, which extends prior work demonstrating the usefulness of queueing theory in synthetic and native gene circuits. We conclude with an investigation of how synchronization and entrainment may be sensitive to the presence of multiple proteolytic pathways in a cell that couple weakly through crosstalk.

<sup>1</sup>This work was supported by NSF Grant 1330180.

**12:15PM B41.00006 Effect of correlations between minima on a complex energy landscape**

, SAI TEJA PUSULURI, Department of physics, Ohio University, ALEX H LANG, Computational Neurobiology Laboratory, Salk Institute, PANKAJ MEHTA, Department of physics, Boston University, HORACIO E CASTILLO, Department of physics, Ohio University — We recently modeled cellular interconversion dynamics[1] by using an epigenetic landscape model[2] inspired by neural network models[3]. Given an arbitrary set of patterns, the model can be used to construct an energy landscape in which those patterns are the global minima. We study the possible stable states and metastable states of the landscapes thus constructed. We consider three different cases: i) choosing the patterns to be random and independently distributed ii) choosing a set of patterns directly derived from the experimental cellular transcription factor expression data for a representative set of cell types in an organism and iii) choosing randomly generated trees of hierarchically correlated patterns, inspired by biology. For each of the three cases, we study the energy landscapes. In particular we study the basins of attraction of both the stable states and the metastable states, we compute the configurational entropy as a function of energy, and we demonstrate how those results depend on the correlations between the patterns.

**References**

- [1] Pusuluri et.al (2015) arXiv:1505.03889.
- [2] Lang et.al (2014) PLoS computational biology 10, e1003734.
- [3] Kanter et.al (1987) Physical Review A 35, 380392.

**Monday, March 14, 2016 11:15AM - 2:15PM –**

**Session B42 DPOLY: Physics of Copolymers | 345 - Chaitanya Ullal, Rensselaer Polytechnic Institute**

**12:15PM B42.00006 Frank-Kasper sigma phase stabilized by tailored architectures of block copolymers.**

, WEIHUA LI, MEIJIAO LIU, NAN XIE, FENG QIU, State Key Laboratory of Molecular Engineering of Polymers, Department of Macromolecular Science, Fudan University, AN-CHANG SHI, Department of Physics, McMaster University — Block copolymer self-assembly forms diverse interesting ordered morphologies, of which the spherical phase is of particular interest because it resembles the similar space symmetry as atomic crystals and has a tunable period on nanoscale. Moreover, the packing lattice of spherical domains dictated by the adjustable competition between the entropic and interfacial energies is programmable. For AB diblock copolymers, it has been known that the stable spherical phase is mainly bcc except for a very narrow region of fcc at the vicinity of the order-disorder transition. When introducing variable number of blocks and architectures to form complex AB-type block copolymers, the A15 phase was predicted as stable. However, a striking experiment observed a new spherical phase, the complex Frank-Kasper sigma phase that consists of 30 spheres in a unit cell, in the PI-*b*-PLA diblock copolymer as well as a SISO tetrablock terpolymer. Inspired by this experiment, we studied the stability of all known spherical phases of fcc, bcc, A15 and sigma in various block copolymers including conformationally asymmetric AB diblock, AB<sub>m</sub> miktoarm, and BABC tetrablock copolymers. We have revealed the formation mechanism of the nonclassical A15 and sigma phases due to the tailored architectures.

**12:27PM B42.00007 From the Disordered State to the Frank-Kasper Sigma Phase: Readily Tuning the Phase Behavior of Block Polymers via Lithium Salt Addition**, MATTHEW IRWIN, ROBERT HICKEY, FRANK BATES, TIMOTHY LODGE, Univ of Minn - Minneapolis — Sphere-forming block copolymers have long been known to assemble onto a body-centered cubic (BCC) lattice, but recent work has demonstrated that with the correct thermal treatments, more exotic morphologies such as dodecagonal quasicrystals or the Frank-Kasper sigma phase can be observed. In this presentation, we show that a similar variety of morphologies can be obtained by simply adding small amounts of lithium bis(trifluoromethane)sulfonimide (LiTFSI), which preferentially partitions into one of the domains. Using small-angle X-ray scattering, we have found that block copolymers, which are disordered when neat, can form spheres with liquid-like packing, BCC crystals, the Frank-Kasper sigma phase, or hexagonally close packed crystals upon increasing the salt loading. This work demonstrates a unique, alternative route to highly segregated sphere-forming block copolymers and examines the universality of the formation of these complex morphologies.

**Monday, March 14, 2016 11:15AM - 2:15PM —**  
**Session B41 DBIO: Systems Biology** 344 - Josh Shaevitz, Princeton University

**12:27PM B41.00007 The Power Spectrum of Ionic Nanopore Currents: The Role of Ion Correlations**, MIRA ZORKOT, RAMIN GOLESTANIAN, DOUWE BONTHUIS, University of Oxford — Measuring the ionic current passing through a nanometer-scale membrane pore has emerged over the past decades as a versatile technique to study molecular transport. These measurements suffer from high noise levels that typically exhibit a power law dependence on the frequency. A thorough theoretical understanding of the power spectrum is essential for the optimisation of experimental setups and for the use of measurement noise as a novel probe of the nanopore's microscopic properties. We calculate the power spectrum of electric-field-driven ion transport through nanopores using both linearized mean-field theory and Langevin dynamics simulations. With only one fitting parameter, the linearized mean-field theory accurately captures the dependence of the simulated power spectrum on the pore radius and the applied electric field. Remarkably, the linearized mean-field theory predicts a plateau in the power spectrum at low frequency  $f$ , which is confirmed by the simulations at low ion concentration. At high ion concentration, however, the power spectrum follows a power law that is reminiscent of the  $1/f$  dependence found experimentally at low frequency. Based on simulations with and without ion-ion interactions, we attribute the low-frequency power law dependence to ion-ion correlations

**12:39PM B41.00008 Statistical Models of Adaptive Immune populations**, ZACHARY SETHNA, CURTIS CALLAN, Princeton University, ALEKSANDRA WALCZAK, THIERRY MORA, Ecole Normale Suprieure — The availability of large ( $10^4$ - $10^6$  sequences) datasets of B or T cell populations from a single individual allows reliable fitting of complex statistical models for naïve generation, somatic selection, and hypermutation. It is crucial to utilize a probabilistic/informational approach when modeling these populations. The inferred probability distributions allow for population characterization, calculation of probability distributions of various hidden variables (e.g. number of insertions), as well as statistical properties of the distribution itself (e.g. entropy). In particular, the differences between the T cell populations of embryonic and mature mice will be examined as a case study. Comparing these populations, as well as proposed mixed populations, provides a concrete exercise in model creation, comparison, choice, and validation.

**Monday, March 14, 2016 11:15AM - 2:15PM —**  
**Session B42 DPOLY: Physics of Copolymers I** 345 - Chaitanya Ullal, Rensselaer Polytechnic Institute

**12:39PM B42.00008 Characterization of Lithium Polysulfide Salts in Homopolymers and Block Copolymers<sup>1</sup>**, DUNYANG WANG, KEVIN WUJCIK, NITASH BALSARA, University of California Berkeley — Ion-conducting polymers are important for solid-state batteries due to the promise of better safety and the potential to produce higher energy density batteries. Nanostructured block copolymer electrolytes can provide high ionic conductivity and mechanical strength through microphase separation. One of the potential use of block copolymer electrolytes is in lithium-sulfur batteries, a system that has high theoretical energy density wherein the reduction of sulfur leads to the formation of lithium polysulfide intermediates. In this study we investigate the effect of block copolymer morphology on the speciation and transport properties of the polysulfides. The morphology and conductivities of polystyrene-*b*-poly(ethylene oxide) (SEO) containing lithium polysulfides were studied using small-angle X-ray scattering and ac impedance spectroscopy. UV-vis spectroscopy is being used to determine nature of the polysulfide species in poly(ethylene oxide) and SEO.

<sup>1</sup>Department of Energy, Soft Matter Electron Microscopy Program and Battery Materials Research Program

**12:51PM B42.00009 Congruent Lamellar-to-Disorder Phase Transitions in Diblock Copolymer-Homopolymer Ternary Blends**, ROBERT HICKEY, TIMOTHY GILLARD, MATTHEW IRWIN, TIMOTHY LODGE, FRANK BATES, University of Minnesota — Symmetric ternary blends of AB diblock copolymers and the corresponding A and B homopolymers are predicted to be characterized by a multicritical Lifshitz point within mean-field theory. Previous studies have shown that fluctuations destroy the predicted Lifshitz point and lead to a bicontinuous microemulsion ( $B_{\mu}E$ ) channel, which separates the lamellar and 2-phase regions in the ternary phase prism. Here, we establish the existence of a line of congruent first-order lamellar-to-disorder transitions when appropriate amounts of poly(cyclohexylethylene) (C) and poly(ethylene) (E) homopolymers are mixed with the corresponding symmetric CE diblock copolymer. We present complimentary optical transmission, small-angle X-ray scattering, transmission electron microscopy (TEM), and rheological results obtained using two experimental protocols: (1) fixing the CE volume fraction and varying the C/E ratio, and (2) setting the C/E ratio at the condition of congruency and varying CE volume fraction from 0 to 1. These results establish a quantitative and facile method for identifying the detailed phase behavior in the vicinity of the  $B_{\mu}E$ , and provide fresh insight into the nature of such mixtures near the nominal Lifshitz conditions. Surprisingly, well-ordered lamellae are revealed by TEM at compositions within 1% of the  $B_{\mu}E$  channel, suggesting a remarkably close approach to the predicted, mean-field unbinding transition. Moreover, the width of the  $B_{\mu}E$  narrows to about 1% under congruent conditions.

**Monday, March 14, 2016 11:15AM - 2:15PM —**  
**Session B41 DBIO: Systems Biology** 344 - Josh Shaevitz, Princeton University

**12:51PM B41.00009 Networks In Real Space: Characteristics and Analysis for Biology and Mechanics**, CARL MODES, MARCELO MAGNASCO, The Rockefeller University, ELENI KATIFORI, University of Pennsylvania — Functional networks embedded in physical space play a crucial role in countless biological and physical systems, from the efficient dissemination of oxygen, blood sugars, and hormonal signals in vascular systems to the complex relaying of informational signals in the brain to the distribution of stress and strain in architecture or static sand piles. Unlike their more-studied abstract cousins, such as the hyperlinked internet, social networks, or economic and financial connections, these networks are both constrained by and intimately connected to the physicality of their real, embedding space. We report on the results of new computational and analytic approaches tailored to these physical networks with particular implications and insights for mammalian organ vasculature.

**1:03PM B41.00010 A kinetic model for chemical neurotransmission<sup>1</sup>**, GUILLERMO RAMIREZ-SANTIAGO, Instituto de Matematicas, UNAM Juriquilla, ALEJANDRO MARTINEZ-VALENCIA, FRANCISCO FERNANDEZ DE MIGUEL, Instituto de Fisiologia Celular, UNAM — Recent experimental observations in presynaptic terminals at the neuromuscular junction indicate that there are stereotyped patterns of cooperativeness in the fusion of adjacent vesicles. That is, a vesicle in hemifusion process appears on the side of a fused vesicle and which is followed by another vesicle in a priming state while the next one is in a docking state. In this talk we present a kinetic model for this morphological pattern in which each vesicle state previous to the exocytosis is represented by a kinetic state. This chain states kinetic model can be analyzed by means of a Master equation whose solution is simulated with the stochastic Gillespie algorithm. With this approach we have reproduced the responses to the basal release in the absence of stimulation evoked by the electrical activity and the phenomena of facilitation and depression of neuromuscular synapses. This model offers new perspectives to understand the underlying phenomena in chemical neurotransmission based on molecular interactions that result in the cooperativity between vesicles during neurotransmitter release.

<sup>1</sup>DGAPA grants IN118410 and IN200914 and Conacyt grant 130031

## Monday, March 14, 2016 11:15AM - 2:15PM –

Session B42 DPOLY: Physics of Copolymers I 345 - Chaitanya Ullal, Rensselaer Polytechnic Institute

**1:03PM B42.00010 Unbinding Transition of the  $\alpha$ -BN Phase of BABCB Tetra-block Terpolymers**, ASHKAN DEHGHAN, McMaster University, HURMIZ SHAMANA, University of Guelph, CHRIS GUBBELS, AN-CHANG SHI, McMaster University — We study the phase behaviour of BABCB/B multiblock terpolymer/homopolymer blends using real-space self-consistent field theory. We focus on the effects of the added homopolymers on the structure of the  $\alpha$ -BN phase, formed in the pure BABCB system. In the  $\alpha$ -BN phase, the A and C blocks form spheres sitting on a three dimensional layered structure, resembling that of graphite. Our results demonstrate that the added homopolymers would aggregate in the regions between the layers in the  $\alpha$ -BN phase. We use this property of the added homopolymers as a mechanism for separating the layers. By examining the effects of homopolymer/multiblock interactions and their relative degree of polymerization on the overall phase behaviour of the system, we identified a critical homopolymer concentration at which the layers composed of A/C spheres unbind to form free standing sheets, resembling the structure of graphene.

**1:15PM B42.00011 Simulation of free energies of bicontinuous morphologies formed through block copolymer/homopolymer self-assembly**, POORNIMA PADMANABHAN, Cornell University, FRANCISCO MARTINEZ-VERACOECHEA, None, FERNANDO ESCOBEDO, Cornell University — Different types of bicontinuous phases can be formed from A-B diblock copolymers by the addition of A-type homopolymers over a range of compositions and relative chain lengths. Particle-based molecular simulations were used to study three bicontinuous phases – double gyroid (G), double diamond (D) and plumber's nightmare (P) - near their triple point of coexistence. For 3-D ordered phases, the stability of the morphology formed in simulation is highly sensitive to box size whose exact size is unknown a-priori. Accurate free energy estimates are required to ascertain the stable phase, particularly when multiple competing phases spontaneously form at the conditions of interest. A variant of thermodynamic integration was implemented to obtain free energies and hence identify the stable phases and their optimal box sizes by tracing a reversible path that connects the ordered and disordered phases. Clear evidence was found of D-G and D-P phase coexistence, consistent with previous predictions for the same blend using Self-consistent field theory. Our simulations also allowed us to examine the microscopic details of these coexisting bicontinuous phases and detect key differences between the microstructure of their nodes and struts.

## Monday, March 14, 2016 11:15AM - 2:15PM –

Session B41 DBIO: Systems Biology 344 - Josh Shavitz, Princeton University

**1:15PM B41.00011 Analysis of aggregation of platelets in thrombosis**, are key players in thrombus formation by first rolling over collagen bound von Willebrand factor followed by formation of a platelet aggregate. The first adhered platelets bind additional platelets until the whole injury is sealed off by a platelet aggregate. The coagulation plug by creating a tight fibrin network, and then wound contraction takes place because of morphological changes in platelet activation and aggregation mainly through fibrinogen polymerization into fibrin fibers. The process includes multiple steps and local shear-rate which regulate and control the process. Coagulation can be divided into two pathways: the intrinsic and the extrinsic. The intrinsic pathway is initiated by the exposure of a negatively charged. It is able to activate factor XII, using a complex of high-molecular-weight kininogen as cofactors. Thrombin is the final enzyme that is needed to convert fibrinogen into fibrin with the exposure of tissue factor to the circulating blood, which is the major initiator of coagulation. There are several steps in the coagulation cascade, resulting in large amounts of thrombin. It is dependent on the presence of pro-coagulant surfaces such as phospholipids—which include phosphatidylserine (PS)—on their outer membrane. PS-bearing surfaces are able to increase the concentration and co-localizing coagulation factors. Aggregation of platelets are analyzed and compared to adhesion of platelets.

replacing MAR16-2015-020003.

**1:27PM B41.00012 Oxidant Signaling in Cells Revealed by Single Rare-Earth Based Nanoparticle Imaging**, CEDRIC BOUZIGUES, MOUNA ABDESSELEM, RIVO RAMODIHARILAFY, THIERRY GACOIN, Ecole Polytechnique, PIERRE-LOUIS THARAUX, PARCC - Inserm - HEGP, ANTIGONI ALEXANDROU, Ecole Polytechnique — The spatio-temporal organization of signaling pathways controls the cell response. Reactive oxygen species (ROS) are second messengers involved in the control of numerous normal and pathological processes and their local concentration is thus tightly regulated. However, the dynamics of ROS production and organization is mostly unknown, due to the lack of efficient probes. We developed single ROS sensitive Eu<sup>3+</sup>-doped nanoparticle imaging to quantitatively probe the intracellular ROS response. We revealed specific temporal patterns of ROS production under different types of stimulation (PDGF and ET-1) and quantitatively identified mechanisms of transactivation, which notably control the dynamics of the cell response. By using a microfluidic system, we apply spatially controlled stimulations and displayed the maintenance of asymmetric ROS concentration in the cell under a PDGF gradient. We then developed a ratiometric method using a nanoparticle mix, to quantitatively detect ROS with a 500 ms temporal resolution. We thus elucidate molecular mechanisms responsible for the control of the oxidant production kinetics. Altogether, our results reveal regulation mechanisms controlling ROS spatio-temporal organization, which can be crucial for the buildup of the cell response.

## Monday, March 14, 2016 11:15AM - 2:15PM –

Session B42 DPOLY: Physics of Copolymers I 345 - Chaitanya Ullal, Rensselaer Polytechnic Institute

**1:27PM B42.00012 Sequence-Specific Copolymer Compatibilizers designed via a Genetic Algorithm<sup>1</sup>**, VENKATESH MEENAKSHISUNDARAM, TARAK PATRA, JUI-HSIANG HUNG, DAVID SIMMONS, Univ of Akron — For several decades, block copolymers have been employed as surfactants to reduce interfacial energy for applications from emulsification to surface adhesion. While the simplest approach employs symmetric diblocks, studies have examined asymmetric diblocks, multiblock copolymers, gradient copolymers, and copolymer-grafted nanoparticles. However, there exists no established approach to determining the optimal copolymer compatibilizer sequence for a given application. Here we employ molecular dynamics simulations within a genetic algorithm to identify copolymer surfactant sequences yielding maximum reductions in the interfacial energy of model immiscible polymers. The optimal copolymer sequence depends significantly on surfactant concentration. Most surprisingly, at high surface concentrations, where the surfactant achieves the greatest interfacial energy reduction, specific non-periodic sequences are found to significantly outperform any regularly blocky sequence. This emergence of polymer sequence-specificity within a non-sequenced environment adds to a recent body of work suggesting that specific sequence may have the potential to play a greater role in polymer properties than previously understood.

<sup>1</sup> We acknowledge the W. M. Keck Foundation for financial support of this research

**1:39PM B42.00013 Effect of the Degree of Hydrogen Bonding on Asymmetric Lamellar Phase Transformation in Binary Block Copolymer Blends**, JONGHEON KWAK, SUNG HYUN HAN, HONG CHUL MOON, POSTECH, VICTOR PRYAMITSYN, VENKAT GANESAN, University of Texas, JIN KON KIM, POSTECH — A binary mixture of two block copolymers whose blocks are capable of forming the hydrogen bonding allows one to obtain various microdomains that could not be expected for neat block copolymer. For instance, we reported that the binary blend of asymmetric polystyrene-*block*-poly(2-vinylpyridine) copolymer (as-PS-*b*-P2VP) and polystyrene-*block*-polyhydroxystyrene copolymer (as-PS-*b*-PHS) blends where the hydrogen bonding occurred between P2VP and PHS showed asymmetric lamellar microdomains. Since asymmetric lamellar microdomains are formed due to the interface curvature change by favorable hydrogen bonding interaction between the hydroxyl group and nitrogen atom, a large ratio of lamellar width (thus, enhanced asymmetry) could potentially be achieved by increasing the degree of the hydrogen bonding. We employed two kinds of binary blends (polystyrene-*block*-poly(4-vinylpyridine) (as-PS-*b*-P4VP)/as-PS-*b*-PHS and as-PS-*b*-P2VP/as-PS-*b*-PHS). It was observed by SAXS and TEM that as-PS-*b*-P4VP/as-PS-*b*-PHS blend which exhibits much stronger hydrogen bonding formed asymmetric lamellar morphology at more asymmetric volume fraction where as-PS-*b*-P2VP/as-PS-*b*-PHS blend could not form and the experimental results show qualitative agreement with the SST model prediction.

**Monday, March 14, 2016 11:15AM - 2:15PM —**  
**Session B41 DBIO: Systems Biology** 344 - Josh Shaevitz, Princeton University

**1:39PM B41.00013 Regulatory inhibition of biological tissue mineralization through post-nucleation shielding<sup>1</sup>**, JOSHUA CHANG, National Institutes of Health, ROBERT MIURA, New Jersey Institute of Technology — In vertebrates, insufficient availability of calcium and phosphate ions in extracellular fluids leads to loss of bone density and neuronal hyper-excitability. To counteract this problem, calcium ions are present at high concentrations throughout body fluids at concentrations exceeding the saturation point. This condition leads to the opposite situation where unwanted mineral sedimentation may occur. Remarkably, ectopic or out-of-place sedimentation into soft tissues is rare, in spite of the thermodynamic driving factors. This fortunate fact is due to the presence of auto-regulatory proteins that are found in abundance in bodily fluids. Yet, many important inflammatory disorders such as atherosclerosis and osteoarthritis are associated with this undesired calcification. Hence, it is important to gain an understanding of the regulatory process and the conditions under which it can go awry. We adapted mean-field classical nucleation theory to the case of surface-shielding in order to study the regulation of sedimentation of calcium phosphate salts in biological tissues.

<sup>1</sup>Mathematical Biosciences Institute, NSF DMS-1021818, National Institutes of Health, Rehab Medicine

**1:51PM B41.00014 E.coli in weak magnetic field in different media**, SAMINA MASOOD, University of Houston Clear Lake — We study the growth of E-coli in a weak magnetic field, both in a liquid and a solid medium. We use LB broth for that purpose at the room temperature and study the growth in different types of magnetic field. We grow it over the bar magnets and within the magnetic field generated by the Helmholtz coils. It has been clearly noticed that the growth of bacteria is clearly affected with the magnetic field and the different types of magnetic field affect differently.

**Monday, March 14, 2016 11:15AM - 2:15PM —**  
**Session B42 DPOLY: Physics of Copolymers I** 345 - Chaitanya Ullal, Rensselaer Polytechnic Institute

**1:51PM B42.00014 Microphase-separated structures within randomly end-linked copolymer networks**, DI ZENG, RYAN HAYWARD, Univ of Mass - Amherst — Self-assembly within randomly cross-linked or end-linked copolymer networks provides a robust method to generate co-continuous nanometer-scale structures. Here, we investigate self-assembly within copolymer networks prepared by end linking of several different pairs of telechelic polymers in a common solvent. For sufficiently high levels of immiscibility between the constituent polymers, removal of solvent leads to microphase separation into disordered nanoscale structures. Using a variety of characterization methods, including transmission electron microscopy, small-angle X-ray scattering, differential scanning calorimetry, and dynamic mechanical analysis, we find that these networks exhibit co-continuous morphologies over a wide range of volume fraction of the two components, with a characteristic length scale that can be tuned by adjusting the molecular weight of the starting polymers.

**2:03PM B42.00015 Effects of Blockiness on the phase behavior of random copolymers**, GORDON VANDERWOUDE, AN-CHANG SHI, McMaster University — Theoretical study of random block copolymers remains a challenging topic due in part to the sheer enormity of their phase space. In this study we use the self-consistent field theory to investigate the phase behaviour of linear (AB)*n*-type and (AB)*n*-C-type multiblock copolymers with randomly distributed A and B blocks. In particular, we examine the effect of blockiness of the random copolymers on the formation of ordered phases. The blockiness can be quantified by the average length of individual A or B blocks, which can be taken as a measure of the heterogeneity of the random copolymers. We observed that the critical value of the  $\chi$  parameter, at which the order-disorder transition occurs, decreases with increasing blockiness in the (AB)*n* copolymers. We also observed that the phase behaviour of the (AB)*n*-C copolymers depends strongly on the blockiness of the random chain. In particular, the blockiness governs whether or not the A/B blocks can phase separate within the A/B domains, thus dictating whether the (AB)*n*-C behaves as A/B-C diblock copolymers or as ABC terpolymers. The theoretical phase diagrams will be compared with available experiments.

**Monday, March 14, 2016 11:15AM - 2:15PM —**  
**Session B41 DBIO: Systems Biology** 344 - Josh Shaevitz, Princeton University

**2:03PM B41.00015 Comparative Study of Bacterial Growth in Magnet Fields** , DEREK SMITH, SAMINA MASOOD, University of Houston - Clear Lake — It has been shown that magnetic fields affect bacterial growth. A comparative study of growth rates for gram-positive and gram-negative bacteria with different types of magnetic fields is done. Special focus is placed upon growth within liquid media, and the effect of magnetic fields relative to the chosen growth medium is considered.

**Monday, March 14, 2016 11:15AM - 2:03PM —**

**Session B43 GSNP GSOF: Avalanches in Granular and Other Particle-based Materials II** 346

- Bob Behringer, Duke University

**11:15AM B43.00001 Global and local avalanches in cohesive and non cohesive granular material: crackling and seismicity** , JONATHAN BARES, LMGC Montpellier, France — Commonly, granular materials yield or flow if sufficiently large stress is applied, leading to avalanche-like behavior. For experimentally wedge split cohesive granular material and sheared 2D and 3D grains, we seek to understand the dynamics of these burst of activity from the local to the global scale. Whether the system rearranges locally like in the case of a fracture front propagating in a cohesive material or in the whole system like in the case of sheared granular medium, similar free scale statistics are observed for the intensity of the rearrangements. We present first an experimental setup that allows growing well-controlled tensile cracks in brittle heterogeneous solids of tunable microstructure. Also, force networks and displacement fields are measured both on two and three-dimensional sheared material for cyclically sheared photoelastic and hydrogel particles. Avalanches, their size, location and duration are extracted at the global scale from the rapid variation of the stored energy whereas at the local scale they are measured from the energy drop, displacement and acoustic activity. Statistics of those different quantities are computed and correlated to test their intrinsic entanglement and analyze their universal dynamics.

**11:51AM B43.00002 Experimental Avalanches in a Rotating Drum.**<sup>1</sup> , ALINE HUBARD, Levich Institute of City College of New York, COREY O'HERN, Department of Mechanical Engineering & Materials Science, Department of Applied Physics, and Department of Physics, Yale University, MARK SHATTUCK, Levich Institute and Physics Department of The City College of New York and CUNY Graduate Center — We address the question of universality in granular avalanches and the system size effects on it. We set up an experiment made from a quasi-two-dimensional rotating drum half-filled with a monolayer of stainless-steel spheres. We measure the size of the avalanches created by the increased gravitational stress on the pile as we quasi-statically rotate the drum. We find two kinds of avalanches determined by the drum size. The size and duration distributions of the avalanches that do not span the whole system follow a power law and the avalanche shapes are self-similar and nearly parabolic. The distributions of the avalanches that span the whole system are limited by the maximal amount of potential energy stored in the system at the moment of the avalanche.

<sup>1</sup>NSF CMMI-1462439, CMMI-1463455

**12:03PM B43.00003 Stability of Granular Packings Jammed under Gravity: Avalanches and Unjamming**<sup>1</sup> , CARL MERRIGAN, Brandeis University , SUMIT BIRWA, TIFR Hyderabad, SHUBHA TEWARI, UMass Amherst, BULBUL CHAKRABORTY, Brandeis University — Granular avalanches indicate the sudden destabilization of a jammed state due to a perturbation. We propose that the perturbation needed depends on the entire force network of the jammed configuration. Some networks are stable, while others are fragile, leading to the unpredictability of avalanches. To test this claim, we simulated an ensemble of jammed states in a hopper using LAMMPS. These simulations were motivated by experiments with vibrated hoppers where the unjamming times followed power-law distributions<sup>2</sup>. We compare the force networks for these simulated states with respect to their overall stability. The states are classified by how long they remain stable when subject to continuous vibrations. We characterize the force networks through both their real space geometry and representations in the associated force-tile space<sup>3</sup>, extending this tool to jammed states with body forces.

<sup>1</sup>Supported by NSF Grant DMR1409093 and DGE1068620

<sup>2</sup>Lozano, C., Zuriguel, I., Garcimartín, A. (2015). Stability of clogging arches in a silo submitted to vertical vibrations. Physical Review E, 91(6), 062203.

<sup>3</sup>Sarkar, S., Bi, D., Zhang, J., Behringer, R. P., Chakraborty, B. (2013). Origin of rigidity in dry granular solids. Physical review letters, 111(6), 068301.

**12:15PM B43.00004 Structure of jammed configurations and their relation to unjamming times**<sup>1</sup> , SUMIT KUMAR BIRWA, TIFR Centre for Interdisciplinary Sciences, Hyderabad, CARL MERRIGAN, BULBUL CHAKRABORTY, Brandeis University, SHUBHA TEWARI, University of Massachusetts, Amherst — The distribution of the times for the cessation of flow of grains falling under gravity in a vertical hopper is known to be exponential. Recent experiments have shown, however, that the time lapse between avalanches follows a power-law distribution when the hopper is unjammed using periodic vertical vibrations<sup>2</sup>. The reasons for this distribution of the unjamming times, which indicates the time needed for an applied continuous perturbation to induce another avalanche, are not well understood. We report on a numerical simulation of granular hopper flow using LAMMPS<sup>3</sup> in which we seek to understand the origin and scope of this behavior. We find that cessation of flow is related to the formation of a stable arch that spans the system. However, the actual structure of the jammed configuration varies and is closely related to the unjamming time. We find that the symmetry of the arches is an important parameter in determining the strength of the jammed configurations. Using different force thresholds, we have characterized the contact networks around the arches which provides stability to the packed structure and analyzed the strength of various jammed configurations.

<sup>1</sup>Supported by NSF Grant DMR1409093 and DGE1068620

<sup>2</sup>I. Zuriguel et al., Scientific reports 4, 7324 (2014).

<sup>3</sup><http://lammps.sandia.gov/>

**12:27PM B43.00005 Intermittent Flow of Granular Matter in an Annular Geometry** , TED BRZINSKI, KAREN E. DANIELS, NC State University — Granular solids can be subjected to a finite stress below which the response is elastic. Above this yield stress, however, the material fails catastrophically, undergoing a rapid plastic deformation. In the case of a monotonically increasing stress the material exhibits a characteristic stick-slip response. We investigate the statistics of this intermittent failure in an annular shear geometry, driven with a linear-ramp torque in order to generate the stick-slip behavior. The apparatus is designed to allow visual access to particle trajectories and inter-particle forces (through the use of photoelastic materials). Additionally, twelve piezoelectric sensors at the outer wall measure acoustic emissions due to the plastic deformation of the material. We vary volume fraction, and use both fixed and deformable boundaries. We measure how the distribution of slip size and duration are related to the bulk properties of the packing, and compare to systems with similar governing statistics.

**12:39PM B43.00006 Effect of interstitial fluid on event-size distribution for granular hoppers.** , JUHA KOIVISTO, DOUGLAS DURIAN, Univ of Pennsylvania — The discharge of granular hoppers is avalanche-like in that flow proceeds until probabilistically interrupted by the formation of a stable arch over the hole. The average event size appears to diverge at a critical hole size, thus defining a putative clogging transition. However, we now believe that instead it grows exponentially as a power of the hole diameter, so in fact all hoppers are susceptible to clogging<sup>1</sup>. To investigate the influence of grain dynamics on arch formation, we conducted a series of experiments where the event size distribution was measured for grains in a system that was totally submerged in water. We find that the distribution is exponential, just as for dry non-cohesive grains in air. However, for a given hole the number of grains in the average event decreases roughly with a factor of two, and the critical hole size increases by 10%. Thus, submerged hoppers are more susceptible to clogging and dynamics play a role. In air, the “effective temperature” set by rms grain speed helps to prevent arch formation.

<sup>1</sup>C.C. Thomas et al., Phys. Rev. Lett. 114, 178001 (2015).

**12:51PM B43.00007 Non-local rheology for dense granular flows in avalanches** , ADRIEN IZZET, ERIC CLEMENT, BRUNO ANDREOTTI, ESPCI — A local constitutive relation was proposed to describe dense granular flows (GDR MiDi, EPJE 2004). It provides a rather good prediction of the flowing regime but does not foresee the existence of a creep regime as observed by Komatsu et al. (PRL 2001). In the context of a 2D shear cell, a relaxation length for the velocity profile was measured (Bouzid et al., PRL 2013) which confirmed the existence of a flow below the standard Coulomb yield threshold. A correction for the local rheology was proposed. To test further this non-local constitutive relation, we built an inclined narrow channel within which we monitor the flow from the side. We managed to observe the creep regime over five orders of magnitude in velocity and fit the velocity profiles in the depth with an asymptotic solution of the non-local equation. However, the boundary condition at the free surface needs to be selected in order to calibrate the non-local rheology over the whole range of stresses in the system. In this perspective, we complement the experimental results with 2D simulations of hard and frictional discs on an inclined plane in which we introduce a surface friction force proportional to the effective pressure in the granular. We analyze these results in the light of the non-local rheology.

**1:03PM B43.00008 Jamming and chaotic dynamics in different granular systems** , HOMAYOON MAGHSOODI, ERIK LUIJTEN, Northwestern University — Although common in nature and industry, the jamming transition has long eluded a concrete, mechanistic explanation. Recently, Banigan *et al.* (Nat. Phys. **9**, 288–292, 2013) proposed a method for characterizing this transition in a granular system in terms of the system’s chaotic properties, as quantified by the largest Lyapunov exponent. They demonstrated that in a two-dimensional shear cell the jamming transition coincides with the bulk density at which the system’s largest Lyapunov exponent changes sign, indicating a transition between chaotic and non-chaotic regimes. To examine the applicability of this observation to realistic granular systems, we study a model that includes frictional forces within an expanded phase space. Furthermore, we test the generality of the relation between chaos and jamming by investigating the relationship between jamming and the chaotic properties of several other granular systems, notably sheared systems (Howell, D., Behringer R. P., Veje C., Phys. Rev. Lett. **82**, 5241–5244, 1999) and systems with a free boundary. Finally, we quantify correlations between the largest Lyapunov vector and collective rearrangements of the system to demonstrate the predictive capabilities enabled by adopting this perspective of jamming.

**1:15PM B43.00009 3D imaging of particle-scale rotational motion in cyclically driven granular flows** , MATT HARRINGTON, University of Pennsylvania, DYLAN POWERS, University of Maryland, ERIC COOPER, Pomona College, WOLFGANG LOSERT, University of Maryland — Recent experimental advances have enabled three-dimensional (3D) imaging of motion, structure, and failure within granular systems. 3D imaging allows researchers to directly characterize bulk behaviors that arise from particle- and meso-scale features. For instance, segregation of a bidisperse system of spheres under cyclic shear can originate from microscopic irreversibilities and the development of convective secondary flows. Rotational motion and frictional rotational coupling, meanwhile, have been less explored in such experimental 3D systems, especially under cyclic forcing. In particular, relative amounts of sliding and/or rolling between pairs of contacting grains could influence the reversibility of both trajectories, in terms of both position and orientation. In this work, we apply the Refractive Index Matched Scanning technique to a granular system that is cyclically driven and measure both translational and rotational motion of individual grains. We relate measured rotational motion to resulting shear bands and convective flows, further indicating the degree to which pairs and neighborhoods of grains collectively rotate.

**1:27PM B43.00010 Characterizing local forces and rearrangements inside a gravity-driven granular flow** , EMMA THACKRAY, KERSTIN NORDSTROM, Mount Holyoke College — While the gravity-driven flow of a granular material in a silo geometry can be modeled by the Beverloo equation, the mesoscale-level particle rearrangements and interactions that drive this flow are not well-understood. We have constructed a quasi-two-dimensional system of bidisperse, millimeter-scale disks with photoelastic properties that make force networks within the material visible. The system is contained in an acrylic box with an adjustable bottom opening. We can approach the clogging transition by adjusting this opening and by adding external forcing to the top of the flowing pile. By placing the system between cross-polarizers, we can obtain high-speed video of this system during flow, and extract intensity signals that can be used to identify and quantify localized, otherwise indeterminate forces. We can simultaneously track individual particle motions, which can be used to identify shear transformation zones in the system. We are therefore able to correlate local forces with rearrangements within the system, and characterize the evolution of this interplay on the approach to the clogging transition.

**1:39PM B43.00011 Dynamic structural network evolution in compressed granular systems.** , LIA PAPADOPOULOS, University of Pennsylvania, JAMES PUCKETT, Gettysburg College, KAREN DANIELS, North Carolina State University, DANIELLE BASSETT, University of Pennsylvania — The heterogeneous dynamic behavior of granular packings under shear or compression is not well-understood. In this study, we use novel techniques from network science to investigate the structural evolution that occurs in compressed granular systems. Specifically, we treat particles as network nodes, and pressure-dependent forces between particles as layer-specific network edges. Then, we use a generalization of community detection methods to multilayer networks, and develop quantitative measures that characterize changes in the architecture of the force network as a function of pressure. We observe that branchlike domains reminiscent of force chains evolve differentially as pressure is applied: topological characteristics of these domains at rest predict their coalescence or dispersion under pressure. Our methods allow us to study the dynamics of mesoscale structure in granular systems, and provide a direct way to compare data from systems under different external conditions or with different physical makeup.

**1:51PM B43.00012 Self organization and shear-jamming in magnetic photoelastic particles** , MEREDITH COX, DONG WANG, Duke University, JONATHAN BARES, LMGC Montpellier, France, BOB BEHRINGER, Duke University — Many experimental studies of simple particles in granular systems have been conducted, but the behavior of complex particles in such systems has not been addressed. There has been a growing interest in functionalized microparticles, and the study of these complex particles may reveal interesting analogues between micro- and macroparticles. We perform experiments to investigate magnetic particles in a 2D granular material close to the jamming transition. We incrementally compress and shear photoelastic particles containing magnets and image the interparticle forces in each compression using a photoelastic technique. To track the orientation of individual particles, we draw UV-visible bars on each particle and image each compression of the system under ultraviolet light. We repeat the experimental procedure using varying ratios of magnetic to nonmagnetic particles from 0% magnetic to 100% magnetic. By using custom software to resolve particle deformations, we extract particle contact and pressure.

**Monday, March 14, 2016 11:15AM - 2:15PM –**

**Session B44 GQI: Quantum Characterization, Verification and Validation I** 347 - Elham Kashefi,  
University of Edinburgh

**11:15AM B44.00001 Towards a Model Selection Rule for Quantum State Tomography<sup>1</sup>**, TRAVIS SCHOLTEN, ROBIN BLUME-KOHOUT, Sandia Natl Labs — Quantum tomography on large and/or complex systems will rely heavily on model selection techniques, which permit on-the-fly selection of small efficient statistical models (e.g. small Hilbert spaces) that accurately fit the data. Many model selection tools, such as hypothesis testing or Akaike's AIC, rely implicitly or explicitly on the Wilks Theorem, which predicts the behavior of the loglikelihood ratio statistic (LLRS) used to choose between models. We used Monte Carlo simulations to study the behavior of the LLRS in quantum state tomography, and found that it disagrees dramatically with Wilks' prediction. We propose a simple explanation for this behavior; namely, that boundaries (in state space and between models) play a significant role in determining the distribution of the LLRS. The resulting distribution is very complex, depending strongly both on the true state and the nature of the data. We consider a simplified model that neglects anisotropy in the Fisher information, derive an almost analytic prediction for the mean value of the LLRS, and compare it to numerical experiments. While our simplified model outperforms the Wilks Theorem, it still does not predict the LLRS accurately, implying that alternative methods may be necessary for tomographic model selection.

<sup>1</sup>Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE

**11:27AM B44.00002 Experimental Demonstration of Self-Guided Quantum Tomography**, ROBERT J. CHAPMAN, School of Electrical and Computer Engineering, RMIT University, CHRISTOPHER FERRIE, EQuS, School of Physics, University of Sydney, ALBERTO PERUZZO, School of Electrical and Computer Engineering, RMIT University — Robust and precise quantum state characterization is critical for future quantum experiments and technologies, and yet is a fundamentally challenging task. Standard and adaptive quantum tomography procedures are impractical for systems being prepared today due to the exponential scaling of quantum state space. These techniques are sensitive to statistical noise and require highly precise measurement settings. We present an experimental demonstration of autonomous and robust self-guided quantum tomography. Self-guided quantum tomography iteratively learns a quantum state using a stochastic gradient ascent algorithm. As a result it is robust against statistical noise and measurement errors. In addition, self-guided quantum tomography does not require any computationally expensive optimization, necessary for adaptive quantum tomography, or post-processing, required for standard quantum tomography. We demonstrate the robustness of self-guided quantum tomography by engineering the level of statistical noise and experimental errors, achieving measurement fidelities greater than standard quantum tomography in a range of one- and two-qubit experiments. Our demonstration opens pathways towards robust quantum state characterization in current and near-future experiments, where standard techniques are already impractical.

**11:39AM B44.00003 Improved precision-guaranteed quantum tomography<sup>1</sup>**, TAKANORI SUGIYAMA, Dep. of Systems Innovation, Osaka University — Quantum tomography is one of the standard tool in current quantum information experiments for verifying that a state/process/measurement prepared in the lab is close to an ideal target. Precision-guaranteed quantum tomography (Sugiyama, Turner, Murao, PRL 111, 160406 2013) gives rigorous error bars on a result estimated from arbitrary finite data sets from any given informationally complete tomography experiments. The rigorous error bars were derived with a real-valued concentration inequality called Hoeffding's inequality. In this talk, with a vector-valued concentration inequality, we provide an improved version of the error bars of precision-guaranteed quantum tomography. We examine the new error bars for specific cases of multi-qubit systems and numerically show that the degree of improvement becomes large as the dimension of the system increases.

<sup>1</sup>Supported by JSPS Research Fellowships for Young Scientists H27-276 and JSPS Postdoctoral Fellowships for Research Abroad H25-32

**11:51AM B44.00004 Gate Set Tomography on two qubits**, ERIK NIELSEN, ROBIN BLUME-KOHOUT, JOHN GAMBLE, KENNETH RUDINGER, Sandia National Laboratories — Gate set tomography (GST) is a method for characterizing quantum gates that does not require pre-calibrated operations, and has been used to both certify and improve the operation of single qubits. We analyze the performance of GST applied to a simulated two-qubit system, and show that Heisenberg scaling is achieved in this case. We present a GST analysis of preliminary two-qubit experimental data, and draw comparisons with the simulated data case. Finally, we will discuss recent theoretical developments that have improved the efficiency of GST estimation procedures, and which are particularly beneficial when characterizing two qubit systems. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

**12:03PM B44.00005 Hamiltonian tomography for quantum many-body systems with arbitrary couplings<sup>1</sup>**, SHENG-TAO WANG, Univ of Michigan - Ann Arbor, DONG-LING DENG, Condensed Matter Theory Center and Joint Quantum Institute, University of Maryland, College Park, LUMING DUAN, Univ of Michigan - Ann Arbor — Characterization of qubit couplings in many-body quantum systems is essential for benchmarking quantum computation and simulation. We propose a tomographic measurement scheme to determine all the coupling terms in a general many-body Hamiltonian with arbitrary long-range interactions, provided the energy density of the Hamiltonian remains finite. Different from quantum process tomography, our scheme is fully scalable with the number of qubits as the required rounds of measurements increase only linearly with the number of coupling terms in the Hamiltonian. The scheme makes use of synchronized dynamical decoupling pulses to simplify the many-body dynamics so that the unknown parameters in the Hamiltonian can be retrieved one by one. We simulate the performance of the scheme under the influence of various pulse errors and show that it is robust to typical noise and experimental imperfections.

<sup>1</sup>This work is supported by the IARPA MUSIQ program, the ARO and the AFOSR MURI program.

**12:15PM B44.00006 Quantum Compressed Sensing Using 2-Designs**, YI-KAI LIU, NIST, SHELBY KIMMEL, University of Maryland — We develop a method for quantum process tomography that combines the efficiency of compressed sensing with the robustness of randomized benchmarking. Our method is robust to state preparation and measurement errors, and it achieves a quadratic speedup over conventional tomography when the unknown process is a generic unitary evolution. Our method is based on PhaseLift, a convex programming technique for phase retrieval. We show that this method achieves approximate recovery of almost all signals, using measurements sampled from spherical or unitary 2-designs. This is the first positive result on PhaseLift using 2-designs. We also show that exact recovery of all signals is possible using measurements sampled from unitary 4-designs. Previous positive results for PhaseLift required spherical 4-designs, while PhaseLift was known to fail in certain cases when using spherical 2-designs.

**12:27PM B44.00007 Scalable randomized benchmarking of non-Clifford gates<sup>1</sup>**, ANDREW CROSS, EASWAR MAGESAN, LEV BISHOP, JOHN SMOLIN, JAY GAMBETTA, IBM T J Watson Res Ctr — Randomized benchmarking is a widely used experimental technique to characterize the average error of quantum operations. Benchmarking procedures that scale to enable characterization of  $n$ -qubit circuits rely on efficient procedures for manipulating those circuits and, as such, have been limited to subgroups of the Clifford group. However, universal quantum computers require additional, non-Clifford gates to approximate arbitrary unitary transformations. We define a scalable randomized benchmarking procedure over  $n$ -qubit unitary matrices that correspond to protected non-Clifford gates for a class of stabilizer codes. We present efficient methods for representing and composing group elements, sampling them uniformly, and synthesizing corresponding  $\text{poly}(n)$ -sized circuits. The procedure provides experimental access to two independent parameters that together characterize the average gate fidelity of a group element.

<sup>1</sup>We acknowledge support from ARO under contract W911NF-14-1-0124.

**12:39PM B44.00008 Benchmarking of Quantum Control in ESR**, GUANRU FENG, KYUNGDEOCK PARK, FRANKLIN H CHO, BRANDON BUONACORSI, ROBABEH RAHIMI, JONATHAN BAUGH, RAYMOND LAFLAMME, Institute for Quantum Computing, University of Waterloo — Quantum error correction is essential for realizing scalable quantum computation. Key ingredients for quantum error correction are highly polarized ancilla qubits and high-fidelity quantum control. While NMR quantum processors have demonstrated high control fidelity, the requirement to prepare highly polarized spin qubits on demand is a major challenge. Electron-nuclear hyperfine coupled spin systems provide a possible solution: electrons can be fully polarized at accessible fields and temperatures, and their polarization is typically reset much faster than nuclei by spin relaxation. This makes open system cooling methods, such as heat bath algorithm cooling, possible. In this talk, I will describe our recent efforts to improve the precision of microwave control in a custom electron spin resonance spectrometer. In particular, we use randomized benchmarking of quantum gates to quantify control errors, and carefully take into account the resonator transfer function in correcting pulses. Moreover, we implement a protocol that distinguishes coherent and incoherent errors, which gives deeper insight into the nature of the remaining control imperfections and how to address them.

**12:51PM B44.00009 Informational completeness in bounded-rank quantum-state tomography<sup>1</sup>**, CHARLES BALDWIN, IVAN DEUTSCH, AMIR KALEV, University of New Mexico — Quantum-state tomography is a demanding task, however, it can be made more efficient by applying prior information about the system. A common prior assumption is that the state being measured is pure, or close to pure, since most quantum information protocols require pure states. Measurements of pure states can be constructed to be more efficiently than measurements of an arbitrary state, and for these types of measurements, there exists two different notions of informational completeness. One notion, called strict-completeness, is more useful for practical applications since it is compatible with convex optimization and is robust to noise. We present a unified framework for both notions of completeness for a certain type of measurements. These are measurements that allow algebraic reconstruction of a few density matrix elements. The framework also aids in the construction of new strictly-complete measurements. Moreover, the results are easily generalized to the case when the prior information is the state has bounded rank.

<sup>1</sup>This work was supported by NSF Grants PHY- 1212445, PHY-1521016, and PHY-1521431

**1:03PM B44.00010 The power of being positive: Robust state estimation made possible by quantum mechanics<sup>1</sup>**, AMIR KALEV, CHARLES BALDWIN, Univ of New Mexico — Quantum-state tomography (QST) is generally expensive to implement experimentally. Nevertheless, in state-of-the-art experiments in quantum information science the goal is not to produce arbitrary states but states that have very high purity. Including this prior information in QST results in more manageable tomography protocols. In the context of pure-state tomography, and more generally, of bounded-rank states (states with rank  $\leq r$ ) tomography, a natural notion of informational completeness emerges, *rank- $r$  completeness*. The purpose of this contribution is two fold. First, to prove and emphasize the significance of a less intuitive, yet more powerful, notion of completeness for practical QST, *rank- $r$  strict-completeness*. This notion is made possible due to the positive semidefinite property of density matrices. Strictly-complete quantum measurements ensure a robust estimation of the state of the system, regardless of the convex estimator we use. Thus, pragmatically, quantum state tomography should be done using these kind of measurements. Second, to argue, based on strong numerical indication, that it is fairly straightforward to experimentally implement such measurements by measuring only few random orthonormal bases. For example, in our numerical experi

<sup>1</sup>This work was supported by NSF Grants PHY-1212445, PHY-1521016, and PHY-1521431

**1:15PM B44.00011 Bayesian mean estimation for finite two-photon experiments**, BRIAN WILLIAMS, PAVEL LOUGOVSKI, Oak Ridge National Lab — Estimations of quantum probabilities are commonly made utilizing frequency based methods to invert Born's rule where  $X$  is found  $k$  out of  $n$  times,  $P(X) = |\langle \psi | X | \psi \rangle|^2 \approx k/n$ . For an infinite measurement number the maximum likelihood estimation (MLE) represents the true probability. Unfortunately, the number of measurements in any experiment is finite. Given this, better estimates are provided by Bayesian mean estimation (BME). We present a novel method utilizing an experiment-specific probability distribution to make fully informed estimations of any quantum probability, efficiency parameter, or complete density matrix. Our method accounts for the finite measurement number, inter-basis parameter dependence, and estimate physicality. No knowledge of the pathway/detector efficiencies or the photon number generated by the source is required. Only knowledge of the raw singles and coincidence counts is needed. We present our estimation procedure for a single basis experiment, the extension to multiple bases, the application to state tomography to estimate strictly physical quantum states, simulation results comparing MLE and BME estimates, and experimental application of our method using our numerical tomography package TOMOHAK based on slice sampling.

**1:27PM B44.00012 How to construct the optimal Bayesian measurement in quantum statistical decision theory<sup>1</sup>**, FUYUHIKO TANAKA, Osaka Univ — Recently, much more attention has been paid to the study aiming at the application of fundamental properties in quantum theory to information processing and technology. In particular, modern statistical methods have been recognized in quantum state tomography (QST), where we have to estimate a density matrix (positive semidefinite matrix of trace one) representing a quantum system from finite data collected in a certain experiment. When the dimension of the density matrix gets large (from a few hundred to millions), it gets a nontrivial problem. While a specific measurement is often given and fixed in QST, we are also able to choose a measurement itself according to the purpose of QST by using quantum statistical decision theory. Here we propose a practical method to find the best projective measurement in the Bayesian sense. We assume that a prior distribution (e.g., the uniform distribution) and a convex loss function (e.g., the squared error) are given. In many quantum experiments, these assumptions are not so restrictive. We show that the best projective measurement and the best statistical inference based on the measurement outcome exist and that they are obtained explicitly by using the Monte Carlo optimization.

<sup>1</sup> the Grant-in-Aid for Scientific Research (B) (No. 26280005)

**1:39PM B44.00013 Experimental Estimation of Average Fidelity of a Clifford Gate on a 7-qubit Quantum Processor**, DAWEI LU, University of Waterloo, HANG LI, Tsinghua University, DENIS-ALEXANDRE TROTTIER, University of Waterloo, JUN LI, University of Science and Technology of China, AHARON BRODUTCH, ANTHONY KRISMANICH, AHMAD GHAVAMI, GARY DMITRIENKO, University of Waterloo, GUILU LONG, Tsinghua University, JONATHAN BAUGH, RAYMOND LAFLAMME, University of Waterloo, UNIVERSITY OF WATERLOO TEAM, TSINGHUA UNIVERSITY COLLABORATION, USTC COLLABORATION — The traditional approach of characterizing a given quantum gate via quantum process tomography (QPT) requires exponential number of experiments. Therefore, estimating the average fidelity of the quantum gate by QPT is not practical for large-scale systems. In this talk, I will discuss about how to certify a Clifford gate within polynomial complexity using a twirling protocol. In particular, we adopted this method in NMR and certified a 7-qubit quantum Clifford gate with only 1600 experiments (in contrast, QPT requires millions of experiments). This Clifford gate is important as it generates maximal coherence from single coherence, and non-trivial for benchmarking the coherent control in experiment. We show that the average fidelity of this gate is over 87% after accounting for the decoherence effect, and to date this is the largest experimental gate-characterization. This twirling protocol is efficient and scalable, and can also be extended to other systems straightforwardly.

**1:51PM B44.00014 Crosstalk characterization by eigenvalue estimation: Theory<sup>1</sup>**, MARCUS DA SILVA, Raytheon BBN Technologies — As qubit systems continue to grow and long coherence times become routine, the dominating sources of error shift away from decoherence and towards control errors. One pervasive source of control errors is crosstalk – where control fields intended for one qubit leak onto other qubits. In this talk we describe a method to quantify crosstalk by estimating the eigenvalues of the system's evolution using a technique known as "spectrum estimation". We discuss the wide applicability of the method, and demonstrate similar accuracy scaling to the robust phase estimation algorithm of Kimmel, Low, and Yoder.

<sup>1</sup>We acknowledge funding from ARO under contract W911NF-14-C-0048.

**2:03PM B44.00015 Crosstalk characterization in superconducting qubits by eigenvalue estimation: Experiment<sup>1</sup>**, MATTHEW WARE, KIN CHUNG FONG, COLM A. RYAN, BRIAN HASSIK, THOMAS OHKI, MARCUS P. DA SILVA, Raytheon BBN Technologies, RAYTHEON BBN TECHNOLOGIES TEAM — Superconducting qubit devices offer a promising path towards a scalable quantum computer. As these systems continue to grow in size and complexity, crosstalk errors, which build up during long control sequences, lead to an overall loss in control fidelity. In this talk we explore the use of eigenvalue estimation (a.k.a. "spectrum estimation") in superconducting systems as a high-accuracy method to detect and quantify crosstalk between qubits, and demonstrate how these techniques allow for quick identification and estimation of system crosstalk.

<sup>1</sup>We acknowledge funding from ARO under contract W911NF-14-C-0048.

**Monday, March 14, 2016 11:15AM - 2:15PM –**  
**Session B45 GQI: Semiconductor Qubits: Multidot Qubits and Dynamical Control** 348 - Vanita Srinivasa, Laboratory for Physical Sciences/University of Maryland, College Park, MD

**11:15AM B45.00001 Multiple quantum dot spin qubits**, SEIGO TARUCHA, The University of Tokyo & Riken Center for Emergent Matter Science — To date various techniques of implementing spin qubits and entangling gates have been developed with quantum dots (QDs). The necessary step for further scaling up the qubit system is to increase the number of QDs with a well-controlled charge state to prepare multiple qubits and improve the fidelity of the qubit gates as well. I will first review spin-1/2 qubit gates with triple QDs for operating three qubits, local and non-local entangling gates, and SWAP gates. I show that the fidelity of these spin manipulations is significantly increased by decreasing the data acquisition time. Secondly I will refer to quadruple and quintuple QDs to implement multiple spin qubits. For the triple QD we use two sets of two coupled dots in the spin blockade regime to demonstrate operation of three individual spin qubits. We use an exchange coupling between the neighboring dots to make two sets of SWAPs and an inhomogeneous Zeeman field difference between the neighboring dots (between the remote dots) to make local (non-local) control of S-T<sub>0</sub> oscillations. We apply the same technique for the quadruple QD to coherently manipulate individual four spins. We finally discuss a way to further scale up the qubit system using multiple QDs.

**11:51AM B45.00002 A new look at encoded-qubit quantum dot quantum computing in silicon**, CHARLES TAHAN, YUN-PIL SHIM, RUSKO RUSKOV, Laboratory for Physical Sciences — Although the properties of spin-based qubits are specified by the material system they reside in, it's possible to modify those properties by encoding a qubit into multiple physical spins. Here we consider new operating regimes for encoded spin qubits and discuss their relevance to spin-based quantum computing and qubit-qubit coupling, especially in silicon quantum dot systems. We will also briefly discuss recent developments in g-factor theory in silicon quantum dots and their possible implications.

**12:03PM B45.00003 High quality exchange rotations in spin qubits using symmetric gating<sup>1</sup>**, F. MARTINS, F. K. MALINOWSKI, P. D. NISSEN, C. M. MARCUS, F. KUEMMETH, Center for quantum devices, Niels Bohr Institute, University of Copenhagen, Denmark, E. BARNES, Department of Physics, Virginia Tech / Condensed Matter Theory Center and Joint Quantum Institute, Department of Physics, University of Maryland, USA, G. C. GARDNER, S. FALLAHI, M. J. MANFRA, Department of Physics and Astronomy and Birck Nanotechnology Center, Purdue University, USA — We present results on a singlet-triplet qubit implemented in a GaAs/AlGaAs heterostructure and we show that exchange oscillations can be realized either by tilting the double well potential, the conventional method, or by symmetrically lowering the barrier, as originally suggested by Loss and DiVincenzo. The two methods are compared here. We find that lowering the barrier between dots has much less relative exchange noise compared to tilting the potential. Since exchange rotations are sensitive to electrical noise and relatively insensitive to nuclear noise, this yields significantly enhanced free induction decay times and quality factors. Our results are comparable to those reported recently in silicon quantum dot devices, obtained using similar techniques.

<sup>1</sup>Support through IARPA-MQCO, LPS-MPO-CMTC, Army Research Office, and the Danish National Research Foundation is acknowledged

**12:15PM B45.00004 Charge noise mitigation in triple-dot encoded spin qubits**, EMILY PRITCHETT, HRL Laboratories — The immediate scalability of electrons confined to semiconductor quantum dots makes them one of the most attractive platforms for quantum information processing; however, 1/f charge noise associated with electrical confinement has been a leading source of noise in quantum dot systems. Recently, there has been a surge of experimental and theoretical work aimed at charge noisemitigation in quantum dot systems implementing AC- or DC-control of triple dots at "sweet spots". In this talk, we compare the symmetric operation point (SOP)DC control technique implemented in Reed, et al. [arXiv:1508.01223] to the resonant exchange (RX) AC control technique [Medford, et al., PRL 111, 050501 (2013), Taylor, et al., PRL 111, 050502 (2013), Russ, et al., Phys. Rev. B 91, 235411 (2015)]. Numerical results suggest that both DC and AC triple-dot control can offer a comparably substantial reduction in charge noise; however, the validity of the rotating wave approximation forces a trade-off between speed and accuracy for RX qubits, while the performance of SOP qubits actually improves at shorter gate times.

**12:27PM B45.00005 The validity of the RWA and gate operation speedup by violating RWA in resonant-driven qubit systems<sup>1</sup>**, YANG SONG, Condensed Matter Theory Center, Dept. of Physics, Univ. of Maryland — The rotating wave approximation (RWA) is ubiquitously used in understanding (quasi)resonant driven systems and designing pulses for state evolution. Following the practice in atomic and NMR physics, a wide range of semiconducting qubit systems are driven resonantly to manipulate the qubit, including single-spin/resonant exchange (RX)/various singlet-triplet(ST)/spin-charge hybrid qubits. The purpose of this talk is twofold: (I) Examine the validity of RWA in different qubit systems and analyze the error in terms of quantum computation; (II) Present faster gate operations by going into RWA-invalid regime for resonant-driven qubits (esp. for ST and RX types). We measure the RWA-induced infidelity and discuss it in view of the fault-tolerant error correction threshold and operation speeds. Applying the analytical extension (two orders higher than RWA) greatly reduces the infidelity, in the regime where the RWA is attempted to be used. Moreover, we show that the resonant-driven system is not limited by the Rabi-like weak coupling limit and the associated slow gate speed, much smaller than the level splitting (e.g., the small Zeeman energy gradient in ST qubits). We demonstrate the universal one qubit gates for driving strength up to a few level splitting, achieving fast control with only simple sinusoidal pulses. We also solve for the 'shifted sinusoidal' pulses needed for ST qubits where the exchange coupling cannot change signs.

<sup>1</sup>In collaboration with Xin Wang, Jason Kestner and Sankar Das Sarma, and supported by LPS-MPO-CMTC and IARPA- MQCO

**12:39PM B45.00006 Leakage of The Quantum Dot Hybrid Qubit in The Strong Driving Regime<sup>1</sup>**, YUAN-CHI YANG, MARK FRIESEN, S. N. COPPERSMITH, Univ of Wisconsin, Madison — Recent experimental demonstrations of high-fidelity single-qubit gates suggest that the quantum dot hybrid qubit is a promising candidate for large-scale quantum computing. The qubit is comprised of three electrons in a double quantum dot, and can be protected from charge noise by operating in an extended sweet-spot regime. Gate operations are based on exchange interactions mediated by an excited state. However, strong resonant driving causes unwanted leakage into the excited state. Here, we theoretically analyze leakage caused by strong driving, and explore methods for increasing gate fidelities.

<sup>1</sup>This work was supported in part by ARO (W911NF-12-0607), NSF (PHY-1104660), ONR (N00014-15-1-0029), and the University of Wisconsin-Madison.

**12:51PM B45.00007 Tenfold increase in the Rabi decay time of the quantum dot hybrid qubit**, BRANDUR THORGRIMSSON, University of Wisconsin-Madison, DOHUN KIM, Yonsei University, Seoul, South Korea, C.B. SIMMONS, DANIEL R. WARD, RYAN H. FOOTE, D. E. SAVAGE, M. G. LAGALLY, MARK FRIESEN, S. N. COPPERSMITH, M. A. ERIKSSON, University of Wisconsin-Madison — The quantum dot hybrid qubit is formed from three electrons in a double quantum dot. In previous work, we showed that the hybrid qubit has the speed of a charge qubit and the stability of a spin qubit. Here, we show that the hybrid qubit is also highly tunable, and can be tuned into regimes with desirable coherence properties. By changing the interdot tunnel rate by only 25%, from 5 GHz to 6.25 GHz, we are able to increase the Rabi decay time by a factor of ten, from 18 ns to 177 ns. We attribute this improvement to the refinement of an extended sweet spot in the energy dispersion of the hybrid qubit, where the qubit is less susceptible to charge noise, which is a dominant source of decoherence. This work was supported in part by ARO (W911NF-12-0607) and NSF (DMR-1206915 and PHY-1104660). Development and maintenance of the growth facilities used for fabricating samples is supported by DOE (DE-FG02-03ER46028). This research utilized NSF-supported shared facilities at the University of Wisconsin-Madison.

**1:03PM B45.00008 Effect of Charge Noise on Landau-Zener Interferometry in double quantum dots**, ZHENYI QI, MARK FRIESEN, SUSAN COPPERSMITH, MAXIM VAVILOV, Univ of Wisconsin, Madison — We study the effect of charge noise on the dynamics of semiconductor quantum dot qubits. Recent experiments have demonstrated relatively long coherence times in these systems; however at the same time, the visibility of the Landau-Zener interference pattern is relatively low. We argue that the electromagnetic noise of the environment affects the coherence of the qubit near the charge degeneracy point, including the singlet-triplet avoided level crossing, and results in the reduced visibility of the Landau-Zener interferometry when the singlet-triplet avoided level crossing happens in the vicinity of the charge degeneracy point. Using a master equation, we describe the evolution of the density matrix for the qubit assuming weak coupling of the quantum dot to its electromagnetic environment and compare our results to experimental data.

**1:15PM B45.00009 Noise-induced collective quantum state preservation in spin qubit arrays<sup>1</sup>**, EDWIN BARNES, Department of Physics, Virginia Tech and Condensed Matter Theory Center, University of Maryland, DONG-LING DENG, ROBERT THROCKMORTON, YANG-LE WU, Condensed Matter Theory Center, University of Maryland — The hyperfine interaction with nuclear spins (or, Overhauser noise) has long been viewed as a leading source of decoherence in individual quantum dot spin qubits. We show that in a coupled multi-qubit system consisting of as few as four spins, interactions with nuclear spins can have the opposite effect where they instead preserve the collective quantum state of the system. This noise-induced state preservation can be realized in a linear spin qubit array using current technological capabilities. Our proposal requires no control over the Overhauser fields in the array; only experimental control over the average interqubit coupling between nearest neighbors is needed, and this is readily achieved by tuning gate voltages. Our results illustrate how the role of the environment can transform from harmful to helpful in the progression from single-qubit to multi-qubit quantum systems.

<sup>1</sup>Work supported by LPS-MPO-CMTC and IARPA-MQCO

**1:27PM B45.00010 Decoupling a spin qubit from high-frequency Larmor dynamics of a GaAs nuclear spin bath<sup>1</sup>**, FILIP K. MALINOWSKI, FREDERICO MARTINS, PETER D. NISSEN, MARK S. RUDNER, CHARLES M. MARCUS, FERDINAND KUEMMETH, Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, EDWIN BARNES, Department of Physics, Virginia Tech, SAEED FALLAHI, GEOFFREY C. GARDNER, MICHAEL J. MANFRA, Department of Physics and Astronomy and Birck Nanotechnology Center, Purdue University — We present a technique of decoupling a spin qubit in a GaAs/AlGaAs heterostructure from low- and high-frequency noise arising from hyperfine interaction of electrons with nuclear spins. We use Carr-Purcell-Meiboom-Gill sequences in which we synchronize the repetition rate of  $\pi$  pulses to difference Larmor frequencies of  $^{69}\text{Ga}$ ,  $^{71}\text{Ga}$  and  $^{75}\text{As}$  nuclei. This decouples the qubit both from low-frequency noise due to diffusion of nuclear spins and from noise at selected high frequencies, allowing us to apply more than a thousand  $\pi$  pulses in a sequence. We demonstrate a coherence time of a singlet-triplet qubit of 0.87 ms, i.e. five orders of magnitude longer than the inhomogeneous dephasing time intrinsic to GaAs.

<sup>1</sup>Support through IARPA-MQCO, Army Research Office, LPS-MPO-CMTC, the Villum Foundation and the Danish National Research Foundation is acknowledged.

**1:39PM B45.00011 Noise filtering of composite pulses for singlet-triplet qubits<sup>1</sup>**, XIN WANG, XU-CHEN YANG, City University of Hong Kong — Dynamically corrected gates are useful measures to combat decoherence in spin qubit systems. They are, however, mostly designed assuming the static-noise model and may thus be considered low-frequency noise filters. In this talk we carefully examine the applicability of a particular type of dynamically corrected gates, namely the SUPCODE designed for singlet-triplet qubits, under realistic  $1/f^\alpha$  noises. Through randomized benchmarking, we have found that SUPCODE offers improvement of the gate fidelity for  $\alpha > 1$  and the improvement becomes exponentially more pronounced with the increase of the noise exponent  $\alpha$  up to 3. On the other hand, for small  $\alpha$  SUPCODE will not offer any improvement. We also present the computed filter transfer functions for the SUPCODE gates for nuclear and charge noise respectively and have found that they are consistent with the finding from the benchmarking.

<sup>1</sup>The work is supported by grants from City University of Hong Kong (Projects No. 9610335 and No. 7200456).

**1:51PM B45.00012 Dynamical Decoupling with pulse errors for ensembles of interacting spins**, E. S. PETERSEN, A. M. TYRSHKIN, S. A. LYON, Princeton University — Dynamical decoupling (DD) is a well-known approach for decoupling quantum (spin) systems from their environments. Theoretically, the performance of DD pulse sequences is often analyzed using a single spin approximation in which environmental noise is included through single spin operators. This approach has successfully analyzed the effectiveness of many popular DD pulse sequences (like CPMG and XY4) to cancel environmental noise even in the presence of unavoidable pulse errors. However, this methodology does not describe the effect of DD on the spin-spin interactions present in experiments involving large numbers of spins. Here, we go beyond the usual single-spin model, extending the analysis of DD sequences to include such spin-spin interactions. We find that when using certain popular DD sequences (like CPMG), coherence times of ensembles with dipolar interactions between spins can be drastically influenced by pulse errors. While sequences with ideal pulses do not decouple the spin-spin interactions, the presence of even small pulse errors can partially (or even greatly) decouple the spin-spin interactions thus leading to longer coherence times. Furthermore, the extent that these interactions are decoupled is highly dependent on the type of DD sequence used, and not necessarily the number of pulses involved. These calculations explain results of past experiments (Tyrshkin et al, arxiv: 1011.1903).

**2:03PM B45.00013 Dynamic field-frequency lock for tracking magnetic field fluctuations in electron spin resonance experiments**, ABRAHAM ASFAW, ALEXEI TYRSHKIN, STEPHEN LYON, Department of Electrical Engineering, Princeton University, Princeton NJ 08544 — Global magnetic field fluctuations present significant challenges to pulsed electron spin resonance experiments on systems with long spin coherence times. We will discuss results from experiments in which we follow instantaneous changes in magnetic field by locking to the free induction decay of a proton NMR signal using a phase-locked loop. We extend conventional field-frequency locking techniques used in NMR to follow slow magnetic field drifts by using a modified Carr-Purcell-Meiboom-Gill (CPMG) pulse sequence in which the phase of the  $\pi$ -pulses follows the phase of the proton spins at all times. Hence, we retain the ability of the CPMG pulse sequence to refocus local magnetic field inhomogeneities without refocusing global magnetic field fluctuations. In contrast with conventional field-frequency locking techniques, our experiments demonstrate the potential of this method to dynamically track global magnetic field fluctuations on timescales of about 2 seconds and with rates faster than a kHz. This frequency range covers the dominant noise frequencies in our electron spin resonance experiments as previously reported.

## Monday, March 14, 2016 11:15AM - 2:03PM –

Session B46 GIMS: Instrumentation I: Detectors, Sensors, Signal Processing & Analysis 311 - James Matey, NIST

**11:15AM B46.00001 Contemporary Issues in Ultra-Low Alpha Particle Counting**, MICHAEL GORDON, IBM TJ Watson Research Center — Single-Event Upsets (SEU) in CMOS devices are caused by the passage of ionizing radiation either from terrestrial neutrons or from the natural alpha particle radiation within the materials surrounding the transistors. Interactions of the neutrons with the silicon cause spallation reactions which emit energetic highly ionizing elements. Alpha particles, on the other hand, can upset the devices through direct ionization rather than through a nuclear reaction as in the case of the neutrons. In order to minimize the alpha-particle component of SEU, the radiation from the materials within a distance 100  $\mu\text{m}$  of the transistors, currently needs to have an alpha particle emissivity of less than 2 alpha particles per khr per square centimeter. Many alpha particle detectors have background levels that are larger than this, which can make these measurements inaccurate and time consuming. This talk will discuss what is involved in making alpha particle emissivity measurements of materials used in the semiconductor industry using an ultra-low background commercially-available ionization detector. Detector calibration and efficiency, radon adsorption on the samples, and the effect of surface charge on electrically insulating samples will be discussed.

**11:27AM B46.00002 TRIASSIC: the Time-Resolved Industrial Alpha-Source Scanning Induced Current microscope**, ARTHUR PALLONE, Norwich University — Time-resolved ion beam induced current (TRIBIC) microscopy yields useful information such as carrier mobility and lifetimes in semiconductors and defect locations in devices; however, traditional TRIBIC uses large, expensive particle accelerators that require specialized training to operate and maintain. The time-resolved industrial alpha-source scanning induced current (TRIASSIC) microscope transforms TRIBIC by replacing the particle accelerator facility with an affordable, tabletop instrument suitable for use in research and education at smaller colleges and universities. I will discuss the development of, successes with, setbacks to and future directions for TRIASSIC.

**11:39AM B46.00003 Superconducting Nuclear Recoil Sensor for Directional Dark Matter Detection<sup>1</sup>**, ANN JUNGHANS, KEVIN BALDWIN, MARKUS HEHLEN, Los Alamos National Laboratory, RANDY LAFLER, DINESH LOOMBA, NGUYEN PHAN, University of New Mexico, NINA WEISSE-BERNSTEIN, Los Alamos National Laboratory — The Universe consists of 72% dark energy, 23% dark matter and only 5% of ordinary matter. One of the greatest challenges of the scientific community is to understand the nature of dark matter. Current models suggest that dark matter is made up of slowly moving, weakly interacting massive particles (WIMPs). But detecting WIMPs is challenging, as their expected signals are small and rare compared to the large background that can mimic the signal. The largest and most robust unique signature that sets them apart from other particles is the day-night variation of the directionality of dark matter on Earth. This modulation could be observed with a direction-sensitive detector and hence, would provide an unambiguous signature for the galactic origin of WIMPs. There are many studies underway to attempt to detect WIMPs both directly and indirectly, but solid-state WIMP detectors are widely unexplored although they would present many advantages to prevalent detectors that use large volumes of low pressure gas. We present first results of a novel multi-layered architecture, in which WIMPs would interact primarily with solid layers to produce nuclear recoils that then induce measureable voltage pulses in adjacent superconductor layers.

<sup>1</sup>This work was supported by the U.S. Department of Energy through the LANL Laboratory Directed Research and Development Program.

**11:51AM B46.00004 It may be possible to use Speech Recognition Algorithms to sort through Particle Detection**, RICHARD KRISKE, University of Minnesota — There are some similarities between recognizing speech and written language and in recognizing Particle interaction and decays. In the Viterbi Algorithm or speech recognition, a target word is recursively compared with the unknown utterance. Say one remembered the word Motion in a song and wanted to find that song. First the letter M is typed in and the most common words with M show up say it is the word "Menards", then an "O" is typed in and statistically the most common word is now "Movies", now the "t" is typed in and the most common word is "Motley Crue" finally all the letters are typed in and the song that matches is "Motion Lyrics". We all recognize the Algorithm and perhaps a few have realized that this Algorithm could also be applied to Decay Chains in Particle Scattering and Detection. Also there may come a day when perhaps Neutrinos where transmitted with the purpose of Communication, one system would be to use a type of "Morse Code", but another could be to use Decay Chains themselves. Perhaps the sender could tune the Energy such that the information received would rely on the Energy being transmitted, since it may be that only a few of the particles are received, too few for "Morse Code" to work.

**12:03PM B46.00005 Bayesian 2D Current Reconstruction from Magnetic Images**, COLIN B. CLEMENT, MATTHEW K. BIERBAUM, KATJA NOWACK, JAMES P. SETHNA, Cornell University — We employ a Bayesian image reconstruction scheme to recover 2D currents from magnetic flux imaged with scanning SQUIDS (Superconducting Quantum Interferometric Devices). Magnetic flux imaging is a versatile tool to locally probe currents and magnetic moments, however present reconstruction methods sacrifice resolution due to numerical instability. Using state-of-the-art blind deconvolution techniques we recover the currents, point-spread function and height of the SQUID loop by optimizing the probability of measuring an image. We obtain uncertainties on these quantities by sampling reconstructions. This generative modeling technique could be used to develop calibration protocols for scanning SQUIDS, to diagnose systematic noise in the imaging process, and can be applied to many tools beyond scanning SQUIDS.

**12:15PM B46.00006 ABSTRACT WITHDRAWN —**

**12:27PM B46.00007 Detection of zeptojoule microwave pulses using an electrothermal bifurcation**, JOONAS GOVENIUS, RUSSELL LAKE, KUAN TAN, MIKKO MÖTTÖNEN, Department of Applied Physics, Aalto University, Finland — We utilize electrothermal feedback for the threshold detection of weak 8.4 GHz microwave pulses containing approximately  $200 \times h \times (8.4 \text{ GHz}) \approx 1.1 \times 10^{-21} \text{ J}$  of energy. The feedback couples the electrical and thermal degrees of freedom in the central component of our detector, a metallic nanowire that absorbs the incoming microwave radiation and transduces the temperature change into a radio-frequency electrical signal. We can tune the feedback in situ, which provides access to both positive and negative feedback regimes with rich nonlinear dynamics. In particular, strong positive feedback leads to the emergence of two metastable electron temperature states in the millikelvin range. We use these states in the threshold detection protocol.

**12:39PM B46.00008 Micro-Hall devices for magnetic, electric and photo-detection**, A. GILBERTSON, Imperial College, H. SADEGHI, Lancaster University, V. PANCHAL, O. KAZAKOVA, National Physical Laboratory, C.J. LAMBERT, Lancaster University, S.A. SOLIN<sup>1</sup>, L.F. COHEN, Imperial College — Multifunctional mesoscopic sensors capable of detecting local magnetic ( $B$ ), electric ( $E$ ), and optical fields can greatly facilitate image capture in nano-arrays that address a multitude of disciplines. The use of micro-Hall devices as  $B$ -field sensors [1] and, more recently as  $E$ -field sensors [2] is well established. Here we report the real-space voltage response of InSb/AlInSb micro-Hall devices to not only local  $E$ -, and  $B$ -fields but also to photo-excitation using scanning probe microscopy. We show that the ultrafast generation of localised photocarriers results in conductance perturbations analogous to those produced by local  $E$ -fields. Our experimental results are in good agreement with tight-binding transport calculations in the diffusive regime. At room temperature, samples exhibit a magnetic sensitivity of  $>500 \text{ nT}/\sqrt{\text{Hz}}$ , an optical noise equivalent power of  $>20 \text{ pW}/\sqrt{\text{Hz}}$  ( $\lambda = 635 \text{ nm}$ ) comparable to commercial photoconductive detectors, and charge sensitivity of  $>0.04 \text{ e}/\sqrt{\text{Hz}}$  comparable to that of single electron transistors. [1] Boero, G.; Demierre, M.; Besse, P. A.; Popovic, R. S. *Sensors and Actuators A-Physical* **2003**, *106* (1-3), 314-320. [2] Barbolina, I. I. et al. *Applied Physics Letters* **2006**, *88* (1), 013901.

<sup>1</sup>Work done while on sabbatical from Washington University. Co-founder of PixelEXX, a start-up whose focus is imaging nano-arrays.

**12:51PM B46.00009 Understanding the TERS Effect with On-line Tunneling and Force Feedback Using Multiprobe AFM/NSOM with Raman Integration**, AARON LEWIS, Hebrew University of Jerusalem. Dept. of Applied Physics, Jerusalem, Israel, RIMMA DEKHTER, PATRICIA HAMRA, YOSHI BAR-DAVID, HESHAM TAHA, Nanonics Imaging Ltd., Jerusalem, Israel — Tip enhanced Raman scattering (TERS) has evolved in several directions over the past years. The data from this variety of methodologies has now accumulated to the point that there is a reasonable possibility of evolving an understanding of the underlying cause of the resulting effects that could be the origin of the various TERS enhancement processes. The objective of this presentation is to use the results thus far with atomic force microscopy (AFM) probes with noble metal coating, etching, transparent gold nanoparticles with and without a second nanoparticle [Wang and Schultz, ANALYST 138, 3150 (2013)] and tunneling feedback probes [R. Zhang et. al., NATURE 498, 82 (2013)]. We attempt at understanding this complex of results with AFM/NSOM multiprobe techniques. Results indicate that TERS is dominated by complex quantum interactions. This produces a highly confined and broadband plasmon field with all  $k$  vectors for effective excitation. Normal force tuning fork feedback with exposed tip probes provides an excellent means to investigate these effects with TERS probes that we have shown can circumvent the vexing problem of jump to contact prevalent in conventional AFM methodology and permit on-line switching between tunneling and AFM feedback modes of operation.

**1:03PM B46.00010 A Cantilever Torque Magnetometer for Measuring Hall Conductivity**, SAMUEL MUMFORD, E. M. LEVENSON-FALK, Stanford University, AMIR YACOBY, Harvard University, AHARON KAPITULNIK, Stanford University — We propose a cantilever-based torque magnetometer of Corbino-disc patterned samples in magnetic field. Applying a voltage difference across the disc, a magnetic dipole moment is created which will interact with the magnetic field, exerting a torque on the cantilever. A circulating current will flow in the presence of potential difference between the two edges of the disc which is placed at the end of a vibrating cantilever. The induced magnetic dipole moment will interact with the magnetic field, creating a torque. The measured torque yields information about the transverse conductance of the ring - hence  $\sigma_{xy}$ .

**1:15PM B46.00011 Carbon Nanotube Bolometer for Absolute FTIR Spectroscopy**, SOLOMON WOODS, NIST, JORGE NEIRA, Jung Research and Development Corp., NATHAN TOMLIN, JOHN LEHMAN, NIST — We have developed and calibrated planar electrical-substitution bolometers which employ absorbers made from vertically-aligned carbon nanotube arrays. The nearly complete absorption of light by the carbon nanotubes from the visible range to the far-infrared can be exploited to enable a device with read-out in native units equivalent to optical power. Operated at cryogenic temperatures near 4 K, these infrared detectors are designed to have time constant near 10 ms and a noise floor of about 10 pW. Built upon a micro-machined silicon platform, each device has an integrated heater and thermometer, either a carbon nanotube thermistor or superconducting transition edge sensor, for temperature control. We are optimizing temperature-controlled measurement techniques to enable high resolution spectral calibrations using these devices with a Fourier-transform spectrometer.

**1:27PM B46.00012 Optical design of a compact near-infrared multispecies gas sensor**, JOSHUA LARSON, FATIMA TOOR, Univ of Iowa — In this work we present the design of a compact and cost effective near infrared (NIR) gas sensor system that can detect nitrous oxide ( $\text{NO}_x$ ), ammonia ( $\text{NH}_3$ ), and methane ( $\text{CH}_4$ ) simultaneously. These three gases were chosen as they are environmental pollutants and their monitoring is especially important in agricultural states like Iowa. As a first step in our design process, we have developed a Matlab model based on Beer-Lambert's law to generate sample sensor data for each of the gases at different concentrations. The data measured from the sensor system will be as a function of time instead of wavelength, so we performed Fourier Transform analysis on the sensor data to convert it to voltage versus time. The simulated sensor data will enable to design software algorithms to separate the absorption signals for each of the three gases. As a second step, we have developed a lab-based sensor system comprising of three components: (i) a NIR lead sulfide ( $\text{PbS}$ ) photodiode, (ii) an LED that emits 1900 nm to 2600 nm, and (iii) an optical cavity where the gases are introduced. We are designing the optical cavity using ray optics COMSOL finite element method simulator using the principles of a compact chaotic cavity that will allow the LED light to have a path length of greater than 100 m within the cavity, enabling high sensitivity gas detection. Our end goal is to have an autonomous drone mounted device that is simple and inexpensive to use. We plan to license this technology to agricultural equipment manufacturers.

**1:39PM B46.00013 Enthalpy of sublimation as measured using a silicon oscillator.**, HAMZA SHAKEEL, J.M. POMEROY, National Institute of Standards and Technology — In this study, we report the enthalpy of sublimation of common gases (nitrogen, oxygen, argon, carbon dioxide, neon, krypton, xenon, and water vapor) using a large area silicon oscillator with a sub-ng ( $\approx 0.027 \text{ ng/cm}^2$ ) mass sensitivity. The double paddle oscillator design enables high frequency stability (17 ppb) at cryogenic temperatures and provides a consistent technique for enthalpy measurements. The enthalpies of sublimation are derived from the rate of mass loss during programmed thermal desorption and are detected as a change in the resonance frequency of the self-tracking oscillator. These measured enthalpy values show excellent agreement with the accepted literature values.

**1:51PM B46.00014 Conversion of far ultraviolet to visible radiation: absolute measurements of the conversion efficiency of tetraphenyl butadiene<sup>1</sup>**, ROBERT E. VEST, National Institute of Standards and Technology, MICHAEL A. COPLAN, University of Maryland, CHARLES W. CLARK, Joint Quantum Institute — Far ultraviolet (FUV) scintillation of noble gases is used in dark matter and neutrino research<sup>2</sup> and in neutron detection.<sup>3</sup> Upon collisional excitation, noble gas atoms recombine into excimer molecules that decay by FUV emission. Direct detection of FUV is difficult. Another approach is to convert it to visible light using a wavelength-shifting medium. One such medium, tetraphenyl butadiene (TPB) can be vapor-deposited on substrates. Thus the quality of thin TPB films can be tightly controlled. We have measured the absolute efficiency of FUV-to-visible conversion by 1  $\mu\text{m}$ -thick TPB films vs. FUV wavelengths between 130 and 300 nm, with 1 nm resolution. The energy efficiency of FUV to visible conversion varies between 1% and 5%. We make comparisons with other recent results.<sup>4</sup>

<sup>1</sup>Work performed at the NIST SURF III Synchrotron Ultraviolet Radiation Facility,

<sup>2</sup>"Liquid noble gas detectors for low energy particle physics," V. Chepel and H. Araújo, *JINST* **8**, R04001 (2013)

<sup>3</sup>"Noble gas excimer scintillation following neutron capture in boron thin films," J. C. McComb, *et al.*, *J. Appl. Phys.* **115**, 144504 (2014)

<sup>4</sup>"Fluorescence efficiency and visible re-emission spectrum of tetraphenyl butadiene films at extreme ultraviolet wavelengths," V. M. Gehman, *et al.*, *Nuc. Inst. Meth. A* **654**, 116 (2011)

## Monday, March 14, 2016 11:15AM - 2:15PM – Session B47 DCMP: Molecular Assembly on Surfaces 312 -

**11:15AM B47.00001 Supra-molecular networks for CO<sub>2</sub> capture<sup>1</sup>**, JERZY SADOWSKI, JOHN KESTELL, Brookhaven National Laboratory — Utilizing capabilities of low-energy electron microscopy (LEEM) for non-destructive interrogation of the real-time molecular self-assembly, we have investigated supramolecular systems based on carboxylic acid-metal complexes, such as trimesic and mellitic acid, doped with transition metals. Such 2D networks can act as host systems for transition-metal phthalocyanines (MPc; M = Fe, Ti, Sc). The electrostatic interactions of CO<sub>2</sub> molecules with transition metal ions can be tuned by controlling the type of TM ion and the size of the pore in the host network. We further applied infrared reflection-absorption spectroscopy (IRRAS) to determine of the molecular orientation of the functional groups and the whole molecule in the 2D monolayers of carboxylic acid. The kinetics and mechanism of the CO<sub>2</sub> adsorption/desorption on the 2D molecular network, with and without the TM ion doping, have been also investigated.

<sup>1</sup>This research used resources of the Center for Functional Nanomaterials, which is the U.S. DOE Office of Science User Facility, at Brookhaven National Laboratory under Contract No. DE-SC0012704.

**11:27AM B47.00002 Experimental and Computational Comparison of the Self-Assembled Nanostructures of Pentacene Derivatives on Gold**, AMANDA LARSON, RYAN MILLER, JUN WANG<sup>1</sup>, KARSTEN POHL, University of New Hampshire — Pentacene derivatives can tailor the standard pentacene molecule for unique properties beneficial to organic photovoltaic devices. Increased solubility, photo-oxidative resistance, thermal stability and tailor-able HOMO-LUMO gaps make novel pentacene derivatives enticing for further study. Scanning tunneling microscopy and density functional theory was used to examine the atomic interface between gold and the pentacene derivatives: 6,13-dichloropentacene (DCP) and 5,6,7-trithiapentacene-13-one (TTPO), electron donors exhibiting self-assembled monolayer structures on gold surfaces. Comparing DCP, TTPO and pentacene highlights the effects of differing substituents to the self-assembled structures. In particular, the unique 3-dimensional angular assembly of TTPO is examined and clarified through use of extensive computation. The lateral arrangement of the molecule is unique, causing the thiol substituent side of the molecule to be angled down towards the gold surface, while the long-axis of TTPO is parallel to the gold surface; distinctive from previously observed pentacene and pentacene derivative assemblies. By understanding the differences in self-assembly of similar molecules, we are developing novel pathways towards molecular control of organic-metal interfaces.

<sup>1</sup>\*current ORNL

**11:39AM B47.00003 Molecular assembly and organic film growth on complex intermetallic surfaces.**<sup>1</sup>, ABDULLAH AL-MAHBOOB, HEM RAJ SHARMA, Department of Physics, University of Liverpool, UK, JERZY T SADOWSKI, Center for Functional Nanomaterials, Brookhaven National Laboratory, USA, JULIAN LEDIEU, VINCENT FOURNE, Institut Jean Lamour, Universit  de Lorraine, France, RONAN MCGRATH, Department of Physics, University of Liverpool, UK — We extensively studied the role of molecular symmetry and symmetry/structures of wide ranges of substrate-surfaces from non-periodic to periodic to quasi-crystalline in nucleation, growth and phase transition in films made of organic molecular materials. Recently, most interest in quasicrystals is due to the generalization of aperiodic ordering to several classes of systems. Compared to periodic materials, these provide a closer approximation to an isotropic first Brillouin zone, which is of great importance to the design of new functional materials. Here, we present results obtained from our ongoing study of interface mediated molecular assembly extended on complex intermetallic surfaces with specific examples of C<sub>60</sub> and Zn-phthalocyanine on quasicrystalline and approximant surfaces. We employed in-situ real-time low-energy electron microscopy (LEEM) for investigation of the processes in assembly and film growth and post-growth STM study and DFT calculations to understand structural details and growth mechanism.

<sup>1</sup>Research were carried out in part at the Center for Functional Nanomaterials, Brookhaven National Lab, USA; partly at Institut Jean Lamour, Universit  de Lorraine, France; and partly at the Surface Science Research Centre, University of Liverpool, UK.

**11:51AM B47.00004 A theoretical and experimental investigation on the adsorption of pentacene on the Cu(322) surface**, JERONIMO MATOS, University of Central Florida, MICHELE SAUVAGE-SIMKIN, Synchrotron SOLEIL and UR1-CNRS, ALESSANDRO COATI, Synchrotron SOLEIL, YVES GARREAU, Synchrotron SOLEIL and Universit  Paris Diderot, ALINA VLAD, Synchrotron SOLEIL, KATHRIN MULLER, Max Planck Institut fr Festk rperforschung, AZZEDINE BENDOUNAN, Synchrotron SOLEIL, ABDELKADER KARA, University of Central Florida — In this study, complementary techniques including density functional theory (DFT), grazing incidence x-ray diffraction (GIXD), and scanning tunneling microscopy (STM) are used to study the surface distortions induced by the adsorption of pentacene on the stepped Cu(322) surface. GIXD measurements are performed for the clean Cu(322) surface and at various coverages of pentacene, up to one monolayer. For the one monolayer case, reciprocal space maps from GIXD measurement suggest the reconstruction of the steps to double the step width and height, with two pentacene molecules present at each terrace. Complementary DFT calculations are carried out, with and without the self-consistent inclusion of vdW interactions, using the optB88-vdW and PBE functionals. Our investigation illustrates a prototype method for conducting future benchmarking studies to assess the accuracy of the current self-consistent vdW functionals when applied to organic molecule adsorption.

**12:03PM B47.00005 Coverage Dependent Assembly of Anthraquinone on Au(111)**, BRAD CONRAD, Appalachian State Univ, ANDREW DELOACH, North Carolina State University, THEODORE EINSTEIN, University of Maryland - College Park, DANIEL DOUGHERTY, North Carolina State University — A study of adsorbate-adsorbate and surface state mediated interactions of anthraquinone (AnQ) on Au(111) is presented. We utilize scanning tunneling microscopy (STM) to characterize the coverage dependence of AnQ structure formation. Ordered structures are observed up to a single monolayer (ML) and are found to be strongly dependent on molecular surface density. While the complete ML forms a well-ordered close-packed layer, for a narrow range of sub-ML coverages irregular close-packed islands are observed to coexist with a disordered pore network linking neighboring islands. This network displays a characteristic pore size and at lower coverages, the soliton walls of the herringbone reconstruction are shown to promote formation of distinct pore nanostructures. We will discuss these nanostructure formations in the context of surface mediated and more direct adsorbate interactions.

**12:15PM B47.00006 Self-Assembly of Glycine on Cu (001): The tale of Temperature and Polarity**, LIFANG XU, Institute of Physics, Chinese Academy of Sciences, JING XU, Department of Physics, Renmin University of China, ZHESHUAI LIN, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, SHENG MENG, ENGE WANG, Institute of Physics, Chinese Academy of Sciences — Glycine on Cu(001) is used as an example to illustrate the critical role of molecular polarity and finite temperature effect in self-assembly of bio-molecules at a metal surface. A unified picture for glycine self-assembly on Cu(001) is derived based on full polarity compensation considerations. Temperature plays a non-trivial role: the ground-state structure at 0 K is absent at room temperature, where intermolecular hydrogen bonding overweighs competing molecule-substrate interactions. The unique p(24) structure predicted as the most stable structure was confirmed by ab initio molecular dynamics simulations, whose scanning tunneling microscopy images and anisotropic free-electron-like dispersion are in excellent agreement with experiments. Moreover, the rich self-assembling patterns including the heterochiral and homochiral phases, and their interrelationships are entirely governed by the same mechanism.

**12:27PM B47.00007 Interaction of porphyrins with low coordinated sites on the MgO(001) surface**, OSMAN BARIS MALCIOGLU, MICHEL BOCKSTEDTE, Solid State Physics, FAU Erlangen-Nrnberg, Erlangen Germany — The functionalization of metal oxide surfaces with porphyrins is achieved via site selective linker groups and a specific metal center in the macrocycle. Metal oxide surfaces like MgO(001) have got a rather inert pristine surface and reactive low coordinated sites such as steps and kink-sites. Recently the metallization of H2TPP with Mg via low coordinated sites on MgO(001) has been demonstrated. The underlying mechanisms, however, remain unclear. Here we address this issue. We study the adsorption of H2TPP on MgO(001) and its interaction with low coordinated sites employing ab initio molecular dynamics simulations. We find that H2TPP is mobile on the surface due to steric hindrance from phenyl rings preventing physisorption of the macrocycle, until a step or kink site is encountered. Upon encountering such a site, H2TPP anchors itself to form a rather stable complex, and spontaneously deprotonates from the macrocycle. We discuss the electronic and structural properties of the adsorbate complex, the intermediate and the metallized porphyrins using (hybrid) TDDFT and many body perturbation theory, identifying various effects that can be used to uniquely identify presence of such complexes.

**12:39PM B47.00008 Molecular lifting, twisting, and curling during metal-assisted polycyclic hydrocarbon dehydrogenation.**, DAVIDE CURCIO, LUCA OMICIUOLO, Univ of Trieste - Trieste, Italy, MONICA POZZO, London Centre for Nanotechnology, University College London, UK, PAOLO LACOVIG, SILVANO LIZZIT, Elettra-Sincrotrone Trieste S.C.p.A., Trieste, Italy, NAILA JABEEN, Univ of Trieste - Trieste, Italy, LUCA PETACCIA, Elettra-Sincrotrone Trieste S.C.p.A., Trieste, Italy, DARIO ALFE, London Centre for Nanotechnology, University College London, UK, ALESSANDRO BARALDI, Univ of Trieste - Trieste, Italy — Through a combined experimental and theoretical approach, we show that coronene molecules adsorbed on Ir(111) undergo major changes in conformation during the dissociation process, which brings the molecules from a flat configuration to graphene, through a series of exotic configurations. The complex reaction path involves the tilting upwards of the molecules, which subsequently experience a rotation with respect to the surface. During the lifting, the C-C strain is initially relieved, while as the dehydrogenation proceeds, the molecules experience a progressive increase in the average interatomic distance, and gradually settle to form peculiar dome shaped nanographenes. This reaction mechanism can provide new insight into the surface assisted break-up mechanism of PAHs, which has been demonstrated to be an effective strategy for the synthesis of low dimensional carbon-based materials. Beside the peculiarity of the reaction pathway, using these processes we envisage the unique possibility of creating new structures with different functionalities by encapsulating single atoms below the carbon dome.

**12:51PM B47.00009 Predictive Modeling of Metal-Organic Chains with Active Metal Site**, NASEEM UD DIN, DUY LE, TALAT RAHMAN, Univ of Central Florida — Creation, stabilization, characterization and control of single atom transition metal (TM) sites may lead to significant advancement of the next-generation catalyst. Motivated by the experimental results of Skomski et al. [1], we have performed density functional theory based calculations of TM-dipyridyltetrazine (DT) chains in which TM atoms are stabilized and separated by the DT molecules. Our calculations show that the formation energies of the chains are high, suggesting that these chains can easily be synthesized and stabilized. Moreover, by calculating the adsorption energies of CO, O<sub>2</sub> and O atom on the metal atom sites of the chains we found that these molecules/atoms strongly bond to TM atoms Mo, Cr, Fe and Co occupying these sites, suggesting that these TM-DT chains are potential candidates for CO oxidation catalyst. Details of reaction pathway (energetic and kinetic) of CO oxidation on the chains will be also presented and discussed. [1] D. Skomski, C.D. Tempas, K.A. Smith, and S.L. Tait, "Redox-Active On-Surface Assembly of Organic Chains with Single-Site Pt(II)," *Journal of the American Chemical Society* **136**, 9862-9865 (2014).

**1:03PM B47.00010 The impact of functional group on the electronic structure of coordination center<sup>1</sup>**, ZAHRA HOOSHMAND GHAREHBAGH, DUY L, TALAT S RAHMAN, University of Central Florida — While 9, 10 dicyano-anthracene (DCA) forms a coordination network on Cu(111) surface with Cu adatom coordinated by three DCA molecules [1], its isomers, 9,10-diisocyno-anthracene forms, surprisingly, molecular rows on the same surface [2]. To understand the impact of functional groups on the electronic structure of the coordination center, we have carried out density functional theory based calculations of the electronic structure of a set of naphthalene molecules with different functional groups (N, CN, NC, NH<sub>2</sub>, COH, COOH) adsorbed on Cu(111), with and without a Cu adatom. Our results show that while the interaction between the naphthalene backbone and the Cu(111) surface is dominated by van der Waals (vdW) forces, in all cases considered the functional group forms a covalent bond with the Cu (ad)atom (on) of the surface. The calculated differential charge redistribution shows that the strongest covalent bond is formed by the NC group, which differs remarkably from that formed by the CN group, while the vdW interaction is very similar in both cases. These results provide insights into the different surface coordination behavior of molecules with above-mentioned functional groups. 1. Pawin, G., et al., *A Surface Coordination Network Based on Substrate-Derived Metal Adatoms with Local Charge Excess*. *Angewandte Chemie International Edition*, 2008. 47(44): p. 8442-8445. 2. L. Bartels, Private communication.

<sup>1</sup>Work support in part by NSF Grant CHE-1310327

**1:15PM B47.00011 Spin-Polarized Hybridization at the interface between different 8-hydroxyquinolates and the Cr(001) surface**, JINGYING WANG, ANDREW DELOACH, DANIEL B DOUGHERTY, Department of Physics, North Carolina State University, DOUGHERTY LAB TEAM — Organic materials attract a lot of attention due to their promising applications in spin-tronic devices. It is realized that spin-polarized metal/organic interfacial hybridization plays an important role to improve efficiency of organic spintronic devices. Hybridized interfacial states help to increase spin injection at the interface. Here we report spin-resolved STM measurements of single tris(8-hydroxyquinolinato) aluminum molecules adsorbed on the antiferromagnetic Cr(001). Our observations show a spin-polarized interface state between Alq3 and Cr(001). Tris(8-hydroxyquinolinato) chromium has also been studied and compared with Alq3, which exhibits different spin-polarized hybridization with the Cr(001) surface state than Alq3. We attribute the differences to different character of molecular orbitals in the two different quinolates.

**1:27PM B47.00012 Adsorption of thiophene on Pt, Pd, Au, and Rh(100) surfaces with the role of the van der Waals' interaction**, WALTER MALONE, JERONIMO MATOS, ABDELKADER KARA, University of Central Florida — We explore the adsorption of thiophene (C<sub>4</sub>H<sub>4</sub>S) on Pt(100), Au(100), Pd(100), and Rh(100) surfaces using density functional theory with and without self-consistent van der Waals interactions (vdWs). The six functionals we use are PBE, optB86b-vdW, optB88-vdW, optPBE-vdW, revPBE-vdW, and rPW86-vdW2. We examine a variety of adsorption sites with the molecule's plane both parallel and perpendicular to the surface. In the case of parallel adsorption the highest binding energy occurs when the molecule is centered over a hollow site with the sulfur atom near an atop site. The highest adsorption energy for perpendicular configurations is achieved when the sulfur atom lies over a bridge site and the carbon atoms near hollow sites. We find that for thiophene on the coinage metals the vdW functionals predict higher adsorption energies than those predicted by the PBE functional. On the other hand, for thiophene on the reactive transition metal substrates only optB86b-vdW, optB88-vdW, and optPBE-vdW result in an enhancement in the adsorption energy over the PBE value. We also explore some of the electronic properties of the system including charge transfer and change in the work function. Our results indicate that adsorption characteristics depends heavily on the functional used and geometry.

**1:39PM B47.00013 Manipulating the dipole layer of polar organic molecules on metal surfaces via different charge-transfer channels**, MENG-KAI LIN, Natl Tsing Hua Univ, YASUO NAKAYAMA, Department of Pure and Applied Chemistry, Tokyo University of Science, YING-JIE ZHUANG, CHIN-YUNG WANG, Natl Tsing Hua Univ, TUN-WEN PI, National Synchrotron Radiation Research Center (NSRRC), HISAO ISHII, Graduate School of Advanced Integration Science, Chiba University, S.-J. TANG, Natl Tsing Hua Univ — The key properties of organic films such as energy level alignment (ELA), work functions, and injection barriers are closely linked to this dipole layer. Using angle resolved photoemission spectroscopy (ARPES), we systemically investigate the coverage-dependent work functions and spectra line shapes of occupied molecular orbital states of a polar molecule, chloroaluminum phthalocyanine (CIAIPc), grown on Ag(111) to show that the orientations of the first CIAIPc layer can be manipulated via the molecule deposition rate and post annealing, causing ELA at organic-metal interface to differ for about 0.3 eV between Cl-up and Cl-down configuration. Moreover, by comparing the experimental results with the calculations based on both gas-phase model and realistic model of CIAIPc on Ag(111), we evidence that the different orientations of CIAIPc dipole layers lead to different charge-transfer channels between CIAIPc and Ag, a key factor that controls the ELA at organic-metal interface.

**1:51PM B47.00014 Coulomb blockade and charge ordering in a few layers of TTF-TCNQ investigated by low-temperature STM/STS<sup>1</sup>**, SEOKMIN JEON, PETRO MAKSYMOWYCH, Oak Ridge National Laboratory — In contrast to the vast effort on bulk crystal phases of the prototypical organic charge-transfer complex, TTF-TCNQ, study of low-dimensional phases has been limited to monolayer phases on substrates. In this state, however, none of the physics of the bulk phase is observed owing to the overwhelming effect of the substrate. We investigate the molecular structure and electronic properties of a few layers of TTF-TCNQ grown on Au(111) and Ag(111) using STM/STS at 4.3 K. By decoupling the molecular electronic state from the metal surface, we have made the first observation of the effect of confinement on the electronic properties of TTF-TCNQ. STS reveals a plethora of sharp features due to molecular orbitals, each influenced by charge-transfer between the molecules. We hypothesize the existence of a Mott-insulator state in 3-layer islands, with a Coulomb gap of ~1 eV. In contrast, the corresponding bulk phase is a Peierls insulator with a gap of ~20 meV. The root cause of the nanoscale phase is traced to simultaneous electron confinement and structural frustration, which dramatically modify the energy balance of self-ionization allowing for integer charge transfer. These studies open broad opportunities to explore correlated electron physics in molecular systems.

<sup>1</sup>This research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

**2:03PM B47.00015 The evolution of phases and electronic states in potassium doped coronene film<sup>1</sup>**, CHAOQIANG XU, XUDONG XIAO, Department of Physics, The Chinese University of Hong Kong, Shatin, Hong Kong, China — Alkali-metal-doped hydrocarbon materials have been found to exhibit improved superconductivity transition temperature  $T_c$  relative to the traditional organic superconductors. However, theoretical attempts to understand the superconductivity mechanism in this class of materials are still hindered by the limited experimental information available. In our study, we employed scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) to detect both the structures and the electronic properties of the doped hydrocarbon films at molecular scale. By gradually increasing potassium doping level, the evolution of structures and electronic properties in potassium doped coronene film was then investigated. Particularly, a splitting of the lowest unoccupied molecular orbital (LUMO) state was observed when the LUMO was brought to the Fermi level, giving direct evidence of electronic correlation effect in this system. Our results should contribute to a better understanding of the interaction between coronene molecules and potassium atoms and may shed some light to understand the superconductivity properties of this system.

<sup>1</sup>Research Grants Council of Hong Kong (Grant No. 404613)

**Monday, March 14, 2016 11:15AM - 2:03PM –**  
**Session B48 GQI: Quantum Optics with Superconducting Circuits** 349 - Irfan Siddiqi, University of California, Berkeley

**11:15AM B48.00001 Electromagnetically induced transparency in a tunable three-dimensional transmon<sup>1</sup>**, TIEFU LI, QICHUN LIU, Institute of Microelectronics, Tsinghua University, XIAOQING LUO, Beijing Computational Science Research Center, HU ZHAO, Institute of Microelectronics, Tsinghua University, WEI XIONG, ZHEN CHEN, Beijing Computational Science Research Center, YINGSHAN ZHANG, J. S. LIU, WEI CHEN, Institute of Microelectronics, Tsinghua University, FRANCO NORI, Center for Emergent Matter Science (CEMS), RIKEN, J. S. TSAI, Department of Physics, Tokyo University of Science, J. Q. YOU, Beijing Computational Science Research Center — Electromagnetically induced transparency (EIT) has been realized in atomic systems, but fulfilling the EIT conditions for artificial atoms made from superconducting circuits is a more difficult task. Here we report an experimental observation of the EIT in a tunable three-dimensional transmon by probing the cavity transmission. We tune the transmon to adjust its damping rates to fulfill the EIT conditions. From the experimental observations, we clearly identify the EIT and Autler-Townes splitting (ATS) regimes as well as the transition regime in between. Also, the experimental data demonstrate that the threshold  $\Omega_{AIC}$  determined by the Akaike information criterion can describe the EIT-ATS transition better than the threshold  $\Omega_{EIT}$  given by the EIT theory.

<sup>1</sup>This work is supported by the NSAF Grant No. U1330201, the NSFC Grant No. 91421102, and the MOST 973 Program Grant Nos. 2014CB848700 and 2014CB921401.

**11:27AM B48.00002 Resonance fluorescence from an artificial atom in squeezed vacuum, Part 1: Efficient fluorescence detection<sup>1</sup>**, A. EDDINS, D.M. TOYLI, Quantum Nanoelectronics Laboratory, UC Berkeley, S. PURI, S. BOUTIN, Departement de Physique, Université de Sherbrooke, D. HOVER, V. BOLKHOVSKY, MIT Lincoln Laboratory, W.D. OLIVER, MIT Lincoln Laboratory and Research Laboratory of Electronics, Massachusetts Institute of Technology, A. BLAIS, Departement de Physique, Université de Sherbrooke, I. SIDDIQI, Quantum Nanoelectronics Laboratory, UC Berkeley — The accurate prediction of the fluorescence spectrum of a single atom under coherent excitation, comprising canonical phenomena such as the Mollow triplet, is a fundamental success of quantum optics. Despite considerable efforts, experiments demonstrating a strong modification to the resonance fluorescence spectrum resulting from driving an atomic system with non-classical squeezed light have remained elusive, in part due to challenges in efficient coupling. In this talk, we discuss how we strongly couple microwave-frequency squeezed light to a superconducting artificial atom and detect the resulting fluorescence using a Josephson traveling-wave parametric amplifier (JTWPA). Whereas alternative detection techniques require extensive experimental hardware and long averaging times to resolve fluorescence, the large dynamic range and GHz bandwidth of the JTWPA facilitate direct detection of the Mollow triplet with a spectrum analyzer in minutes, enabling a systematic study with respect to the properties of squeezed vacuum.

<sup>1</sup>This work is funded by the ARO and ONR.

**11:39AM B48.00003 Resonance fluorescence from an artificial atom in squeezed vacuum, Part 2: Squeezing characterization through fluorescence<sup>1</sup>**, D.M. TOYLI, A. EDDINS, Quantum Nanoelectronics Laboratory, UC Berkeley, S. PURI, S. BOUTIN, Departement de Physique, Université de Sherbrooke, D. HOVER, V. BOLKHOVSKY, MIT Lincoln Laboratory, W.D. OLIVER, MIT Lincoln Laboratory and Research Laboratory of Electronics, Massachusetts Institute of Technology, A. BLAIS, Departement de Physique, Université de Sherbrooke, I. SIDDIQI, Quantum Nanoelectronics Laboratory, UC Berkeley — The accurate prediction of the fluorescence spectrum of a single atom under coherent excitation, comprising canonical phenomena such as the Mollow triplet, is a fundamental success of quantum optics. Despite considerable efforts, experiments demonstrating a strong modification to the resonance fluorescence spectrum resulting from driving an atomic system with non-classical squeezed light have remained elusive, in part due to challenges in efficient coupling. In this second of two talks, we discuss observations of the dramatic dependence of the Mollow triplet spectrum on the phase of the squeezed vacuum environment and measurements of subnatural fluorescence linewidths that demonstrate up to 3.5 dB of squeezing below the standard vacuum limit. In addition to realizing two seminal predictions for resonance fluorescence in squeezed vacuum, our work provides simple and robust metrological tools for characterizing squeezed light at microwave frequencies.

<sup>1</sup>This work is funded by the ARO and ONR.

**11:51AM B48.00004 Stochastic path integral approach to continuous quadrature measurement of a single fluorescing qubit<sup>1</sup>**, ANDREW N. JORDAN, AREEYA CHANTASRI, University of Rochester, BENJAMIN HUARD, École Normale Supérieure-PSL Research University — I will present a theory of continuous quantum measurement for a superconducting qubit undergoing fluorescent energy relaxation. The fluorescence of the qubit is detected via a phase-preserving heterodyne measurement, giving the cavity mode quadrature signals as two continuous qubit readout results. By using the stochastic path integral approach to the measurement physics, we obtain the most likely fluorescence paths between chosen boundary conditions on the state, and compute approximate correlation functions between all stochastic variables via diagrammatic perturbation theory. Of particular interest are most-likely paths describing increasing energy during the fluorescence. Comparison to Monte Carlo numerical simulation and experiment will be discussed.

<sup>1</sup>This work was supported by US Army Research Office Grants No. W911NF-09-0-01417 and No. W911NF-15-1-0496, by NSF grant DMR-1506081, by John Templeton Foundation grant ID 58558, and by the DPSTT Project Thailand

**12:03PM B48.00005 Two-mode squeezing in a broadband parametric amplifier** , J. A. GROVER, A. KAMAL, S. GUSTAVSSON, F. YAN, T. P. ORLANDO, W. D. OLIVER, Research Laboratory of Electronics, MIT, D. HOVER, V. BOLKHOVSKY, J. L. YODER, MIT Lincoln Laboratory, C. MACKLIN, K. O'BRIEN, I. SIDDIQI, University of California Berkeley — The Josephson traveling wave parametric amplifier (JTWPA) exhibits gains of greater than 20 dB over a frequency range of a few gigahertz. In addition to being a quantum-limited amplifier over a wide frequency range, the JTWPA is a source of broadband squeezed radiation. We report the observation of broadband squeezing of microwave light generated by a JTWPA by measuring cross correlations between modes separated by up to one gigahertz in frequency. Employing a chain of two JTWPAs, the first as a squeezer and the second as a quantum-limited preamplifier, ensures a high-efficiency measurement of squeezing. We also discuss progress towards employing such two-mode squeezed radiation to realize high-fidelity dispersive readout of superconducting qubits.

This research was funded in part by the U.S. Army Research Office Grant No. W911NF-14-1-0682 and by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA) and by the Assistant Secretary of Defense for Research & Engineering via MIT Lincoln Laboratory under Air Force Contract No. FA8721-05-C-0002.

**12:15PM B48.00006 Displacement of squeezed propagating microwave states** , KIRILL G. FEDOROV, LING ZHONG, STEFAN POGORZALEK, PETER EDER, MICHAEL FISCHER, JAN GOETZ, FRIEDRICH WULSCHNER, EDWARD XIE, EDWIN MENZEL, FRANK DEPPE, ACHIM MARX, RUDOLF GROSS, Walther-Meißner-Institut; Technische Universität München; Nanosystems Initiative Munich — Displacement of propagating squeezed states is a fundamental operation for quantum communications. It can be applied to fundamental studies of macroscopic quantum coherence and has an important role in quantum teleportation protocols with propagating microwaves. We generate propagating squeezed states using a Josephson parametric amplifier and implement displacement using a cryogenic directional coupler. We study single- and two-mode displacement regimes. For the single-mode displacement we find that the squeezing level of the displaced squeezed state does not depend on the displacement amplitude. Also, we observe that quantum entanglement between two spatially separated channels stays constant across 4 orders of displacement power. We acknowledge support by the German Research Foundation through SFB 631 and FE 1564/1-1, the EU project PROMISCE, and Elite Network of Bavaria through the program ExQM.

**12:27PM B48.00007 Engineering Non-Classical Light with Non-Linear Microwaveguides** , ARNE GRIMSMO, Univ of Sherbrooke, AASHISH CLERK, McGill University, ALEXANDRE BLAIS, Univ of Sherbrooke — The quest for ever increasing fidelity and scalability in measurement of superconducting qubits to be used for fault-tolerant quantum computing has recently led to the development of near quantum-limited broadband phase preserving amplifiers in the microwave regime. These devices are, however, more than just amplifiers: They are sources of high-quality, broadband two-mode squeezed light. We show how bottom-up engineering of Josephson junction embedded waveguides can be used to *design* novel squeezing spectra. Furthermore, the entanglement in the two-mode squeezed output field can be imprinted onto quantum systems coupled to the device's output. These broadband microwave amplifiers constitute a realization of non-linear waveguide QED, a very interesting playground for non-equilibrium many-body physics.

**12:39PM B48.00008 Topological quantum states of light in coupled microwave cavities** , RUICHAO MA, JOHN C. OWEN, AMAN LACHAPPELLE, TAEKWAN YOON, DAVID SCHUSTER, JONATHAN SIMON, University of Chicago — We present a unique photonic platform to explore quantum many-body phenomena in coupled cavity arrays. We create tight binding lattices with arrays of evanescently coupled three-dimensional coaxial microwave cavities. Topologically non-trivial band structures are engineered by utilizing the chiral coupling of the cavity modes to ferrite spheres in a magnetic field. We develop robust, minimal methods to completely characterize the tight-binding Hamiltonian, including all onsite disorder, tunnel coupling, local dissipation and effective flux, using only spectroscopic measurement on specific sites. These efforts pave the way to realize low-disorder, long-coherence, topological tight binding models, where the many-body states can be spectroscopically driven and probed in temporally- and spatially- resolved measurements. Using techniques from circuit QED, effective onsite photon-photon interactions may be introduced by coupling to superconducting qubits. This will allow us to explore the interplay between topology and coherent interaction in these artificial strongly-correlated photonic quantum materials.

**12:51PM B48.00009 Quantum optics with nonlinearly coupled superconducting resonators** , VADIRAJ A.M., C.W.S. CHANG, POL FERNANDEZ-DIAZ, C.M. WILSON, Institute for Quantum Computing, University of Waterloo, Waterloo, Canada — Superconducting circuits provide a robust platform for studying fundamental aspects of light-matter interaction in the circuit QED architecture. Here, we study a novel circuit that couples two superconducting resonators via a nonlinear interaction mediated by a superconducting quantum interference device (SQUID). The interaction hamiltonian has a form analogous to optomechanical systems with the photon number in one resonator coupling to the current in the other. However, the nonlinear coupling constant can be many orders of magnitude larger than in typical optomechanical systems. This can potentially bring the system into a new regime of single-photon coupling between the resonators, enabling novel physics. We will present preliminary results in this direction.

**1:03PM B48.00010 Experimental investigation of a steady-state dynamical phase transition in a Jaynes-Cummings dimer** , JAMES RAFTERY, DARIUS SADRI<sup>1</sup>, Princeton University, STEPHAN MANDT, Columbia University, HAKAN TÜRECİ, ANDREW HOUCK, Princeton University — Experimental progress in circuit-QED has made it possible to study non-equilibrium many-body physics using strongly correlated photons. Such open and driven systems can display new types of dynamical phase transitions [1]. A steady state transition has also been predicted for a Jaynes-Cummings dimer where the photon current between the two cavities acts as an order parameter [2]. Here, we discuss the theory and report measurements of the steady-state behavior of a circuit-QED dimer with in situ tunable inter-cavity coupling and on-site photon-photon interaction. [1] J. Raftery, D. Sadri, S. Schmidt, H. E. Türeci, and A. A. Houck, Phys. Rev. X 4, 031043 (2014). [2] S. Mandt, D. Sadri, A. A. Houck, and H. E. Türeci, New J. Phys. 17 (2015) 053018.

<sup>1</sup>Recently deceased

**1:15PM B48.00011 Fock-state stabilization in superconducting circuits using biased Josephson junctions** , JEAN-RENE SOUQUET, AASHISH CLERK, McGill Univ — The ability to prepare and stabilize non-trivial states is a crucial ingredient for quantum information processing. Here, we analyze theoretically a simple scheme for stabilizing Fock states in a superconducting circuit using the nonlinearity inherent in a voltage-biased Josephson junction. Unlike a recent demonstration of Fock state stabilization [1], our protocol does not require any microwave driving. We also discuss how the same system can be used to generate propagating single-photon states with high fidelity, again without the use of microwave drives or pulses.

[1] E. T. Holland, B. Vlastakis, R. W. Heeres, M. J. Reagor, U. Vool, Z. Leghtas, L. Frunzio, G. Kirchmair, M. H. Devoret, M. Mirrahimi, R. J. Schoelkopf. Phys. Rev. Lett. 115, 180501 (2015).

**1:27PM B48.00012 Steady-state response of coupled non-linear superconducting quantum oscillators** , MATTHEW ELLIOTT, ERAN GINOSSAR, Advanced Technology Institute, University of Surrey — Analytic solutions of non-linear, dissipative quantum systems can provide access to parameter regimes where numerical simulation is unfeasible. In particular, they are useful when these systems are driven at high powers but influenced by quantum fluctuations. We find exact solutions of a Fokker-Planck equation from which we derive the response characteristics of coupled linear and non-linear oscillators under the influence of both coherent and parametric driving. By working in an experimentally feasible parameter regime for superconducting quantum circuits, we model a realistic driven cavity-transmon system and obtain the steady-state frequency response of both cavity and transmon at a range of drive powers, comparing our results with recent experimental data. We show that this method can also be extended to investigate the behaviour of a resonator with a quartic non-linearity which is driven coherently and parametrically, revealing the structure of bifurcations in the steady-state solutions.

**1:39PM B48.00013 Dressed-state engineering for continuous detection of itinerant microwave photons** , KAZUKI KOSHINO, Tokyo Medical and Dental University, ZHIRONG LIN, KUNIHITO INOMATA, RIKEN Center for Emergent Matter Science, TSUYOSHI YAMAMOTO, NEC Smart Energy Research Laboratories, YASUNOBU NAKAMURA, University of Tokyo — Microwave quantum optics using superconducting qubits and transmission lines enables various quantum-optical phenomena that have not been reached in the visible light domain. However, the lack of an efficient detector for itinerant microwave photons has been a long-standing problem. A promising approach is to use the deterministic switching of a  $\Lambda$  system induced by individual photons. Recently, we realized a  $\Lambda$  system by the dressed-state engineering of a qubit-resonator system and achieved a detection efficiency  $\sim 66\%$ . However, this detector should be operated in the time-gated mode, since the drive field to generate the  $\Lambda$ -type transition must be turned off during the qubit readout. Here, we propose a scheme for continuous detection of itinerant microwave photons. In the proposed device, a superconducting qubit is coupled dispersively to two resonators: one is used to form a  $\Lambda$  system that deterministically captures incoming photons and the other is used for continuous monitoring of the event. The proposed device enables continuous operation of the photon detector, preserving the advantages of our previous scheme, such as a high detection efficiency, insensitivity to the signal pulse shape, and short dead times after detection.

**1:51PM B48.00014 Observation of quantum-limited heat conduction over macroscopic distances<sup>1</sup>** , MIKKO MOTTONEN, MATTI PARTANEN, KUAN YEN TAN, JOONAS GOVENIUS, RUSSELL LAKE, MIIKA MAKELA, TUOMO TANTTU, QCD Labs, Department of Applied Physics, Aalto University, Finland — The emerging quantum technological devices, such as the quantum computer, call for extreme performance in thermal engineering at the nanoscale. Importantly, quantum mechanics sets a fundamental upper limit for the flow of information and heat, which is quantified by the quantum of thermal conductance. We present experimental observations of quantum-limited heat conduction over macroscopic distances extending to a meter. We achieved this striking improvement of four orders of magnitude in the distance by utilizing microwave photons travelling in superconducting transmission lines. Thus it seems that quantum-limited heat conduction has no fundamental restriction in its distance. This work lays the foundation for the integration of normal-metal components into superconducting transmission lines, and hence provides an important tool for circuit quantum electrodynamics, the basis of the emerging superconducting quantum computer. In particular, our results may lead to remote cooling of nanoelectronic devices with the help of a far-away in-situ-tunable heat sink.

<sup>1</sup>European Research Council (ERC) is acknowledged for funding under the grant no. 278117 (SINGLEOUT)

**Monday, March 14, 2016 11:15AM - 2:15PM –**  
**Session B50 DAMOP: Driven and Dissipative Atomic Systems** Hilton Baltimore Holiday Ballroom 1 - Ryan Wilson, Joint Quantum Institute, University of Maryland

**11:15AM B50.00001 Self-organization of atoms coupled to a chiral reservoir** , ZACHARY ELDREDGE, Univ of Maryland-College Park, DARRICK CHANG, ICFO, Barcelona, ALEXEY GORSHKOV, Univ of Maryland-College Park — Recently, there has been increasing interest in the properties of confined light in the vicinity of tapered optical nanofibers. Interesting avenues have been suggested concerning cold atoms trapped on the fiber by evanescent light fields. It has been shown that the interaction between atoms coupled to this one-dimensional reservoir leads to equations of motion possessing self-organized stable solutions which exhibit striking many-body dynamics. Finally, it has also been observed that spin-orbit coupling due to the extreme confinement of the light leads to a directionality in the coupling to the fiber. In this paper we explore the implications of a chiral interaction on self-organization and show that the overall configuration exhibits similar behavior to the symmetric case but undergoes dramatic changes in some regions of parameter space. We also present proposals for experimental realizations of our model as well as signatures of chiral behavior.

**11:27AM B50.00002 Novel Infrared Dynamics of Cold Atoms on Hot Graphene** , SANGHITA SENGUPTA, VALERI KOTOV, DENNIS CLOUGHERTY, Univ of Vermont — The low-energy dynamics of cold atoms interacting with macroscopic graphene membranes exhibits severe infrared divergences when treated perturbatively. These infrared problems are even more pronounced at finite temperature due to the (infinitely) many flexural phonons excited in graphene. We have devised a technique to take account (resummation) of such processes in the spirit of the well-known exact solution of the independent boson model. Remarkably, there is also similarity to the infrared problems and their treatment (via the Bloch-Nordsieck scheme) in finite temperature “hot” quantum electrodynamics and chromodynamics due to the long-range, unscreened nature of gauge interactions. The method takes into account correctly the strong damping provided by the many emitted phonons at finite temperature. In our case, the inverse membrane size plays the role of an effective low-energy scale, and, unlike the above mentioned field theories, there remains an unusual, highly nontrivial dependence on that scale due to the 2D nature of the problem. We present detailed results for the sticking (atomic damping rate) rate of cold atomic hydrogen as a function of the membrane temperature and size. We find that the rate is very strongly dependent on both quantities.

**11:39AM B50.00003 Periodically driven system coupled to a fermionic bath: A Keldysh approach** , DONG E. LIU, Microsoft Research Station Q, ALEX LEVCHENKO, Department of Physics, University of Wisconsin-Madison, ROMAN M. LUTCHYN, Microsoft Research Station Q — We develop a Keldysh approach to study a time-periodically driven system with dissipation. We apply this approach to a periodically driven metallic system coupled to a normal metal and a superconducting bath. After integrating out the fermionic bath degrees of freedom and incorporating its effects exactly through self-energy, we find non-equilibrium Green functions for the driven system which take into account effect of the bath. Our formalism allows one to evaluate non-equilibrium distribution function for particles in the periodically-driven system as well as other observable quantities (e.g. tunneling density of states). In the case of a superconducting bath, we study interplay of the proximity-induced superconducting pairing correlations and the dissipation due to light-excited quasiparticles.

**11:51AM B50.00004 Two coupled nonlinear cavities in a driven-dissipative environment** , BIN CAO, KHAN MAHMUD, MOHAMMAD HAFEZI, Joint Quantum Institute, Univ of Maryland-College Park — We investigate two coupled nonlinear cavities that are driven coherently in a dissipative environment. This is the simplest setting containing a good number of features of an array of coupled cavity quantum simulator with Kerr nonlinearity which gives rise to many strongly correlated phases. We find analytical solution for the steady state using the generalized P representation and expressing the master equation in the form of Fokker-Planck equation. A comparison shows a good match of the analytical and numerical solutions across different regimes. We investigate the quantum correlations in the steady state by solving the full master equation numerically, analyzing its second-order coherence, entanglement entropy and Liouvillian gap as a function of drive and detuning. This gives us insights into the nature of bistability and how the tunneling-induced bistability emerges in coupled cavities when going beyond a single cavity. We can understand much of the semiclassical physics in terms of the underlying phase space dynamics of a driven and damped classical pendulum. Furthermore, in the semiclassical analysis, we find steady state solutions with different number density in the two wells that can be considered an analog of double well self-trapped states.

## 12:03PM B50.00005 Non-equilibrium Steady-State Behavior in a Scale-Free Quantum Network

, JIANSHI ZHAO, CRAIG PRICE, QI LIU, NATHAN GEMELKE, The Pennsylvania State University — We describe the nonequilibrium dynamics of a cold atomic gas held in a spatially random optical potential and gravity, subject to a controlled amount of dissipation in the form of an extremely slow dark-state laser cooling process. Reaching local kinetic temperatures below the 100nK scale, such systems provide a novel context for observing the non-equilibrium steady-state (NESS) behavior of a disordered quantum system. For sufficiently deep potentials and strong dissipation, this system can be modeled by a self-organized version of directed percolation, and exhibits power-law decay of phase-space density with time due to the presence of absorbing clusters with a wide distribution of entropy and coupling rates. In the absence of dissipation, such a model cannot apply, and we observe the crossover to exponential loss of phase-space density. We provide measurements of the power-law decay constant by observing the non-equilibrium motion of atoms over a ten-minute period, consistent with  $\gamma = 0.31 \pm 0.04$ , and extract scaling of the absorbed number with dissipation rate, showing another power-law behavior, with exponent  $0.5 \pm 0.2$  over two decades of optical excitation probability.

## 12:15PM B50.00006 Steady States in Fermionic Interacting Dissipative Floquet Systems

, KARTHIK SEETHARAM, CHARLES BARDYN, Caltech, NETANEL LINDNER, Technion, MARK RUDNER, University of Copenhagen, GIL REFAEL, Caltech — The possibility to drive quantum systems periodically in time offers unique ways to deeply modify their fundamental properties, as exemplified by Floquet topological insulators. It also opens the door to a variety of non-equilibrium effects. Resonant driving fields, in particular, lead to excitations which can expose the system to heating. We previously demonstrated that the analog of thermal states can be achieved and controlled in a fermionic Floquet system in the presence of phonon scattering, spontaneous emission, and an energy filtered fermionic bath. However, interactions play an important role in thermalization and present additional sources of heating. We analyze the effects of weak interactions in the presence of dissipation and the role of coherences in determining the steady state of the driven system. Interactions generically create additional excitations and, in contrast to phonons, may sustain inter-Floquet-band coherences at steady state.

## 12:27PM B50.00007 How should we understand non-equilibrium many-body steady states?

, MOHAMMAD MAGHREBI, ALEXEY GORSHKOV, University of Maryland — : Many-body systems with both coherent dynamics and dissipation constitute a rich class of models which are nevertheless much less explored than their dissipationless counterparts. The advent of numerous experimental platforms that simulate such dynamics poses an immediate challenge to systematically understand and classify these models. In particular, nontrivial many-body states emerge as steady states under non-equilibrium dynamics. In this talk, I use a field-theoretic approach based on the Keldysh formalism to study nonequilibrium phases and phase transitions in such models. I show that an effective temperature generically emerges as a result of dissipation, and the universal behavior including the dynamics near the steady state is described by a thermodynamic universality class. In the end, I will also discuss possibilities that go beyond the paradigm of an effective thermodynamic behavior.

## 12:39PM B50.00008 Dissipation induced topological insulators: A recipe

, MOSHE GOLDSTEIN, Tel Aviv University, Israel — It has recently been realized that driven-dissipative dynamics, which usually tends to destroy subtle quantum interference and correlation effects, could actually be used as a resource. By proper engineering of the reservoirs and their couplings, one may drive a system towards a desired quantum-correlated steady state, even in the absence of internal Hamiltonian dynamics. An intriguing class of quantum phases is characterized by topology, including the quantum Hall effect and topological insulators and superconductors. Which of these noninteracting topological states can be achieved as the result of purely dissipative Lindblad-type dynamics? Recent studies have only provided partial answers to this question. In this talk I will present a general recipe for the creation, classification, and detection of states of the integer quantum Hall and 2D topological insulator type as the outcomes of coupling a system to reservoirs, and show how the recipe can be realized with ultracold atoms and other quantum simulators. The mixed states so created can be made arbitrarily close to pure states, and the construction may be generalized to other topological phases.

## 12:51PM B50.00009 Engineering non-Hermitian optical potentials for Polariton Condensation

, SAEED KHAN, Department of Electrical Engineering, Princeton University, LI GE, Department of Engineering Science and Physics, College of Staten Island, CUNY, HAKAN TURECI, Department of Electrical Engineering, Princeton University — We present a theoretical study of incoherently pumped exciton-polariton condensates in general cavity geometries, based on an analysis of the linear non-Hermitian modes of the (optical) pump induced potential. An analytical description is obtained for how the threshold pump power for condensation into a specific mode depends quantitatively on the relative spatial profiles of that mode and the pump. Specifically, we show that for a general pump profile, modes which best organize to balance the amplification from the pump against the repulsive pump potential achieve the lowest threshold power [1]. Reversing this idea, choosing the spatial profile of the pump provides control over which spatial mode condenses at lowest power. Our work hence provides a scheme to engineer non-Hermitian optical potentials for preferential polariton condensation into a specific mode, by an appropriate choice of pump profile. This approach has recently been used to achieve condensation in the flat band of a Lieb chain of micropillar cavities, where the flat band has energy above the ground state and hence cannot be studied in systems in thermal equilibrium [2].

### References:

- [1] L. Ge, *et. al.*, arXiv: 1311.4847 (2013)
- [2] F. Baboux *et. al.*, arXiv: 1505.05652 (2015)

## 1:03PM B50.00010 Collective phases of strongly interacting cavity photons

, RYAN WILSON, United States Naval Academy, Annapolis, MD 21402, MICHAEL FOSS-FEIG, KHAN MAHMUD, MOHAMMAD HAFEZI, Joint Quantum Institute & Joint Center for Quantum Information and Computer Science, University of Maryland, College Park, MD 20742 — We study the steady state phases of the Bose-Hubbard model in the presence of dissipation and coherent driving, which in the limit of strong interactions maps onto a driven-dissipative XX spin- $\frac{1}{2}$  model with transverse and longitudinal fields. Using a site-decoupled mean-field approximation, we identify phases with antiferromagnetic and spin density wave order, in addition to limit cycle phases, where oscillatory dynamics persist indefinitely. We also identify collective bistable phases, where the system supports two steady states among spatially uniform, antiferromagnetic, and limit cycle phases. We compare these mean-field results to exact quantum trajectories for one dimensional cavity arrays. The quantum results exhibit short-range antiferromagnetic and spin density wave order, in good qualitative agreement with the mean-field predictions. In the bistable regime, this system exhibits real-time collective switching between macroscopically distinguishable states. We present a clear physical picture for these dynamics, and establish a simple relationship between the switching times and properties of the quantum Liouvillian.

## 1:15PM B50.00011 Driven-dissipative bosons in open boundary and inhomogeneous cavity arrays

, KHAN W. MAHMUD, University of Maryland, RYAN M. WILSON, United States Naval Academy, MICHAEL FOSS-FEIG, MOHAMMAD HAFEZI, University of Maryland — We study the driven-dissipative Bose-Hubbard model, which describes the physics of coherently pumped photonic cavity arrays as well as strongly interacting ultracold bosons in an optical lattice in a driven dissipative setting. We investigate many-body states and their quantum correlations on finite size lattices with open boundary conditions, a set up which is experimentally relevant. We show that the effects of hard boundaries on the steady-states are nontrivial, and explain the results in terms of finite system size excitations and the underlying phases of a thermodynamically large system. Furthermore, we explore the effects of trap inhomogeneity, such as an external harmonic trap, quantifying the breakdown of local density approximation for finite system size. We use a mixed state version of matrix product states algorithm for the numerical investigation.

**1:27PM B50.00012 Flying over decades**, JUDITH HOELLER, MENA ISSLER<sup>1</sup>, Graduate Student, ATAC IMAMOGLU, Professor — Levy flights have been extensively used in the past three decades to describe non-Brownian motion of particles. In this presentation I give an overview on how Levy flights have been used across several disciplines, ranging from biology to finance to physics. In our publication we describe how a single electron spin 'flies' when captured in quantum dot using the central spin model. At last I motivate the use of Levy flights for the description of anomalous diffusion in modern experiments, concretely to describe the lifetimes of quasi-particles in Josephson junctions.

<sup>1</sup>Finished PhD at ETH in Spring 2015

**1:39PM B50.00013 Multiple timescale analysis of dynamical evolution near two coalescing eigenvalues in open quantum systems**, SAVANNAH GARMON, Osaka Prefecture University, GONZALO ORDONEZ, Butler University — Recently the physics of coalescing eigenvalues at an exceptional point (EP) has been studied in a wide range of physical contexts, including open quantum systems. At an EP  $N$  at which  $N$  eigenvalues coalesce the Hamiltonian can no longer be diagonalized but instead only reduced to a Jordan block of dimension  $N$ . In order to describe the survival probability  $P(t)$  for an initially prepared state in the vicinity of two coalescing levels, we further subdivide the EP2 case into the EP2A and EP2B [1], where the EP2A involves the coalesce of two virtual bound states to form a resonance/anti-resonance pair and the EP2B occurs when two resonances collide to form two new resonances. We show that in the vicinity of the EP2B the usual exponential decay appearing for resonances on intermediate timescales is modified as  $P(t) \sim te^{-\Gamma t}$ . However, the long-time evolution near the EP2B follows a  $1/t^3$  power law decay. Meanwhile the evolution for the EP2A is non-exponential on all timescales, and may be strongly influenced by continuum threshold effects [2]. [1] S. Garmon, M. Gianfreda, and N. Hatano, Phys. Rev. A 92, 022125 (2015). [2] S. Garmon, T. Petrosky, L. Simine and D. Segal, Fortschr. Phys. 61, 261 (2013). [3] N. Hatano and G. Ordóñez, J. Math. Phys. 55, 122106 (2014).

**1:51PM B50.00014 Quantum Spontaneous Stochasticity**, THEODORE DRIVAS, GREGORY EYINK, The Johns Hopkins University — Classical Newtonian dynamics is expected to be deterministic, but recent fluid turbulence theory predicts that a particle advected at high Reynolds-numbers by "nearly rough" flows moves nondeterministically. Small stochastic perturbations to the flow velocity or to the initial data lead to persistent randomness, even in the limit where the perturbations vanish! Such "spontaneous stochasticity" has profound consequences for astrophysics, geophysics, and our daily lives. We show that a similar effect occurs with a quantum particle in a "nearly rough" force, for the semi-classical (large-mass) limit, where spreading of the wave-packet is usually expected to be negligible and dynamics to be deterministic Newtonian. Instead, there are non-zero probabilities to observe multiple, non-unique solutions of the classical equations. Although the quantum wave-function remains split, rapid phase oscillations prevent any coherent superposition of the branches. Classical spontaneous stochasticity has not yet been seen in controlled laboratory experiments of fluid turbulence, but the corresponding quantum effects may be observable by current techniques. We suggest possible experiments with neutral atomic-molecular systems in repulsive electric dipole potentials.

**2:03PM B50.00015 Current-carrying quasi-steady states in a periodically driven many-body system**, MARK RUDNER, Niels Bohr Institute, Copenhagen University, NETANEL LINDNER, Technion, EREZ BERG, Weizmann Institute — We investigate many-body dynamics in a one-dimensional interacting periodically driven system, based on a partially-filled version of Thouless topologically quantized adiabatic pump. The corresponding single particle Floquet bands are chiral, with the Floquet spectrum realizing nontrivial cycles around the quasienergy Brillouin zone. For non-integer filling the system is gapless; here the driving cannot be adiabatic and the system is expected to rapidly absorb energy from the driving field. We identify parameter regimes where scattering between Floquet bands of opposite chirality is exponentially suppressed, opening a long time window where the many-body evolution separately conserves the occupations of the two chiral bands. Within this intermediate time regime we predict that the system reaches a quasi-steady state with uniform crystal momentum occupation within each Floquet band. This state furthermore carries a non-vanishing current given directly by the difference of densities in the right and left moving chiral bands. This remarkable behavior, which holds for both bosons and fermions, may be readily studied experimentally in recently developed cold atom systems.

## Monday, March 14, 2016 11:15AM - 2:15PM —

Session B51 FIAP: Materials: Synthesis, Growth, and Processing Hilton Baltimore Holiday Ballroom 2 - Seunghun Lee, University of Maryland

**11:15AM B51.00001 The impact of neutral impurity concentration on charge drift mobility<sup>1</sup>**, HAO MEI, GUOJIAN WANG, DONGMING MEI, GANG YANG, YUTONG GUAN, Univ of South Dakota — High-purity germanium crystals are being grown using the Czochralski technique at the University of South Dakota. The carrier concentration, mobility and resistivity are measured by Hall Effect system. Many factors contribute to the overall mobility. We investigated the impact of neutral impurity concentration on charge drift mobility. Several samples with measured mobility larger than 35000 cm<sup>2</sup>/Vs from the grown crystals were used for this investigation. With the measured mobility and the ionized impurity concentration, we were able to calculate the neutral impurity concentration by the Matthiessen's rule. The correlations between the neutral impurity concentrations with the radius of the crystals were studied. We report that the concentration of neutral impurity constrains charge draft mobility for high-purity germanium crystals and the non-uniform distribution of neutral impurity could result in an anisotropy of draft time distribution in a given germanium detector.

<sup>1</sup>This work is supported by DOE grant DE-FG02-10ER46709 and the state of South Dakota.

**11:27AM B51.00002 Influences of solid/liquid boundary layer thickness and tilting angle on zone-refinement of germanium crystals**, GANG YANG, YUTONG GUAN, HAO MEI, GUOJIAN WANG, DONGMING MEI, University of South Dakota — In zone-refining of metals, solid/liquid (S/L) boundary layer thickness has an influence on segregation coefficient of impurity atoms. Additionally, the segregation of impurity elements during zone refining can be maximized by adjusting the zone refinement tube with a proper angle. In this paper, we report the influences of S/L boundary layer thickness on the segregation coefficients of boron, phosphor, aluminum and gallium, which have been identified as four main impurities in germanium crystal by Photothermal Ionization Spectroscopy (PTIS). The thickness of S/L boundary layer was found by using a well-known model to fit the experimental data. The optimized segregation coefficients have been used to calculate the impurity distribution along the purified ingot. In addition, we have also optimized the tilting angle of the germanium ingot to investigate the impact on the segregation. This work is supported by DOE grant DE-FG02-10ER46709 and the state of South Dakota.

**11:39AM B51.00003 The Electronic Properties of Nanoscale Meta-lattice Made by High Pressure CVD**, ZHAOHUI HUANG, VINCENT CRESPI, Pennsylvania State University — Meta-lattice can be defined as an artificial 3D superlattice with periodic structural modulation occurred at 10nm scale. One viable route to synthesize can be as follows: A template is first prepared by close-packed nanometer-sized silica spheres, then Si/Ge or a binary semiconductor is infiltrated into voids by high pressure chemical vapor deposition (CVD). Later silica spheres can be removed by chemical method, and voids in the inverse meta-lattice offer the opportunity for a second infiltration. Due to the characteristic length of voids, meta-lattice provides a platform to test novel mesoscopic electronic and thermal phenomena. A meta-lattice solid can show novel physical properties that each constituent infiltrate material does not have. Since a significant portion of atoms are located on the surface, the interface structure details are expected to play a critical role. Here we investigate Si/Ge inverse meta-lattices with or without silica template present. Tight-binding, DFT and GW/BSE techniques are employed to look into the electronic and optical properties.

**11:51AM B51.00004 Aluminum Nitride Grown by Atomic Layer Epitaxy Characterized with Real-Time Grazing Incidence Small Angle X-ray Scattering**, VIRGINIA ANDERSON, NEERAJ NEPAL, SCOOTER JOHNSON, US Naval Research Laboratory, ZACHARY ROBINSON, The College at Brockport, State University of New York, ALEXANDER DEMASI, Boston University, JENNIFER HITE, US Naval Research Laboratory, KARL LUDWIG, Boston University, CHARLES EDDY, US Naval Research Laboratory — Aluminum nitride, gallium nitride, and indium nitride are being considered for many applications, and are currently being used commercially for LEDs. These III-nitride films are conventionally deposited by metalorganic chemical vapor deposition and molecular beam epitaxy. Research into depositing III-nitrides with atomic layer epitaxy (ALE) is underway as it is a fabrication friendly technique for thin films at lower temperatures. AlN deposited with ALE at 500°C have been shown to have good crystallinity, but relatively high carbon and oxygen impurities, and understanding the film deposition mechanism is an ongoing project.<sup>1</sup> Grazing incidence small angle x-ray scattering (GISAXS) is sensitive to surface features, making it useful for real time monitoring of deposition processes. AlN was monitored by GISAXS while being deposited with ALE using trimethylaluminum and hydrogen/nitrogen plasma at the Brookhaven National Synchrotron Light Source and the Cornell High Energy Synchrotron Source. The GISAXS of AlN ALE at nominally 400°C, 450°C, and 500°C was compared to ex situ characterization with XPS and AFM.

<sup>1</sup>N. Nepal et al., *Appl. Phys. Lett.* **103** 082110 (2013)

**12:03PM B51.00005 Parallel Stitching of Two-Dimensional Materials**, XI LING, YUXUAN LIN, MILDRED DRESSSELHAUS, TOMS PALACIOS, JING KONG, Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, DEPARTMENT OF ELECTRICAL ENGINEERING AND COMPUTER SCIENCE, MASSACHUSETTS INSTITUTE OF TECHNOLOGY TEAM — Large scale integration of atomically thin metals (e.g. graphene), semiconductors (e.g. transition metal dichalcogenides (TMDs)), and insulators (e.g. hexagonal boron nitride) is critical for constructing the building blocks for future nanoelectronics and nanophotonics. However, the construction of in-plane heterostructures, especially between two atomic layers with large lattice mismatch, could be extremely difficult due to the strict requirement of spatial precision and the lack of a selective etching method. Here, we developed a general synthesis methodology to achieve both vertical and in-plane “parallel stitched” heterostructures between a two-dimensional (2D) and TMD materials, which enables both multifunctional electronic/optoelectronic devices and their large scale integration. This is achieved via selective “sowing” of aromatic molecule seeds during the chemical vapor deposition growth. MoS<sub>2</sub> is used as a model system to form heterostructures with diverse other 2D materials. Direct and controllable synthesis of large-scale parallel stitched graphene-MoS<sub>2</sub> heterostructures was further investigated. Unique nanometer overlapped junctions were obtained at the parallel stitched interface, which are highly desirable both as metal-semiconductor contact and functional devices/systems, such as for use in logical integrated circuits (ICs) and broadband photodetectors.

**12:15PM B51.00006 Solution-Processed hybrid Sb<sub>2</sub>S<sub>3</sub> planar heterojunction solar cell**, WENXIAO HUANG, ISMAIL BORAZAN, DAVID CARROLL, Wake Forest Univ — Thin-film solar cells based on inorganic absorbers permit a high efficiency and stability. Among or those absorber candidates, recently Sb<sub>2</sub>S<sub>3</sub> has attracted extensive attention because of its suitable band gap (1.5eV ~1.7 eV), strong optical absorption, low-cost and earth-abundant constituents. Currently high-efficiency Sb<sub>2</sub>S<sub>3</sub> solar cells have absorber layer deposited on nanostructured TiO<sub>2</sub> electrodes in combination with organic hole transport material (HTM) on top. However it's challenging to fill the nanostructured TiO<sub>2</sub> layer with Sb<sub>2</sub>S<sub>3</sub> and subsequently by HTM, this leads to uncovered surface permits charge recombination. And the existing of Sb<sub>2</sub>S<sub>3</sub>/TiO<sub>2</sub>/HTM triple interface will enhance the recombination due to the surface trap state. Therefore, a planar junction cell would not only have simpler structure with less steps to fabricate but also ideally also have a higher open circuit voltage because of less interface carrier recombination. By far there is limited research focusing on planar Sb<sub>2</sub>S<sub>3</sub> solar cell, so the feasibility is still unclear. Here, we developed a low-toxic solution method to fabricate Sb<sub>2</sub>S<sub>3</sub> thin film solar cell, then we studied the morphology of the Sb<sub>2</sub>S<sub>3</sub> layer and its impact to the device performance. The best device with a structure of FTO/TiO<sub>2</sub>/Sb<sub>2</sub>S<sub>3</sub>/P3HT/Ag has PCE over 5% which is similar or higher than yet the best nanostructure devices with the same HTM. Furthermore, based on solution engineering and surface modification, we improved the Sb<sub>2</sub>S<sub>3</sub> film quality and achieved a record PCE. .

**12:27PM B51.00007 Visible Aligned Carbon Nanotube-MoS<sub>2</sub> Hybrids**, RUI WANG, Department of Physics & Astronomy, Vanderbilt University, Nashville, TN 37235, USA, TU HONG, TIANJIAO WANG, Department of Electrical Engineering & Computer Science, Vanderbilt University, Nashville, TN 37235, USA, AHMAD IFFAT ALI, Department of Chemical & Biomolecular Engineering, Vanderbilt University, Nashville, TN 37235, USA, DEVPAUL SINGH CHANI, Pope John Paul II High School, Hendersonville, TN 37075, USA, YAQIONG XU<sup>1</sup>, Department of Physics & Astronomy, Vanderbilt University, Nashville, TN 37235, USA — Single-walled carbon nanotubes (SWNTs) have gained great interest due to their excellent electrical, mechanical and thermal properties. Recent progress in two-dimensional (2D) materials has opened up new horizons in the realm of physics and engineering that could lead to the revolution of future electronics and optoelectronics. Various hybrid structures have been developed for different applications. Here we report a facile method to synthesize ultrathin 2D hybrids between horizontally-aligned SWNT and monolayer molybdenum sulfide (MoS<sub>2</sub>) through chemical vapor deposition (CVD). These hybrid structures can be imaged under an optical microscope; and their Raman mapping indicates that MoS<sub>2</sub> flakes are partially grown on top of SWNTs. Moreover, strong photocurrent signals have been observed in SWNT-MoS<sub>2</sub> hybrids through scanning photocurrent measurements. These fundamental studies may provide a new way to fabricate 2D hybrids for future electronics and optoelectronics.

<sup>1</sup>Department of Electrical Engineering & Computer Science, Vanderbilt University, Nashville, TN 37235, USA

**12:39PM B51.00008 Synthesis and electrical characterization of Rhenium Diselenide**, BYEONGGIL KANG, YOUNGCHAN KIM, SKKU Advanced Institute of Nanotechnology(SAINT), Sungkyunkwan University, Suwon, 440-746, Korea, CHANGGU LEE, Department of Mechanical Engineering and SKKU Advanced Institute of Nanotechnology(SAINT), Sungkyunkwan University, Suwon, 440-746, Korea, GRAPHENE ENGINEERING LAB. TEAM — Rhenium diselenide (ReSe<sub>2</sub>) as the one of new members of 2-dimensional transition metal dichalcogenide (TMDC) material possesses a high potential for optoelectronic applications. In this work, we report a synthesis method thin single crystalline ReSe<sub>2</sub> via chemical vapor deposition (CVD) and the electrical characterization. The structure of the synthesized ReSe<sub>2</sub>, which has triclinic symmetry, is characterized by transmission electron microscope (TEM). Also, the synthesized ReSe<sub>2</sub> show Raman spectrum characteristics with peaks having same position regardless of the sample thickness due to the low symmetry. We fabricate bottom-gated field effect transistors (FET) with ambipolar behavior and on/off ratio 10<sup>5</sup> and carrier mobility of 0.21cm<sup>2</sup>/Vs (hole) and 0.20cm<sup>2</sup>/Vs (electron).

**12:51PM B51.00009 Growth and Characterization of TMDs (MoS<sub>2</sub>, MoSe<sub>2</sub>, WS<sub>2</sub>, WSe<sub>2</sub> & MoTe<sub>2</sub>) and Their Alloys on Various Substrates**, DAVID BARROSO, ARIANA NGUYEN, SAHAR NAGHIBI, MICHAEL GOMEZ, INGRID LIAO, CHUN-YU HUANG, I-HSI LU, EDWIN PRECIADO, THOMAS EMPANTE, WILLIAM COLEY, DOMINIC MARTINEZ, AIMEE MARTINEZ, Univ of California - Riverside — Transition Metal Dichalcogenides (TMDs) have been of interest over the past years due to their exciting semiconducting properties. In the bulk, TMDs possess a native indirect bandgap and transition to a direct bandgap as they approach the monolayer limit. The bandgaps range from 1.15 eV to 1.95 eV depending on composition. Using organic liquids and/or inorganic powders as precursors, CVD growth has been realized for MX<sub>2</sub> TMDs (M = Mo, W; X = S, Se) and their alloys at tunable compositions. I will present the effect of tuning parameters such as temperature, gas flow, time of heat and hold on the resultant single-layer films. Different precursors can lead to different overall film structures and enable different growth conditions. The films can either be made homogeneous in bandgap or gradients of material/bandgap can be grown. The use of different substrates (dielectric, ferroelectric, piezoelectric, semiconducting, insulating, patterned) allows an additional degree of freedom and sets the stage for subsequent experiments. I will talk about preparation methods tailored toward direct applicability of surface acoustic spectroscopy, scanning photocurrent microscopy, and ferroelectric gating of the single-layer films.

**1:03PM B51.00010 Interfacial reaction between metal-insulator transition material NbO<sub>2</sub> thin film and wide band gap semiconductor GaN**, AGHAM POSADAS, University of Texas at Austin, ALEXANDER KVIT, University of Wisconsin - Madison, ALEXANDER DEMKOV, University of Texas at Austin — Materials that undergo a metal-insulator transition (MIT) are potentially useful for a wide variety of applications including electronic and opto-electronic switches, memristors, sensors, and coatings. In most such materials, the MIT is driven by temperature. In one such material, NbO<sub>2</sub>, the MIT mechanism is primarily of the Peierls-type, in which the dimerization of the Nb atoms without electron correlation causes the transition from metallic to semiconducting. We describe our initial work at combining NbO<sub>2</sub> and GaN in epitaxial form, which could be potentially useful in resistive switching devices operating at very high temperatures. We grow NbO<sub>2</sub> films on GaN(0001)/Si(111) substrates using reactive molecular beam epitaxy from a metal evaporation source and molecular oxygen. X-ray diffraction shows that the films are found to grow with a single out of plane orientation but with three symmetry-related orientation domains in the plane. In situ x-ray photoelectron spectroscopy confirms that the phase pure NbO<sub>2</sub> is formed but that a chemical reaction occurs between the GaN and NbO<sub>2</sub> during the growth forming a polycrystalline interfacial layer. We perform STEM-EELS analysis of the film and the interface to further elucidate their chemical and structural properties.

**1:15PM B51.00011 Impact of Crystalline Structure on the Temperature Dependence of Resistivity<sup>1</sup>**, YUTONG GUAN, GANG YANG, DONGMING MEI, The University of South Dakota — Since HPGe radiation detectors work under cryogenic temperature, the electrical properties at low temperature are essential for the detector performance. In this study, the resistivity of two types of HPGe, i.e. single crystal from Czochralski growth and poly-crystal from zone refining, was investigated in the temperature range from 4.2 to 100K. It was found that there was a turning point on the resistivity vs temperature curves for both types of crystals. However, the turning points for them were significantly different: 30K for single crystalline while 60K for polycrystalline. In order to explore the reason, microstructures of both types of crystals were investigated by optical microscopy. The results showed a very good agreement between electrical properties and microstructures.

<sup>1</sup>This work is supported by DOE grant DE-FG02-10ER46709 and the state of South Dakota.

**1:27PM B51.00012 Atomistic simulations of activated processes in nanoparticles synthesis<sup>1</sup>**, FEDERICO GIBERTI, GIULIA GALLI, Institute for Molecular Engineering, The University of Chicago — Core-shell and Janus nanoparticles are promising building blocks for new, highly efficient solar cells. One of the most common synthetic pathways to produce such nanostructures is the use of cation exchange reactions. Although widely used, these procedures are not completely understood. We employed classical Molecular Dynamics and Monte Carlo simulations to understand these transformation at the molecular level; in particular we investigated the conversion from CdSe (sphalerite) to PbSe (rocksalt) NPs with 2-3 nm diameter. In order to recover the equilibrium free energy surfaces we used state of the art enhanced sampling techniques, including Metadynamics. The formation of hybrid core-shell structures resulted to be an activated process, where the limiting step is the transition of a sphalerite to a rocksalt PbSe nucleus. We found that the barrier height and the stability of the two phases depend on the size of the PbSe nucleus, suggesting that the process could proceed via a two step mechanism, where a small sphalerite nucleus is formed first, and it then transforms to a rocksalt nucleus. Our results give insight into possible manipulation processes at the molecular scale, which could be used to stabilize metastable NPs and tune their physical and chemical properties.

<sup>1</sup>This work was supported by the DOE grant No. DE-FG02-06ER46262

**1:39PM B51.00013 3D Functional Elements Deep Inside Silicon with Nonlinear Laser Lithography**, ONUR TOKEL, AHMET TURNALI, Bilkent University, EMRE ERGECEN, Massachusetts Institute of Technology, IHOR PAVLOV, FATIH OMER ILDAY, Bilkent University — Functional optical and electrical elements fabricated on silicon (Si) constitute fundamental building blocks of electronics and Si-photonics. However, since the highly successful established lithography are geared towards surface processing, elements embedded inside Si simply do not exist. Here, we present a novel direct-laser writing method for positioning buried functional elements inside Si wafers. This new phenomenon is distinct from previous work, in that the surface of Si is not modified. By exploiting nonlinear interactions of a focused laser, permanent refractive index changes are induced inside Si. The imprinted index contrast is then used to demonstrate a plethora of functional elements and capabilities embedded inside Si[1]. In particular, we demonstrate the first functional optical element inside Si, the first information-storage capability inside Si, creation of high-resolution subsurface holograms, buried multilevel structures, and complex 3D architectures in Si, none of which is currently possible with other methods. This new approach complements available techniques by taking advantage of the real estate under Si, and therefore can pave the way for creating entirely new multilevel devices through electronic-photonics integration. [1]Tokel, O., arxiv.org/abs/1409.28

**1:51PM B51.00014 Circular photogalvanic effect in silicon nanowires**, SAJAL DHARA, E. J. MELE, RITESH AGARWAL, University of Pennsylvania — Circular photogalvanic effect (CPGE), the generation of a photocurrent whose magnitude and polarity depends on chirality of optical excitation, is demonstrated in the visible optical range in silicon nanowires, a bulk non-gyrotropic material with weak spin-orbit coupling. CPGE, which is absent in bulk Si is found to arise from interband transitions only at the metal-semiconductor contacts to Si nanowires where inversion symmetry is broken by a Schottky electric field. Furthermore, by applying a bias voltage that modulates this field, the sign and magnitude of the CPGE can be controlled. From excitation energy dependent measurements and symmetry considerations, it is argued that the [110] surface states due to Si chains that are not aligned with the nanowire growth direction and the Schottky field produce an artificial gyrotropic optical medium that supports CPGE. This work reveals the role of the surface states in the generation of chirality-dependent photocurrents in silicon with a purely orbital-based mechanism, and also opens up new possibilities of engineering new functionalities in Si that can be integrated with conventional electronics.

**2:03PM B51.00015 Fabrication of self-forming silver network as transparent conductive electrode with photoresist**, CHAOBIN YANG, JUAN M MERLO, MICHAEL J BURNS, KRZYSZTOF KEMPA, MICHAEL J NAUGHTON, Boston College — It has been reported that a metal wire network, obtained by sputtering with a self-cracking gel film mask, can function as a TCO replacement, perhaps reducing end device cost [1]. Toward further process simplification and cost reduction, we are investigating various electroless deposition schemes to template a wire network electrode. We report here that a conventional photoresist film can be prepared with a network of microcracks and can be used as a mask to electrolessly deposit metal, e.g. silver. With this method, no vacuum chambers are required, and undeposited metal can even be recycled for additional depositions. [1] B. Han, K. Pei, Y. Huang, X. Zhang, Q. Rong, Q. Lin, Y. Guo, T. Sun, C. Guo, D. Carnahan, M. Giersig, Y. Wang, J. Gao, Z. Ren, and K. Kempa, *Adv. Mater.* 26, 873 (2014).

**Monday, March 14, 2016 11:15AM - 2:15PM –**

**Session B52 DAMOP: Optomechanics and Hybrid Systems I: Novel Systems** Hilton Baltimore Holiday Ballroom 3 - Tom Purdy, NIST

**11:15AM B52.00001 Exploring the Macroscopic Quantum Physics of Motion with Superfluid He-4**, LAURA DE LORENZO, AARON PEARLMAN, KEITH SCHWAB, Caltech — We demonstrate the use of superfluid helium-4 as an extremely low loss optomechanical element. We form an optomechanical system with a cylindrical niobium superconducting TE<sub>011</sub> resonator whose 40 cm<sup>3</sup> inner cylindrical cavity is filled with <sup>4</sup>He. Coupling is realized via the variations in permittivity resulting from the density profile of the acoustic modes. Acoustic losses in helium-4 below 500 mK are governed by the intrinsic nonlinearity of sound, leading to an attenuation which drops as T<sup>4</sup>, indicating the possibility of quality factors (Q) over 10<sup>10</sup> at 10 mK. In our lowest loss mode, we demonstrate this T<sup>4</sup> law at temperatures down to 50 mK, realizing an acoustic Q of 1.35\*10<sup>8</sup> at 8.1 kHz. When coupled with a low phase noise microwave source, we expect this system to be utilized as a probe of macroscopic quantized motion, for precision measurements to search for fundamental physical length scales, and as a continuous gravitational wave detector. Our estimates suggest that a resonant superfluid acoustic system could exceed the sensitivity of current broad-band detectors for narrow-band sources such as pulsars. De Lorenzo, L. A. and Schwab, K. C., *New J. Phys.* 16, 113020 (2014).

**11:27AM B52.00002 Mechanical Resonance and Damping Properties of Gallium Nitride Nanowires in Selected-Area Growth Arrays Measured via Optical Bragg Scattering<sup>1</sup>**, JOHN HOULTON, Univ of Colorado - Boulder, M. D. BRUBAKER, K. A. BERTNESS, NIST Boulder, C. T. ROGERS, Univ of Colorado - Boulder — We report the use of optical Bragg scattering to measure the mechanical resonance frequencies and quality factors (Q) of gallium nitride (GaN) nanowires (NWs) in selected-area growth arrays. The GaN NWs are grown by catalyst-free molecular beam epitaxy on silicon (111) wafers. Hexagonal arrays of approximately 100 GaN NWs with pitch spacings of 400 - 1000 nm have been prepared. The NWs contained in such arrays have diameters ranging from 100-300 nm and lengths from 3 - 10 μm. A diode laser operating at 640 nm and 2 mW of optical power is used to perform Bragg scattering homodyne detection to passively read out the thermally induced Brownian mechanical motion of the NWs. The first order cantilever-mode mechanical resonance frequencies of these NWs have been measured to be between 2 - 12 MHz. We find that the optical readout via Bragg scattered light allows the simultaneous detection of all lowest order mechanical resonances in a given array. Q factors ranging from 1,000 - 12,000 have been seen at room temperature and 10<sup>-5</sup> Torr pressures. Qs as high as 25,000 have been seen at temperatures of 80 K. These results show that the narrow mechanical resonances observed in freely-grown GaN NWs can also be seen in NWs prepared via selected-area growth.

<sup>1</sup>We gratefully acknowledge funding via NIST MSE Grant # 1553451

**11:39AM B52.00003 Ultra-thin superconducting film coated silicon nitride nanowire resonators for low-temperature applications**, ABHILASH SEBASTIAN, NIKOLAY ZHELEV, ROBERTO DE ALBA, JEEVAK PARPIA, Cornell University — We demonstrate fabrication of high stress silicon nitride nanowire resonators with a thickness and width of less than 50 nm intended to be used as probes for the study of superfluid <sup>3</sup>He. The resonators are fabricated as doubly-clamped wires/beams using a combination of electron-beam lithography and wet/dry etching techniques. We demonstrate the ability to suspend (over a trench of depth ~8 μm) wires with a cross section as small as 30 nm, covered with a 20 nm superconducting film, and having lengths up to 50 μm. Room temperature resonance measurements were carried out by driving the devices using a piezo stage and detecting the motion using an optical interferometer. The results show that metalizing nano-mechanical resonators not only affects their resonant frequencies but significantly reduce their quality factor (Q). The devices are parametrically pumped by modulating the system at twice its fundamental resonant frequency, which results in observed amplification of the signal. The wires show self-oscillation with increasing modulation strength. The fabricated nanowire resonators are intended to be immersed in the superfluid <sup>3</sup>He. By tracking the resonant frequency and the Q of the various modes of the wire versus temperature, we aim to probe the superfluid gap structure.

**11:51AM B52.00004 Optomechanics with superfluid He4 thin films**, CHRISTOPHER BAKER, GLEN HARRIS, DAVID MCAUSLAN, YAUHEN SACHKOU, XIN HE, EOIN SHERIDAN, WARWICK BOWEN, Univ of Queensland — Cavity optomechanics focuses on the interaction between confined light and a mechanical degree of freedom. Vibrational modes of superfluid helium-4 have recently been identified as an attractive mechanical element for cavity optomechanics, thanks to their ultra-low dissipation arising from superfluids viscosity free flow. Here we propose and demonstrate an approach to superfluid optomechanics based on femtogram thin films of superfluid helium condensed on the surface of a microscale microtoroid optical whispering gallery mode resonator. Excitations within the film, known as third sound, manifest as surface waves with a restoring force provided by the van der Waals interaction. We experimentally probe the thermodynamics of these superfluid excitations in real-time, and demonstrate both laser cooling and amplification of the thermal motion. In addition, we propose and demonstrate an entirely new approach to optical forcing based on the atomic recoil of superfluid helium-4. This technique utilizes the thermomechanical effect of superfluids, whereby frictionless fluid flow is generated in response to a local heat source. Using this technique, we achieve superfluid forces on a microtoroid mechanical mode an order of magnitude greater than the equivalent radiation pressure force.

**12:03PM B52.00005 Strong coupling and parametric amplification in mechanical modes of graphene**, JOHN MATHEW, Tata Institute of Fundamental Research, Mumbai, India, RAJ PATEL, Tata Institute of Fundamental Research, Mumbai, India, Birla Institute of Technology & Science, Pilani - K.K.Birla Goa Campus, India, ABHINANDAN BORAH, RAJAMANI VIJAYARAGHAVAN, MANDAR DESHMUKH, Tata Institute of Fundamental Research, Mumbai, India — We demonstrate strong dynamical coupling and parametric amplification in mechanical modes of a graphene drum using an all electrical configuration. Low tension in the system allows large electrostatic tunability of the modes thus enabling dynamic pumping experiments. In the strong coupling regime a red detuned pump gives rise to new eigenmodes having highly tunable mode splitting (cooperativity ~60) with coherent energy transfer. The coupling is also used to amplify the modes under the action of a blue detuned pump. In addition, self-oscillations and parametric amplification of the fundamental vibrational mode is demonstrated with a gain of nearly 3. The low mass and high frequency of these atomically thin resonators could prove useful for studying mode coupling in the quantum regime.

**12:15PM B52.00006 Observation of vacuum-enhanced electron spin resonance of optically levitated nanodiamonds** , TONGCANG LI, THAI HOANG, JONGHOON AHN, JAEHOON BANG, Purdue University — Electron spins of diamond nitrogen-vacancy (NV) centers are important quantum resources for nanoscale sensing and quantum information. Combining such NV spin systems with levitated optomechanical resonators will provide a hybrid quantum system for many novel applications. Here we optically levitate a nanodiamond and demonstrate electron spin control of its built-in NV centers in low vacuum. We observe that the strength of electron spin resonance (ESR) is enhanced when the air pressure is reduced. To better understand this novel system, we also investigate the effects of trap power and measure the absolute internal temperature of levitated nanodiamonds with ESR after calibration of the strain effect. Our results show that optical levitation of nanodiamonds in vacuum not only can improve the mechanical quality of its oscillation, but also enhance the ESR contrast, which pave the way towards a novel levitated spin-optomechanical system for studying macroscopic quantum mechanics. The results also indicate potential applications of NV centers in gas sensing.

**12:27PM B52.00007 Piezo-optomechanical circuits** , KRISHNA COIMBATORE BALRAM<sup>1</sup>, MARCELO DAVANCO, B. ROBERT ILIC, KARTIK SRINIVASAN, NIST - Natl Inst of Stds & Tech — Coherent links between the optical, radio frequency (RF), and mechanical domains are critical for applications ranging from quantum state transfer between the RF and optical domains to signal processing in the acoustic domain for microwave photonics. We develop such a piezo optomechanical circuit platform in GaAs, in which localized and interacting 1550 nm photons and 2.4 GHz phonons are combined with photonic and phononic waveguides. GaAs allows us to exploit the photoelastic effect to engineer cavities with strong optomechanical coupling ( $g_0/2\pi \approx 1.1$  MHz) and the piezoelectric effect to couple RF fields to mechanical motion through surface acoustic waves, which are routed on-chip using phononic crystal waveguides. This platform enables optical readout of electrically-injected mechanical states with an average coherent intracavity phonon number as small as  $\approx 0.05$  and the ability to drive mechanical motion with equal facility through either the optical or electrical channel. This is used to demonstrate a novel acoustic wave interference effect in which optically-driven motion is completely cancelled by electrically-driven motion, and vice versa. As an application of this, we present time-domain measurements of optically-controlled acoustic pulse propagation.

<sup>1</sup>Secondary Affiliation is Maryland Nanocenter, University of Maryland, College Park, MD

**12:39PM B52.00008 Magneto-optical coupling in whispering gallery mode resonators** , JAMES HAIGH, Hitachi Cambridge Laboratory, Cambridge, CB3 0HE, UK, STEFAN LANGENFELD, NICHOLAS LAMBERT, JEREMY BAUMBERG, Cavendish Laboratory, University of Cambridge, Cambridge, CB3 0HE, UK, ANDREW RAMSAY, Hitachi Cambridge Laboratory, Cambridge, CB3 0HE, UK, ANDREAS NUNNENKAMP, ANDREW FERGUSON, Cavendish Laboratory, University of Cambridge, Cambridge, CB3 0HE, UK — We demonstrate that yttrium iron garnet microspheres support optical whispering gallery modes similar to those in non-magnetic dielectric materials. The direction of the ferromagnetic moment tunes the resonant optical frequency via the Voigt effect, dependent on the angle of the magnetization with respect to the plane of the whispering gallery mode. This parametric coupling of the magnetization to the optical mode may enable analogous experiments to those performed in cavity optomechanics. In addition, the Faraday effect couples the two ordinarily linear polarized modes, split by the geometrical birefringence due to the boundary conditions at the surface. This results in a polarization rotation of the light emitted from the cavity. Our results extend recent work on the strong coupling of microwave photons to magnetization dynamics into the optical domain. An understanding of the magneto-optical coupling in whispering gallery modes, where the propagation direction rotates with respect to the magnetization, is fundamental to the emerging field of cavity optomagnonics. [arXiv:1510.06661].

**12:51PM B52.00009 Quartz-superconductor quantum electromechanical system** , MATT WOOLLEY, MUHAMMAD EMZIR, UNSW Australia, GERARD MILBURN, MARKUS JERGER, University of Queensland, MAXIM GORYACHEV, MIKE TOBAR, University of Western Australia, ARKADY FEDOROV, University of Queensland — Quartz bulk acoustic wave oscillators support mechanical modes with very high resonance frequencies and extremely high quality factors. As such, they provide an appealing platform for quantum optics experiments with phonons, gravitational wave detection, and tests of quantum mechanics. We propose to cool and measure the motion of a quartz oscillator using a transmon, with the coupling mediated by a tuneable superconducting LC circuit. The mechanical motion ( $\sim 250$  MHz) is resonantly coupled to the LC circuit ( $\sim 250$  MHz) by a piezoelectric interaction, the LC circuit is coupled to the transmon ( $\sim 8$  GHz) via sideband transitions, and there is a smaller direct coupling between the quartz oscillator and the transmon. By driving the transmon on its red sideband, the mechanical and electrical oscillators may be cooled close to their quantum ground state. By observing the fluorescence of the qubit, the occupations of the oscillators may be determined via the motional sidebands they induce. A minimal model of this system consists of a qubit coupled to two oscillators, which are themselves mutually coupled. The steady-state of the system and the qubit fluorescence spectrum are evaluated analytically using a perturbative projection operator technique, and verified numerically.

**1:03PM B52.00010 Single photon frequency conversion and channelization based on microwave piezo-optomechanical devices.** , LINRAN FAN, CHANGLIN ZOU, MENNO POOT, RISHENG CHENG, HONG TANG, Yale University — Cavity optomechanics holds very promising potentials for quantum information processing, as it provides both a convenient method to manipulate photons and a platform to bridge different quantum system. Especially, the integration of microwave devices with cavity optomechanics draws great interest as such a hybrid platform can provide strong electrical actuation, ultra-sensitive optical readout, and parametric mechanical signal amplification simultaneously in a single device. This hybrid platform enables great functionalities in manipulating photons, and builds direct link between microwave photon and optical photon, which is important for future quantum network. Aluminum nitride (AlN) is ideal for such hybrid platform. Besides low optical and mechanical loss, AlN possesses strong piezoelectric effect, which gives rise to strong coupling between microwave cavities and mechanical resonators. We will present our recent progress in developing integrated AlN hybrid platform for photon manipulation, such as optical amplification and absorption, cascaded optical delay, single photon frequency shifting, etc.

**1:15PM B52.00011 Displacement linear detection down to thermal fluctuations of a silicon nitride membrane with self-mixing technique<sup>1</sup>** , LORENZO BALDACCI, ALESSANDRO PITANTI, LUCA MASINI, ANDREA ARCANGELI, DANIEL NAVARRO URRIOS, NEST, Istituto Nanoscienze - CNR and Scuola Normale Superiore, ALESSANDRO TREDICUCCI, NEST, Istituto Nanoscienze - CNR and Dipartimento di Fisica E. Fermi, Universit'a di Pisa, SOULMAN RESEARCH GROUP TEAM — Active optomechanical systems exploit the interaction between photons and mechanical vibrations inside a laser cavity. A compound cavity made of a laser diode and an external vibrating reflector is a suitable platform, due to its ease of construction and coupling modulation. Here we use it as a linear displacement detector, by studying the motion of a silicon nitride suspended membrane as the external mirror of a near infrared laser diode. The membrane vibrations cause fluctuations in the laser optical power, which are collected by a photodiode and measured with a spectrum analyzer. The dynamics of the membrane driven by a piezo actuator was investigated in a homodyne configuration. The high Q-factor ( $\sim 10^5$  at low pressure) of the fundamental mechanical mode at 74 kHz enabled direct measurement of thermal motion at room temperature, which holds an average displacement of 20 pm. Therefore, compound cavity systems can be employed as table-top, cost-effective displacement linear detectors. Furthermore, nonlinear optomechanical interactions could be observed, with new possibilities in the study of non-Markovian quantum properties at the mesoscale.

<sup>1</sup>Work supported by European Research Council, advanced grant No. 321122 SouLMan

**1:27PM B52.00012 Microwave cavity piezo-opto-mechanical resonators based on film thickness modes operating beyond 10 GHz**, XU HAN, HONG TANG, Yale University — Micromechanical resonators, which support and confine microwave frequency phonons on a scale comparable to optical wavelength, provide a valuable intermediate platform facilitating interactions among electrical, optical, and mechanical domains. High-frequency mechanical resonances ease the refrigeration conditions for reaching quantum mechanical ground state and also hold promise for practical device applications. However, efficient actuation of the highly stiff mechanical motions above gigahertz frequencies remains a challenging task. Here, we demonstrate a high-performance piezo-opto-mechanical resonator operating at 10.4 GHz by exploiting the acoustic thickness mode of an aluminum nitride micro-disk. In contrast to the in-plane mechanical modes, the thickness mode can be easily scaled to high frequencies with low mechanical and optical dissipations. A high  $f \cdot Q$  product of  $1.9 \times 10^{13}$  Hz is achieved in ambient air at room temperature. Moreover, strong piezo-electro-mechanical coupling can be achieved by coupling the thickness mode with a microwave resonator, making it possible for coherent signal conversion. The thickness mode-based piezo-opto-mechanical resonators can be expected to serve as essential elements for advanced hybrid information networks.

**1:39PM B52.00013 Slot-mode optomechanical crystals with enhanced coupling and multimode functionality**<sup>1</sup>, KAREN GRUTTER, MARCELO DAVANCO, KARTIK SRINIVASAN, NIST - Natl Inst of Stds & Tech — A number of cavity optomechanics applications involve multiple interacting optical and mechanical modes. A key challenge in such systems is developing multimode platforms with both flexibility in the optical and mechanical designs and interactions as strong as those shown in single-mode systems. We thus present slot-mode optomechanical crystals, in which photonic and phononic crystal nanobeams separated by a narrow slot couple optomechanically. We pattern these beams to confine a low-loss optical mode in the slot and a mechanical breathing mode at the center of the mechanical beam. This structure has large optomechanical coupling rates and great design flexibility toward multimode systems. We demonstrate this in  $\text{Si}_3\text{N}_4$  slot-mode devices, with 980 nm optical modes coupling to mechanical modes at 3.4 GHz, 1.8 GHz, and 400 MHz. We use  $\text{Si}_3\text{N}_4$  tensile stress to shrink slot widths to 24 nm, greatly enhancing optomechanical coupling. Finally, with this platform, we develop multimode systems with three-beam geometries, in which two different mechanical modes couple to one optical mode and two different optical modes couple to one mechanical mode.

<sup>1</sup>The authors acknowledge funding from DARPA (MESO) and the National Research Council Research Associateship Program

**1:51PM B52.00014 Nonlinearly Coupled Superconducting Lumped Element Resonators**, MICHELE C. COLLODO, ANTON POTOČNIK, ANTONIO RUBIO ABADAL, MINTU MONDAL, MARKUS OPPLIGER, ANDREAS WALLRAFF, Laboratory for Solid State Physics, ETH Zurich — We study SQUID-mediated tunable coupling between two superconducting on-chip resonators in the microwave frequency range. In this circuit QED implementation, we employ lumped-element type resonators, which consist of Nb thin film structured into interdigitated finger shunt capacitors and meander inductors. A SQUID, functioning as flux dependent and intrinsically nonlinear inductor, is placed as a coupling element together with an interdigitated capacitor between the two resonators (cf. A. Baust *et al.*, Phys. Rev. B **91** 014515 (2015)). We perform a spectroscopic measurement in a dilution refrigerator and find the linear photon hopping rate between the resonators to be widely tunable as well as suppressible for an appropriate choice of parameters, which is made possible due to the interplay of inductively and capacitively mediated coupling. Vanishing linear coupling promotes nonlinear effects ranging from onsite- to cross-Kerr interaction. A dominating cross-Kerr interaction related to this configuration is notable, as it induces a unique quantum state. In the course of analog quantum simulations, such elementary building blocks can serve as a precursor for more complex geometries and thus pave the way to a number of novel quantum phases of light

**2:03PM B52.00015 Microwave Reentrant Cavities for Quantum Devices**<sup>1</sup>, NATALIA C. CARVALHO, JEREMY BOURHILL, DANIEL CREEDON, MAXIM GORYACHEV, ARC Centre of Excellence for Engineered Quantum Systems, The University of Western Australia, SERGE GALLIOU, FEMTO-ST Institute, MICHAEL TOBAR, ARC Centre of Excellence for Engineered Quantum Systems, The University of Western Australia — A microwave reentrant cavity is a device able to provide a very sensitive high-Q microwave mode. Its design can be highly advantageous for electromechanical devices and quantum measurements. In this sense, a tuneable device based on a narrow-gap superconducting reentrant cavity is under development. The resonant frequency is able to be fine-tuned over a range larger than 500 MHz at 10 mK with an electrical Q-factor of  $10^5$ . Such a cavity could possibly accommodate a transmon qubit to control and manipulate its quantum state. We are also working on the investigation of bulk acoustic wave (BAW) resonators in microwave reentrant cavities. BAW resonators offer a promising way to process quantum information through the coupling between microwaves and acoustic phonons. Thus, we are developing a device able to excite phonons through non-linearities and the piezoelectricity of the plano-convex quartz crystal. We will detail our experiments that work towards cooling gram scale phonon resonances to the quantum ground state.

<sup>1</sup>Funded by ARC Grant No. CE110001013 (Australia) and National Counsel of Technological and Scientific Development (Brazil)

**Monday, March 14, 2016 11:15AM - 2:15PM —**

**Session B53 DFD GSOF: Drops, Bubbles and Interfacial Fluid Mechanics** Hilton Baltimore Holiday Ballroom 4 - Siddhartha Das, University of Maryland-College Park

**11:15AM B53.00001 ABSTRACT WITHDRAWN —**

**11:27AM B53.00002 Acoustical vortices on a Chip for 3D single particle manipulation and vorticity control**<sup>1</sup>, ANTOINE RIAUD, CNRS Nord pas de Calais, JEAN-LOUIS THOMAS, OLIVIER BOU MATAR, CNRS Paris, MICHAEL BAUDOIN, CNRS Nord pas de Calais — Surface acoustic waves offer most of the basic functions required for on-chip actuation of fluids at small scales: efficient flow mixing, integrated pumping, particles separation, droplet displacement, atomization, division and fusion. Nevertheless some more advanced functions such as 3D particles manipulation and vorticity control require the introduction of some specific kind of waves called acoustic vortices. These helical waves propagate spinning around a phase singularity called the dark core. On the one hand, the beam angular momentum can be transferred to the fluid and create point-wise vorticity for confined mixing, and on the other the dark core can trap individual particles in an acoustic well for single object manipulation. In this presentation, I will show how acoustical vortices on-a-chip can be synthesized with a programmable electronics and an array of transducers<sup>2</sup>. I will then highlight how some of their specificities<sup>3</sup> can be used for acoustical tweezing and twisting.

<sup>1</sup>This work is supported by ANR Project No. ANR-12-BS09-0021-01 and ANR-12-BS09-0021-02, and Rgion Nord Pas de Calais.

<sup>2</sup>A. Riaud, J.-L. Thomas, E. Charron, A. Bussonniere, O. Bou Matar, M. Baudoin Phys. Rev. Applied 4, 034004 (2015)

<sup>3</sup>A. Riaud, J.-L. Thomas, O. Bou Matar, M. Baudoin Phys. Rev. E - Accepted for publication

**11:39AM B53.00003 Coalescence-induced jumping of nanoscale droplets on super-hydrophobic surfaces**, ZHI LIANG, PAWEL KEBLINSKI, Rensselaer Polytechnic Institute, NANOSCALE SCIENCE AND ENGINEERING CENTER TEAM — The coalescence-induced jumping of tens of microns size droplets on super-hydrophobic surfaces has been observed in both experiments and simulations. However, whether the coalescence-induced jumping would occur for smaller, particularly nanoscale droplets, is an open question. Using molecular dynamics simulations, we demonstrate that in spite of the large internal viscous dissipation, coalescence of two nanoscale droplets on a super-hydrophobic surface can result in a jumping of the coalesced droplet from the surface with a speed of a few m/s. Similar to the coalescence-induced jumping of microscale droplets, we observe that the bridge between the coalescing nano-droplets expands and impacts the solid surface, which leads to an acceleration of the coalesced droplet by the pressure force from the solid surface. We observe that the jumping velocity decreases with the droplet size and its ratio to the inertial-capillary velocity is a constant of about 0.126, which is close to the minimum value of 0.111 predicted by continuum-level modeling of Enright et al. [R. Enright, N. Miljkovic, J. Sprittles, K. Nolan, R. Mitchell, and E. N. Wang, ACS Nano 8, 10352 (2014)].

**11:51AM B53.00004 Droplet climbing on a pre-wetted conical fibre**, ZHEN JIAN, ERQIANG LI, S. T. THORODDSEN, King Abdullah University of Science and Technology (KAUST) — We study the motion of a droplet on a wet conical fibre. The conical fibres are fabricated with a glass-puller, with tip diameters of several  $\mu\text{m}$ . With liquid is fed through the hollow fibre and travels up the outside of the cone, forming a droplet, which is initially attached near the tip. This drop grows in size and then detaches and moves on the fibre, at velocities up to 0.25 m/s. We focus on the regime with small Bond number  $Bo = \rho g R^2 / \sigma$  and capillary number  $Ca = \mu U / \sigma$ , where the droplet motion is driven by the pressure gradient due to the continuous curvature change along the conical fibre. High-speed imaging and numerical simulations via the Gerris code are employed to investigate the dynamics of the droplet detachment and climbing. Our focus is on the interface profile near the tip, the mechanism of droplet formation and climbing, and the velocity field in the thin liquid layer on the cone.

**12:03PM B53.00005 Electro-osmotic flow in bicomponent fluids<sup>1</sup>**, ANDREI BAZARENKO, MARCELLO SEGA, University of Vienna — The electroosmotic flow (EOF) is a widely used technique that uses the action of external electric fields on solvated ions to move fluids around in microfluidics devices. For homogeneous fluids, the characteristics of the flow can be well approximated by simple analytical models, but in multicomponent systems such as oil-in-water droplets one has to rely to numerical simulations. The purpose of this study is to investigate physical properties of the EOF in a bicomponent fluid by solving the coupled equations of motions of explicit ions in interaction with a continuous model of the flow. To do so we couple the hydrodynamics equations as solved by a Shan-Chen Lattice-Boltzmann method<sup>2</sup> to the molecular dynamics of the ions<sup>3</sup>. The presence of explicit ions allows us to go beyond the simple Poisson-Boltzmann approximations, and investigate a variety of EOF regimes.

<sup>1</sup>ETN-COLLDENSE (H2020-MCSA-ITN-2014, Grant No. 642774)

<sup>2</sup>X. Shan, and H. Chen, Phys. Rev. E, 47, 1815-1819 (1993)

<sup>3</sup>M. Segal, M. Sbragaglia, S. S. Kantorovich and A. Ivanov, Soft Matter, 9, 10092-10107 (2013)

**12:15PM B53.00006 Electrohydrodynamics of toroidal droplets**, ALEXANDROS FRAGKOPOULOS, ERIC BERGER, Georgia Institute of Technology, EKAPOPAIRAM, King Mongkut's Institute of Technology Ladkrabang, ALBERTO FERNANDEZ-NIEVES, Georgia Institute of Technology — Toroidal droplets are unstable and always transform into spherical droplets due to surface tension. This can happen via Rayleigh-Plateau instabilities, or via the shrinking of the handle. Interestingly, charging a toroidal droplet can cause expansion, rather than shrinking, of the handle. In this talk, we will discuss the use of particle image velocimetry to obtain the velocity profile inside both neutral and charged toroidal droplets as they transform into the spherical shape. In particular, we quantify the effect of surface stresses on the velocity field and, consequently, on the shape of the interface as the droplet evolves by either shrinking or expanding.

**12:27PM B53.00007 Study of the (1 + 1)D Long Wavelength Steady States of the Bénard Problem For Ultrathin Films**, CHENGZHE ZHOU, SANDRA TROIAN, California Institute of Technology, 1200 E California Blvd., MC 128-95, Pasadena, CA — We investigate the stationary states of the (1 + 1)D equation  $h_t + [h^3 h_{xxx} + h^2 \gamma_x(h)]_x = 0$  for thin films of thickness  $h(x, t)$  where  $x$  is the spatial variable and  $t$  is time. The variable  $\gamma(h)$ , denotes the surface tension along the gas/liquid interface of the slender bilayer confined between two substrates enforcing thermal conduction within the gap. Equilibrium solutions include flat films, droplets, trenches/ridges and positive periodic steady states (PPSS), the latter conveniently parameterized by a generalized interfacial pressure and the global extremum in shape. We derive perturbative solutions describing PPSS shapes near the stability threshold including their minimal period, average height and free energy. Weakly nonlinear analysis confirms that flat films always undergo a supercritical unstable pitch-fork bifurcation. Globally, our numerical simulations indicate at most one non-trivial PPSS per given period and volume. The free energy of droplet states is also always lower than the relevant corresponding PPSS, suggesting that initial flat films tend to redistribute mass into droplet-like configurations. By solving the linearized eigenvalue problem, we also confirm the unstable nature of PPSS solutions far from the stability threshold.

**12:39PM B53.00008 Collective oscillations and coupled modes in confined microfluidic droplet arrays<sup>1</sup>**, ULF D. SCHILLER, Department of Materials Science and Engineering, Clemson University, JEAN-BAPTISTE FLEURY, RALF SEEMANN, Experimental Physics, Saarland University, GERHARD GOMPPER, Institute of Complex Systems, Forschungszentrum Jülich — Microfluidic droplets have a wide range of applications ranging from analytic assays in cellular biology to controlled mixing in chemical engineering. Ensembles of microfluidic droplets are interesting model systems for non-equilibrium many-body phenomena. When flowing in a microchannel, trains of droplets can form microfluidic crystals whose dynamics are governed by long-range hydrodynamic interactions and boundary effects. In this contribution, excitation mechanisms for collective waves in dense and confined microfluidic droplet arrays are investigated by experiments and computer simulations. We demonstrate that distinct modes can be excited by creating specific 'defect' patterns in flowing droplet trains. While longitudinal modes exhibit a short-lived cascade of pairs of laterally displacing droplets, transversely excited modes form propagating waves that behave like microfluidic phonons. We show that the confinement induces a coupling between longitudinal and transverse modes. We also investigate the life time of the collective oscillations and discuss possible mechanisms for the onset of instabilities. Our results demonstrate that microfluidic phonons can exhibit effects beyond the linear theory, which can be studied particularly well in dense and confined systems.

<sup>1</sup>This work was supported by Deutsche Forschungsgemeinschaft under grant no. SE 1118/4.

**12:51PM B53.00009 Drop impact on inclined superhydrophobic surfaces<sup>1</sup>**, WONJAE CHOI, SANI LECLEAR, JOHNATHON LECLEAR, . ABHIJEET, University of Texas at Dallas, KYOO-CHUL PARK, Harvard University — We report an empirical study and dimensional analysis on the impact patterns of water drops on inclined superhydrophobic surfaces. While the classic Weber number determines the spreading and recoiling dynamics of a water drop on a horizontal / smooth surface, for a superhydrophobic surface, the dynamics depends on two distinct Weber numbers, each calculated using the length scale of the drop or of the pores on the surface. Impact on an inclined superhydrophobic surface is even more complicated, as the velocity that determines the Weber number is not necessarily the absolute speed of the drop but the velocity components normal and tangential to the surface. We define six different Weber numbers, using three different velocities (absolute, normal and tangential velocities) and two different length scales (size of the drop and of the texture). We investigate the impact patterns on inclined superhydrophobic surfaces with three different types of surface texture: (i) posts, (ii) ridges aligned with and (iii) ridges perpendicular to the impact direction. Results suggest that all six Weber numbers matter, but affect different parts of the impact dynamics, ranging from the Cassie-Wenzel transition, maximum spreading, to anisotropic deformation.

<sup>1</sup>We acknowledge financial support from the Office of Naval Research (ONR) through Contract 3002453812.

**1:03PM B53.00010 Spreading of water nanodroplets on graphene**, JOSEPH ANDREWS, SHAYANDEV SINHA, PETER CHUNG, SIDDHARTHA DAS, Univ of Maryland-College Park — Understanding the wetting of 2D materials is central to the successful application of these materials in a variety of disciplines that involve the interaction of a liquid with such layered substrates. Recent studies focusing on wetting statics and contact angle selection on graphene-coated solids indicate a wetting translucent behavior of graphene. However, little research has been done on the wetting dynamics of graphene-coated systems. Here, we simulate the wetting dynamics of water drops on free-standing graphene layers using a molecular dynamics framework. We employ the extended simple point charge (SPC/E) model to simulate the water drops. Our simulations are validated against the experimental results of water drop contact angles on graphite. Unlike many existing MD studies, we obtain the results starting from a physical consideration of spherical water drops. We observe the half power law for the spreading dynamics, i.e.,  $r \sim t^{1/2}$  ( $r$  is the spreading radius and  $t$  is the spreading time). Identical spreading laws have been identified for Lennard Jones (LJ) nanodroplets on non-layered surfaces; therefore, we establish that the change in the nature of the substrate (non-layered to 2D) and the liquid (LJ to water) does not alter the physics of wetting dynamics of nanodroplets.

**1:15PM B53.00011 Domain and rim growth kinetics in stratifying foam films**, YIRAN ZHANG, SUBINUER YILIXIATI, VIVEK SHARMA, University of Illinois at Chicago — Foam films are freely standing thin liquid films that typically consist of two surfactant-laden surfaces that are ~5 nm – 10 micron apart. Sandwiched between these interfacial layers is a fluid that drains primarily under the influence of viscous and interfacial forces, including disjoining pressure. Interestingly, a layered ordering of micelles inside the foam films (thickness <100 nm) leads to a stepwise thinning phenomena called stratification, which results in a thickness-dependent variation in reflected light intensity, visualized as progressively darker shades of gray. Thinner, darker domains spontaneously grow within foam films. During the initial expansion, a rim forms near the contact line between the growing thinner domain and the surrounding region, which influences the dynamics of domain growth as well as stratification. Using newly developed interferometry digital imaging optical microscopy (IDIOM) technique, we capture the rim evolution dynamics. Finally, we also develop a theoretical model to describe both rim evolution and domain growth dynamics.

**1:27PM B53.00012 Drop formation, pinch-off dynamics and liquid transfer of simple and complex fluids**, JELENA DINIC, VIVEK SHARMA, University of Illinois at Chicago — Liquid transfer and drop formation processes underlying jetting, spraying, coating, and printing – inkjet, screen, roller-coating, gravure, nanoimprint hot embossing, 3D – often involve formation of unstable columnar necks. Capillary-driven thinning of such necks and their pinchoff dynamics are determined by a complex interplay of inertial, viscous and capillary stresses for simple, Newtonian fluids. Micro-structural changes in response to extensional flow field that arises within the thinning neck give rise to additional viscoelastic stresses in complex, non-Newtonian fluids. Using FLOW-3D, we simulate flows realized in prototypical geometries (dripping and liquid bridge stretched between two parallel plates) used for studying pinch-off dynamics and influence of microstructure and viscoelasticity. In contrast with often-used 1D or 2D models, FLOW-3D allows a robust evaluation of the magnitude of the underlying stresses and extensional flow field (both uniformity and magnitude). We find that the simulated radius evolution profiles match the pinch-off dynamics that are experimentally-observed and theoretically-predicted for model Newtonian fluids and complex fluids.

**1:39PM B53.00013 Simulations of high and low viscosity micro-scale droplets splashing on a dry surface**, ARNOUT BOELEN, ANDRZEJ LATKA, JUAN DE PABLO, University of Chicago — When a droplet hits a dry surface at atmospheric pressure with a high enough impact velocity, it splashes and breaks apart into many smaller droplets. However, when the ambient gas pressure is reduced, splashing is suppressed. This is contrary to intuition, which suggests a more violent splash should occur at lower gas densities due to reduced drag forces. Although splashes of high and low viscosity liquids visually look very different, they also obey the pressure effect. In this study the effect of viscosity on splashing is investigated, to get a better understanding of the pressure effect in general. Simulation results are presented comparing splashing of low viscosity ethanol with high viscosity silicone oil in air. The droplets are several hundred microns large. The simulations are 2D, and are performed using a Volume Of Fluid approach. The contact line is described using the Generalized Navier Boundary Condition. Both the gas phase and the liquid phase are assumed to be incompressible. The results of the simulations show good agreement with experiments, including reproduction of the pressure effect, and suggest that the same scaling laws that apply to lamella formation in simple drop deposition, also apply to splashing droplets.

**1:51PM B53.00014 Dynamics of Wetting and Wicking on Rough Surfaces**, DION ANTAO, DANIEL PRESTON, SOLOMON ADERA, YANGYING ZHU, EVELYN WANG, Massachusetts Institute of Technology — Micro/nano engineering of surfaces to enhance the performance of phase-change heat transfer processes has recently gained wide interest. Interfacial phenomena at the micro/nanoscale play an important role in defining the dynamic wetting and wicking characteristics of the surfaces. Here we report experiments that characterize the dynamic wetting and wicking processes on microstructured silicon surfaces. We investigated cylindrical micropillar arrays in a square pattern with various diameter, pitch, and height to characterize key interfacial behavior over a wide range of surface roughness. The experiments were performed by dipping the microstructured sample vertically into a reservoir of de-ionized water and the spreading dynamics were captured with a high speed camera. We observed that both wetting and wicking exhibit a power law dependence on time, however they occur at different time scales. The instantaneous (~10-100 ms) wetting behavior occurs due to the interfacial tensions, and the resultant force acting at the three-phase contact line. The longer time scale (>100 ms) wicking behavior results from the balance of the capillary pressure generated within the microstructure and the viscous pressure loss from flow through the micropillar array. We develop analytical models to predict these different time scale behavior and compare them to experimental results. This work provides insight into key dynamic processes affecting micro/nanostructure enhanced phase-change heat transfer devices.

**2:03PM B53.00015 ABSTRACT WITHDRAWN —**

**Monday, March 14, 2016 11:15AM - 2:15PM —**

**Session B54 FIAP DMP: Optical Properties of Semiconductor Nanostructures II** Hilton Baltimore Holiday Ballroom 5 - Alexander Efros, Naval Research Lab

**11:15AM B54.00001 Experimental evidence of  $\alpha \rightarrow \beta$  phase transformation in SiC quantum dots and their size-dependent luminescence**, XIAOXIAO GUO, Department of Physics, Southeast University, DEJIAN DAI, Department of Physics, Southeast University, Nanjing 211189, PR China, BAOLU FAN, Department of Physics, Southeast University, JIYANG FAN, Department of Physics, Southeast University, Nanjing 211189, PR China — Silicon carbide (SiC) quantum dots (QDs) have attracted great interest due to their wide application in photonics, optoelectronics, and life sciences. SiC is an outstanding wide-bandgap semiconductor for applications in high power, high temperature, and high frequency electronic devices owing to its superior physical and mechanical properties. As a wide-bandgap semiconductor, SiC has over 250 crystalline structures, and some polytypes have been found in the presolar meteorites. Phase transformation can occur among different SiC polytypes under extreme conditions such as high pressure or high temperature. It remains unknown whether phase transformation can occur under normal conditions. We demonstrate that the  $\alpha \rightarrow \beta$  phase transformation can occur at ambient temperature and pressure in nanoscale SiC. The microstructural characterization and light absorption and emission spectroscopy demonstrate the occurrence of this phase transformation. It is found that the quantum-confinement luminescence dominates in larger SiC QDs and the surface-defect luminescence dominates in ultrasmall SiC QDs. The rare phenomenon of photon absorption accompanied by emission or absorption of multiple phonons has been observed, demonstrating the indirect-bandgap nature of the SiC QDs.

**11:27AM B54.00002 Two-photon absorption in 3-100nm diameter Silicon nanocrystals in solution**, BRANDON FUREY<sup>1</sup>, MICHAEL DOWNER<sup>2</sup>, YIXUAN YU<sup>3</sup>, BRIAN KORGEL<sup>4</sup>, University of Texas at Austin — Silicon nanocrystals (nc-Si) exhibit efficient photoluminescence (PL) that has applications in non-toxic bio-imaging. Two-photon absorption (TPA) is an important process for exciting PL in the tissue transparency spectral window, but absolute TPA coefficients have not been measured as a continuous function of nc size or excitation wavelength. Previous TPA studies have focused on nc-Si embedded in an oxide matrix or on porous Si surfaces at selected discrete wavelengths [1]. However, recently free standing, ligand-stabilized nc-Si with diameters ranging from 3 to 100 nm that are soluble in liquids, including water, and suitable for bio-imaging have become available [3]. We will present calibrated TPA spectra for free standing nc-Si over a wide range of nc diameters, based on measurements with tunable femtosecond laser pulses. We will compare indirect TPA measurements based on collection and detection of PL with direct TPA measurements based on attenuation of the incident beam. [1] P. Zhang, Z. Zhang, K. Chen et al., Nanoscale Res. Lett. 9 (28), 1 (2014) [2] C.M. Hessel, J. Wei, B. Korgel et al., Chem. Mater. 24 (2), 393 (2012)

<sup>1</sup>Department of Physics

<sup>2</sup>Department of Physics

<sup>3</sup>Department of Chemical Engineering

<sup>4</sup>Department of Chemical Engineering

**11:39AM B54.00003 ABSTRACT WITHDRAWN —**

**11:51AM B54.00004 Stimulated emission and lasing from all-inorganic perovskite quantum dots**, HANDONG SUN, YUE WANG, Nanyang Technological University, XIAOMING LI, ZENG HAIBO, Nanjing University of Science and Technology — We present superior optical gain and lasing properties in a new class of emerging quantum materials, the colloidal all-inorganic cesium lead halide perovskite quantum dots (IPQDs) ( $\text{CsPbX}_3$ ,  $X = \text{Cl, Br, I}$ ). Our result has indicated that such material system show combined merits of both colloidal quantum dots and halide perovskites. Low-threshold and ultrastable stimulated emission was demonstrated under atmospheric condition. The flexibility and advantageous optical gain properties of these  $\text{CsPbX}_3$  IPQDs were manifested by demonstration of an optically pumped micro-laser. The nonlinear optical properties including the multi-photon absorption and resultant photoluminescence of the  $\text{CsPbX}_3$  nanocrystals were investigated. A large two-photon absorption cross-section of up to  $\sim 1.2105 \text{ GM}$  is determined from 9 nm-sized  $\text{CsPbBr}_3$  nanocrystals. Moreover, low-threshold frequency-upconverted stimulated emission by two-photon absorption was observed from the thin films of close-packed  $\text{CsPbBr}_3$  nanocrystals. We further realize the three-photon pumped stimulated emission in green spectra range from colloidal IPQD.

**12:03PM B54.00005 Control of Photo- and Electro-generated Excited States of Colloidal Quantum Dots**, XIAOGANG PENG, Zhejiang Univ — Colloidal semiconductor nanocrystals (quantum dots) as solution-processible photo- and electro-excited emitters are promising and may impact many industrial sectors. Both photoluminescence and electroluminescence are based on generation and relaxation of the excited states. Thus, properties of excited states should be the key for design, synthesis, understanding, and applications of emitters. Specifically, as promising emissive materials, colloidal quantum dots rely heavily on their excited-state properties, instead of solely the ground-state properties.

**12:15PM B54.00006 Self-assembled single-mode micro-lasers of "giant" CdSe/CdS core/shell quantum dots**, CHEN LIAO, JIAYU ZHANG, Advanced Photonic Center, Southeast University — So-called giant quantum dots (g-QDs) as optical gain media have attracted much attention due to their near elimination of nonradiative Auger effects. In the present work, phase-pure wurtzite CdSe/CdS core/shell QDs with controlled shell thickness are successfully synthesized, and the threshold of amplified spontaneous emission (ASE) of the films of this series of QDs is measured. The threshold of ASE is decreased dramatically with the CdS shell growth towards 11 monolayers (MLs) ( $21 \mu\text{J}/\text{cm}^2$ ), but increased with the further shell growth. The effects of the overlap degree of electron and hole wave functions, surface states, and absorption cross-section are discussed to explain the ASE properties of the QDs. Moreover, the low-threshold gain of the CdSe/CdS core/shell (11 MLs) g-QDs is exploited to fabricate micro-lasers solely by deposition of small droplets of QDs solution onto glass substrates. The evaporation dynamics of the droplets are governed by the coffee-ring effect which leads to the formation of well defined micron-size rings. The self-assembled coffee-ring micro-lasers display single-mode operation and a very low threshold of  $3 \mu\text{J}/\text{cm}^2$ . Herein, an innovative, simple and reliable method to produce micro-lasers based on CdSe/CdS g-QDs is presented.

**12:27PM B54.00007 Red shift in the photoluminescence of colloidal carbon quantum dots induced by photon reabsorption**, WENXIA ZHANG, JIYANG FAN, Department of Physics, Southeast University, Nanjing 211189, Peoples Republic of China, DEPARTMENT OF PHYSICS, SOUTHEAST UNIVERSITY, NANJING 211189, PEOPLES REPUBLIC OF CHINA TEAM — We synthesize the colloidal carbon/graphene quantum dots 1-9 nm in diameter through a novel alkaline-assisted method and deeply studied their photoluminescence properties. Surprisingly, the luminescence properties of a fixed collection of carbon dots can be systematically changed as the concentration varies. A model based on photon reabsorption is proposed which explains well the experiment. Infrared spectral study indicates that the surfaces of the carbon dots are totally terminated by three bonding-types of oxygen atoms, which result in their ultra-high hydrophilicity. Our result clarifies the mystery of distinct emission colors in carbon dots and indicates that photon reabsorption can strongly affect the luminescence properties of colloidal nanocrystals. This mechanism can be generalized to help understand the complex luminescence properties of other colloidal quantum dots. and should be seriously considered, otherwise, distinct conclusions may be drawn if different concentrations of quantum dots have been utilized in studying their luminescence properties.

**12:39PM B54.00008 Tunable Emission in Inverted Type-I CdS/CdSe Core/Crown Semiconductor Nanoplatelets**, PEDRO LUDWIG HERNANDEZ-MARTINEZ<sup>1</sup>, Nanyang Technological University, SAVAS DELIKANLI, BURAK GUZELTURK<sup>2</sup>, TALHA ERDEM, YUSUF KELESTEMUR, MURAT OLUTAS, MEHMET ZAFER AKGUL, Bilkent University, HILMI VOLKAN DEMIR<sup>3</sup>, Nanyang Technological University — In this work, we present the tunable optical properties of an inverted Type-I core/crown nanoplatelet heterostructure. We show that the emission peak of the resulting CdS/CdSe hetero-nanoplatelets can be tuned continuously between the peak emission wavelengths of the core only CdS nanoplatelets (421 nm) and CdSe nanoplatelets (515 nm). In these inverted Type-I nanoplatelets, the unique continuously tunable emission is enabled by adjusting the lateral width of the CdSe crown, around the core CdS nanoplatelet. As a proof-of-concept, we generate white light by using color conversion concept with CdS/CdSe hetero-nanoplatelets, which have finely tuned thin crowns. This results in a color rendering index of 80.

<sup>1</sup>Bilkent University

<sup>2</sup>Nanyang Technological University

<sup>3</sup>Bilkent University

**12:51PM B54.00009 Nonradiative Auger recombination of biexcitons in CdSe/CdS core-shell nanocrystal quantum dots**, ROMAN VAXENBURG, George Mason University, Fairfax, VA 22030, USA, ANNA RODINA, Ioffe Institute, St. Petersburg, 194021, Russia, EFRAT LIFSHITZ, Technion Israel Institute of Technology, Haifa, 32000, Israel, ALEXANDER EFROS, Naval Research Laboratory, Washington, DC 20375, USA — Semiconductor nanocrystals are known for their applicative potential as light-emitting components in lasers and LEDs, as well as light absorbers in solar cells. The performance of these nanocrystal-based devices, however, strongly depends on the dissipative nonradiative Auger recombination. The study of dynamics of the Auger processes is therefore of key importance in connection with the performance of nanocrystals devices. Here we report on a theoretical study of the Auger recombination dynamics of biexcitons in CdSe/CdS core-shell nanocrystals. Biexcitons can decay by the Auger process via negative or positive trion recombination channels. We study the dependence of the rate of each one of these channels on the angular momentum of the initial biexciton state, nanocrystal geometry, and temperature. We observe that the overall dependence of the rates of both channels is strongly oscillating with nanocrystal geometry, indicating large differences in the Auger rates in nanocrystals of similar size. We find that the rate of the negative trion channel is independent of the initial biexciton angular momentum and is generally slower than the rate of the positive trion channel, which, in contrast, is sensitive to the biexciton angular momentum. Further, we demonstrate that by variation of temperature the Auger rate can be varied across a wide range of values.

**1:03PM B54.00010 Dangling Bond Magnetic Polaron in CdSe nanocrystals**, ALEXANDER EFROS, Naval Research Lab, ANNA RODINA, Ioffe Physico-Technical Institute, RAS — In this work we study theoretically the effect of the spins of the surface dangling bonds on the PL of CdSe nanocrystals (NCs). [1] We show that spins of dangling bonds open new recombination channels for the dark exciton recombination which is connected with flip-flip and flip-flop spin-assisted recombination of the dark exciton. Calculations show that at low temperatures the interaction between dangling bonds and NC excitons leads to the dynamical polarization of the dangling bond spins along the anisotropic axis following by the formation of a dangling bond magnetic polaron. An increase of the temperature, or of the external magnetic field perpendicular to the anisotropic axis, destroys the polaron state. This results in a shift of the transition energy and an increase of its recombination rate. Thus thermal depolarization of the polaron state may explain the small activation energies observed in the temperature dependences of the exciton lifetimes in CdSe NCs. The exchange interaction of the electron spin with spins of the surface dangling bonds explains also radiative recombination of the dark excitons in nanowires, nanorods and nanoplatelets. [1] A. Rodina and A.I. Efros, Nano Lett. v. 15, 4214-4222 (2015)

**1:15PM B54.00011 Superradiance in Spherical Layered Nanostructures**, SERGUEI GOUPALOV, Jackson State Univ — We propose a design of a spherically symmetric nanostructure consisting of alternate concentric semiconductor and dielectric layers. The exciton states in different semiconductor layers of such a structure interact via the common electro-magnetic field of light. We show that, if the exciton states in  $N$  semiconductor layers are in resonance with one another, then superradiant states can emerge under optical excitation of such a structure. We discuss the conditions under which superradiance can be observed and show that they strongly depend on the valence-band structure of the semiconductor layers.

**1:27PM B54.00012 Macrocrystals of Colloidal Quantum Dots in Anthracene: Exciton Transfer and Polarized Emission**, ZELIHA SORAN-ERDEM, TALHA ERDEM, Bilkent University, PEDRO LUDWIG HERNANDEZ-MARTINEZ<sup>1</sup>, Nanyang Technological University, MEHMET ZAFER AKGUL, Bilkent University, NIKOLAI GAPONIK, TU Dresden, HILMI VOLKAN DEMIR<sup>2</sup>, Nanyang Technological University — We systematically investigate the exciton energy transfer from anthracene host (donor) to quantum dots (acceptor) in a centimeter-scale macrocrystal of nonpolar colloidal quantum dots incorporated into anthracene. The decrease in photoluminescence lifetime of the donor anthracene indicate a strong energy transfer with increasing quantum dot concentration in the macrocrystals. In addition, anisotropic emission from the isotropic quantum dots in anthracene macrocrystals was observed. The quantum dots inside the anthracene host acquired a polarization ratio of  $\sim 1.5$  at 0 degree collection angle, and this increases to  $\sim 2.5$  at the collection angle of 60 degree. Finally, a proof-of-concept application of these excitonic macrocrystals as tunable color converters was employed in light-emitting diodes.

<sup>1</sup>Bilkent University

<sup>2</sup>Bilkent University

**1:39PM B54.00013 Optical Properties of the Defect State Luminescence of Zn<sub>2</sub>SnO<sub>4</sub> Nanowires**<sup>1</sup>, BAICHHABI YAKAMI, UMA PAUDYAL, SHASHANK NANDYALA, GAURAB RIMAL, University of Wyoming, JASON K. COOPER, Lawrence Berkeley National Laboratory, JIAJUN CHEN, University of New Orleans, TEYU CHIEN, WENYONG WANG, JON M PIKAL, University of Wyoming, DEPARTMENT OF ELECTRICAL AND COMPUTER ENGINEERING TEAM, DEPARTMENT OF PHYSICS AND ASTRONOMY TEAM — Nanowires (NWs) are a promising option for sensitized solar cells, sensors & display technology. Most of the work thus far has focused on binary oxides for these NWs, but ternary oxides have advantages in additional control of optical and electronic properties. Here we report on the diffuse reflectance, Low Temperature (LT) and Room Temperature (RT) photoluminescence (PL), PL excitation and Time Resolved PL (TRPL) of Zinc Tin Oxide (ZTO) NWs grown by Chemical Vapor Deposition. Our results show two broad peaks centered at 640 nm & 450 nm. The complex emission spectra was studied by Time Resolved Emission Spectroscopy (TRES) and Intensity dependent PL. The intensity dependent TRPL shows that 640 nm states decay much slower than the 450 nm states. We propose an energy band model for the NWs containing donor and acceptor states in the band gap with the associated transitions between these states that are consistent with our results. The effect of annealing in air and vacuum is carried out to study the origin of defect states in these NWs. .

<sup>1</sup>Department of Energy

**1:51PM B54.00014 Photoluminescence of Sequential Infiltration Synthesized ZnO nanostructures.**<sup>1</sup> , LEONIDAS OCOLA, Argonne Natl Lab, DAVID GOSZTOLA, ANGEL YANGUAS-GIL, Argonne National Laboratory, AINE CONNOLLY, Vassar College — We have investigated a variation of atomic layer deposition (ALD), called sequential infiltration synthesis (SiS), as an alternate method to incorporate ZnO and other oxides inside polymethylmethacrylate (PMMA) and other polymers. Energy dispersive spectroscopy (EDS) results show that we synthesize ZnO up to 300 nm inside a PMMA film. Photoluminescence data on a PMMA film shows that we achieve a factor of 400X increase in photoluminescence (PL) intensity when comparing a blank Si sample and a 270 nm thick PMMA film, where both were treated with the same 12 alternating cycles of H<sub>2</sub>O and diethyl zinc (DEZ). PMMA is a well-known ebeam resist. We can expose and develop patterns useful for photonics or sensing applications first, and then convert them afterwards into a hybrid polymer-oxide material. We show that patterning does indeed affect the photoluminescence signature of native ZnO. We demonstrate we can track the growth of the ZnO inside the PMMA polymer using both photoluminescence and Raman spectroscopy and determine the point in the process where ZnO is first photoluminescent and also at which point ZnO first exhibits long range order in the polymer.

<sup>1</sup>This work was supported by the Department of Energy under Contract No. DE-AC02-06CH11357. Use of the Center for Nanoscale Materials was supported by the U. S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

**2:03PM B54.00015 X-ray Analysis of Self-assembled Nano-Dielectrics** , LI ZENG, Northwestern University, RICCARDO TURRISI, University of Milano-Bicocca, JONATHAN EMERY, MARK HERSAM, TOBIN MARKS, MICHAEL BEDZYK, Northwestern University — Organic thin-film transistors (OTFTs) are viewed as the new generation thin-film transistors (TFT) for future low-cost, printable, flexible electronics. A class of materials called self-assembled nano-dielectrics (SAND) with phosphoric acid-based-electron (PAE) building blocks sandwiched between ultrathin layers of high-*k* inorganic oxide materials has been synthesized. These materials show exceptional large capacitance, insulating properties, and are also suitable for ambient atmosphere fabrication. The hybrid nature of these materials combines the distinct properties of both the organic and inorganic components and can be incorporated into the low-operating voltage semiconductor-based OTFT. Despite the great performance and flexibility of SANDs, fundamental aspects of dielectric behavior remain unexplored. Particularly, the behaviors of the Br counteranions that exist within PAE building blocks are poorly understood. Therefore, long-period X-ray Standing Wave (LP-XSW), which is a powerful technique sensitive to heavy atom distributions, was used to characterize SAND deposited on synthetic Si/Mo multilayer substrates. The elemental distributions of Br and reference elements were extracted from the analysis of XSW data. These accurate measurements are important for better understanding of counteranions distributions, charge transportation, dipole-semiconductors interactions, and future device modeling and engineering.

## Monday, March 14, 2016 11:15AM - 2:15PM –

**Session B55 DBIO: Complex Microbial Communities** Hilton Baltimore Holiday Ballroom 6 - Jeff Gore, Massachusetts Institute of Technology

**11:15AM B55.00001 Evolution of Metabolic Dependency**<sup>1</sup> , WENYING SHOU, Fred Hutchinson Cancer Research Center — Microbes are often found to have lost their ability to make essential metabolites (auxotrophs) and instead rely on other individuals for these metabolites. How might metabolic dependency evolve to be so common? When microbes live inside a host (endosymbionts), amply host metabolites support auxotrophic endosymbionts. If the host transmits only a small number of endosymbionts to its offspring, then auxotrophic endosymbionts can rise to high frequency simply by chance. On the other hand, auxotrophs have also been observed in abundant free-living bacteria found in ocean water where nutrient supply is low. How might auxotrophs rise to an appreciable frequency in a large population when nutrient supply is low? We have found commonly-encountered conditions that facilitate the evolution of metabolic dependency. Metabolic interactions can in turn shape spatial organization of microbial communities (Momeni et al. (2013) eLife 2, 00230; Momeni et al. (2013) eLife 2, 00960; Estrela and Brown (2013) PLoS Comput Biol 9, e1003398; Muller et al. (2014) PNAS 111, 1037-1042). Rapid evolution of metabolic dependency can contribute to the complexity of microbial communities.

<sup>1</sup>Evolution of metabolic dependency

**11:51AM B55.00002 Visualizing the population dynamics of microbial communities in the larval zebrafish gut**<sup>1</sup> , RAGHUVeer PARTHASARATHY, The University of Oregon — In each of our digestive tracts, trillions of microbes representing hundreds of different species colonize local environments, reproduce, and compete with one another. The resulting ecosystems influence many aspects their hosts development and health. Little is known about how gut microbial communities vary in space and time: how they grow, fluctuate, and respond to various perturbations. To address this and investigate microbial colonization of the vertebrate gut, we apply light sheet fluorescence microscopy to a model system that combines a realistic *in vivo* environment with a high degree of experimental control: larval zebrafish with defined subsets of commensal bacterial species. Light sheet microscopy enables three-dimensional imaging with high resolution over the entire intestine, providing visualizations that would be difficult or impossible to achieve with other techniques. Quantitative analysis of image data enables measurement of bacterial abundances and distributions. I will describe this approach and focus especially on recent experiments in which a colonizing bacterial species is challenged by the invasion of a second species, which leads to the decline of the first group. Imaging reveals dramatic population collapses that differentially affect the two species due to their different biogeographies and morphologies. The collapses are driven by the peristaltic motion of the zebrafish intestine, indicating that the physical activity of the host environment can play a major role in mediating inter-species competition. role in mediating inter-species competition.

<sup>1</sup>Supported by the National Science Foundation under grant no. 0922951 and the National Institutes of Health under award number 1P50GM098911.

**12:27PM B55.00003 Forming Stable Complex Communities: Random vs. Evolved Interactions** , DAVID KESSLER, Bar Ilan Univ — We examine the problem of constructing a stable complex community of competing species. We first investigate the case of a randomly generated set of interactions and investigate the different regimes. Here, May showed that if the interactions are not very weak, the system typically does not a steady-state with all species present. We show from simulation that the system typically goes to a non-steady state for interaction strengths above an order 1 multiple of the critical May strength. When demographic stochasticity is added, the system typically jumps from one invadable state to another. For extremely strong competition however, the system does revert to one of a number of steady state. Our model contains, as special cases, the celebrated neutral island theories of Wilson-MacArthur and Hubbell. Moreover, we show that slight deviations from perfect neutrality may lead to each of the phases, as the Hubbell point appears to be quadracritical. If, however, the system is allowed to evolve its set of interactions, each new species inheriting its interactions from its parent species, then the system can produce an interaction matrix which is capable of supporting a large number ( $\sim 100$ ) of coexisting species. The key to evolutionary success turns out to be how the child species interacts with its parent.

**1:03PM B55.00004 Adaptive landscapes: Top-down and bottom-up perspectives** , BENJAMIN KERR, University of Washington — Sewall Wright introduced the metaphor of the adaptive landscape, a map from genotype to fitness, more than 80 years ago to help describe his view of adaptive evolution. This metaphor has been immensely popular and has been used in a variety of incarnations. However, a systematic study of the genotype-fitness map presents significant problems. The space of possible genotypes is vast, and the mapping is likely dependent on both environment and the composition of genotypes in a population. In this talk, I will discuss some of these problems and present experimental strategies for uncovering features of adaptive landscapes. In particular, I will discuss how population structure can be used as an experimental variable to elucidate landscape topography and how a combination of experimental evolution and genetic engineering can reveal important landscape features in changing environments. I will also present some potential applications of this work to the problem of antibiotic resistance and potential implications for evolutionary rescue in the face of global climate change. For some of these topics, the classic notion of the adaptive landscape must itself be adapted; however, I propose that there are fruitful ways to continue to apply this metaphor.

**1:39PM B55.00005 Principles of Virus-Microbe Dynamics: From Ecology to Evolution and Back Again** , JOSHUA WEITZ, Georgia Institute of Technology — Viruses are ubiquitous in the environment and can function like microbial predators, regulating the density and diversity of microbes present in a community. However, efforts to understand the dynamics of complex virus-microbe communities remain in their infancy. In this talk, I present examples of the interplay between evolutionary and ecological dynamics arising due to virus-microbe interactions. I begin by introducing canonical models of virus-microbe population dynamics in the context of observed oscillations of *E. coli* and associated phage. I then present a series of examples in which novel features observed in time series data arising from phage interactions with *E. coli* and *V. cholerae* can be understood when considering both population and evolutionary dynamics together. I conclude by presenting our recent efforts to extend the results of laboratory experiments to an environmental context, with significantly higher diversity of both viruses and microbes. Despite this increase in diversity, I show how network theoretic methods can reveal common principles underlying the dynamic coexistence of complex virus and host communities. Building on these findings, I describe new efforts to infer who infects whom directly from time series of multi-strain communities.

**Monday, March 14, 2016 12:00PM - 2:15PM –**

**Session B60 APS: Meet Your Future: An Interactive Session on Industrial Careers for Physicists**

Hilton Baltimore Key Ballroom 3/4 -

**12:00PM B60.00001 Meet Your Future: An Interactive Session on Industrial Careers for Physicists –**

**Monday, March 14, 2016 2:30PM - 5:30PM –**

**Session C1 DCMF: New Developments in Iron Chalcogenide Superconductors** Ballroom I - Ming Yi,

University of California Berkeley

**2:30PM C1.00001 Frustrated Magnetism and Superconductivity in the Iron Chalcogenides<sup>1</sup>** ,

QIMIAO SI, Rice Univ — While studies in the early stage on the iron-based superconductors (FeSCs) focused on the iron pnictides, considerable efforts in the more recent past have also been directed towards iron chalcogenides. These studies are giving us renewed hope for even higher transition temperatures in the iron-based materials. In this talk, I will discuss several theoretical issues on the microscopic physics of the iron chalcogenides that teach us much about the overall physics of the FeSCs. One is the proposal we made on the orbital selective Mott phase [1], for which considerable evidence has come from ARPES [2] and other experiments. The second issue concerns magnetism, in particular the correlation-induced magnetic frustration effect. A major puzzle arises in bulk FeSe, which shows a structural phase transition similar to that seen in the iron pnictides but, unlike the latter, does not exhibit any static antiferromagnetic order. We studied the effect of magnetic frustration associated with the bilinear-biquadratic spin-exchange interactions [3]. Based on the derived phase diagram, we proposed that the structural transition in FeSe originates from an Ising-nematic order of an antiferro-quadrupolar phase. Within this picture, we have predicted that the collective modes of this quadrupolar state show  $(\pi, 0)$  magnetic fluctuations, which have since been verified by inelastic neutron scattering experiments [4]. These results considerably expand on the notion [5] regarding the importance of the bad-metal behavior, and provide a substantially broadened perspective on the magnetic and nematic correlations in the FeSCs. Finally, implications of the frustrated magnetism for superconductivity [5] will also be discussed. References: [1] R. Yu and Q. Si, Phys. Rev. Lett. 110, 146402 (2013). [2] M. Yi et al., Nature Commun. 6, 7777 (2015). [3] R. Yu and Q. Si, Phys. Rev. Lett. 115, 116401 (2015). [4] M. Rahn et al., Phys. Rev. B 91, 180501(R) (2015); Q. Wang et al., arXiv:1502.07544. [5] Q. Si and E. Abrahams, Phys. Rev. Lett. 101, 076401 (2008). [6] E. Nica, R. Yu and Q. Si, arXiv:1505.04170.

<sup>1</sup>Work supported in part by the NSF Grant No. DMR-1309531 and the Robert A. Welch Foundation Grant No. C-1411.

**3:06PM C1.00002 On nematicity, magnetism and superconductivity in FeSe<sup>1</sup>** , ANNA BÖHMER, Ames

Laboratory, U.S. Department of Energy, Iowa State University, Ames, Iowa 50011 — FeSe is unique among iron-based superconductors, notably regarding the interrelationships of structure, magnetism, and superconductivity. At ambient pressure, FeSe exhibits a tetragonal-to-orthorhombic (nematic) phase transition at  $T_s = 90$  K, similar to other iron-based materials, but unlike them, no long-range magnetic order. One consequence is the unique possibility to study the in-plane resistivity anisotropy, arguably the most investigated nematic property, without interfering effects from the Fermi surface reconstruction induced by antiferromagnetic order. Recent findings pose the question whether nematicity in FeSe is driven by magnetic fluctuations, as often assumed in other iron-based systems. In particular, magnetic fluctuations, which are prominent at low temperatures, are not observed above  $T_s$  in FeSe by NMR [1,2], even though indicated by inelastic neutron scattering. The pressure-temperature phase diagram, recently obtained in new comprehensiveness using vapor-grown single crystals [3], shows that the structural transition is suppressed at 2 GPa and a new, likely magnetic phase is stabilized above 0.8 GPa, where  $T_c$  has a local maximum. Various theoretical scenarios have been proposed to explain this nematic transition far away from the magnetic order. Surprisingly, the degree of the orthorhombic distortion does not decrease below the superconducting transition at  $T_c = 8$  K, suggesting that nematic and superconducting channels do not compete [4]. Our new results on the superconducting state under pressure, show a non-monotonic pressure dependence of the upper critical field, which is well explained by the Fermi surface evolution. Further, we have successfully detwinned FeSe crystals and measured the in-plane resistivity anisotropy and elastoresistivity coefficients and compared them with model calculations of inelastic scattering from spin fluctuations. [1] Böhrer et al., PRL 114, 027001 (2015) [2] Baek et al., Nat. Mat. 14, 210 (2015) [3] Terashima et al., JPSJ 84, 063701 (2015) [4] Böhrer et al., PRB 87 180505 (2013)

<sup>1</sup>This work was supported by the Ames Laboratory, US DOE, under Contract No.DE-AC02-07CH11358.

**3:42PM C1.00003 What Makes the  $T_c$  of FeSe/SrTiO<sub>3</sub> so High ?<sup>1</sup>**, DUNG-HAI LEE, Department of Physics, University of California, Berkeley — Raising the superconducting transition temperature to a point where applications are practical is one of the most important challenges in science. In the history of high  $T_c$  superconductivity there are two landmark events: the discovery of copper-oxide superconductor in 1986, and the discovery of iron-based superconductor in 2006. For the Fe-based superconductors the record of  $T_c$  was 55 K [1] until 2012. In the interface system composed of an one unit cell thick FeSe film grown on the TiO<sub>2</sub> terminated (001) surface of SrTiO<sub>3</sub> an anomalously large superconducting-like energy gap was seen by scan tunneling microscopy for [2]. Later ARPES works show the gap opening temperature can reach nearly the liquid nitrogen boiling temperature [3-7]. More recently several FeSe-related bulk and thin film high  $T_c$  systems have been discovered. This talk reviews some of the recent experimental [7] and theoretical [8] progresses in the study of the mechanism for high temperature superconductivity in this interface system. It offers the author's personal view of why  $T_c$  is so high and how to further increase it [910]. References:

1. Z.A. Ren *et al.*, Chin. Phys. Lett. **25**, 2215-2216 (2008).
2. Q.Y. Wang *et al.*, Chin. Phys. Lett. **29**, 037402 (2012).
3. D.F. Liu *et al.*, Nature Commun. **3**, 931 (2012).
4. S. He *et al.*, Nature Materials **12**, 605-610 (2013).
5. S. Tan *et al.*, Nature Materials **12**, 634-640 (2013).
6. R. Peng *et al.*, Nature Commun. **5**, 5044 (2014).
7. J.J. Lee *et al.*, Nature **515**, 245 (2014).
8. Zixiang Li *et al.*, to be published.
9. D.-H. Lee, Chin. Phys. B, 2015, 24 (**11**): 117405 doi: 10.1088/1674-1056/24/11/117405
10. Much of the contents of this talk are stimulated by the collaborative work with Z-X Shen and his ARPES group members and T. Deveraux and his group members.

<sup>1</sup>DHL was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, grant DE-AC02-05CH11231.

**4:18PM C1.00004 What makes the nematic phase of FeSe different than other iron-based superconductors?**<sup>1</sup>, RAFAEL FERNANDES, University of Minnesota — Most iron-based superconductors display, in their normal state, a transition to a magnetic stripe state that is either accompanied or preceded by a tetragonal-to-orthorhombic transition. The proximity between these two transitions has led to the proposal that they correspond to a two-stage melting of the magnetic stripe state, resulting in a vestigial orthorhombic-paramagnetic nematic phase. Despite the success of this scenario to describe many iron-based materials, the simplest of them, FeSe, displays a high-temperature nematic transition but no long-range magnetic order. Interestingly, in its monolayer form, FeSe displays the highest  $T_c$  of all iron-based materials, raising the question of whether the nematic state of its bulk form could be related to the superconducting state of its monolayer form. In this talk, we investigate theoretically the microscopic origin of the nematic phase of FeSe. By extending the standard RPA formalism, we compare the orbital-order susceptibility and the spin-driven nematic susceptibility of a generic multi-orbital Hubbard model. We find that the former cannot in general drive the nematic transition, and that high-energy magnetic fluctuations play a fundamental role in stabilizing the nematic state in the absence of long-range magnetic order. Focusing on FeSe, we identify two features that distinguish it from all other iron-based materials: a very small Fermi energy and a large degeneracy of the magnetic ground state. We show that both effects enhance the nematic transition temperature at the same time as they suppress the magnetic transition. These results may explain why, in FeSe, the onset of nematic order does not require strong magnetic fluctuations, in contrast to other iron-based materials. Finally, we discuss how the interplay between magnetic fluctuations and small Fermi energy in FeSe can lead to the emergence of different types of Pomeranchuk instabilities, and discuss their experimental manifestations.

<sup>1</sup>This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under award number DE-SC0012336

**4:54PM C1.00005 Tuning the electronic structure of bulk FeSe with chemical pressure using quantum oscillations and angle resolved photoemission spectroscopy (ARPES)**, AMALIA COLDEA, University of Oxford — FeSe is a unique and intriguing superconductor which can be tuned into a high temperature superconducting state using applied pressure, chemical intercalation and surface doping. In the absence of magnetism, the structural transition in FeSe is believed to be electronically driven, with the orbital degrees of freedom playing an important part [1]. This scenario supports the stabilization of a nematic state in FeSe, which manifests as a Fermi surface deformation in the presence of strong interactions, as detected by ARPES [1]. Another manifestation of the nematicity is the enhanced nematic susceptibility determined from elastoresistance measurements under applied strain [1]. Isovalent Sulphur substitution onto the Selenium site constitutes a chemical pressure, which subtly modifies the electronic structure of FeSe, suppressing the structural transition without inducing high temperature superconductivity [3]. I will present the evolution of the electronic structure with chemical pressure in FeSe, as determined from quantum oscillations [1,2] and ARPES studies [3] and I will discuss the suppression of the nematic electronic state and the role of electronic correlations. Experiments were performed at high magnetic field facilities in Tallahassee, Nijmegen and Toulouse and Diamond Light Source, UK. This work is mainly supported by EPSRC, UK (EP/I004475/1, EP/I017836/1) and I acknowledge my collaborators from Refs. [1-3]. [1] Phys. Rev. B **91**, 155106 (2015); [2] Phys. Rev. Lett. **115**, 027006 (2015); [3] Phys. Rev. B **92**, 121108 (2015).

**Monday, March 14, 2016 2:30PM - 5:30PM —**

**Session C2 DCMP: Novel Electronic Phenomena in Graphene** Ballroom II - Nikolai Zhitenev, Center for Nanoscale Science and Technology, NIST, MD

**2:30PM C2.00001 Creating and Probing Graphene Electron Optics with Local Scanning Probes<sup>1</sup>**, JOSEPH STROSCIO, Center for Nanoscale Science and Technology, NIST, Gaithersburg, MD 20899 — Ballistic propagation and the light-like dispersion of graphene charge carriers make graphene an attractive platform for optics-inspired graphene electronics where gate tunable potentials can control electron refraction and transmission. In analogy to optical wave propagation in lenses, mirrors and metamaterials, gate potentials can be used to create a negative index of refraction for Veselago lensing and Fabry-Pérot interferometers. In circular geometries, gate potentials can induce whispering gallery modes (WGM), similar to optical and acoustic whispering galleries [1] albeit on a much smaller length scale. Klein scattering of Dirac carriers plays a central role in determining the coherent propagation of electron waves in these resonators. In this talk, I examine the probing of electron resonators in graphene confined by linear and circular gate potentials with the scanning tunneling microscope (STM). The tip in the STM tunnel junction serves both as a tunable local gate potential, and as a probe of the graphene states through tunneling spectroscopy. A combination of a back gate potential,  $V_g$ , and tip potential,  $V_b$ , creates and controls a circular pn junction that confines the WGM graphene states. The resonances are observed in two separate channels in the tunneling spectroscopy experiment: first, by directly tunneling into the state at the bias energy  $eV_b$ , and, second, by tunneling from the resonance at the Fermi level as the state is gated by the tip potential. The second channel produces a fan-like set of WGM peaks, reminiscent of the fringes seen in planar geometries by transport measurements. The WGM resonances split in a small applied magnetic field, with a large energy splitting approaching the WGM spacing at 0.5 T. These results agree well with recent theory on Klein scattering in graphene electron resonators [2]. [1]. Y. Zhao, J. Wyrick, F. D. Natterer, J. F. Rodriguez-Nieva *et al.*, Science **348**, 672 (2015). [2]. J. F. Rodriguez-Nieva, L. S. Levitov, *arXiv:1508.06609*.

<sup>1</sup>This work is done in collaboration with Y. Zhao, J. Wyrick, F.D. Natterer, J. F. Rodriguez-Nieva, C. Lewandoswski, K. Watanabe, T. Taniguchi, N. B. Zhitenev, and L. S. Levitov

**3:06PM C2.00002 Electronic Veselago lensing in graphene PN junctions.**, CORY DEAN, Columbia University — Ballistic electrons in a uniform 2D electron gas (2DEG) behave in close analogy to light propagating through an optical medium. In the absence of impurity scattering, electrons follow straight-line trajectories, while the associated de Broglie wavelength can give rise to interference and diffraction. Here we present measurements of ballistic graphene devices in which a graphite gate is used to realize an atomically-smooth junction. We demonstrate unambiguous signatures of negative refraction across a PN junction, paving the way for electron optics inspired by Veselago lensing. Comparison with theoretical simulations reveals the importance of the junction profile towards this effort. Opportunities for future device designs that may take advantage of these effects will be discussed.

**3:42PM C2.00003 Quantum transport in graphene-based van der Waals heterostructures**, PABLO JARILLO-HERRERO, MIT —.

**4:18PM C2.00004 Observation of the hydrodynamic Dirac fluid and the breakdown of the Wiedemann-Franz law in graphene<sup>1</sup>**, KIN CHUNG FONG, Raytheon BBN Technology — Interactions between particles in quantum many-body systems can lead to collective behavior described by hydrodynamics. One such system is the electron-hole plasma in graphene near the charge neutrality point which can form a strongly coupled Dirac fluid. This charge neutral plasma of quasi-relativistic fermions is expected to exhibit a substantial enhancement of the thermal conductivity, due to decoupling of charge and heat currents within hydrodynamics. Employing high sensitivity Johnson noise thermometry, we report the breakdown of the Wiedemann-Franz law in graphene, with a thermal conductivity an order of magnitude larger than the value predicted by Fermi liquid theory. This result is a signature of the Dirac fluid, and constitutes direct evidence of collective motion in a quantum electronic fluid. This research is performed in collaboration with J. Crossno, J. K. Shi, K. Wang, X. Liu, A. Harzheim, A. Lucas, S. Sachdev, P. Kim, T. Taniguchi, K. Watanabe, and T. A. Ohki.

<sup>1</sup>Funding supported by Raytheon BBN Technologies

**4:54PM C2.00005 Negative local resistance due to viscous electron backflow in graphene**, DENIS BANDURIN, School of Physics and Astronomy, University of Manchester, Manchester M13 9PL, UK — Theoretical and experimental studies of systems in which particles undergo frequent mutual collisions date back to more than two centuries ago. Transport in such systems is described by hydrodynamic theory that was found very successful in explaining the response of classical liquids and gases to external fields. It has been argued for a long time that collective behavior of charge carriers in solids can be also described by hydrodynamic approach. However, there has been almost no direct evidence to hydrodynamic electron transport so far. This is because the conditions at which the hydrodynamic effects become observable are very strict: the electron-electron scattering length should provide the shortest spatial scale in the problem. First of all, this requires ultra clean systems where the scattering at impurities is diminished. Second, the electron-phonon scattering rate should be smaller than that of electron-electron scattering. Due to weak electron-phonon coupling high mobility graphene devices offer an ideal system to study electron hydrodynamics. To amplify the hydrodynamic effects we employed a special measurement geometry. The idea is that in case of hydrodynamic electron flow, vortices emerge in the spatial electric current distribution near the current injection contact. That results in a development of a negative voltage drop at the nearby contacts. We were able to detect such negative signal over the range of temperatures when the electronic system is in a hydrodynamic regime. Finally, we performed a rheological study of electron liquid in graphene. The electron viscosity was found to be an order of magnitude larger than that of honey which is in good agreement with many-body calculation.

**Monday, March 14, 2016 2:30PM - 5:30PM —**  
**Session C3 GMAG: Antiferromagnetic Spintronics** Ballroom III - Axel Hoffmann, Argonne Natl Lab

**2:30PM C3.00001 Electrical switching of an antiferromagnet<sup>1</sup>**, TOMAS JUNGWIRTH, Institute of Physics, Academy of Sciences of the Czech Republic and University of Nottingham UK — Louis Néel pointed out in his Nobel lecture that while abundant and interesting from theoretical viewpoint, antiferromagnets did not seem to have any applications. Indeed, the alternating directions of magnetic moments on individual atoms and the resulting zero net magnetization make antiferromagnets hard to control by tools common in ferromagnets. Strong coupling would be achieved if the externally generated field had a sign alternating on the scale of a lattice constant at which moments alternate in AFMs. However, generating such a field has been regarded unfeasible, hindering the research and applications of these abundant magnetic materials. We have recently predicted that relativistic quantum mechanics may offer staggered current induced fields with the sign alternating within the magnetic unit cell which can facilitate a reversible switching of an antiferromagnet by applying electrical currents with comparable efficiency to ferromagnets. Among suitable materials is a high Néel temperature antiferromagnet, tetragonal-phase CuMnAs, which we have recently synthesized in the form of single-crystal epilayers structurally compatible with common semiconductors. We demonstrate electrical writing and read-out, combined with the insensitivity to magnetic field perturbations, in a proof-of-concept antiferromagnetic memory device. References: [1] J. Zelezny, *et al.*, Phys. Rev. Lett. **113**, 157201 (2014). [2] P. Wadley, *et al.*, Nat. Commun. **4**, 2322 (2013). [3] P. Wadley *et al.* <http://arxiv.org/abs/1503.03765>. [4] T. Jungwirth, X. Marti, P. Wadley, J. Wunderlich, <http://arxiv.org/abs/1509.05296>.

<sup>1</sup>We acknowledge support from European Research Council Advanced Grant no. 268066

**3:06PM C3.00002 Interconnections between magnetic state and transport currents in anti-ferromagnetic  $\text{Sr}_2\text{IrO}_4$** , MAXIM TSOI, The University of Texas at Austin — Interconnections between magnetic state and transport currents in ferromagnetic (F) heterostructures are the basis for spintronic applications, e.g. tunneling magnetoresistance and spin-transfer torque phenomena provide a means to read and write information in magnetic memory devices like STTMRAM. Similar interconnections were proposed [1] to occur in systems where F-components are replaced with antiferromagnets (AFM). We demonstrated experimentally the existence of such interconnections in antiferromagnetic Mott insulator  $\text{Sr}_2\text{IrO}_4$ : first, we found [2] a very large anisotropic magnetoresistance (AMR) which can be used to monitor (read) the magnetic state of AFM; second, we demonstrated [3] the feasibility of reversible resistive switching driven by high-density currents/high electric fields which can be used for writing in AFM memory applications. These results support the feasibility of AFM spintronics where antiferromagnets are used in place of ferromagnets. This work was supported in part by C-SPIN, one of six centers of STARnet, a Semiconductor Research Corporation program, sponsored by MARCO and DARPA, and by NSF grants DMR-1207577, DMR-1265162 and DMR-1122603. [1] A. S. Núñez et al., Phys. Rev. B 73, 214426 (2006); [2] C. Wang et al., Phys. Rev. X 4, 041034 (2014); [3] C. Wang et al, PRB 92, 115136 (2015).

**3:42PM C3.00003 Spin-Hall effects in metallic antiferromagnets.**<sup>1</sup>, WEI ZHANG, Argonne National Laboratory — Materials possessing new parameters for efficient and tunable spin Hall effects are being explored, among which antiferromagnets have become one of the most promising candidates. Two distinct properties of antiferromagnets are the microscopic spin magnetic moment ordering and the intrinsic anisotropy. Thus the natural question arises whether these two unique features of antiferromagnets can become new degrees of freedom for tuning their spin Hall effects. We performed experimental studies using spin pumping and inverse spin Hall detection on prototypical CuAu-I-type metallic antiferromagnets, PtMn, IrMn, PdMn, and FeMn, in which we observed increasing spin Hall effects for the alloys with heavier elements included<sup>2</sup>. In particular, PtMn shows a large spin Hall effect that is comparable to Pt. We also demonstrated that the spin transfer torques from the antiferromagnets are large enough to excite ferromagnetic resonance of an adjacent ferromagnetic layer. We conclude that the sign and magnitude of the spin Hall effects in these antiferromagnets are determined by the atomic spin-orbit coupling of the heavy elements (e.g. Pt and Ir) as well as the large spin magnetic moments of Mn. In addition, by using epitaxial growth, we investigated the influence of the different crystalline and magnetic orientations on the anisotropic spin Hall effects of these antiferromagnets. Most of the experimental results were further corroborated by first-principles calculations, which determine the intrinsic spin Hall effect contribution and suggest pronounced anisotropies. Thus metallic antiferromagnets may become an active component for manipulating spin dependent transport properties in spintronic concepts<sup>3</sup>.

<sup>1</sup>Work at Argonne was supported by the U.S. DOE, OS, Materials Sciences and Engineering Division. Work at Center for Nanoscale Materials was supported by DOE, OS-BES (DE-AC02-06CH11357). Work at Jülich was supported by SPP 1538 Programme of the DFG.

<sup>2</sup> W. Zhang *et al*, Phys. Rev. Lett. 113, 196602 (2014); Phys. Rev. B 92, 144405 (2015).

<sup>3</sup> This work was done in collaboration with: M. Benjamin Jungfleisch, Frank Freimuth, Joseph N. Sklenar, Wanjun Jiang, John E. Pearson, Yuriy Mokrousov, John B. Ketterson, and Axel Hoffmann

**4:18PM C3.00004 Spin Transport by Collective Spin Excitations**<sup>1</sup>, P CHRIS HAMMEL, Ohio State University — We report studies of angular momentum transport in insulating materials. Our measurements reveal efficient spin pumping from high wavevector  $k$  spin waves in thin film  $\text{Y}_3\text{Fe}_5\text{O}_{12}$  (YIG): spin pumping is independent of wavevector up to  $k \sim 20 \mu\text{m}^{-1}$  [1]. Optical detection of YIG FMR by NV centers in diamond reveals a role for spin waves in this insulator-to-insulator spin transfer process [2]. Spin transport is typically suppressed by insulating barriers, but we find that fluctuating antiferromagnetic correlations enable efficient spin transport at nm-scale thicknesses in insulating antiferromagnets, even in the absence of long-range order, and that the spin decay length increases with the strength of the antiferromagnetic correlations [3,4]. [1] S.A. Manuilov, C.H. Du, R. Adur, H.L. Wang, V.P. Bhallamudi, F.Y. Yang and P.C. Hammel, Applied Physics Letters 107 042405 (2015); [2] C.S. Wolfe, V.P. Bhallamudi, H.L. Wang, C.H. Du, S. Manuilov, R.M. Teeling-Smith, A.J. Berger, R. Adur, F.Y. Yang and P.C. Hammel, Physical Review B Rapid Communication 89 180406 (2014); [3] H.L.Wang, C.H. Du, P.C. Hammel and F.Y. Yang, Physical Review Letters 113 097202 (2014); [4] H.L.Wang, C.H. Du, P.C. Hammel and F.Y. Yang, Physical Review B 91 220410 (2015).

<sup>1</sup>This research is supported by the U.S. DOE through Grants DE-FG02-03ER46054 and DE-SC0001304, by the NSF MRSEC program through Grant No. 1420451 and by the Army Research Office through Grant W911NF0910147.

**4:54PM C3.00005 Mechanism of spin current transfer through antiferromagnetic dielectrics**, VASYL TYBERKEVYCH, Oakland University — The mechanisms of spin current (SC) transfer are well-studied in both metallic systems, where SC is carried mostly by spin-polarized electrons, and in ferromagnetic (FM) dielectrics, where propagating spin waves (magnons) are responsible for the spin transfer. The possibility of SC transfer through *antiferromagnetic dielectrics* (AFMD) is much less investigated, although recent experimental studies by H. Wang *et al.* [H. Wang *et al.*, Phys. Rev. Lett. 113, 097202 (2014)] demonstrated extraordinary high efficiency of SC transfer in tri-layer FM-AFMD-Platinum (YIG-NiO-Pt) systems measured by the inverse spin Hall effect (ISHE). Perhaps the most unexpected result of these studies was that, with the increase of the thickness of the AFMD layer, the ISHE voltage, first, *increased*, and, then, exponentially decayed with the characteristic decay length of  $\lambda \sim 10$  nm. Moreover, the excitation frequency, equal to the ferromagnetic resonance (FMR) frequency of the YIG layer, was rather low compared to the frequencies of the antiferromagnetic resonance in the AFMD, which rules out the eigenmodes of the AFMD layer as potential carriers of the spin current. Here we propose a possible mechanism of SC transfer through the AFMD with a biaxial anisotropy, which explains all previous experimental findings and opens a new way of manipulating spin currents using anisotropic AFMD materials. We show, that spin current can be carried by *evanescent* AFMD modes non-resonantly excited at the FM-AFMD interface. The decay length of the evanescent modes is defined by the AFMD anisotropy and determines the SC penetration depth into the AFMD. Furthermore, the anisotropy of the AFMD leads to the coupling between the spin subsystem and the crystal lattice of the AFMD, which makes possible exchange of angular momentum between these subsystems. We demonstrate that, under certain realistic conditions, the angular momentum flows from the lattice to the spin subsystem, in which case the AFMD layer acts as a *spin current amplifier*. The enhancement or the suppression of the spin current by the AFMD lattice depends on the phase shift between the two evanescent AFMD modes and, thus, can be controlled by the method of excitation.

**Monday, March 14, 2016 2:30PM - 5:30PM –**  
**Session C4 DCOMP DPOLY FIAP: Bridging Time and Length Scales: From Nano Assemblies to Bio-Polymers** Ballroom IV - Dvora Perahia, Clemson University

**2:30PM C4.00001 Going up in time and length scales in modeling polymers**, GARY S. GREEST, Sandia National Laboratories — Polymer properties depend on a wide range of coupled length and time scales, with unique macroscopic viscoelastic behavior stemming from interactions at the atomistic level. The need to probe polymers across time and length scales and particularly computational modeling is inherently challenging. Here new paths to probing long time and length scales including introducing interactions into traditional bead-spring models and coarse graining of atomistic simulations will be compared and discussed. Using linear polyethylene as a model system, the degree of coarse graining with two to six methylene groups per coarse-grained bead derived from a fully atomistic melt simulation were probed. We show that the degree of coarse graining affects the measured dynamic. Using these models we were successful in probing highly entangled melts and were able reach the long-time diffusive regime which is computationally inaccessible using atomistic simulations. We simulated the relaxation modulus and shear viscosity of well-entangled polyethylene melts for scaled times of 500 s. Results for plateau modulus are in good agreement with experiment. The long time and length scale is coupled to the macroscopic viscoelasticity where the degree of coarse graining sets the minimum length scale instrumental in defining polymer properties and dynamics. Results will be compared to those obtained from simple bead-spring models to demonstrate the additional insight that can be gained from atomistically inspired coarse grained models. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energys National Nuclear Security Administration under contract DE-AC04-94AL85000.

**3:06PM C4.00002 Multi-scale modelling and dynamics**, FLORIAN MLLER-PLATHE, Technische Universitt Darmstadt, Germany, and Princeton University USA — Moving from a fine-grained particle model to one of lower resolution leads, with few exceptions, to an acceleration of molecular mobility, higher diffusion coefficient, lower viscosities and more. On top of that, the level of acceleration is often different for different dynamical processes as well as for different state points. While the reasons are often understood, the fact that coarse-graining almost necessarily introduces unpredictable acceleration of the molecular dynamics severely limits its usefulness as a predictive tool. There are several attempts under way to remedy these shortcoming of coarse-grained models. On the one hand, we follow bottom-up approaches. They attempt already when the coarse-graining scheme is conceived to estimate their impact on the dynamics. This is done by excess-entropy scaling. On the other hand, we also pursue a top-down development. Here we start with a very coarse-grained model (dissipative particle dynamics) which in its native form produces qualitatively wrong polymer dynamics, as its molecules cannot entangle. This model is modified by additional temporary bonds, so-called slip springs, to repair this defect. As a result, polymer melts and solutions described by the slip-spring DPD model show correct dynamical behaviour. Read more: "Excess entropy scaling for the segmental and global dynamics of polyethylene melts", E. Voyiatzis, F. Müller-Plathe, and M.C. Böhm, Phys. Chem. Chem. Phys. **16**, 24301–24311 (2014). [DOI: 10.1039/C4CP03559C] "Recovering the Reptation Dynamics of Polymer Melts in Dissipative Particle Dynamics Simulations via Slip-Springs", M. Langeloth, Y. Masubuchi, M. C. Böhm, and F. Müller-Plathe, J. Chem. Phys. **138**, 104907 (2013). [DOI: 10.1063/1.4794156].

**3:42PM C4.00003 Role of Ionic Clusters in Dynamics of Ionomer Melts: From Atomistic to Coarse Grained Simulations<sup>1</sup>**, ANUPRIYA AGRAWAL, Research Assistant Professor, Washington University in St. Louis — Ionomers, polymers decorated with ionizable groups, have found application in numerous technologies where ionic transport is required. The ionic groups associate into random clusters resulting in substantial effect on structure, dynamics and transport of these materials. The effects of topology, size and dynamics of these aggregates however remain an open question. Here we probe cluster formation correlated with polymer dynamics through a model system of randomly sulfonated polystyrene (SPS) melts with molecular dynamics (MD) simulations over a broad time and length scales ranging from that within the ionic clusters through polymer segmental dynamics to the motion of the entire molecules. The cluster evolution was probed by fully atomistic studies. We find ladder-like aggregates that transform to globule-like with increasing the dielectric constant of media for sodium neutralized SPS. With increasing dielectric constant, the size of the aggregates decrease and their number increases. Concurrently, the mobility of the polymer increases. The counterion radius and valency affect both morphology and dynamics as is evident in the calculated static and dynamic structure factors. It is further manifested in the results of viscosity obtained through non-equilibrium molecular dynamics technique. Finally, to access larger length scales a three bead coarse-grained model to describe sulfonated styrene that we have developed will be discussed in view of the outstanding challenges in ionic polymers.

<sup>1</sup>Supported in part by DOE Grant No. DE-SC007908. This work was carried out in collaboration with Dvora Perahia and Gary Grest while I was a postdoc at Clemson University. I gratefully acknowledge both of them for their support and encouragement.

**4:18PM C4.00004 Protein free energy landscapes from long equilibrium simulations**, STEFANO PIANA-AGOSTINETTI, D.E. Shaw Research — Many computational techniques based on molecular dynamics (MD) simulation can be used to generate data to aid in the construction of protein free energy landscapes with atomistic detail. Unbiased, long, equilibrium MD simulations—although computationally very expensive—are particularly appealing, as they can provide direct kinetic and thermodynamic information on the transitions between the states that populate a protein free energy surface. It can be challenging to know how to analyze and interpret even results generated by this direct technique, however. I will discuss approaches we have employed, using equilibrium MD simulation data, to obtain descriptions of the free energy landscapes of proteins ranging in size from tens to thousands of amino acids.

**4:54PM C4.00005 Electrostatic Interactions and Self-Assembly in Polymeric Systems<sup>1</sup>**, ANDREY DOBRYNIN, Univ of Akron — Electrostatic interactions between macroions play an important role in different areas ranging from materials science to biophysics. They are main driving forces behind layer-by-layer assembly technique that allows self-assembly of multilayer films from synthetic polyelectrolytes, DNA, proteins and nanoparticles. They are responsible for complexation and reversible gelation between polyelectrolytes and proteins. In this talk, using results of the molecular dynamics simulations and analytical calculations, I will demonstrate what effect electrostatic interactions, counterion condensation and polymer solvent affinity have on a collapse of polyelectrolyte chain in a poor solvent conditions for the polymer backbone, on complexations and reversible gelation between polyelectrolytes and polyampholytes (unstructured proteins), on microphase separation transitions in spherical and planar charged brushes, and on a layer-by-layer assembly of charged nanoparticles and linear polyelectrolytes on charged surfaces.

<sup>1</sup>NSF DMR-1004576 DMR-1409710

**Monday, March 14, 2016 2:30PM - 5:18PM –**

**Session C5 GMAG DMP: Frustrated Magnetism: Theory** 301 - Gang Chen, Fudan University

**2:30PM C5.00001 Functional renormalization group - a new approach to frustrated quantum magnetism**, JOHANNES REUTHER, Freie Universitaet Berlin — The experimental and theoretical investigation of quantum spin systems has become one of the central disciplines of contemporary condensed matter physics. From an experimental viewpoint, the field has been significantly fueled by the recent synthesis of novel strongly correlated materials with exotic magnetic or quantum paramagnetic ground states. From a theoretical perspective, however, the numerical treatment of realistic models for quantum magnetism in two and three spatial dimensions still constitutes a serious challenge. This particularly applies to frustrated systems, which complicate the employment of established methods. This talk intends to propagate the pseudofermion functional renormalization group (PFFRG) as a novel approach to determine large size ground state correlations of a wide class of spin Hamiltonians. Using a diagrammatic pseudofermion representation for quantum spin models, the PFFRG performs systematic summations in all two-particle fermionic interaction channels, capturing the correct balance between classical magnetic ordering and quantum fluctuations. Numerical results for various frustrated spin models on different 2D and 3D lattices are reviewed, and benchmarked against other methods if available.

**3:06PM C5.00002 Filling constraints for spin-orbit coupled insulators in symmorphic and non-symmorphic crystals**, HARUKI WATANABE, Massachusetts Institute of Technology, HOI CHUN PO, ASHVIN VISHWANATH, UC Berkeley, MICHAEL ZALATEL, Station Q — We determine conditions on the filling of electrons in a crystalline lattice to obtain the equivalent of a band insulator - a gapped insulator with neither symmetry breaking nor fractionalized excitations. We allow for strong interactions, which precludes a free particle description. Previous approaches that extend the Lieb-Schultz-Mattis argument invoked spin conservation in an essential way, and cannot be applied to the physically interesting case of spin-orbit coupled systems. Here we introduce two approaches, the first an entanglement based scheme, while the second studies the system on an appropriate flat Bieberbach manifold to obtain the filling conditions for all 230 space groups. These approaches only assume time reversal rather than spin rotation invariance. The results depend crucially on whether the crystal symmetry is symmorphic. Our results clarify when one may infer the existence of an exotic ground state based on the absence of order, and we point out applications to experimentally realized materials. Extensions to new situations involving purely spin models are also mentioned.

**3:18PM C5.00003 Quantum Dimer Model: Phase Diagrams**, GARRY GOLDSTEIN, Cambridge University, CLAUDIO CHAMON, Boston university, CLAUDIO CASTELNOVO, Cambridge University — We present new theoretical analysis of the Quantum Dimer Model. We study dimer models on square, cubic and triangular lattices and we reproduce their phase diagrams (which were previously known only numerically). We show that there are several types of dimer liquids and solids. We present preliminary analysis of several other models including doped dimers and planar spin ice, and some results on the Kagome and hexagonal lattices.

**3:30PM C5.00004 Characterizing excitation statistics in fractionalized phases through spectral functions**, SIDDHARDH C. MORAMPUDI, FRANK POLLMANN, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany, ARI M. TURNER, Johns Hopkins University, Baltimore, USA — Characterizing topologically ordered phases of matter involves identifying the statistics of their emergent anyonic excitations. We show that the exchange statistics of excitations show characteristic signatures in experimentally relevant spectral functions. Drawing motivation from models of gapped quantum spin liquids and fractional Chern insulators which possess fractionalized anyonic excitations, we consider a model with gapped two particle and three particle abelian anyonic excitations. We show that the low energy part of spectral functions can show a robust behaviour from which the statistics of the excitations can be obtained.

**3:42PM C5.00005 From Möbius aromaticity to gapped spin liquids**, CHENG-CHIEN CHEN, Argonne National Laboratory, LUKAS MUECHLER, TITUS NEUPERT, Princeton University, JOSEPH MACIEJKO, University of Alberta, ROBERTO CAR, Princeton University — Motivated by the concept of Mobius aromatics in organic chemistry, the Hubbard model on ring-shaped molecules has been shown previously to support a fragile Mott insulator (FMI) ground state, which is distinct from a conventional insulator through its nontrivial transformation properties under point-group symmetry operations. In this talk, we discuss two-dimensional lattices of weakly-coupled FMI molecules belonging to multi-dimensional irreducible representations of the molecular point group. The low-energy effective Hamiltonians map onto quantum compass models with broken spin SU(2) symmetry. On the triangular lattice, the ground state develops long-range magnetism, which corresponds to a charge-ordered state of the molecules. On the honeycomb lattice, interestingly, we find a non-degenerate gapped spin-liquid ground state that preserves all spatial symmetries but transforms nontrivially under point-group operations. Our microscopic model therefore realizes an intrinsically interacting fermionic symmetry protected topological (SPT) phase.

**3:54PM C5.00006 Tetrahedral Spin Crystal to a Chiral Spin Liquid: Frustration-induced quantum melting**, ARUN PARAMAKANTI, CIARAN HICKEY, University of Toronto, LUKASZ CINCIO, Perimeter Institute, ZLATKO PAPIC, University of Leeds — Motivated by the recent interest in interacting topological phases, we study the Haldane-Hubbard model which is shown to host a Mott insulating state with chiral tetrahedral magnetic texture. Frustration-induced melting of this spin crystal leads to a chiral spin liquid. We discuss the properties of these phases, and the Chern-Simons-Higgs theory of the intervening exotic quantum critical point.

**4:06PM C5.00007 Symmetric tensor networks and practical simulation algorithms to sharply identify classes of quantum phases distinguishable by short-range physics<sup>1</sup>**, YING RAN, SHENGHAN JIANG, Boston College — Phases of matter are sharply defined in the thermodynamic limit. One major challenge of accurately simulating quantum phase diagrams of interacting quantum systems is due to the fact that numerical simulations usually deal with the energy density, a local property of quantum wavefunctions, while identifying different quantum phases generally rely on long-range physics. In this paper we construct generic fully symmetric quantum wavefunctions under certain assumptions using a type of tensor networks: projected entangled pair states, and provide practical simulation algorithms based on them. We find that quantum phases can be organized into crude classes distinguished by short-range physics, which is related to the fractionalization of both on-site symmetries and space-group symmetries. Consequently, our simulation algorithms, which are useful to study long-range physics as well, are expected to be able to sharply determine crude classes in interacting quantum systems efficiently. Examples of these crude classes are demonstrated in half-integer quantum spin systems on the kagome lattice. Limitations and generalizations of our results are discussed.

<sup>1</sup>the Alfred P. Sloan fellowship and National Science Foundation under Grant No. DMR-1151440

**4:18PM C5.00008 Numerical studies of AKLT valence bond solids in one, two and three dimensions**, KEOLA WIERSCHEM, KEVIN BEACH, The University of Mississippi — The fixed-point valence bond solids of Affleck, Kennedy, Lieb and Tasaki (the so-called AKLT states) have become archetypes of symmetry protected topological order. These states are constructed by first placing  $M$  valence bonds on each pair of neighboring lattice points, and then symmetrizing the  $Mz$  resulting spin-1/2 degrees of freedom at each lattice site into a combined spin- $S$  degree of freedom with  $2S = Mz$  (where  $M$  is the multiplicity of the AKLT state and  $z$  is the lattice coordination number). Using Monte Carlo sampling of the AKLT wavefunctions in the loop gas framework, we directly calculate correlation functions and energy gap estimators for these states in one, two and three dimensions. We also study the behavior of the so-called strange correlator, which has been proposed as a measure of symmetry protected topological order.

**4:30PM C5.00009 Theory of supersymmetry “protected” topological phases of isostatic lattices and highly frustrated magnets**, MICHAEL LAWLER, Binghamton University — I generalize the theory of phonon topological band structures of isostatic lattices to highly frustrated antiferromagnets. I achieve this with a discovery of a many-body supersymmetry (SUSY) in the phonon problem of balls and springs which also applies to geometrically frustrated magnets. The Witten index of the SUSY model, when restricted to the single body problem (meaningful for linearized phonons), is then shown to be the Calladine-Kane-Lubensky index of mechanical structures that forms the cornerstone of the phonon topological band structure theory. “Spontaneous supersymmetry breaking” is then identified as the need to gap all modes in the bulk to create the topological state. The many-body SUSY formulation shows that the topology is not restricted to a band structure problem but extends to systems of coupled bosons and fermions that are in principle also realizable in solid state systems. The analogous supersymmetry of the magnon problem turns out to be particularly useful for highly frustrated magnets with the kagome family of antiferromagnets an analog of topological isostatic lattices. Thus, a solid state realization of the theory of phonon topological band structure may be found in highly frustrated magnets. However, our results show that this topology is protected not

**4:42PM C5.00010 Non-Kondo Mechanism of Resistivity Minimum in Frustrated Itinerant Magnets**, CRISTIAN BATISTA, T-Division and CNLS, Los Alamos National Laboratory, ZHENTAO WANG, Department of Physics and Astronomy, Rice University, KIPTON BARROS, T-Division and CNLS, Los Alamos National Laboratory, GIA-WEI CHERN, Department of Physics, University of Virginia — Frustration can induce novel phenomena in the transport properties of itinerant magnets. The "amount of frustration" is typically quantified by the  $|\Theta_{CW}|/T_C$  ratio. A large value of this ratio corresponds to a broad temperature regime  $T_C < T < \Theta_{CW}$ , where the spins are in spin liquid state, i.e., the magnetic structure factor is not flat, as in the gas ( $T > \Theta_{CW}$ ) state and it does not contain Bragg peaks, as in the ordered or "solid" state at  $TT_C$ . We demonstrate that when interaction between magnetic moments is mediated by the conduction electrons, the electronic resistivity increases upon lowering temperature, due to enhanced scattering rate for  $k \leq 2k_F$ . To illustrate this phenomenon we consider a triangular Kondo lattice model with classical local moments. By using both analytical and numerical methods, we unambiguously demonstrate that the electronic resistivity grows upon lowering temperature inside the spin liquid regime. This growth necessarily leads to a resistivity minimum when electron-electron and electron-phonon scattering are included. We note that the origin of this resistivity minimum is radically different from the well-known minimum induced by the Kondo effect.

**4:54PM C5.00011 Vortex Crystals with Chiral Stripes in Itinerant Magnets**, RYO OZAWA, Dept. of Appl. Phys., Univ. of Tokyo, SATORU HAYAMI, KIPTON BARROS, Theoretical Division and CNLS, Los Alamos National Lab., GIA-WEI CHERN, Dept. of Phys., Univ. of Virginia, YUKITOSHI MOTOME, Dept. of Appl. Phys., Univ. of Tokyo, CRISTIAN D. BATISTA, Theoretical Division and CNLS, Los Alamos National Lab. — Noncoplanar spin textures in itinerant magnets are generating increasing interest because of the associated spin Berry phase, which induces a tremendous effective magnetic field on the itinerant electrons. Such noncoplanar spin textures appear frequently in itinerant magnets, even with vanishingly small spin-orbit coupling. We explore a generic condition for noncoplanar spin ordering, with a focus on "frustration" in itinerant magnets, that is characterized by multiple global maxima in the magnetic susceptibility. In a simple square Kondo lattice model, we find that a noncoplanar vortex-antivortex crystal with a one-dimensional modulation of spin scalar chirality becomes stable in a wide range of electron filling fraction [1]. The unexpected result is obtained by careful analyses of higher-order terms in the perturbative expansion in terms of the Kondo exchange coupling and the degree of noncoplanarity, as well as numerical simulation based on the Langevin and stochastic Landau-Lifshitz-Gilbert dynamics with the kernel polynomial method. [1] R. Ozawa, S. Hayami, K. Barros, G.-W. Chern, Y. Motome, and C. D. Batista, preprint (arXiv:1510.06830).

**5:06PM C5.00012 Lifting mean field degeneracies in anisotropic spin systems<sup>1</sup>**, YURIY SIZYUK, NATALIA PERKINS, Univ of Minn - Minneapolis, PETER WOLFLE, Karlsruhe Institute of Technology — We propose a method for calculating the fluctuation contribution to the free energy of anisotropic spin systems with generic bilinear superexchange magnetic Hamiltonian based on the Hubbard-Stratonovich transformation. We show that this contribution splits the set of mean field degenerate states with rotational symmetry, and chooses states with the order parameter directed along lattice symmetric directions as the true ground states. We consider the simple example of Heisenberg-compass model on cubic lattice to show that depending on the relative strength of the compass and Heisenberg interactions the spontaneous magnetization is pinned to either one of the cubic directions or one of the cubic body diagonals with a intermediate phase in between where the minima and maxima of the free energy interchange.

<sup>1</sup>DMR-1005932, DMR-1511768, and NSF PHY11-25915

**Monday, March 14, 2016 2:30PM - 5:30PM –**  
**Session C6 GMAG DMP: Magnetic Characterization and Imaging** 302 - Vojtech Uhler, UCSD

**2:30PM C6.00001 Exploring 360 domain walls in ferromagnetic nanostructures using circular magnetic fields<sup>1</sup>**, ANANDAKUMAR SARELLA, F. I. KAYA, K. E. AIDALA, Mt Holyoke Coll — Ferromagnetic nanostructures can exhibit intriguing magnetic states, such as the metastable 360 domain wall (DW), in which two 180 DWs combine to form a nearly flux closed state in sufficiently thin structures. These composite structures have potential to maximize storage densities due to their minimal stray fields. We study a straightforward method to nucleate 360 DWs in nanorings, nanowires, using in-plane circular fields, as if from a current carrying wire passing through the substrate in close proximity to the nanostructures. Our simulations, using OOMMF, predict that the vortex state of a ring with appropriate geometry will reverse from CW to CCW through an intermediate state consisting of pairs of 360 DWs. We examine the dependence of the switching field and intermediate states on geometric properties such as the diameter, thickness, and width of the ring. Using the local circular field, we can also nucleate 360 DWs in nanowires, pinning the location of the DWs at notches spaced as close as 100 nm apart, suggesting high density storage. We are currently studying these structures experimentally using AFM/MFM. We generate the circular field by passing current through AFM tip and image the resulting magnetic states with MFM.

<sup>1</sup>NSF grants No. DMR 1208042 and 1207924. Simulations were run on the Odyssey cluster, Research Computing Group at Harvard.

**2:42PM C6.00002 Quantitative X-Ray Magnetic Microscopy: from parallel stripe domains to buried topological defects<sup>1</sup>**, MARIA VELEZ, C. BLANCO-ROLDAN, C. QUIROS, F. VALDES-BANGO, L. M. ALVAREZ-PRADO, J. I. MARTIN, J. M. ALAMEDA, Universidad de Oviedo-CINN, SPAIN, A. HIERRO-RODRIGUEZ, U. Porto, Portugal, M. DUCH, N. TORRAS, J. ESTEVE, IMB - CNM, CSIC, SPAIN, A. SORRENTINO, R. VALCARCEL, E. PEREIRO, S. FERRER, Alba Synchrotron, SPAIN — Magnetic transmission X-ray microscopy (TXM) is a powerful imaging technique that can produce element specific images of magnetic domains with nanometric lateral resolution. Here we present a novel imaging method in which the angular dependence of the magnetic contrast in a series of high resolution TXM images is used to obtain quantitative descriptions of the magnetization (canting angles and sense). This has been applied first to analyze parallel stripe domains in weak perpendicular anisotropy ferromagnetic NdCo<sub>5</sub> layers of different thickness, and in NdCo<sub>5</sub>/Permalloy bilayers. Then, our method has been used to identify complex topological defects (merons or 1/2 skyrmions) in a NdCo<sub>5</sub> film that are only partially replicated by the Permalloy overlayer [1]. Meron propagation in trilayers (across the thickness) and in hexagonal networks (across bifurcations) will be discussed in terms of their topological characteristics (chirality and polarity). [1] C. Blanco-Roldan et al. Nature Communications 6 (2015) 8196

<sup>1</sup>Work supported by Spanish grant FIS2013- 45469

**2:54PM C6.00003 Soft x-ray ptychography studies of nanoscale magnetic and structural correlations in thin SmCo5 films<sup>1</sup>**, P. FISCHER, MSD LBNL Berkeley CA 94720, X. SHI, ALS LBNL Berkeley CA 94720, V. NEU, D. ELEFANT, IFW Dresden Germany, J.C.T. LEE, D.A. SHAPIRO, M. FARMAND, T. TYLISZCZAK, W. SHIU, S. MARCHESINI, S. ROY, S.D. KEVAN, ALS LBNL Berkeley CA 94720 — Soft x-ray ptychographic imaging was applied to probe an amorphous 50 nm thin SmCo5 film prepared by off-axis pulsed laser deposition and exhibiting a strong perpendicular magnetic anisotropy. Amplitude and phase contrast images, retrieved at photon energies near the cobalt L3 resonance, were used to identify and characterize magnetic and structural features with a spatial resolution of about 10 nm. Aside from the common magnetic labyrinth domain pattern, nanoscale structural inclusions were identified that are primarily located in close proximity to the magnetic domain walls. X-ray absorption spectroscopy suggests that these inclusions are nanocrystalline Sm2Co17 phases with nominally in-plane magnetic anisotropy. Our results indicate that x-ray ptychographic imaging enables fruitful studies of magnetic and structural correlations at length scales relevant to emerging magnetic and spintronic devices.

<sup>1</sup>Supported by the Director of the Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DEAC02-05CH11231.

### **3:06PM C6.00004 Asymmetric and Stochastic Behavior in Magnetic Vortices Studied by Soft X-ray Microscopy**

<sup>1</sup>, MI-YOUNG IM, LBNL — Asymmetry and stochasticity in spin processes are not only long-standing fundamental issues but also highly relevant to technological applications of nanomagnetic structures to memory and storage nanodevices. Those nontrivial phenomena have been studied by direct imaging of spin structures in magnetic vortices utilizing magnetic transmission soft x-ray microscopy (BL6.1.2 at ALS). Magnetic vortices have attracted enormous scientific interests due to their fascinating spin structures consisting of circularity rotating clockwise ( $c = +1$ ) or counter-clockwise ( $c = -1$ ) and polarity pointing either up ( $p = +1$ ) or down ( $p = -1$ ). We observed a symmetry breaking in the formation process of vortex structures in circular permalloy (Ni<sub>80</sub>Fe<sub>20</sub>) disks. The generation rates of two different vortex groups with the signature of  $cp = +1$  and  $cp = -1$  are completely asymmetric. The asymmetric nature was interpreted to be triggered by intrinsic Dzyaloshinskii-Moriya interaction (DMI) arising from the spin-orbit coupling due to the lack of inversion symmetry near the disk surface and extrinsic factors such as roughness and defects. We also investigated the stochastic behavior of vortex creation in the arrays of asymmetric disks. The stochasticity was found to be very sensitive to the geometry of disk arrays, particularly interdisk distance. The experimentally observed phenomenon couldn't be explained by thermal fluctuation effect, which has been considered as a main reason for the stochastic behavior in spin processes. We demonstrated for the first time that the ultrafast dynamics at the early stage of vortex creation, which has a character of classical chaos significantly affects the stochastic nature observed at the steady state in asymmetric disks. This work provided the new perspective of dynamics as a critical factor contributing to the stochasticity in spin processes and also the possibility for the control of the intrinsic stochastic nature by optimizing the design of asymmetric disk arrays.

<sup>1</sup>This work was supported by the Director, Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231, by Leading Foreign Research Institute Recruitment Program through the NRF

### **3:42PM C6.00005 Ultrasensitive Scanning Transmission X-ray Microscopy: Pushing the Limits of Time Resolution and Magnetic Sensitivity**

HENDRIK OHLDA, SLAC - Natl Accelerator Lab — Understanding magnetic properties at ultrafast timescales is crucial for the development of new magnetic devices. Samples of interest are often thin film magnetic multilayers with thicknesses in the range of a few atomic layers. This fact alone presents a sensitivity challenge in STXM microscopy, which is more suited toward studying thicker samples. In addition the relevant time scale is of the order of 10 ps, which is well below the typical x-ray pulse length of 50–100 ps. The SSRL STXM is equipped with a single photon counting electronics that effectively allows using a double lock-in detection at 476 MHz (the x-ray pulse frequency) and 1.28 MHz (the synchrotron revolution frequency) to provide the required sensitivity. In the first year of operation the excellent spatial resolution, temporal stability and sensitivity of the detection electronics of this microscope has enabled researchers to acquire time resolved images of standing as well as traveling spin waves in a spin torque oscillator in real space as well as detect the real time spin accumulation in non magnetic Copper once a spin polarized current is injected into this material. The total magnetic moment is comparable to that of a single nanocube of magnetic Fe buried under a micron of non-magnetic material.

### **3:54PM C6.00006 ABSTRACT WITHDRAWN —**

### **4:06PM C6.00007 Magnetorheology of hybrid colloids measured by spin coating and classical rheometry.<sup>1</sup>**

RAHEEMA MUHAMMAD ASLAM, University of Navarra, Spain, KESHWAD SHAHRIVAR, JUAN DE VICENTE LVAREZ-MANZANEDA, University of Granada, Spain, WENCESLAO GONZALEZ-VIAS, University of Navarra, Spain — Hybrid colloids composed of micron-sized ferromagnetic and diamagnetic particles constitute a promising category of magnetorheological fluids with enhanced field-induced apparent yield stress. However, the physical mechanism explaining this stress enhancement is currently lacking. For the first time, we measure and compare the magnetic field-dependent viscosity of hybrid diluted colloids using spin-coating [] and magnetorheometry []. In the former technique, a magnetic field is applied during the spin coating of the colloidal suspension involving evaporation of the solvent. The viscosity of the colloidal suspension at applied field can be derived from the surface coverage of the dry spin-coated deposits and from the viscosity of the colloid at zero field. In the latter, its viscosity is measured with a torsional parallel plate magnetorheometer under uniaxial magnetic fields aligned in the gradient direction of a steady shearing flow. The experimental results under different conditions and the effect of each component on the magnetorheological properties of the resulting colloid will be discussed. [] M. Pichumani et al., Soft Matter, 2013, 9, 3220-3229 [] Juan de Vicente et al., Soft Matter, 2011, 7, 3701-3710

<sup>1</sup>This work is partly supported by the Spanish MINECO (FIS201454101-P).

### **4:18PM C6.00008 Accuracy of MRI-based Magnetic Susceptibility Measurements**

STEPHEN RUSSEK, HANNAH ERDEVIG, KATHRYN KEENAN, KARL STUPIC, NIST - Boulder — Magnetic Resonance Imaging (MRI) is increasingly used to map tissue susceptibility to identify microbleeds associated with brain injury and pathologic iron deposits associated with neurologic diseases such as Parkinson's and Alzheimer's disease. Field distortions with a resolution of a few parts per billion can be measured using MRI phase maps. The field distortion map can be inverted to obtain a quantitative susceptibility map. To determine the accuracy of MRI-based susceptibility measurements, a set of phantoms with paramagnetic salts and nano-iron gels were fabricated. The shapes and orientations of features were varied. Measured susceptibility of 1.0 mM GdCl<sub>3</sub> solution in water as a function of temperature agreed well with the theoretical predictions, assuming Gd<sup>3+</sup> is spin 7/2. The MRI susceptibility measurements were compared with SQUID magnetometry. The paramagnetic susceptibility sits on top of the much larger diamagnetic susceptibility of water (-9.04 × 10<sup>-6</sup>), which leads to errors in the SQUID measurements. To extract out the paramagnetic contribution using standard magnetometry, measurements must be made down to low temperature (2K). MRI-based susceptometry is shown to be as or more accurate than standard magnetometry and susceptometry techniques.

**4:30PM C6.00009 Neutron interferometry with cold stage<sup>1</sup>**, TAI SIYA MINEEVA, Institute for Quantum Computing, M. ARIF, M.G. HUBER, National Institute of Standards and Technology, C.B. SHAHI, Tulane University, C.W. CLARK, Joint Quantum Institute, D.G. CORY, J. NSOFINI, D. SARENAC, D.A. PUSHIN, Institute for Quantum Computing — Neutron interferometry (NI) is amongst the most precise methods for characterizing neutron interactions by measuring the relative difference between two neutron paths, one of which contains a sample-of-interest. Because neutrons carry magnetic moment and are deeply penetrating, they are excellent probes to investigate properties of magnetic materials. The advantage of NI is its unique sensitivity which allows to directly measure magnetic and structural transitions in materials. Up to now NI has been sparingly used in material research due to its sensitivity to environmental noise. However, recent successes in implementing Quantum Error Correction principles lead to an improved NI design making it robust against mechanical vibrations. Following these advances, a new user facility at the National Institute for Standards and Technology was built to study condensed matter applications, biology and quantum physics. Incorporating cold sample stage inside NI is the first of its kind experiment which can be carried out on large range of temperatures down to 4K. Upon successful realization, it will open new frontiers to characterize magnetic domains, phase transitions and spin properties in a variety of materials such as, for example, iron-based superconductors and spintronic materials.

<sup>1</sup>Supported in part by CERC, CIFAR, NSERC and CREATE.

**4:42PM C6.00010 Relaxometry imaging of superparamagnetic magnetite nanoparticles at ambient conditions**, AMIT FINKLER, DOMINIK SCHMID-LORCH, THOMAS HÄBERLE, 3. Physikalisches Institut, Universität Stuttgart, FRIEDEMANN REINHARD, Technische Universität München, ANDREA ZAPPE, 3. Physikalisches Institut, Universität Stuttgart, MICHAEL SLOTA, 1. Physikalisches Institut, Universität Stuttgart, LAPO BOGANI, Department of Materials, University of Oxford, JÖRG WRACHTRUP, 3. Physikalisches Institut, Universität Stuttgart — We present a novel technique to image superparamagnetic iron oxide nanoparticles via their fluctuating magnetic fields. The detection is based on the nitrogen-vacancy (NV) color center in diamond, which allows optically detected magnetic resonance (ODMR) measurements on its electron spin structure. In combination with an atomic-force-microscope, this atomic-sized color center maps ambient magnetic fields in a wide frequency range from DC up to several GHz [1], while retaining a high spatial resolution in the sub-nanometer range [2]. We demonstrate imaging of single 10 nm sized magnetite nanoparticles using this spin noise detection technique. By fitting simulations (Ornstein-Uhlenbeck process) to the data, we are able to infer additional information on such a particle and its dynamics, like the attempt frequency and the anisotropy constant [3]. This is of high interest to the proposed application of magnetite nanoparticles as an alternative MRI contrast agent or to the field of particle-aided tumor hyperthermia. [1] E. Schäfer-Nolte et al., Phys. Rev. Lett. **113**, 217204 (2014) [2] P. Maletinsky et al., Nat. Nanotech. **7**, 320 (2012) [3] D. Schmid-Lorch et al., Nano Lett. **15**, 4942 (2015)

**4:54PM C6.00011 ABSTRACT WITHDRAWN —**

**5:06PM C6.00012 Measurements of magnetic spin excitations in Permalloy microstructures using nitrogen-vacancy magnetometry**, H.J. JASON LIU, SEUNGHA YOON<sup>1</sup>, ROBERT MCMICHAEL, Center for Nanoscale Science and Technology, National Institute of Standards and Technology — The magnetic properties of nitrogen-vacancy (NV) centers in diamond have enabled emerging applications in fields ranging from cell biology to quantum computing. An NV center is a lattice defect, which behaves like a spin-1 system. NV centers can be prepared in the  $m_z = 0$  state by excitation with green light, and the spin state can be detected by the center's fluorescence of red light. The Zeeman splitting of the  $m_z = 1$  state, combined with a spin coherence time that can approach 1 ms, makes the NV center a sensitive, atom-sized magnetometer. Recently, NV centers have been used to measure spin wave excitations and vortex core dynamics in a Permalloy microdisk. In this talk, we present current NV center measurements on Permalloy micro and nanostructures that build on previous work. Permalloy structures were fabricated on top of a microstrip antenna and the measurements were conducted on a home-built confocal microscope. Preliminary measurements show photoluminescence contrast of ~12% and field detectivity on the order of T/Hz<sup>1/2</sup>. This allows for fine field mapping of stray magnetic fields produced by micro and nanostructures, which are typically a few milliteslas in magnitude.

<sup>1</sup>Maryland Nanocenter, University of Maryland

**5:18PM C6.00013 Using NV-centers in diamond for optical magnetic sensing in superconductors<sup>1</sup>**, N M NUSRAN, K R JOSHI, K CHO, R PROZOROV, Ames Laboratory and Iowa State University — Magnetic field-dependent fluorescence of nitrogen vacancy (NV) centers in diamond has recently emerged as a promising technology for nanoscale sensing including non-invasive sensitive magnetometry and mapping of the magnetic field distribution. In particular, NV-sensing can be used to study magnetic phenomena in superconductors. After detailed introduction of this novel magneto-sensing technique, we will present results of magnetic measurements on several superconductors, including Ba<sub>1-x</sub>K<sub>x</sub>Fe<sub>2</sub>As<sub>2</sub> and type-I materials. Details of the superconducting phase transition, the Meissner state, magnetic flux distribution upon field penetration, exit and trapping will be discussed.

<sup>1</sup>This work was supported by the U.S. Department of Energy, Office of Basic Energy Science, Materials Science and Engineering Division and was performed at the Ames Laboratory, Iowa State University under contract DE-AC02-07CH11358.

**Monday, March 14, 2016 2:30PM - 5:30PM —**

**Session C7 APS SPS: Undergraduate Research/SPS III** 303 - Crystal Bailey, American Physical Society

**2:30PM C7.00001 Guiding brine shrimp through mazes by solving reaction diffusion equations.**, KRISHMA SINGAL, FLAVIO FENTON, None — Excitable systems driven by reaction diffusion equations have been shown to not only find solutions to mazes but to also to find the shortest path between the beginning and the end of the maze. In this talk we describe how we can use the Fitzhugh-Nagumo model, a generic model for excitable media, to solve a maze by varying the basin of attraction of its two fixed points. We demonstrate how two dimensional mazes are solved numerically using a Java Applet and then accelerated to run in real time by using graphic processors (GPUs). An application of this work is shown by guiding phototactic brine shrimp through a maze solved by the algorithm. Once the path is obtained, an Arduino directs the shrimp through the maze using lights from LEDs placed at the floor of the Maze. This method running in real time could be eventually used for guiding robots and cars through traffic.

**2:42PM C7.00002 An Agent Based Model for Social Class Emergence**, XIAOXIANG YANG, DANIEL RODRIGUEZ SEGURA, FEI LIN, IRINA MAZILU, Washington and Lee University — We present an open system agent-based model to analyze the effects of education and the society-specific wealth transactions on the emergence of social classes. Building on previous studies, we use realistic functions to model how years of education affect the income level. Numerical simulations show that the fraction of an individuals total transactions that is invested rather than consumed can cause wealth gaps between different income brackets in the long run. In an attempt to incorporate the network effects, we also explore how the probability of interactions among agents depending on the spread of their income brackets affects wealth distribution.

**2:54PM C7.00003 Generation and characterization of high-density gas jets from a 150 micron diameter nozzle in air<sup>1</sup>** , LUKE HAHN, KEVIN BARTAS, YAN TAY, DONGHOON KUK, KI-YONG KIM, Univ of Maryland-College Park — This work characterizes argon and nitrogen gas jets in unconventional atmospheric pressure instead of the conventional vacuum pressure, and then compares the results directly to that of the conventional technique of creating gas jet targets. A Mach-Zehnder interferometer was used to estimate the number density of the gas jet, and a Rayleigh scattering setup was used to determine if either of the techniques formed atomic clusters and if so, estimating relative quantity. The diameter of the cylindrical nozzle used for is around 150  $\mu\text{m}$  with backing pressures ranging from 13 bars to 69 bars. The highest backing pressure gives us a maximum phase shift value of 9 rad, number density  $4.5 \cdot 10^{20} \text{ cm}^{-3}$ . Another characteristic property of these jets is the shock diamond formation due to the flows interaction with atmospheric air particles. The highest number density for a shock diamond was  $\sim 10^{20} \text{ cm}^{-3}$  which does not necessarily occur at higher backing pressure. Also, the distance from the first shock diamond to the nozzle orifice does increase with increasing backing pressure, consistent with a theory. This type of high-density, thin gas jets can be used as a laser target for creating dense plasmas and producing energetic particles and X-rays in the atmospheric conditions.

<sup>1</sup>Work supported by DOE, Fusion Energy Sciences under Award No. DE-SC0010706.

**3:06PM C7.00004 Combination Gravimetric/Volumetric Sorption Instrument for Energy Applications.** , DONALD BETHEA, JACOB BURRESS, Univ of South Alabama — The use of gaseous fuels such as hydrogen and methane (natural gas) will reduce emissions. Unfortunately, the storage of hydrogen and methane at room temperature is difficult because they are both supercritical gases, making the adoption of these fuels cumbersome. One means of overcoming the storage problem is to use physisorption-based systems which exploit the van der Waals interaction between the gas and a nanoporous material to compress the gases to near liquid densities. To measure the amount of gas in these materials, gravimetric or volumetric methods are employed. Gravimetric weighs the amount of gas and volumetric uses differences in gas pressures. Gravimetric systems typically have problems with buoyancy corrections. Volumetric systems normally have larger uncertainties that propagate through the isotherm. A modified system will be presented which allows for both gravimetric and volumetric gas sorption measurements. Additionally, the buoyancy corrections for the gravimetric measurements are significantly small and less than the uncertainties in the measurement. This apparatus can take measurements of most gases at room temperature and up to 200 bar.

**3:18PM C7.00005 Decoherence of nitrogen-vacancy defect spins in diamond from surface spins** , MICHAEL DOMINGUEZ, MICHAEL E. FLATT, Department of Physics and Astronomy, University of Iowa — In recent work[1,2], researchers measured the spin coherence time of intentionally-doped nitrogen-vacancy (NV) spin ensembles. The spin coherence times of these spins depends on their local environment, including their nearness to the surface of the material. We calculated the decoherence time of a deep spin within the material affected by the presence of a sheet of surface spins interacting with the deep spin through the dipolar interaction. These calculations describe the experimental measurements qualitatively, however quantitative agreement requires the assumption these spins extend deeper into the material from the surface layer. [1] J. Cardellino et al., Nat. Nanotechnol. 9, 343 (2014) [2] K. Ohno et al., Appl. Phys. Lett. 101, 082413 (2012). This work was supported by the NIGMS under Award Number R25GM058939

**3:30PM C7.00006 Electrostatic Simulation of Charge Trapping in Carbon Nanotube Vertical Organic Field Effect Transistors<sup>1</sup>** , JENNIFER CRAWFORD, ANDREW RINZLER, SELMAN HERSHFELD, Univ of Florida - Gainesville — The carbon nanotube vertical organic field effect transistor is a vertical sequence consisting of a gate electrode, gate dielectric, thin nanotube network source electrode, organic semiconducting channel and finally the drain electrode. The drain current is modulated by the gate voltage which varies a Schottky barrier between source and channel layers. Hysteresis in the current-voltage characteristic has been observed when a electret charge trapping layer is placed between the nanotube source and the gate dielectric. We provide a model for charge injection into a trapping layer placed in contact with the carbon nanotube film and solve self-consistently for the electrostatics and the occupancy of the traps. For a range of applied gate voltages the simulations demonstrate hysteresis of the carbon nanotubes' charge as a result of the electric field produced by the trapped charge. This affects the current by modulating the Schottky barrier.

<sup>1</sup>This work was supported by the NSF grant DMR-1461019.

**3:42PM C7.00007 Quantum correlations of magnetic impurities by a multiple electron scattering in carbon nanotubes** , DIDIER GAMBOA ANGULO, Universidad Autnoma de Yucatn, GUILLERMO CORDOURIER MARURI, ROMEO DE COSS GMEZ, Centro de Investigacin y de Estudios Avanzados del IPN — In this work we analyze the quantum correlations and polarizations states of magnetic impurities spins, when a multiple electron scattering was taken place. A sequence of non-correlated electrons interacts through scattering producing quantum correlation which will have an impact on the electronic transmission. We consider a short range Heisenberg interaction between ballistic electron and static impurities. We analyze the cases when the electron scattering is produce by one and two impurities, obtaining the electronic transmission rates. Concurrence and fidelity calculations are performed to obtain the level of quantum entanglement and polarization correlations. We also discuss the possible application of this model to metallic and semiconductor carbon nanotubes, which could have important implications on spintronics and quantum information devices.

**3:54PM C7.00008 Exact Diagonalization of a Quantum XXZ Model with Long-Range Interactions<sup>1</sup>** , JUSTIN A. WILLIAMS, DAVID A. SMITH, University of West Florida, C.C.-JOSEPH WANG, None, CHRISTOPHER N. VARNEY, University of West Florida — In recent years, rapid advancement has been made in using ultra-cold gases as quantum spin simulators, with two dimensional lattices becoming a rich target for exploring the exotic states and excitations of spin-1/2 systems on frustrated lattices. When the interaction in the system becomes long-ranged, the spins are frustrated by the long-range interaction. Consequently, the competition between the geometric frustration and the long-range interaction results in the the underlying orders present in the ground state being unclear. Here, we investigate the quantum dipolar XXZ model with exact diagonalization to characterize and contrast the ground state and excitations on square and triangular lattices to provide a baseline for comparison with experiments.

<sup>1</sup>University of West Florida Summer Undergraduate Research Program, University of West Florida Quality Enhancement Plan Award

**4:06PM C7.00009 A Holographic c-Theorem for Schrodinger Spacetimes** , WEISHUN ZHONG, JAMES LIU, University of Michigan — We prove a c-theorem for holographic renormalization group flows in a Schrodinger spacetime that demonstrates that the effective radius  $L(r)$  monotonically decreases from the UV to the IR, where  $r$  is the bulk radial coordinate. This result assumes that the bulk matter satisfies the null energy condition, but holds regardless of the value of the critical exponent  $z$ . We also construct several numerical examples in a model where the Schrodinger background is realized by a massive vector coupled to a real scalar. The full Schrodinger group is realized when  $z=2$ , and in this case it is possible to construct solutions with constant effective  $z(r)=2$  along the entire flow.

**4:18PM C7.00010 The Configuration Space Symmetries in the Quantum Bouncer** , DAVID LOCKERBY, American University — We study a few-body particle system with contact interactions in a quantum bouncer potential well. In principle, the strength of the gravitational field can be extracted from the one-particle energy spectrum, but this is currently experimentally impractical. This project explores how varying the number of particles and tuning the particle interaction strength can improve measurement sensitivity. The analysis exploits the additional symmetries of configuration space that occur either in the unitary limit of contact interactions or when the bouncer potential is decorated with additional infinite delta-barriers.

**4:30PM C7.00011 Exploring Quantum Dynamics of Continuous Measurement with a Superconducting Qubit** , ARIAN JADBABAIE, NEDA FOROUZANI, DIAN TAN, KATER MURCH, Washington University, St. Louis — Weak measurements obtain partial information about a quantum state with minimal backaction. This enables state tracking without immediate collapse to eigenstates, of interest to both experimental and theoretical physics. State tomography and continuous weak measurements may be used to reconstruct the evolution of a single system, known as a quantum trajectory. We examine experimental trajectories of a two-level system at varied measurement strengths with constant unitary drive. Our analysis is applied to a transmon qubit dispersively coupled to a 3D microwave cavity in the circuit QED architecture. The weakly coupled cavity acts as pointer system for QND measurements in the qubits energy basis. Our results indicate a marked difference in state purity between two approaches for trajectory reconstruction: the Bayesian and Stochastic Master Equation (SME) formalisms. Further, we observe the transition from diffusive to jump-like trajectories, state purity evolution, and a novel, tilted form of the Quantum Zeno effect. This work provides new insight into quantum behavior and prompts further comparison of SME and Bayesian formalisms to understand the nature of quantum systems. Our results are applicable to a variety of fields, from stochastic thermodynamics to quantum control.

**4:42PM C7.00012 A simple table-top experiment demonstrating mechanical oscillation of a macroscopic object driven by radiation pressure.** , GRACE JESENSKY, DOMINIC DAMS, OLEKSIY KHOMENKO, WOO-JOONG KIM, Seattle Univ — We have implemented a Michelson's interferometer to demonstrate the resonant motion of a cm-sized cantilever due to radiation pressure of a laser diode (5 mW or less). The mechanical oscillation is found to be 2.454 (+/-0.003) kHz and is independently confirmed by dynamic force microscopy in which a piezoelectric transducer (PZT) is employed as a mechanical driver. We will discuss other applications, such as a wavelength meter and short-ranged force measurements, based on our simple table-top experiment.

**4:54PM C7.00013 ABSTRACT WITHDRAWN —**

**5:06PM C7.00014 Transient even and odd order nonlinearity of a YBCO transmission line<sup>1</sup>** , RICHARD HUIZEN, Grand Valley State University, STEPHEN REMILLARD, Hope College — Second (IMD2) and third (IMD3) order intermodulation distortions were found to exhibit dependencies on temperature and magnetic field. A carrier wave at the 890 MHz resonant frequency of the type-II  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  superconducting resonator circuit, with  $T_C = 89\text{K}$ , was introduced into the circuit via an electric coupling antenna. Two off-resonance probe signals were injected into the circuit via a separate magnetic coupling element. The combination of these three signals locally excited synchronous second and third order IMD. A static magnetic field was applied perpendicularly to the film which induced magnetic flux vortices in the sample. Upon removal of the static magnetic field, IMD2 and IMD3 exhibited distinct transient decay modes correlating to temperature. Between 85.0K and 87.5K, IMD3 decayed exponentially. Above 87.5K, IMD3 exhibited bounded exponential growth, while within a narrow temperature range around 87.5K, removal of a static magnetic field strongly suppressed IMD3. IMD2 exhibited exponential decay at all temperatures. Even and odd order microwave nonlinearities were thus shown to result from different, magnetically coupled, physical mechanisms.

<sup>1</sup>Funding for this project was provided by Award number DMR-1206149 from the National Science Foundation.

**5:18PM C7.00015 Magnetic Levitation Experiments with the Electrodynamic Wheel<sup>1</sup>** , VINCENT CORDREY, ANGEL GUTARRA-LEON, NATHAN GAUL, WALERIAN MAJEWSKI, Northern VA Comm College — Our experiments explored inductive magnetic levitation using circular Halbach arrays with the strong variable magnetic field on the outer rim of the ring. Such a system is usually called an Electrodynamic Wheel (EDW). Rotating this wheel around a horizontal axis above a flat conducting surface should induce eddy currents in said surface through the variable magnetic flux. The eddy currents produce, in turn, their own magnetic fields which interact with the magnets of the EDW. We constructed two Electrodynamic Wheels with different diameters and demonstrated that the magnetic interactions produce both lift and drag forces on the EDW which can be used for levitation and propulsion of the EDW. The focus of our experiments is the direct measurement of lift and drag forces to compare with theoretical models using wheels of two different radii.

<sup>1</sup>Supported by grants from the Virginia Academy of Science, Society of Physics Students, Virginia Community College System, and the NVCC Educational Foundation.

**Monday, March 14, 2016 2:30PM - 5:30PM –**  
**Session C12 GSNP GSOF: Intrinsic Localized Modes: Recent Developments and Future Perspectives** 308 - David Campbell, Boston University

**2:30PM C12.00001 From Discrete Breathers to Many Body Localization and Flatbands** , SERGEI FLACH<sup>1</sup>, Center for Theoretical Physics of Complex Systems, Institute for Basic Science, Daejeon, South Korea — Discrete breathers (DB) and intrinsic localized modes (ILM) are synonymic dynamical states on nonlinear lattices - periodic in time and localized in space, and widely observed in many applications. I will discuss the connections between DBs and many-body localization (MBL) and the properties of DBs on flatband networks. A dense quantized gas of strongly excited DBs can lead to a MBL phase in a variety of different lattice models. Its classical counterpart corresponds to a 'nonergodic metal' in the MBL language, or to a nonGibbsian selftrapped state in the language of nonlinear dynamics. Flatband networks are lattices with small amplitude waves exhibiting macroscopic degeneracy in their band structure due to local symmetries, destructive interference, compact localized eigenstates and horizontal flat bands. DBs can preserve the compactness of localization in the presence of nonlinearity with properly tuned internal phase relationships, making them promising tools for control of the phase coherence of waves.

<sup>1</sup>also at: New Zealand Institute of Advanced Study, Massey University, Auckland, New Zealand

**3:06PM C12.00002 Recent advances in the physics of localized states** , YURI KIVSHAR<sup>1</sup>, Nonlinear Physics Center, Australian National University, Canberra, Australia — We will review several examples of the existence and generation of localized states in optics and metamaterials including weakly coupled optical waveguides and arrays of nonlinear “meta-atoms” in metamaterials. We will also mention some recent studies on an interplay of nonlinearity-induced energy localization and edge states in discrete systems appeared in the systems with nontrivial topology

<sup>1</sup>Also at the ITMO University, St. Petersburg, Russia

**3:42PM C12.00003 Shepherding intrinsic localized modes in micro-mechanical arrays** , ALBERT SIEVERS, Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, NY 14853 — The energy profiles of intrinsic localized modes (ILMs) in periodic physical lattices with nonlinear forces resemble those of localized vibrational modes at defects in a harmonic lattice but, like solitons, they can propagate; however, in contrast with solitons they loose energy as they move through the lattice - the more localized the excitation the faster the energy loss. One of our experimental studies with micro-mechanical arrays involves steady state locking of ILMs, and their interactions with impurities. By measuring the linear response spectra of a driven array containing an ILM both the dynamics of bifurcation transitions and the hopping of vibrational energy have been connected to the transition properties of soft modes. Recently the search for a completely mobile ILM has focused attention on minimizing the resonance interaction that occurs between the localized excitation and small amplitude plane wave modes. Via simulations we demonstrate that when more than one type of nonlinear force is present their Fourier components can often be designed to cancel against each other in the k-space region of the plane wave dispersion curve, removing the resonance. The end result is super-transmission for an ILM in a discrete physical lattice. Such an engineered, intrinsic, low loss channel may prove to be a useful property for other physical systems treated within a tight binding approximation. In collaboration with M. Sato.

**4:18PM C12.00004 Localized Modes in Granular Chains** , MASON PORTER, University of Oxford — Granular crystals are tightly-packed lattices (or more disordered arrangements) of solid particles that deform elastically when they contact each other. In the presence of precompression, they can exhibit breather solutions in the form of intrinsic localized modes and defect modes. I'll give an introduction to granular crystals and will then examine breathers in one-dimensional granular crystals (i.e., granular chains) in both models and experiments. I will give examples using both diatomic configurations and homogeneous configurations with defect particles. I will also consider disordered granular chains and discuss recent work on nonlinear Anderson localization and related phenomena in such systems.

**4:54PM C12.00005**

### **Intrinsic Localized Modes in Optical Photonic Lattices and Arrays**

<sup>1</sup> , DEMETRIOS CHRISTODOULIDES, CREOL-College of Optics and Photonics, UCF — Discretizing light behavior requires optical elements that can confine optical energy at distinct sites. One possible scenario in implementing such arrangements is to store energy within low loss high Q-microcavities and then allow photon exchange between such components in time. This scheme requires high-contrast dielectric elements that became available with the advent of photonic crystal technologies. Another possible avenue where such light discretization can be directly observed and studied is that based on evanescently coupled waveguide arrays. As indicated in several studies, discrete systems open up whole new directions in terms of modifying light transport properties. One such example is that of discrete solitons. By nature, discrete solitons represent self-trapped wavepackets in nonlinear periodic structures and result from the interplay between lattice diffraction (or dispersion) and material nonlinearity. In optics, this class of self-localized states has been successfully observed in both one- and two-dimensional nonlinear waveguide arrays. In recent years such photonic lattices have been implemented or induced in a variety of material systems, including those with cubic (Kerr), quadratic, photorefractive, and liquid-crystal nonlinearities. In all cases the underlying periodicity or discreteness can lead to new families of optical solitons that have no counterpart whatsoever in continuous systems. Interestingly, these results paved the way for observations in other physical systems obeying similar evolution equations like Bose-Einstein condensates. New developments in laser writing ultrashort femtosecond laser pulses, now allow the realization of all-optical switching networks in fully 3D environments using nonlinear discrete optics. Using this approach all-optical routing can be achieved using blocking operations. The spatio-temporal evolution of optical pulses in both normally and anomalously dispersive arrays can lead to novel schemes for mode-locking and pulse compression. A strong signature of discrete X-wave formation was also demonstrated in such structures. In the last few years, Anderson localization was unequivocally observed in array systems where the transition from ballistic transport to diffusive, and the cross-over to Anderson localization was studied as a function of disorder and nonlinearity. In recent studies synthetic lattices exhibiting parity-time (PT) symmetry were also considered. The interplay of gain and loss in this latter family of structures leads to counterintuitive characteristics and behavior such as non-reciprocal propagation and power oscillations. The realization of discrete array systems at sub-wavelength scales is another important direction that is nowadays intensively pursued. References 1. D. N. Christodoulides, F. Lederer, and Y. Silberberg, Nature 424, 817- 823 (2003). 2. F. Lederer, G. I. Stegeman, D. N. Christodoulides, G. Assanto, M. Segev and Y. Silberberg, Phys. Reports 463, 1-126 (2008). 3. M Wimmer, A Regensburger, MA Miri, C. Bersch, D.N Christodoulides, and U. Peschel, "Observation of optical solitons in PT-symmetric lattices" Nature Communications 6, 7782 (2015).

<sup>1</sup>Intrinsic Localized Modes in Optical Photonic Lattices and Arrays

**Monday, March 14, 2016 2:30PM - 5:30PM –**

**Session C13 DMP: DMP Prize Session** 309 - Michael E. Flatt, University of Iowa

**2:30PM C13.00001 David Adler Lectureship Award in the Field of Materials Physics: Electrically Tunable Nanoantennas for Control of Absorption, Emission and Scattering<sup>1</sup>** , HARRY ATWATER, California Institute of Technology — Progress in understanding resonant subwavelength structures has fueled an explosion of interest in both fundamental processes and nanophotonic devices for imaging, sensing, solar energy conversion and thermal radiation control. Achieving electronic tunability of the optical properties is also an emerging opportunity to bring nanoscale resonators and antennas to life as dynamic objects. While the optical properties of photonic and plasmonic nanostructures are typically fixed at the time of fabrication, gated field effect tuning of the carrier density in conducting oxides and two-dimensional materials enables the optical dispersion of individual structures to be altered from dielectric to plasmonic, yielding active nano-antenna arrays with electrically tunable absorption, radiative emission and scattering properties.

<sup>1</sup>Supported by U.S. Department of Energy (DOE) Office of Science Basic Energy Sciences

**3:06PM C13.00002 Frank Isakson Prize for Optical Effects in Solids: Optical spectroscopy and mechanisms of superconductivity.** , DIRK VAN DER MAREL<sup>1</sup>, University of Geneva — By its very nature the phenomenon of superconductivity is intimately connected to the electrodynamics properties of a material, both in the normal and in the superconducting state. Optical spectroscopy and electrical transport -corresponding to the zero-frequency limit of the optical response- provide for this reason sensitive tools probing the collective response of a superconducting material. Optical spectroscopy can provide the real and imaginary parts of the optical conductivity of an electron liquid for all frequencies from radiowaves through infrared and visible up to the ultraviolet and even X-ray frequencies. Theory of the optical response is particularly well developed, leading among others to a number of sumrules, providing powerful tools for confronting experiment and theoretical models of superconducting pairing. In this talk examples of sumrules will be discussed relating to the kinetic energy and the Coulomb energy of the paired electrons, and experimental data of addressing these two energies will be presented. The basic understanding of pair formation in the conventional (i.e. BCS) model of superconductivity is, that electrons form pairs as a result of an attractive interaction. On general grounds one then expects the interaction energy to become reduced when the electrons form pairs, while at the same time their kinetic energy increases. Superconductivity is a stable state of matter provided that all contributions together result in a lowering of the total (interaction, kinetic plus other terms if relevant) lowering of energy. In this talk I will demonstrate that these two effects can be observed in the cuprate superconductors, that behave according to aforementioned trends for strongly overdoped cuprates, but that the observed effects have the opposite sign for underdoped and optimally doped cuprates. These observations compare favorably with published numerical calculations based on models of strong electron-electron correlation, not involving the vibrations of the lattice, and where the electron-electron interaction is purely repulsive.

<sup>1</sup>Invited talk because of the Frank Isakson Prize 2016

**3:42PM C13.00003 Frank Isakson Prize Talk: Superfluid and normal-fluid densities in the cuprate superconductors from infrared spectroscopy**<sup>1</sup> , D.B. TANNER, University of Florida — Measurements for a number of cuprate families of optical reflectance over a wide spectral range (far-infrared to ultraviolet) have been analyzed using Kramers-Kronig analysis to obtain the optical conductivity  $\sigma(\omega)$  and (by integration of the real part of the conductivity) the spectral weight of low- and mid-energy excitations. For the Kramers-Kronig analysis to give reliable results, accurate high-frequency extrapolations, based on x-ray atomic scattering functions, were used. When the optical conductivities of the normal and superconducting states are compared, a transfer of spectral weight from finite frequencies to the zero-frequency delta-function conductivity of the superconductor is seen. The strength of this delta function gives the superfluid density,  $\rho_s$ . In a clean metallic superconductor the superfluid density is essentially equal to the conduction electron density. The cuprates in contrast have only about 20% of the *ab*-plane low-energy spectral weight in the superfluid. The rest remains in finite-frequency, midinfrared absorption. In underdoped materials the superfluid fraction is even smaller. There are two ways to measure  $\rho_s$ , using either the partial sum rule for the conductivity or by examination of  $\sigma_2(\omega)$ . Comparison of these two estimates of the superfluid density shows that 98% of the *ab*-plane superfluid density comes from energies below 0.15 eV.

<sup>1</sup>Many students, postdocs, and materials preparers have contributed to this work; to all I am very grateful.

**4:18PM C13.00004 Richard L. Greene Dissertation Award in Experimental Condensed Matter or Materials Physics Talk: Ferromagnetic quantum criticality in YbNi<sub>4</sub>P<sub>2</sub>** , ALEXANDER STEPPKE, University of St. Andrews — In a number of strongly correlated electron systems quantum phase transitions can be observed by the suppression of antiferromagnetic order. In contrast the prototypical continuous quantum phase transition of a metallic ferromagnet is often preempted by a first-order transition or a superconducting state. We show that the Kondo lattice system YbNi<sub>4</sub>P<sub>2</sub> exhibits a ferromagnetically ordered phase with a very low Curie temperature of 0.15K. The compound can be tuned to a ferromagnetic quantum critical point by substitution of phosphorus by arsenic. With thermodynamic studies of specific heat, ac susceptibility and thermal expansion we show strong evidence for the ferromagnetic order and the quantum criticality in the YbNi<sub>4</sub>(P 1-x As x)<sub>2</sub> doping series and the existence of a ferromagnetic quantum critical point at zero applied field for small substitutions.

**4:54PM C13.00005 Richard L. Greene Dissertation Award in Experimental Condensed Matter or Materials Physics Talk: Towards single atom magnets** , SUSANNE BAUMANN, IBM Almaden Research Center — Magnetic anisotropy is a fundamental property of magnetic materials that governs the stability and directionality of their magnetization. At the atomic level, magnetic anisotropy originates from anisotropy in the orbital angular momentum (L) and the spin-orbit coupling that connects the spin moment of a magnetic atom to the spatial symmetry of its ligand field environment. Generally, the ligand field, that is necessary for the anisotropy, also quenches the orbital moment and reduces the total magnetic moment of the atom to its spin component. However, careful design of the coordination geometry of a single atom can restore the orbital moment while inducing uniaxial anisotropy, as we present here for single atoms deposited on top of a thin MgO film. Scanning tunneling spectroscopy and x-ray absorption spectroscopy measurements show a large magnetic anisotropy of 19 meV for iron and 58 meV for cobalt, as well as relaxation times of many milliseconds. These results offer a strategy, based on symmetry arguments and careful tailoring of the interaction with the environment, for the rational design of nanoscopic permanent magnets and single atom magnets.

**Monday, March 14, 2016 2:30PM - 5:30PM –**

**Session C14 FHP FPS: The Author in Dialogue: Steven Weinberg's 'To Explain the World'**

310 - Joseph D. Martin, Michigan State University

**2:30PM C14.00001 Reflections of a whig physicist** , STEVEN WEINBERG, Theory Group, Physics Department, University of Texas at Austin — I argue that a whig interpretation, keeping an eye on present knowledge and methods, is appropriate in the history of science.

**3:06PM C14.00002 Beller Lecture: Is Understanding the Past in Its Own Terms Understanding?** , DAVID WOOTTON, Professor of History at the University of York — History of Science is in a state of intellectual confusion symbolized by its hostility to what is called Whig history. The fundamental issue is whether it is legitimate to use hindsight in the writing of history. In this lecture I will defend retrospective history in three key respects: a) retrospection is generally a legitimate procedure in historical writing, primarily because historical outcomes are often unintended and unpredictable; b) retrospection is particularly legitimate where science is concerned because scientific development is path dependent; c) retrospection is particularly legitimate in history of science because science progresses, and progress can only be identified retrospectively. Defending retrospection is entirely compatible with recognizing that science is culturally specific; thus retrospection need not involve anachronism. See [www.inventionofscience.com](http://www.inventionofscience.com)

**3:42PM C14.00003 To Explain Copernicus: The Islamic Scientific and Religious Contexts** , F. JAMIL RAGEP, McGill University — No one seriously disputes the novelty of Copernicus's monumental decision to put the Earth in motion or its importance for the development of modern science. But that decision can appear quite different when viewed from the perspective of a modern scientist versus that of a contextualist historian. In his recent book *To Explain the World*, Prof. Weinberg places great store on what he calls aesthetic criteria for understanding Copernicus's choice. The historical record, however, is rather ambiguous on the matter, and if anything supports the view that Copernicus came to his aesthetic justifications (such as the beautiful ordering of the planets) after first reaching his heliocentric theory. So if not aesthetics, what did lead him to go against a two-millennium tradition that placed the Earth firmly in the center of the Cosmos? There are no doubt many factors; one of the most intriguing suggestions, well-argued by Noel Swerdlow, is that Copernicus was led to heliocentrism by his rather conservative desire to restore uniform, circular motion to the heavens and remove the irregularities of Ptolemaic astronomy. Swerdlow has also asserted that this has much to do with Islamic predecessors who were attempting to do the same thing, only within a geocentric framework. In this presentation, I will briefly summarize this Islamic scientific context and then explore the religious beliefs that led not only to the questioning of Ptolemaic scientific authority, including his alleged lack of observational diligence, but also ancient philosophical authority, the latter opening up possibilities for alternative cosmologies, at least one of which included the Earth's motion. Finally, evidence will be presented that connects these Islamic contexts with Copernicus's theories and justifications.

**4:18PM C14.00004 The Diagnosis of Error in Histories of Science** , WILLIAM THOMAS, History Associates, Inc. — Whether and how to diagnose error in the history of science is a contentious issue. For many scientists, diagnosis is appealing because it allows them to discuss how knowledge can progress most effectively. Many historians disagree. They consider diagnosis inappropriate because it may discard features of past actors' thought that are important to understanding it, and may have even been intellectually productive. Ironically, these historians are apt to diagnose flaws in scientists' histories as proceeding from a misguided desire to idealize scientific method, and from their attendant identification of deviations from the ideal as, *ipso facto*, a paramount source of error in historical science. While both views have some merit, they should be reconciled if a more harmonious and productive relationship between the disciplines is to prevail. In *To Explain the World*, Steven Weinberg narrates the slow but definite emergence of what we call science from long traditions of philosophical and mathematical thought. This narrative follows in a historiographical tradition charted by historians such as Alexandre Koyre and Rupert Hall about sixty years ago. It is essentially a history of the emergence of reliable (if fallible) scientific method from more error-prone thought. While some historians such as Steven Shapin view narratives of this type as fundamentally error-prone, I do not view such projects as *a priori* illegitimate. They are, however, perhaps more difficult than Weinberg supposes. In this presentation, I will focus on two of Weinberg's strong historical claims: that physics became detached from religion as early as the beginning of the eighteenth century, and that physics proved an effective model for placing other fields on scientific grounds. While I disagree with these claims, they represent at most an overestimation of vintage science's interest in discarding theological questions, and an overestimation of that science's ability to function at all reliably.

**4:54PM C14.00005 to be determined** , JENNIFER OUELLETTE, Gizmodo — No abstract available.

**Monday, March 14, 2016 2:30PM - 5:30PM –**

**Session C15 DCMP DMP: Graphene: Adatoms, Doping, and Magnetism** 314 - Olaf van 't Erve, Naval Research Laboratory

**2:30PM C15.00001 Proximity induced exchange interaction in graphene-YIG devices<sup>1</sup>** , JOHANNES CHRISTIAN LEUTENANTSMEYER, ALEXEY KAVERZIN, MAGDALENA WOJTASZEK, BART J. VAN WEES, University of Groningen, PHYSICS OF NANODEVICES TEAM — The proximity of two materials with radically different properties can give rise to a new physical phenomenon present only in the direct vicinity to the interface. Graphene is a perfect candidate for observing proximity effects as being ultimately thin and therefore ultimately sensitive for such interactions. Ferromagnetism is one of the desired properties for spintronics applications of graphene. It is absent in the pristine state, however, one can artificially induce magnetic ordering by bringing graphene in the proximity of ferrimagnetic insulating material, such as yttrium iron garnet (YIG). In this work we show that a monolayer of graphene placed on top of YIG adopts the exchange interaction induced by YIG and thus becomes ferromagnetic even at room temperatures. The proximity induced exchange interaction results in an effective magnetic field that influences directly the spin transport in graphene seen in a spin precession measurements. We are able to fit the measured Hanle dependences with extended solutions of Bloch diffusion equations and extract the value of the effective exchange field that is around 200 mT. Our findings open up a new route for creating novel all graphene in plane spin valve devices for spintronics applications.

<sup>1</sup>European Unions Seventh Framework Programme n607904-13 Spinograph, n604391 Graphene Flagship, FOM, ZIAM

**2:42PM C15.00002 Magneto-plasmons in graphene in a periodically modulated magnetic field** , YUXUAN JIANG, OWEN VAIL, JEREMY YANG, JAMEY GIGLIOTTI, Georgia Institute of Technology, Atlanta, GA, USA, CLAIRE BERGER, Georgia Institute of Technology, Atlanta, GA, USA/CNRS, Institut Néel, Grenoble, France, WALTER DE HEER, Georgia Institute of Technology, Atlanta, GA, USA, DMITRY SMIRNOV, National High Magnetic Field Laboratory, Tallahassee, FL, USA, ZHIGANG JIANG, Georgia Institute of Technology, Atlanta, GA, USA — We present infrared magneto-spectroscopy study of graphene in a periodically modulated magnetic field. Corrugated trenches are first patterned on SiC substrate using e-beam lithography and plasma etching. Multilayer epitaxial graphene is then grown over the trenches, forming a periodic structure. In the presence of an external magnetic field, the perpendicular component of the field is spatially modulated, and the modulation strength can be tuned by varying the trench packing density or the tilting angle of the field with respect to the substrate. Experimentally, enhanced absorption and salient deviations from single Lorentzian lineshape are observed, resulting from the periodic modulation. The deviated spectra can be well fitted by two Lorentzians, suggestive of the presence of two active modes. In addition, as the packing density of the trenches increases, the coupling between the corrugated graphene structures becomes stronger, resulting in a broadened spectrum.

**2:54PM C15.00003 Theory for disorder-induced magnetodrag in one-channel model for graphene<sup>1</sup>** , NAVNEETH RAMAKRISHNAN, DEREK HO, Center for Advanced 2D Materials, SHAFFIQUE ADAM, Yale-NUS College — Recent work has shown the presence of disorder induced magnetoresistance that persists far away from charge neutrality, even in effective one-band systems [1]. This effect manifests itself in the magnetic field dependence of Coulomb drag, an effect that existing theoretical treatments have not considered [2]. In the presence of disorder, we calculate the magnetodrag as a function of the parameters of the disorder distribution and compare our results with the available experimental data in graphene and 2D electron gases. We comment on the relevance of these results in explaining the large magnetodrag at charge neutrality in graphene.

## References

- [1] J. Ping, I. Yudhistira, N. Ramakrishnan, S. Cho, S. Adam, and M. S. Fuhrer, *Phys. Rev. Lett.* 113, 047206 (2014).
- [2] B. N. Narozhny, A. Levchenko, *arXiv:1505.07468* (2015).

<sup>1</sup>This work is supported by the Singapore National Research Foundation NRF-NRFF2012-01.

**3:06PM C15.00004 Induced magnetism in exfoliated graphene via proximity effect with yttrium iron garnet thin films**, MARIO AMADO, YANG LI, ANGELO DI BERNARDO, Materials Science and Metallurgy, University of Cambridge, UK, ANTONIO LOMBARDO, ANDREA C. FERRARI, Cambridge Graphene Centre, University of Cambridge, UK, JASON ROBINSON, Materials Science and Metallurgy, University of Cambridge, UK — The recent discovery of the quantum anomalous Hall effect (QAHE) in magnetically doped topological insulators cooled below in the millikelvin regime represents breakthrough in the field of spintronics. Theoretically, the QAHE should occur in graphene proximity coupled to a ferromagnetic insulator but with the promise of much higher operating temperatures for practical applications. Hints of proximity-induced magnetism in graphene coupled to yttrium iron garnet (YIG) films have been reported although the QAHE remains unobserved; the lack of a fully developed plateau in graphene/YIG devices can be attributed to poor interfacial coupling and therefore a dramatically reduced magnetic proximity effect. Here we report the deposition and characterisation of epitaxial thin-films of YIG on lattice-matched gadolinium gallium garnet substrates by pulsed laser deposition. Pristine exfoliated graphene flakes transferred mechanically onto the YIG are reported alongside results that correlate the effects of YIG morphology on the electronic and crystal properties of graphene by electrical (low temperature magnetoresistance measurements in Hall-bar-like configuration) and optical (Raman) means.

**3:18PM C15.00005 The magnetic ratchet effect in bilayer graphene**, EDWARD MCCANN, NARJES KHEIRABADI, Physics Department, Lancaster University, Lancaster, LA1 4YB, UK, VLADIMIR FAL'KO, National Graphene Institute, The University of Manchester, Manchester, M13 9PL, UK — Experiments [1] have measured a magnetic ratchet effect for electrons in hydrogenated monolayer graphene, an effect in which a d.c. electric current is generated from an a.c. electric field in the presence of an in-plane magnetic field and spatial asymmetry. Here, we describe the theory of the magnetic ratchet effect in bilayer graphene. The Boltzmann kinetic equation [2,3] is used to relate the d.c. current to the scattering probability of electrons in bilayer graphene. Taking into account details of the low-energy band structure of bilayer graphene, including interlayer hopping parameters, we compare contributions arising from gate- and disorder-induced spatial asymmetry, illustrating that bilayer and multilayer graphenes are natural candidates for the study of non-linear transport effects. [1] C. Drexler et al, Nature Nanotechnology 8, 104 (2013). [2] V. I. Fal'ko, Sov. Phys. Solid State 31, 561 (1989). [3] S. A. Tarasenko, Phys. Rev. B 83, 035313 (2011).

**3:30PM C15.00006 Magnetic nanostructures on graphene**, XIAOJIE LIU, Center for Quantum Science and School of Physics, Northeast Normal University, Changchun, 130117, People's Republic of China., CAI-ZHUANG WANG, Ames Laboratory U. S. Department of Energy, and Department of Physics and Astronomy, Iowa State University, Ames, IA, 50011, U. S. A., HAI-QING LIN, Beijing Computational Science Research Center, Beijing 100084, China, MYRON HUPALO, Ames Laboratory U. S. Department of Energy, and Department of Physics and Astronomy, Iowa State University, Ames, IA, 50011, U. S. A., PATRICIA A. THIEL, Ames Laboratory U. S. Department of Energy, Department of Chemistry and Department of Materials Science and Engineering, Iowa State University, Ames, KAI-MING HO, MICHAEL C. TRINGIDES, Ames Laboratory U. S. Department of Energy, and Department of Physics and Astronomy, Iowa State University, Ames, IA, 50011, U. S. A. — The calculations also show that Fe clusters on graphene exhibit ferromagnetic order but have smaller magnetic moments compared to the corresponding free-standing clusters. By contrast, Mn clusters on graphene exhibit ferrimagnetic coupling and enhanced magnetic moment compared to their free-standing clusters. Adsorption of Fe and Mn nanostructures also induces magnetic moments in graphene, and the induced magnetic moment on each carbon atom in graphene is correlated with the distortion of the graphene lattice. The origin of the magnetic moment changes in the clusters upon adsorption can be attributed to the electron redistribution due to the interaction with graphene.

**3:42PM C15.00007 Understanding Magnetic Trimer Interactions in (Cr,Mn)-Substituted Graphene<sup>1</sup>**, JASON T. HARALDSEN, Department of Physics, University of North Florida, CHARLES B. CROOK, GREGORY HOCHINS, Department of Physics and Astronomy, James Madison University, JIAN-XIN ZHU, Theoretical Division and Center for Integrated Nanotechnologies, Los Alamos National Laboratory, COSTEL CONSTANTIN, Department of Physics and Astronomy, James Madison University, ALEXANDER V. BALATSKY, Institute for Materials Science, Los Alamos National Laboratory — We investigate the magnetic interactions within a graphene superlattice produced by three directly substituted transition-metal atoms (specifically chromium and manganese). Using a first principles approach, we calculate the electronic and magnetic properties for this system assuming an equilateral trimer configuration with varying atomic separations. Through an examination of the electronic band structure, density of states, and Millikan populations (magnetic moment) for each atom, we find that the presence of magnetic impurities establishes a distinct magnetic moment in the graphene lattice, where the interactions are dependent on the spatial and magnetic characteristic between the magnetic atoms and the carbon atoms, which leads to either ferromagnetic or antiferromagnetic behavior. Furthermore, we use magnetization mapping to show that the substituted atoms induce an overall magnetic moment in the graphene lattice, which may help guide the discussion on spintronic graphene.

<sup>1</sup>JTH, CBC, GH, and AVB acknowledge support from the Institute for Materials Science via the United States Basic Energy Sciences (E304)

**3:54PM C15.00008 Controlling Adatom Magnetism on Bilayer Graphene by External Field**, MUKUL KABIR, Indian Institute of Science Education and Research, Pune 411008, India, DHANI NAFDAY, TANUSRI SAHA-DASGUPTA, S. N. Bose National Centre for Basic Sciences, Kolkata 700098, India — We study the effect of external electric field on the magnetic properties of single Fe adatom and Fe dimer hosted on a bilayer graphene surface grown on a SiO<sub>2</sub> substrate within first-principles calculations. We find that electric field perpendicular to the bilayer graphene modulates the charge and spin-state of the single Fe adatom over a wide range. States ranging from  $3d^6$ ,  $S=2$  to  $3d^{10}$ ,  $S=0$  have been observed for Fe adatom, which may be inaccessible under normal condition. This would be of interest in the context of orbitally controlled Kondo effect. Further, for Fe-dimer, we find that a small electric field is able to tune the magnetic exchange coupling. Interestingly, we also observe an unusual magnetostructural coupling for Fe-dimer, which stabilizes a ferrimagnetic state over a fully compensated antiferromagnetic spin configuration.

**4:06PM C15.00009 Novel electronic properties of hydrogenated graphene: A first-principles calculation**, HONG-YAN LU, RUI WANG, SHIH-YANG LIN, C. S. TING, Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, Texas 77204, USA — We studied the electronic properties of some new kinds of hydrogenated graphenes by first-principles calculations. The designed systems, depending on the position and concentration of the hydrogen atoms, may show interesting band structures that are different from that of the pure graphene. For example, we can obtain semiconductor of a gap about 3eV with flat valance and conduction bands, or semimetal with anisotropic Dirac cones in which the position of Dirac points are shifted from K points, or semimetal with flat band crossing the Dirac cone at the Dirac point. The consequences of these features will be presented. We are able to get good metal with considerable density of states at Fermi level. The phonon dispersions and spectra as well as the electron-phonon couplings of such metallic systems are currently being investigated by the first-principles calculation, their superconductivity transition temperatures  $T_c$  should thus be predictable by assuming the electron-phonon coupling as the pairing interaction. We expect that the phonon frequencies are quite large, and the  $T_c$  could be high for some of the metallic systems.

**4:18PM C15.00010 Peculiarity of Thiophene/Graphene interface for organic electronic applications**, SOURAYA GOUMRI-SAID, Al Faisal University — Interfacial study between thiophene molecule and graphene surface is investigated on the basis of density functional theory. The reported HOMO-LUMO energy gaps, adsorption energy as well as binding energy are showing the existence of intermolecular forces accumulated from the attractive van der Waals forces and Pauli repulsion forces. The interface's separation distance is varied from 1.00Å to 2.50Å. It is noted that, subsequently growing intermolecular forces are very sensitive even to a relatively small change in the interface's separation distance between the molecule and the surface. The electronic density of states, dense electrons population of the thiophene/graphene system is found to be at energy Fermi level with appearance of spin-polarization. A slight magnetic behaviour on thiophene molecule, accompanied by a decrease in the magnetization of graphene surface was observed in the presence of the molecule near to the surface.

**4:30PM C15.00011 Adsorption of Nitric Oxide on Carbon Vacancies in Graphene and its Impact on the Conductivity**, JORGE SOFO, SANGZI LIANG, Physics Department, The Pennsylvania State University, GUGANG CHEN, AVETIK HARUTYUNYAN, Honda Research Institute — The conductance of graphene in FET devices increases when exposed to NO with detection limits down to the part-per-quadrillion level. We explore a possible explanation for this phenomena assuming that NO chemisorbs to vacancies and eventually dissociates. We found that adsorption of NO in graphene vacancies is favorable by 5.3 eV. In order to evaluate the conductivity due to these impurities, we obtain a minimum tight binding model with a Wannier transformation of the Kohn-Sham orbitals obtained by DFT. We evaluate the conductivity using the Kubo-Greenwood formula and the kernel polynomial method. We consider vacancies, NO and N chemisorbed in the vacancies, and O as an adatom on graphene. We found that the conductivity stays the same when NO adsorbs into a vacancy, but it increases when the oxygen atom moves away from the nitrogen atom, either leaving or moving to other parts of the surface, with the former giving a larger increase in conductivity.

**4:42PM C15.00012 Using Single Adatoms to Sense Screening by Graphene Charge Carriers**, JONATHAN WYRICK, FABIAN NATTERER, Center for Nanoscale Science and Technology, NIST, YUE ZHAO, Center for Nanoscale Science and Technology, NIST; University of Maryland, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, NIKOLAI ZHITENEV, JOSEPH STROSCIO, Center for Nanoscale Science and Technology, NIST — As electronic devices approach the nanometer scale it becomes increasingly necessary to understand how small numbers of defects interact with one another and ultimately determine the behavior of a device. In the case of devices with graphene exposed at the surface, defects can be modelled and varied by depositing adatoms. We investigate how Co atoms adsorbed on graphene create and modify the electric potential experienced by graphene carriers using scanning tunneling microscopy and spectroscopy at low temperature. When an STM tip is brought into proximity to a biased graphene sample the electric field between tip and sample is screened by graphene's 2D electron gas, resulting in a local top-gating potential under the tip. This potential can be manipulated by varying a backgate voltage and the sample bias, and can be spatially characterized by imaging charging rings that form around defects when the potential changes their charge state. We find that defect charging rings lying near or even crossing adsorbed Co atoms become distorted and can form secondary charging rings around those atoms. To explain these effects we employ a charging model that incorporates a defect resonance, the screened tip potential, and modified screening in regions localized around Co atoms.

**4:54PM C15.00013 Transport measurement of Li doped monolayer graphene**, ALI KHADEMI, EBRAHIM SAJADI, PINDER DOSANJH, JOSHUA FOLK, Department of Physics and Astronomy, University of British Columbia, Vancouver, BC, V6T1Z1, Canada, ALEXANDER STHR, STIVEN FORTI, ULRICH STARKE, Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — Lithium adatoms on monolayer graphene have been predicted to induce superconductivity with a critical temperature near 8 K [1], and recent experimental evidence by ARPES indicates a critical temperature nearly that high [2]. Encouraged by these results, we investigated the effects of lithium deposited at cryogenic temperatures on the electronic transport properties of epitaxial and CVD monolayer graphene down to 3 K. The change of charge carrier density due to Li deposition was monitored both by the gate voltage shift of the Dirac point and by Hall measurements, in low and high doping regimes. In the high doping regime, a saturation density of  $210^{13} \text{ cm}^{-2}$  was observed independent of sample type, initial carrier density and deposition conditions. No signatures of superconductivity were observed down to 3 K. [1] G. Profeta, et al., Nat Phys 8, 131 (2012). [2] B. M. Ludbrook, et al., PNAS 112 (38), 11795–11799 (2015).

**5:06PM C15.00014 Phase transitions of monolayers on graphene**, JOSHUA KAHN, BORIS DZYUBENKO, OSCAR VILCHES, DAVID COBDEN, Department of Physics, University of Washington — We have studied physisorbed layers of monatomic and diatomic gases on graphene. We used devices in which few-layer graphene, ranging from monolayer to trilayer, is suspended across a trench between two platinum contacts and are cleaned by thermal and current annealing. We found that the density of adsorbates is revealed by the conductance, similar to the case with nanotubes. The conductance change for a monolayer can be large. On trilayer graphene the adsorbed gases can be seen to exhibit transitions between two-dimensional phases identical to those on bulk graphite, including incommensurate and commensurate solid, fluid and vapor and multiple layers. New features appear in the conductance at the boundaries of the commensurate phase of Kr. We are able to measure single-particle binding energies very accurately and see how it depends on thickness; investigate the effects of changing disorder by gradually current annealing; and search for new phases in the case of monolayer graphene where atoms adsorbed on both sides can interact. We can map out the 2d phase diagrams very quickly by ohmic heating, which gives nearly instantaneous control of the temperature.

**5:18PM C15.00015 Electronic transport experiments on osmium-adatom-decorated graphene**, JAMIE ELIAS, ERIK HENRIKSEN, Washington University in St. Louis — Monolayer graphene is theoretically predicted to inherit a spin-orbit coupling from a dilute coating of certain transition metal adatoms. To explore these predictions we have constructed a cryogenic probe capable of *in situ* thermal annealing of graphene followed immediately by electronic transport measurements and controlled deposition of sub-monolayer coatings of most any metal. Previously a light coating of indium on graphene was investigated, and found to transfer electrons to graphene and reduce the mobility although no evidence of an induced spin-orbit coupling was seen. We are now depositing osmium and tungsten on graphene devices. Our initial results show an unexpected hole-doping and a sizable increase in resistance of the sample. We will report our progress on characterizing these samples by electronic transport measurements.

## Monday, March 14, 2016 2:30PM - 5:30PM –

Session C16 DCMP DMP: Scanning Tunneling Microscopy/Spectroscopy of Graphene 315 -  
Michael Lodge, University of Central Florida

**2:30PM C16.00001 Imaging nonlocal transport in graphene using scanning gate microscopy<sup>1</sup>**, MALCOLM CONNOLLY, ZIWEI DOU, University of Cambridge, SEI MORIKAWA, Institute of Industrial Science, University of Tokyo, SHU-WEI WANG, CHARLES SMITH, University of Cambridge, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, SATORU MASUBUCHI, TOMOKI MACHIDA, Institute of Industrial Science, University of Tokyo — Nonlocal transport measurements are designed to detect when charge injected by a current probe induces voltages far from the classical current path. While a range of exotic forces can induce nonlocal transport of Dirac fermions in graphene such as bandstructure topology [1], Zeeman spin Hall [2], and many-body interactions [3], it is important to understand the role of density fluctuations around the Dirac point where nonlocality can be most pronounced. We use scanning gate microscopy to image current flow and nonlocal signals directly in high-mobility graphene encapsulated by hexagonal boron nitride. Despite being located several mean-free paths from the current injector, Hall voltage probes parallel with current path display an order of magnitude larger nonlocal signal than expected around the Dirac point. SGM images captured at different carrier density are consistent with current spreading due to percolation. Such long range charge transport should be considered when designing devices and calculating the relaxation length of nonlocal currents. [1] R. V. Gorbachev, et al., Science, 346, 6208, 448-451 (2014) [2] D. A. Abanin, et al., Science, 332, 6027, 328-330 (2011) [3] D. A. Bandurin, arXiv:1509.04165 (2015)

<sup>1</sup>Supported by EPSRC

**2:42PM C16.00002 New Approaches to Edge-Doping Graphene Nanoribbons**, DANIEL J. RIZZO, TOMAS MARANGONI, TING CAO, GIANG D. NGUYEN, HSIN-ZON TSAI, ARASH A. OMRANI, CHRISTOPHER BRONNER, TRINITY JOSHI, GRIFFIN F. RODGERS, WON-WOO CHOI, RYAN R. CLOKE, STEVEN G. LOUIE, FELIX R. FISCHER, MICHAEL F. CROMMIE, UC Berkeley, CROMMIE TEAM<sup>1</sup>, FISCHER TEAM<sup>2</sup>, LOUIE TEAM<sup>3</sup> — Graphene nanoribbons (GNRs) are narrow semiconducting strips of graphene that exhibit novel electronic and magnetic properties. New bottom-up fabrication techniques enable atomic-scale precision in GNR synthesis. The use of these techniques to reliably tune the position and size of GNR band gaps is an important challenge that also has relevance for the question of whether GNRs are viable for future nanotechnologies. We have used scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) to investigate how the geometry of heteroatom incorporation alters the electronic structure of bottom-up fabricated chevron-type GNRs. We find that the addition of nitrogen into the GNR edge via a five-membered ring yields a reduced band gap compared to the behavior of pristine, undoped chevron GNRs.

<sup>1</sup>Performed STM, STS, and nc-AFM measurements

<sup>2</sup>Performed organic synthesis of precursors and designed precursors

<sup>3</sup>Performed calculations of electronic structure

**2:54PM C16.00003 Scanning tunneling microscopy of atomically precise graphene nanoribbons exfoliated onto H:Si(100)**, ADRIAN RADOCEA, University of Illinois at Urbana-Champaign, MOHAMMAD MEHDI POUR, TIMOTHY VO, MIKHAIL SHEKHIREV, ALEXANDER SINITSKII, University of Nebraska - Lincoln, JOSEPH LYDING, University of Illinois at Urbana-Champaign — Atomically precise graphene nanoribbons (GNRs) are promising materials for next generation transistors due to their well-controlled bandgaps and the high thermal conductivity of graphene. The solution synthesis of graphene nanoribbons offers a pathway towards scalable manufacturing. While scanning tunneling microscopy (STM) can access size scales required for characterization, solvent residue increases experimental difficulty and precludes band-gap determination via scanning tunneling spectroscopy (STS). Our work addresses this challenge through a dry contact transfer method that cleanly transfers solution-synthesized GNRs onto H:Si(100) under UHV using a fiberglass applicator. The semiconducting silicon surface avoids problems with image charge screening enabling intrinsic bandgap measurements. We characterize the nanoribbons using STM and STS. For chevron GNRs, we find a 1.6 eV bandgap, in agreement with computational modeling, and map the electronic structure spatially with detailed spectra lines and current imaging tunneling spectroscopy. Mapping the electronic structure of graphene nanoribbons is an important step towards taking advantage of the ability to form atomically precise nanoribbons and finely tune their properties.

**3:06PM C16.00004 LT-STM/STS studies of clean armchair edge**<sup>1</sup>, ZHENG JU, WENHAN ZHANG, WEIDA WU, Department of Physics and Astronomy, Rutgers University, WEIDA WU TEAM — It was predicted and observed that the passivated zigzag edges of graphene host highly localized edge state [1]. This edge state is predicted to be spin-polarized, which is appealing for spintronic applications. In contrast, no edge state was expected at passivated armchair graphene edge. Here we report low temperature scanning tunneling microscopy and spectroscopy (STM/STS) studies of electronic properties of clean monoatomic step edges on cleaved surface of HOPG. Most of step edges are armchair edges, in agreement with previous STM results. We observed only  $(\sqrt{3} \times \sqrt{3})R30^\circ$  superstructure near armchair edges, which has been reported in previous STM studies [2, 3, 4]. On the other hand, no honeycomb superstructure was observed in our STM data. In addition, our STM results reveal an intriguing localized electronic state at clean armchair edges. Spectroscopic and spatial evolution of this edge state will be presented. [1] Fujita et al, JSPJ, 65, 1920, (1996). [2] Niimi et al, PRB, 73, 085421 (2006). [3] Giunta and Kelyt, J. Chem. Phys., 114, 1807 (2001). [4] Sakai, et al, PRB, 81, 235417(2010).

<sup>1</sup>This work is supported by NSF DMR-1506618.

**3:18PM C16.00005 Exotic Charge Polarization near Dirac Cone Merging Transition in Graphene-based Systems**, NOAH WILSON, OWEN MYERS, TARAS LAKOBA, VALERI KOTOV, Univ of Vermont — Extreme strain in graphene yields a fascinating charge distribution around a Coulomb impurity. Graphene's band structure is characterized by gapless Dirac cones but can be made gapped by application of intense strain. The cones become increasingly elliptic continually merging, until the spectrum has an exotic, highly anisotropic, semi-Dirac, nature. This situation can also occur in various artificially engineered lattices. The unusual spectrum leads to an unconventional charge distribution around a Coulomb impurity. Crucially, unlike isotropic graphene, the polarization charge density exhibits long-range oscillatory tails far from the impurity. Such exotic behavior is due to the anisotropy of the polarization, and occurs even at zero chemical potential (i.e. unrelated to Friedel-type physics). The angular and radial functions are intrinsically coupled, hence a litany of distinct angular distributions is observed through multiple distance regimes. The density can approach infinity at angles where it was once close to zero, be negative all around the impurity, or have its polarity fluctuate along different directions. Thus our results could have important implications for STM experiments probing polarization charge around impurities in highly anisotropic Dirac systems.

**3:30PM C16.00006 Experimental Evidence of Giant Non-reciprocity of WGM Modes in Graphene**, YUE ZHAO, Dept. of Physics, South University of Science and Technology of China; Center for Nanoscale Science and Technology, NIST; Maryland Nanocenter, UMD, JONATHAN WYRICK, FABIAN NATTERER, Center for Nanoscale Science and Technology, NIST, JOAQUIN RODRIGUEZ-NIEVA, Dept. of Physics, Massachusetts Institute of Technology, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Material Science, Japan, LEONID LEVITOV, Dept. of Physics, Massachusetts Institute of Technology, NIKOLAI ZHITENEV, JOSEPH STROSCIO, Center for Nanoscale Science and Technology, NIST — Klein scattering in a circular graphene pn junction can lead to Whispering Gallery Mode(WGM) type resonances[1]. Utilizing the electrostatic potential induced by the probe of a scanning tunneling microscope, we create graphene electron resonators defined by circular pn junctions. These quasi-confined WGM states can be probed by tunneling spectroscopy measurements. With small applied magnetic fields, we observe a large energy splitting of the WGM states, displaying a manifestation of non-reciprocity due to Klein scattering of massless Dirac fermions in graphene [2].

1. Y. Zhao, et. al., *Science* 348(6235), 672-675

2. J. F. Rodriguez-Nieva, L. S. Levitov, *arXiv: 150806609*

**3:42PM C16.00007 The synthesis of planar sp<sup>2</sup>-bonded system from molecular building blocks**<sup>1</sup>, XIN ZHANG, HONG LUO, University at Buffalo, GONG GU, University of Tennessee, Knoxville — Biphenyl and pyrene molecules were deposited onto atomically flat Cu (100) surface as building blocks for the synthesis of planar, conjugated, sp<sup>2</sup>-bonded system. In situ STM observation confirmed the formation of highly-ordered lattice structure after annealing under UHV condition, as a result of the substrate-assisted dehydrogenation. The electronic properties of the system were examined by STS and will be presented.

<sup>1</sup>ONR N00014-15-1-2661

**3:54PM C16.00008 Tunneling spectroscopy in metal-hexagonal boron nitride-graphene structures<sup>1</sup>**, U. CHANDNI, Institute for Quantum Information and Matter and Department of Physics, California Institute of Technology, Pasadena, California 91125, USA, K. WATANABE, T. TANIGUCHI, National Institute for Materials Science, 1-1 Namiki, Tsukuba Ibaraki 305-0044, Japan, J. P. EISENSTEIN, Institute for Quantum Information and Matter and Department of Physics, California Institute of Technology, Pasadena, California 91125, USA — Tunneling spectroscopy provides a tool to probe the density of states of various electronic materials. Here, we report vertical tunneling transport in van der Waals heterostructures with hexagonal boron nitride (hBN) as a tunnel barrier between graphene (or graphite) and a metal (Cr/Au) electrode. We observe a strong suppression of tunneling at low biases, with a gap of about 130 meV in the dI/dV spectrum for metal-hBN-graphene (or graphite) structures. In the graphene devices, the finite zero-bias tunnel resistance was found to depend on the electron density of the graphene layer, while the gap remained unaffected. We also tested graphite-hBN-graphite junctions, in which the strong suppression of tunneling at low energies was found to be absent. We interpret the signatures in the context of phonon-mediated processes in such vertical heterostructures.

<sup>1</sup>We acknowledge funding provided by the Institute for Quantum Information and Matter, an NSF Physics Frontiers Center with support of the Gordon and Betty Moore Foundation through Grant GBMF1250.

**4:06PM C16.00009 Modification of Electronic Surface States by Graphene Islands on Cu(111)<sup>1</sup>**, GRADY GAMBREL, The Ohio State University, SHAWNA HOLLEN, University of New Hampshire, STEVEN TJUNG, NANCY SANTAGATA, EZEKIEL JOHNSTON-HALPERIN, JAY GUPTA, The Ohio State University — The interaction of graphene with copper is of interest for graphene applications due to the frequent use of copper in the chemical vapor deposition (CVD) growth of graphene. We grew pristine graphene islands on Cu(111) by dissociating ethylene gas in an ultra high vacuum environment. In situ low-temperature scanning tunneling microscopy (STM) was used to measure the physical and electronic structure of the surface with atomic resolution, enabling us to compare the graphene-covered regions to bare Cu(111). We observed a shift of the Rydberg-like series of images potential states (IPS) to lower energies and a decrease in linewidth in graphene-covered regions, indicating a decrease in local work function and reduced coupling to the copper bulk states. In some cases, the first of these states were split, which may correspond to the dual Rydberg series which has been predicted for graphene. By measuring the dispersion of the Shockley surface state, we found that the band edge and effective mass are influenced by the graphene layer. We will extend these findings [SM Hollen, et al. Phys. Rev B 91, 195425 (2015)] to our study of in situ graphene devices and present preliminary STM and transport data with respect to gate voltage.

<sup>1</sup>Funding for this research was provided by the Center for Emergent Materials: an NSF MRSEC under award number DMR-0820414

**4:18PM C16.00010 Screening of a Coulomb Charge by Dirac Electrons in Graphene<sup>1</sup>**, JINHAI MAO, YUHANG JIANG, GUOHONG LI, Rutgers University, NJ, USA, D. MOLDOVAN, M. RAMEZANI MASIR, F. M. PEETERS, University of Antwerp, Belgium, EVA Y. ANDREI, Rutgers University, NJ, USA — Single-atom vacancies in graphene exhibit a rich variety of electronic phenomena ranging from mid-gap states to Kondo screening. Here we report on a new phenomenon showing that vacancies can host a positive charge which can be built up gradually by applying voltage pulses with the tip of a scanning tunneling microscope. The response of the conduction electrons to this charge, which is monitored with scanning tunneling and Landau level spectroscopy, and compared to numerical simulations, exhibits an unusual electron-hole asymmetry. On the p-doped side screening is weak. In this regime, as the charge is increased its interaction with the conduction electrons undergoes a transition into a regime where itinerant electrons are trapped in quasi-bound states (QBS) resembling an artificial atom. We observe the equivalent of the atomic 1S and 2S states as well as the emergence of a new satellite of the 1S state resulting from the broken sublattice symmetry at the vacancy site. In contrast, on the n-doped side screening is very efficient: as soon as the n-doped regime is entered the charge is screened and the QBS disappear. We show that the QBS are gate tunable and that the trapping mechanism can be turned on and off, providing a new mechanism to control electrons in graphene.

<sup>1</sup>Work supported by DOE-FG02-99ER45742, NSF DMR 1207108, ESF-EUROCORES-EuroGRAPHENE, FWO-VI and the Flemish Methusalem program

**4:30PM C16.00011 Computer simulation of STM images of vertical heterostructures of graphene/hexagonal boron nitride with intercalated atoms<sup>1</sup>**, GUNN KIM, JUNSU LEE, Sejong Univ — Using density functional theory, we did computational simulations of scanning tunneling microscopy of vertical graphene/hexagonal boron nitride heterostructures with an intercalated atom (Li, K, Cr, Mn, Co or Cu). A plane-wave basis set was employed with a kinetic energy of 400 eV. The form of the Perdew-Burke-Ernzerhof type was utilized for the exchange-correlation energy functional. To obtain the more accurate result, the van der Waals interaction was also considered. In the computer-simulated scanning tunneling microscopy (STM) images in the Tersoff-Hamann scheme, we demonstrated that the single impurity atom between Gr and hBN sheets is detectable. We observed three different STM patterns on the graphene side. These can be classified by group 1 (Li, Co, and Cu), group 2 (Cr and Mn), and group 3 (K), which have hexagonal, circular, and wide bright spot patterns around the impurity atom, respectively. Although Co and Cu are both in group 1, the Co atom shows stronger d orbital character than the Cu atom. Interestingly, in the case of the Co atom, the simulated STM images are quite different at bias voltages of -0.1 V and +0.1 V. While C  $p_z$ -Co  $d_{yz}$  hybridization occurs at the bias voltage of -0.1 V, C  $p_z$ -Co  $d_{xz}$  hybridization occurs at the bias voltage of +0.1 V.

<sup>1</sup>GK and JL were supported by the Basic Science Research program (2013R1A2009131) through the National Research Foundation of Korea.

**4:42PM C16.00012 Growth and analysis of polymorphic graphene with STM and LEEM-IV for applications in molecular self-assembly and organic electronics<sup>1</sup>**, MAXWELL GRADY, Univ of New Hampshire, TAISUKE OHTA, BOGDAN DIACONESCU, Sandia National Laboratory, ZHONGWEI DAI, KARSTEN POHL, Univ of New Hampshire — Graphene has aroused tremendous interest due to its remarkable electronic and mechanical properties, and is of interest for use in organic electronic devices such as organic photovoltaic cells. We present an analysis of a novel graphene system grown on Ru(0001) in the presence of atomic hydrogen and carbon vapor using STM and LEEM-IV. Structural studies completed with STM show a wide array of moire superlattice sizes ranging from 0.9 to 3.0 nm. Preliminary LEEM and LEEM-IV results confirm the presence of ordered graphene atop the Ru(0001) surface. Investigation using LEEM-IV provides information about the carbon layer thickness; also, micro-LEED-IV determines the precise atomic reconstruction of the interface region. In this regard, we believe the hydrogen present in the system to be interstitial at the carbon-ruthenium interface thus passivating the ruthenium surface, decoupling, and lifting the carbon layer from the substrate. The structural polymorphism displayed by this system is of interest for the study of directed self-assembly. Control over moire size can aid in future work using graphene as a template for self-assembled growth of organic electronics.

<sup>1</sup>This work was performed in part at CINT (DE-AC04-94AL85000). Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the US DOE NNSA (DE-AC04-94AL85000).

#### 4:54PM C16.00013 Scanning Tunneling Microscopy Studies of Crystalline Hydrogenation of Graphene Grown on Cu(111)<sup>1</sup>

, STEVEN J. TJUNG, GRADY A. GAMBREL, The Ohio State University, SHAWNA M. HOLLEN, University of New Hampshire, JAY A. GUPTA, The Ohio State University — Because of the sensitivity of 2D material surfaces, chemical functionalization can be exploited to tune the electronic structure of these materials. For example, hydrogen bonding to carbon atoms in graphene tunes the material from a semi-metal to a wide-gap insulator. We developed a method for a reproducible epitaxial growth of graphene on Cu(111) in the ultra-high vacuum chamber of a scanning tunneling microscope (STM). We find that hydrogen atoms can be bonded to the graphene in a nanoscale region using a novel field-emission process, whereby physisorbed H<sub>2</sub> is cracked in situ using the STM tip. This method produced crystalline surfaces of hydrogen-terminated graphene with 4.2Å lattice, which has proven difficult to produce using conventional atomic beam methods which typically produced disordered hydrogenation. Additionally, this hydrogenation process is reversible and we are able to recover the pristine graphene by H desorption during STM imaging at a high bias. STM images after the dehydrogenation process showed the same atomic lattice and Moiré pattern as the pristine graphene, with the exception of additional point defects. STM spectra show the suppression of the Cu surface state on the hydrogenated graphene, but the opening of a wide-gap was not observed.

<sup>1</sup>Funded by the Center for Emergent Materials at the Ohio State University, an NSF MRSEC (Grant No. DMR-1420451 and DMR-0820414).

#### 5:06PM C16.00014 Experimental Investigation of the Electronic Properties of Twisted Bilayer Graphene by STM and STS

, LONGJING YIN, JIABIN QIAO, WENXIAO WANG, WEIJIE ZUO, LIN HE, Beijing Normal Univ — The electronic properties of graphene multilayers depend sensitively on their stacking order. A twisted angle is treated as a unique degree of freedom to tune the electronic properties of graphene system. Here we study electronic structures of the twisted bilayers by scanning tunneling microscopy (STM) and spectroscopy (STS). We demonstrate that the interlayer coupling strength affects both the Van Hove singularities and the Fermi velocity of twisted bilayers dramatically. This removes the discrepancy about the Fermi velocity renormalization in the twisted bilayers and provides a consistent interpretation of all current data. Moreover, we report the experimental evidence for non-Abelian gauge potentials in twisted graphene bilayers by STM and STS. At a magic twisted angle, about 1.11, a pronounced sharp peak is observed in the tunnelling spectra due to the action of the non-Abelian gauge fields. Because of the effective non-Abelian gauge fields, the rotation angle could transfer the charge carriers in the twisted bilayers from massless Dirac fermions into well localized electrons, or vice versa, efficiently. This provides a new route to tune the electronic properties of graphene systems, which will be essential in future graphene nanoelectronics.

#### 5:18PM C16.00015 Ab initio study of friction of graphene flake on graphene/graphite or SiC surface<sup>1</sup>

, OGUZ GULSEREN, Bilkent University, CEREN TAYRAN, Gazi University, CEREN SIBEL SAYIN, Bilkent University — Recently, the rich dynamics of graphene flake on graphite or SiC surfaces are revealed from atomic force microscopy experiments. The studies toward the understanding of microscopic origin of friction are getting a lot of attention. Despite the several studies of these systems using molecular dynamics methods, density functional theory based investigations are limited because of the huge system sizes. In this study, we investigated the frictional force on graphene flake on graphite or SiC surfaces from pseudopotential planewave calculations based on density functional theory. In both cases, graphene flake (24 C) on graphite or SiC surface, bilayer flake is introduced by freezing the top layer as well as the bottom layer of the surface slab. After fixing the load with these frozen layers, we checked the relative motion of the flake over the surface. A minimum energy is reached when the flake is moved on graphene to attain AB stacking. We also conclude that edge reconstruction because of the finite size of the flake is very critical for frictional properties of the flake; therefore the saturation of dangling bonds with hydrogen is also addressed. Not only the symmetric configurations remaining parameter space is extensively studied. Supported by TUBITAK Project No: 114F162.

<sup>1</sup>This work is supported by TUBITAK Project No: 114F162.

### Monday, March 14, 2016 2:30PM - 5:30PM –

Session C17 DCMP: Charge Density Waves: Low Dimensional and Organic Conductors 316 - Eva Andrei, Rutgers University

#### 2:30PM C17.00001 Enhancement of charge ordering by dynamic electron-phonon interaction

, ANDREJ SINGER, Department of Physics, University of California San Diego, ERIC FULLERTON, Center for Memory and Recording Research, University of California San Diego, OLEG SHPYRKO, Department of Physics, University of California San Diego — Symmetry breaking and emergence of order is one of the most fascinating phenomena in condensed matter physics and leads to a plethora of intriguing ground states such as in antiferromagnets, Mott insulators, superconductors, and density-wave systems. Exploiting non-equilibrium dynamics of matter following ultrafast external excitation can provide even more striking routes to symmetry-lowered, ordered states, for instance, by accessing hidden equilibrium states in the free-energy landscape or dynamic stabilization of non-equilibrium states. This is remarkable because ultrafast excitation typically creates disorder, reduces the order parameter, and raises the symmetry. Here, we demonstrate for the case of antiferromagnetic chromium that moderate photo-excitation can transiently enhance the charge-density-wave (CDW) order by up to 30% above its equilibrium value, while strong excitation leads to an oscillating, large-amplitude CDW state that persists above the equilibrium transition temperature. Both effects result from dynamic electron-phonon interaction, which provides an efficient mechanism to selectively transform a broad excitation of the electronic order into a well defined, long-lived coherent lattice vibration. This mechanism may be exploited to transiently enhance the order parameter in other systems with coupled electronic and lattice orders. The data was collected at the x-ray free electron laser LCLS at SLAC.

#### 2:42PM C17.00002 Transport studies in the incommensurate charge density wave series RTe<sub>3</sub>

, PHILIP WALMSLEY, SIMON AESCHLIMANN, Stanford University, PAULA GIRALDO GALLO, NHMFL, Florida State University, IAN FISHER, Stanford University — The quasi-2D rare-earth tritelluride compounds (RTe<sub>3</sub>; R=La-Tm) are a model series in which to study incommensurate charge density waves (iCDWs), with the interplay between Fermi surface nesting and electron-phonon coupling forming an open and lively area of research. The slight orthorhombicity in the 2D Te bilayer that forms the Fermi surface favors a single-domain unidirectional iCDW along the c-axis, with a second, perpendicular unidirectional iCDW forming at lower temperatures in the heavier members (R=Tb-Tm). It remains unclear how the lower temperature iCDW disappears with rare earth substitution (chemical pressure) and whether there is an associated quantum phase transition. We present recent transport measurements that study the evolution of the two iCDWs as they are tuned across the enormous phase-space offered by these compounds, with a particular focus on the in-plane anisotropy and Fermi-surface geometry.

#### 2:54PM C17.00003 Magnetic properties of single crystalline HoTe<sub>3</sub>

, M.S. SONG, B.Y. KANG, K.K. CHO, B.K. CHO, Gwangju Inst of Sci & Tech — Charge density waves (CDWs) are in a broken ground state, driven by electronic instabilities in a low-dimensional system with a highly anisotropic electronic structure [1]. As one of the CDW materials, the RTe<sub>3</sub> (R = rare earth elements) compound is a quasi-two-dimensional system. Even if the magnetic properties of RTe<sub>3</sub> in light rare earth elements have been reported [2], magnetic and electronic information in heavy rare earth elements remains unknown. In this study, the magnetic properties of HoTe<sub>3</sub> were investigated and two ferromagnetic transitions were discovered along a direction perpendicular to the stacking axis while RTe<sub>3</sub>. An antiferromagnetic transition temperature was found at T<sub>N</sub> = 4.5 K for H // b and two ferromagnetic transitions were found at T<sub>c1</sub> = 3.5 K and T<sub>c2</sub> = 4.5 K for H ⊥ b.

[1] G. Gruner, Density Waves in Solids -Perseus, Cambridge, MA, (1994.) [2] Yuji Iyeiri, Teppei Okumura, Chishiro Michioka, and Kazuya Suzuki, Physical Review B **67** 144417 (2003)

**3:06PM C17.00004 Temperature-Dependent Studies of Charge Density Wave States in  $\text{TbTe}_3$**  , MICHAEL BOYER, AARON KRAFT, LING FU, BISHNU SHARMA, Clark University, IAN FISHER, Stanford University — We use temperature-dependent scanning tunneling microscopy (STM) to study charge density wave (CDW) states in  $\text{TbTe}_3$ .  $\text{TbTe}_3$  undergoes a bulk CDW transition near 335 K, though x-ray data shows evidence for CDW fluctuations up to 363 K.[1] Our STM measurements characterize the well-established, long-range, unidirectional CDW state ( $q_{\text{cdw}} = 0.71 \text{ c}^*$ ) at 300 K. Our temperature-dependent measurements above  $T_{\text{CDW}}$  show evidence for localized static CDW order which is consistent with x-ray detection of CDW fluctuations above  $T_{\text{CDW}}$ . Surprisingly, we also find evidence for localized static order associated with a second CDW along the a-axis, a CDW state which never establishes long-range coherence in the bulk of  $\text{TbTe}_3$  even at low temperatures. [1] Ru et al., PRB 77, 035114 (2008).

**3:18PM C17.00005 Doping-induced Charge-Density-Wave** , ATSUSHI NOMURA, KAZUHIKO YAMAYA, SHIGERU TAKAYANAGI, KOICHI ICHIMURA, TORU MATSUURA, SATOSHI TANDA, Hokkaido University, HOKKAIDO UNIVERSITY TEAM — Doping is a useful method for searching new characters in solids, as we can see in the discoveries of impurity semiconductors and high-temperature superconductors. If a Charge-Density-Wave (CDW) is induced in materials which do not exhibit a CDW, new CDW properties might be brought there.  $\text{TaSe}_3$  exhibits no CDW transition but a superconductivity transition at about 2 K while it has a quasi-one-dimensional chain structure as well as typical CDW conductors,  $\text{NbSe}_3$ ,  $\text{TaS}_3$ , and  $\text{NbS}_3$ . Therefore,  $\text{TaSe}_3$  is one of the suitable materials for the induction of a CDW by doping, and we tried to induce a CDW in  $\text{TaSe}_3$  by doping Cu. Cu concentration was determined by inductively coupled plasma atomic emission spectroscopy (ICP-AES). The high Cu concentration was consistent with the high value of residual resistance ( $R(4.5 \text{ K})/(R(280 \text{ K}) - R(4.5 \text{ K}))$ ). Single-crystal X-ray diffraction pattern (XRD) showed an expansion of the  $c$ -axis in Cu-doped  $\text{TaSe}_3$ . The temperature dependence of the resistivity showed the anomaly at 80-100 K in Cu-doped  $\text{TaSe}_3$ , which was never observed in pure  $\text{TaSe}_3$ . These results suggest that the Cu-doping induces a CDW. We will discuss the relation between the resistivity anomaly and superconductivity.

**3:30PM C17.00006 ABSTRACT WITHDRAWN —**

**3:42PM C17.00007 Observation of an Excitonic Sound Wave in  $\text{TiSe}_2$  with meV-resolution EELS** , ANSHUL KOGAR, MELINDA RAK, SEAN VIG, ALI HUSAIN, Univ of Illinois - Urbana, YOUNG IL JOE, NIST, PETER ABBAMONTE, Univ of Illinois - Urbana — The charge density wave (CDW) in  $\text{TiSe}_2$  has been attributed to an excitonic instability by many authors. In a conventional CDW material, there exists a soft phonon at the transition temperature, which, below the transition temperature, gives way to the phase and amplitude collective excitations of the CDW order parameter. In  $\text{TiSe}_2$ , a soft phonon has indeed been observed with inelastic X-ray scattering. In the 1960s, though, W. Kohn predicted that one of the signatures of an excitonic instability would be the presence of a soft electronic excitation which similarly gives way to an excitonic sound mode in the condensed phase. In this talk, I will present data showing that the  $\text{TiSe}_2$  exhibits a collective excitation consistent with the excitonic sound wave prediction, which emerges out of the normal phase plasmon. This provides strong evidence that excitonic correlations play a role in the CDW formation in  $\text{TiSe}_2$ . Hence, a more nuanced view of the charge density wave transition in  $\text{TiSe}_2$  is needed where both excitonic effects and electron-phonon coupling must be taken into consideration.

**3:54PM C17.00008 ABSTRACT WITHDRAWN —**

**4:06PM C17.00009 Decay of Bloch oscillations in the charge-density-wave ordered phase of an all electronic charge density wave state** , OLEG MATVEEV, Department of Physics, Georgetown University, Washington, DC , ANDRII SHVAIKA, Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, Lviv, Ukraine, THOMAS DEVEREAUX, Geballe Laboratory for Advanced Materials, Stanford University, Stanford, CA, USA, JAMES FREERICKS, Department of Physics, Georgetown University, Washington, DC — The charge-density-wave phase of the Falicov-Kimball model displays a number of anomalous behavior including the appearance of subgap density of states as the temperature increases. These subgap states should have a significant impact on transport properties, particularly the nonlinear response of the system to a large dc electric field. Using the Kadanoff-Baym-Keldysh formalism, we employ nonequilibrium dynamical mean-field theory to exactly solve for this nonlinear response. We examine both the current and the order parameter of the conduction electrons as the ordered system is driven by a dc electric field.

**4:18PM C17.00010 Ground state in  $\kappa - (\text{BEDT} - \text{TTF})_2\text{Hg}(\text{SCN})_2\text{Br}$  studied by Raman Spectroscopy and Heat Capacity measurements<sup>1</sup>** , N. HASSAN, Johns Hopkins Univ, S. A. TURUNOVA, E.I. ZHILYAEVA, R.N. LYUBOVSKAYA, Institute of Problems of Chemical Physics, Chernogolovka, Russia, N. DRICHKO, Johns Hopkins Univ — Quasi-two-dimensional organic conductor  $\kappa - (\text{BEDT} - \text{TTF})_2\text{Hg}(\text{SCN})_2\text{Br}$  is a Mott insulator ( $T_c \approx 100 \text{ K}$ ) on a triangular lattice which makes it a potential spin liquid candidate. To elucidate its magnetic ground state we study heat capacity and Raman response of single crystals of this material. Our low temperature heat capacity measurements suggest a presence of a linear term in the temperature dependence, which might indicate the existence of gapless spinons. Vibrational Raman response indicates a presence of charge order fluctuations in the insulating state. The low-frequency Raman response is discussed in terms of fluctuations of paired electron crystal state [1]. [1] S. Dayal, R. T. Clay, H. Li, and S. Mazumdar, Phys. Rev. B 83, 245106 (2011)

<sup>1</sup>The work at IQM was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Material Sciences and Engineering, under Grant No. DEFG02-08ER46544.

**4:30PM C17.00011 ABSTRACT WITHDRAWN —**

**4:42PM C17.00012 Raman scattering in an anisotropic triangular spin lattice system** , HIDEO KISHIDA, YUTO NAKAMURA, KAZUSHI MIZUKOSHI, Nagoya University, YUKIHIRO YOSHIDA, Meijo University, GUNZI SAITO, Meijo University and Toyota Physical and Chemical Research Institute — Spin-disordered quantum phases in an anisotropic triangular spin lattice system,  $\kappa - (\text{BEDT} - \text{TTF})_2\text{B}(\text{CN})_4$ , were recently reported [1]. In this compound, the ratio of the two transfer integrals,  $t'/t$ , reaches 1.44 at 298 K and 1.80 at 100 K. Its optical conductivity in the infrared region is anisotropic. The temperature dependence of the optical anisotropy correlates with that of  $t'/t$ . From the experimentally evaluated optical anisotropy, we expect that the values of  $t'/t$  are larger than 1.80 in the lower temperature region. For this compound, we observe the polarization-dependent broad Raman scattering signals below  $600 \text{ cm}^{-1}$  at 10 K. In such a wavenumber region, we have observed the magnetic Raman signals in triangular spin lattice systems such as  $\kappa - (\text{BEDT} - \text{TTF})_2\text{X}$  [2] and  $\beta'$ -type  $\text{Pd}(\text{dmit})_2$  salts [3]. By comparison with them, we discuss the origin of the Raman signals observed for  $\kappa - (\text{BEDT} - \text{TTF})_2\text{B}(\text{CN})_4$ . [1] Y. Yoshida *et al.*, Nat. Phys. 11, 679 (2015). [2] Y. Nakamura *et al.*, J. Phys. Soc. Jpn. 83, 074708 (2014). [3] Y. Nakamura *et al.*, J. Phys. Soc. Jpn. 84, 044715 (2015).

**4:54PM C17.00013 Strong light-field effects in correlated organic conductors.** , SHINICHIRO IWAI, YOHEI KAWAKAMI, YOTA NAITOH, HIROTAKE ITOH, SUMIO ISHIHARA, Tohoku University, KENJI YONEMITSU, Chuo University — Optical responses of organic conductors have attracted much attentions, because they exhibit ultrafast solid-state phase transitions in the conducting and/or dielectric natures upon photo-excitations. In this decade, photoinduced melting of correlated insulators with clear charge gap have been extensively investigated. On the other hand, optical responses of correlated metal has not been studied well. Here, we describe a charge localization induced by the 9.3 MV/cm instantaneous electric field of a 1.5 cycle (7 fs) infrared pulse in an organic conductor  $\alpha$ -(bis[ethylenedithio]-tetrathiafulvalene)<sub>2</sub>I<sub>3</sub>. A large reflectivity change of 30 percent and a coherent charge oscillation along the time axis reflect the opening of the charge ordering gap in the metallic phase. This optical freezing of charges, which is the reverse of the photoinduced melting of electronic orders, is attributed to the 10 percent reduction of  $t$  driven by the strong, high-frequency electric field. Furthermore, the contribution of Coulomb repulsion will be discussed on the basis of the polarization dependence of the pump light and the theory.

**5:06PM C17.00014 Dielectric Properties of Organic Charge-Transfer Salts** , J. K. H. FISCHER, P. LUNKENHEIMER, S. KROHNS, Experimental Physics V, EKM, University of Augsburg, Augsburg, Germany, R. S. MANNA, Experimental Physics VI, EKM, University of Augsburg, Augsburg, Germany, B. HARTMANN, H. SCHUBERT, M. LANG, J. MÜLLER, Phys. Inst. Univ. Frankfurt, SFB/TR 49, Frankfurt, Germany, J. A. SCHLUETER, Materials Research, National Science Foundation, Arlington, Virginia, United States, C. MÉZIÈRE, P. BATAIL, Laboratoire MOLTECH, UMR 6200 CNRS-Université d'Angers, Bt. K, UFR Sciences, Angers, France, A. LOIDL, Experimental Physics V, EKM, University of Augsburg, Augsburg, Germany — The BEDT-TTF-based charge-transfer salts have attracted considerable attention due to their often intriguing dielectric properties. An example is  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu[N(CN)<sub>2</sub>]Cl. It was recently found to exhibit multiferroicity, for which a new electric-dipole driven mechanism was proposed [1]. The polar moment in this system was suggested to arise from the dimerization of the BEDT-TTF molecules, combined with charge order. Another interesting recent example is  $\alpha$ -(BEDT-TTF)<sub>2</sub>I<sub>3</sub>, which shows the signature of relaxor-ferroelectric behavior [2]. Here, we will present an overview of the dielectric properties of the above systems and provide new results on  $\kappa$ -(BEDT-TTF)<sub>2</sub>Hg(SCN)<sub>2</sub>Cl, which also seems to show relaxor-ferroelectric behavior in its charge-ordered state. In addition, we present measurements of  $\delta$ -(EDT-TTF-CONMe<sub>2</sub>)<sub>2</sub>Br. This compound lacks dimerization, but exhibits charge order already at room temperature. [1] P. Lunkenheimer *et al.*, Nat. Mater. **11**, 755 (2012). [2] P. Lunkenheimer *et al.*, Phys. Rev. B **91**, 245132 (2015).

**5:18PM C17.00015 Anisotropic transport and structure of single-crystal molybdenum bronze, Li<sub>0.33</sub>MoO<sub>3</sub>**<sup>1</sup> , SAEED MOSHFEHGYEGANEH, JOSHUA L. COHN, University of Miami, JOHN J. NEUMEIER, Montana State University — We present transport measurements (resistivity, thermopower, thermal conductivity) on single crystals of the quasi-one-dimensional (Q1D), small-gap semiconductor<sup>a</sup> Li<sub>0.33</sub>MoO<sub>3</sub> in the temperature range 150-500 K. The Q1D character of this material is reflected in  $T = 300$  K resistivity ratios,  $\rho_c:\rho_a:\rho_b \simeq 1:20:180$ , and extreme anisotropy in the Seebeck coefficient within the  $a-c$  planes,  $S_c - S_a \simeq 250 \mu\text{V/K}$ . A weak structural anomaly near  $T_s = 355$  K (0.001 Å expansions along  $c^*$  and  $b^*$  directions, comparable contraction along  $a^*$ ) is identified in the temperature-dependent lattice constants from x-ray diffraction, and is coincident with changes in the transport coefficients. Analysis of the transport data at  $T > T_s$  shows that an intrinsic semiconductor model can be applied to explain transport along the most conducting  $c$  axis, but along  $a$  and  $b^*$  the transport is better described by a non-adiabatic, small-polaron picture.

<sup>a</sup> B. T. Collins *et al.*, J. Sol. St. Chem. **76**, 319 (1988).

<sup>1</sup>This material is based upon work supported by the U.S. Department of Energy Office of Basic Energy Sciences grant DE-FG02-12ER46888 (Univ. Miami) and the National Science Foundation under grant DMR-0907036 (Mont. St. Univ.)

## Monday, March 14, 2016 2:30PM - 5:18PM – Session C18 GMAG DMP: Iridates I 317 - Deepak Singh, University of Missouri

**2:30PM C18.00001 Topological and unconventional magnetic states in transition metal oxides**<sup>1</sup> , GREGORY FIETE, University of Texas at Austin — In this talk I describe some recent work on unusual correlated phases that may be found in bulk transition metal oxides with strong spin-orbit coupling. I will focus on model Hamiltonian studies that are motivated by the pyrochlore iridates, though the correlated topological phases described may appear in a much broader class of materials. I will describe a variety of fractionalized topological phases protected by time-reversal and crystalline symmetries: The weak topological Mott insulator (WTMI), the TI\* phase, and the topological crystalline Mott insulator (TCMI). If time permits, I will also discuss closely related heterostructures of pyrochlore iridates in a bilayer and trilayer film geometry. These quasi-two dimensional systems may exhibit a number of interesting topological and magnetic phases.

<sup>1</sup>This work is generously funded by the ARO, DARPA, and the NSF.

**3:06PM C18.00002 Multipolar effects in Eu<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub>** , YILIN WANG, XI DAI, Institute of Physics, Chinese Academy of Sci (CAS) — We use the density functional theory plus the rotationally invariant Hartree-Fock mean-field method to study the magnetic properties of the pyrochlore iridate material Eu<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub> (5d<sup>5</sup>), where the crystal field splitting  $\Delta$ , spin-orbit coupling (SOC)  $\lambda$  and Coulomb interaction  $U$  of Ir atoms are all playing significant roles. We have constructed a  $t_{2g}$  Wannier tight-binding Hamiltonian and calculated the  $U$ - $\lambda$  phase diagram, from which we find a very stable all-in/all-out antiferromagnetic ground state for moderate SOC (0.2-0.5 eV). In this magnetic state, except for the dipole moments, we also find considerable multipolar moments (octupole) and large non-linear magnetic susceptibility. With strong enough SOC, the system reduces to a  $j_{eff} = \frac{1}{2}$  single band Hubbard model, and the ground state changes to another antiferromagnetic configuration without multipolar moments. Our results indicate that the coexisting multipolar order is crucial to stabilize the all-in/all-out state and contributes a lot to the non-linear magnetic susceptibility.

**3:18PM C18.00003 Resonant X-ray scattering studies of magnetic order and excitations in pyrochlore iridates.** , DESMOND MCMORROW, London Center Nanotechnology — The rare-earth pyrochlore iridates (R<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub>, R=rare earth) have been proposed to host a number of exotic electronic states as a consequence of the existence of strong spin-orbit coupling of the Ir<sup>4+</sup> ion in the presence of significant electron correlations. Of crucial importance to understanding whether any of these states can be realized in practice is to determine the effective low-energy Hamiltonian describing the system. Here we report a comprehensive series of resonant X-ray experiments, both elastic (REXS) and inelastic (RIXS), which reveal the nature of the magnetic order and excitations in single crystals of Sm<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub> and Nd<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub>.

**3:54PM C18.00004 ABSTRACT WITHDRAWN —**

**4:06PM C18.00005 The interplay of ferromagnetic and antiferromagnetic exchanges in the 3d-5d transition metal oxides Sr<sub>2</sub>B<sub>2</sub>IrO<sub>6</sub> (B=Ni, Cu, Zn)** , KATHARINA ROLFS, EKATERINA POMJAKUSHINA, SANDOR TOT, VLADIMIR POMJAKUSHIN, KAZIMIERZ CONDER, Paul Scherrer Institute — In the field of strongly correlated electron systems significant attention has been drawn towards the study of compounds based on magnetic 4d and 5d transition metal (TM) oxides. The spin orbit coupling (SOC) within these systems becomes non-negligible compared to the crystal field energies and leads to new exotic ground states, such as the Mott insulating state in Sr<sub>2</sub>IrO<sub>4</sub>. In order to understand the influence of the SOC on the electronic ground state the focus also turned to mixed 3d-5d systems, which gives the possibility to disentangle SOC effects from common charge-spin-orbital physics, as it is present in pure 3d TMOs and could also introduce new properties. One group within these candidates is the group of Ir-based double perovskites A<sub>2</sub>B<sub>2</sub>IrO<sub>6</sub> (B=3d TM). While in a large number of insulating 3d TMOs, the superexchange interactions between magnetic ions being nearest neighbour is adequate to determine the magnetic order, the SOC of 5d elements can change the exchange topology. This is possibly the case for Sr<sub>2</sub>NiIrO<sub>6</sub>, Sr<sub>2</sub>CuIrO<sub>6</sub> and Sr<sub>2</sub>ZnIrO<sub>6</sub>. All compounds are high oxygen pressure compounds, which we successfully synthesised. The influence of the 3d metal on the magnetic properties will be discussed based on bulk magnetisation, transport measurements and neutron diffraction.

**4:18PM C18.00006 Magnetic Orders Proximal to the Kitaev Limit in Frustrated Triangular Systems: Application to Ba<sub>3</sub>IrTi<sub>2</sub>O<sub>9</sub>** , ANDREI CATUNEANU, Department of Physics and Center for Quantum Materials, University of Toronto, JEFFREY RAU, Department of Physics and Astronomy, University of Waterloo, HEUNG-SIK KIM, HAE-YOUNG KEE, Department of Physics and Center for Quantum Materials, University of Toronto — Frustrated transition metal compounds in which spin-orbit coupling (SOC) and electron correlation work together have attracted much attention recently. In the case of 5d transition metals, where SOC is large,  $j_{eff} = 1/2$  bands near the Fermi level are thought to encompass the essential physics of the material, potentially leading to a concrete realization of exotic magnetic phases such as the Kitaev spin liquid. We derive a spin model on a triangular lattice based on  $j_{eff} = 1/2$  pseudo-spins that interact via antiferromagnetic Heisenberg ( $J$ ) and Kitaev ( $K$ ) exchanges, and crucially, an anisotropic ( $\Gamma$ ) exchange. Our classical analysis of the spin model reveals that, in addition to small regions of 120°,  $Z_2$  / dual- $Z_2$  vortex crystal and nematic phases, the stripy and ferromagnetic phases dominate the  $J$ - $K$ - $\Gamma$  phase diagram. We apply our model to the 5d transition metal compound, Ba<sub>3</sub>IrTi<sub>2</sub>O<sub>9</sub>, in which the Ir<sup>4+</sup> ions form layered two-dimensional triangular lattices. By combining our ab-initio and classical analyses, we predict that Ba<sub>3</sub>IrTi<sub>2</sub>O<sub>9</sub> has a stripy ordered magnetic ground state.

**4:30PM C18.00007 Spin-Orbit Induced Emergent Magnetic Phases in Iridium Based Oxides<sup>1</sup>** , INDRA DASGUPTA, Department of Solid State Physics, Indian Association for the Cultivation of Science, Jadavpur, Kolkata 700032 — We shall present our results on the electronic structure of 6H perovskite type quaternary iridates Ba<sub>3</sub>M<sub>2</sub>Ir<sub>2</sub>O<sub>9</sub>, where Ir ions form structural dimers and non magnetic M provides a knob to tailor the valence of Ir. We shall first consider the d<sup>4.5</sup> insulator Ba<sub>3</sub>YIr<sub>2</sub>O<sub>9</sub> and explain the origin of the pressure induced magnetic transition to a spin-orbital liquid (SOL) state in this system. As a next example [2], we shall consider a pentavalent (d<sup>4</sup>) 6H perovskite iridate Ba<sub>3</sub>ZnIr<sub>2</sub>O<sub>9</sub> and argue that the ground state of this system is a realization of novel SOL state. Our results reveal that such a system provides a very close realization of the elusive J=0 state where Ir local moments are generated due to the comparable energy scales of the singlet-triplet splitting driven by spin-orbit coupling (SOC) and the superexchange interaction mediated by strong intra-dimer hopping, however substantial frustrated interdimer exchange interactions induce quantum fluctuations favoring SOL phase at low enough temperature. [1] S.K. Panda, S. Bhowal, Ying Li, S. Ganguly, Roser Valenti, L. Nordstrom, and I. Dasgupta Physical Review B (Rapid Communication), 2015 (Accepted for Publication), [2] A. Nag et. al. arXiv:1506.04312 [cond-mat.str-el]

<sup>1</sup>Department of Science and Technology, Govt. of India

**4:42PM C18.00008 Orbital-selective singlet dimer formation and suppression of double exchange in 4d and 5d systems<sup>1</sup>** , SERGEY STRELTISOV, Institute of Metal Physics, GANG CAO, University of Kentucky, DANIEL KHOMSKII, University of Cologne — One of the main mechanisms of ferromagnetic ordering in conducting materials is the double exchange (DE). It is usually supposed in DE model that the Hund's coupling  $J_H$  is much larger than electron hopping  $t$ ; in this case one stabilizes the state with maximum spin per pair of ions, which finally leads to ferromagnetism in bulk systems. We show that in the dimerized 4d/5d transition metal oxides for which  $J_H$  is reduced and  $t$  is in contrast enhanced, another situation is possible, when formation of the spin-singlets on delocalized orbitals is more favorable. This leads to suppression of the DE and to a strong decrease of the total spin. The model calculations using the dynamical mean-field theory show that this effect survives even in the extended systems, not only for dimers. Such a situation is realized, e.g., in Y<sub>5</sub>Mo<sub>2</sub>O<sub>12</sub>, CrO<sub>2</sub> under pressure and in many other 4d/5d based materials. Another mechanism, which may suppress DE and which is also typical for 4d/5d compounds is the spin-orbit coupling (SOC). We show on the example of Ba<sub>5</sub>Allr<sub>2</sub>O<sub>11</sub>, that in this system it is the combination of molecular-orbital formation and SOC that strongly decreases magnetic moment on Ir.

<sup>1</sup>Civil Research and Development Foundation via FSCX-14-61025-0

**4:54PM C18.00009 Investigation of frustrated antiferromagnet on the honeycomb lattice with an applied field<sup>1</sup>** , SHENXIU LIU, Department of Physics, Stanford University, HONGCHEN JIANG, TOM DEVEREAUX, Stanford Institute of Materials and Energy Sciences, SLAC — Quantum spin-1/2 honeycomb XY antiferromagnet, or the equivalent hard-core boson system, with both nearest-neighbor J<sub>1</sub> and next-nearest-neighbor J<sub>2</sub> interactions is a representative frustrated system possibly hosting new phases of matter. Recent theoretical study suggests that this system may exhibit a series of incompressible states, which host fermionic elementary excitations rather than bosonic excitations, at small fixed filling factors or equivalent magnetic field strength. In this work, we will examine the theoretical prediction by directly studying the frustrated honeycomb J<sub>1</sub>-J<sub>2</sub> XY model, using unbiased grand canonical density-matrix renormalization group technique. By searching for magnetization plateaus with an applied magnetic field, we will ultimately determine the presence of these incompressible states as well as their properties. For a more comprehensive study, different variants of this model, including the honeycomb J<sub>1</sub>-J<sub>2</sub> Heisenberg antiferromagnet, will also be investigated.

<sup>1</sup>this work is supported by the Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract DE-AC02-76SF00515.

**5:06PM C18.00010 Topological magnon bands in pyrochlore iridate thin films** , PONTUS LAURELL, GREGORY A FIETE, University of Texas at Austin — Thin films of pyrochlore iridates (A<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub>) have previously been studied using weak-coupling techniques such as DFT and DMFT. Here we approach the systems from the strong coupling limit. Since the pyrochlore iridates most likely reside in the difficult to access intermediate coupling regime, a strong coupling study should offer a complementary viewpoint to existing studies. We carry out a variational mean field calculation of the magnetic ground state configurations. We show that the all-in/all-out state, known as the bulk ground state, is generically present in the triangular-Kagome-triangular trilayers. This state can also be found in bilayer films, in specific parameter regimes. A linear spin-wave analysis of the magnetic excitations is also carried out. It shows that when the magnetic order is in (or close to) the all-in/all-out state, the lowest magnon band acquires a non-zero Chern number, leading to the prediction that pyrochlore iridate thin films can host the magnon Hall effect.

# Monday, March 14, 2016 2:30PM - 5:30PM –

Session C19 GMAG DMP: Epitaxial Engineering of Magnetic Oxide Thin Films 318 - Mark Huijben, University of Twente

**2:30PM C19.00001 Epitaxial Engineering of Domain Walls and Distortions in Ferrite Heterostructures.** , JULIA MUNDY, UC Berkeley — The defining feature of ferroics is the ability of an external stimulus—electric field, magnetic field, or stress—to move domain walls. These topological defects and their motion enables many useful attributes, e.g., memories that can be reversibly written between stable states as well as enhanced conductivity, permittivity, permeability, and piezoelectricity. Although methods are known to drastically increase their density, the placement of domain walls with atomic precision has until now evaded control. Here we engineer the location of domain walls with monolayer precision and exploit this ability to create a novel multiferroic in which ferroelectricity enhances magnetism at all relevant length scales. Starting with hexagonal  $\text{LuFeO}_3$ , a geometric ferroelectric with the greatest known planar rumpling, we introduce individual extra monolayers of FeO during growth to construct formula-unit-thick syntactic layers of ferrimagnetic  $\text{LuFe}_2\text{O}_4$  within the  $\text{LuFeO}_3$  matrix, i.e.,  $(\text{LuFeO}_3)_m/(\text{LuFe}_2\text{O}_4)_1$  superlattices. The severe rumpling imposed by the neighboring  $\text{LuFeO}_3$  drives the ferrimagnetic  $\text{LuFe}_2\text{O}_4$  into a simultaneously ferroelectric state and reduces the  $\text{LuFe}_2\text{O}_4$  spin frustration. This increases the magnetic transition temperature significantly—to 281 K for the  $(\text{LuFeO}_3)_9/(\text{LuFe}_2\text{O}_4)_1$  superlattice. Moreover,  $\text{LuFeO}_3$  can form charged ferroelectric domain walls, which we align to the  $\text{LuFe}_2\text{O}_4$  bilayers with monolayer precision. Charge transfers to these domain walls to alleviate the otherwise electrostatically unstable polarization arrangement, further boosting the magnetic moment. Our results demonstrate the utility of combining ferroics at the atomic-layer level with attention to domain walls, geometric frustration and polarization doping to create multiferroics by design.

**3:06PM C19.00002 Understanding the Interplay of Polar, Magnetic, and Electronic Order in Ferroic  $(\text{LuFeO}_3)_m/\text{LuFe}_2\text{O}_4$  Superlattices** , ALEJANDRO REBOLA, Cornell University, HENA DAS, Lawrence Berkeley National Laboratory, CRAIG FENNIE, Cornell University — Multiferroics are not only important from a technological point of view but also because of the rich and complex physics that results from the interplay between spin, charge and structural distortions. Hexagonal  $\text{LuFeO}_3$  has recently been understood theoretical and experimentally, and shown to be an improper structural ferroelectric directly analogous to the hexagonal manganites.  $\text{LuFe}_2\text{O}_4$  is structurally homologous to  $\text{LuFeO}_3$ —both are characterized by a  $\text{FeO}_5$  bipyramidal crystal field— but unlike the latter it exhibits a much larger magnetic moment and it is still a matter of debate whether it is ferroelectric. The double Fe-layer in  $\text{LuFe}_2\text{O}_4$  is thought to be charge ordered and highly frustrated, resulting in possible polar, non-polar or anti-polar charge arrangements. Here we first investigate the relation between different charge and magnetic orders and structural distortions in bulk  $\text{LuFe}_2\text{O}_4$  by DFT and Monte Carlo calculations. Then we concentrate on a system that combines both mechanisms—a structural improper ferroelectric and a charge frustrated polar structure— such as the  $(\text{LuFeO}_3)_m/\text{LuFe}_2\text{O}_4$  superlattices.

**3:18PM C19.00003 Strain-mediated control of orbital ordering planes in heteroepitaxial lanthanum manganite thin films** , YONG-JIN KIM, JIN HONG LEE, KAIST, TAE YEONG KOO, Pohang Accelerator Laboratory, Pohang University of Science and Technology, Pohang 790-784, Korea, CHAN-HO YANG, KAIST — Strain engineering which controls the misfit strain of heteroepitaxial thin films leads to distinctive physical properties in contrast to the intrinsic properties of unstrained bulk materials. Perovskite  $\text{LaMnO}_3$  (LMO) has attracted considerable attention due to strong coupling among the lattice, charge, spin and orbital degrees of freedom. Bulk LMO is known to be an A-type antiferromagnetic ( $T_N \sim 140$  K) Mott insulator, and its orbital ordering plane is established due to cooperative Jahn-Teller distortion below  $\sim 750$  K. Previous studies have focused on the orbital ordering planes of the bulk LMO but not researched on correlation between orbital planes and misfit strain. To figure out the strain dependence of orbital ordering planes, we have grown LMO thin films on four different substrates, i.e.,  $\text{DyScO}_3(110)$ ,  $\text{GaScO}_3(110)$ ,  $\text{SrTiO}_3(001)$ , and  $\text{LSAT}(001)$ , using the pulsed laser deposition technique. The films have been characterized by atomic force microscopy and x-ray diffraction. We have performed resonant x-ray scattering to identify orbital ordering plane on each film. We have found that orbital ordering planes can be modulated depending on the misfit strain.

**3:30PM C19.00004 Ferroelectric-ferromagnetic coupling in hexagonal  $\text{YMnO}_3$  film.**<sup>1</sup> , SHAOBO CHENG, MENGLEI LI, SHIQING DENG, SHANYONG BAO, PEIZHE TANG, WENHUI DUAN, JING MA, CEWEN NAN, JING ZHU, Tsinghua University — Simultaneously achieving ferroelectricity and ferromagnetism in a single phase material is an important research topic in recent decades. Here, we demonstrate that with the modulation of oxygen vacancies, the ferroelectric-ferromagnetic coupling can be realized in the typical hexagonal manganite:  $\text{YMnO}_3$ . The first-principles calculations are used to reveal the importance of oxygen vacancies on the alterations of magnetic behaviors for  $\text{YMnO}_3$ . In order to obtain net magnetic moments, the on-top oxygen vacancies of  $\text{MnO}_5$  clusters should be created, thus the initial 2D spin frustration structure of Mn ions will be broken. By growing  $\text{YMnO}_3$  film on  $\text{Al}_2\text{O}_3$  substrate, large in-plane compressive strain is induced, thus we can experimentally realize the on-top oxygen vacancies. With the help of SQUID and spherical aberration corrected TEM, the magnetic moments are experimentally measured and the correlations between the crystal structures and magnetic properties can be clearly understood. Our findings may pave a way for future applications of single phase multiferroic materials.

<sup>1</sup>National 973 Project of China (2015CB654902, 2011CB606405) and Chinese National Natural Science Foundation (11374174, 51390471)

**3:42PM C19.00005 An oxygen-deficiency modulated multiferroic: Cobalt-substituted perovskite**<sup>1</sup> , JUAN MANUEL FLOREZ, Universidad Técnica Federico Santa María; Massachusetts Inst. of Tech. — In this work, we use density functional theory to model recently demonstrated room temperature ferromagnetism and ferroelectricity in polycrystalline and single crystal Cobalt-substituted  $\text{SrTiO}_3$  thin films ( $\text{SrTi}_{0.70}\text{Co}_{0.30}\text{O}_{3-d}$ ), deposited at different oxygen pressures to change their oxygen vacancy concentration. The modeling indicates an origin for both magnetism and electric polarization in the interactions between oxygen vacancies and the B-site cations. The magnetization saturation increases with the oxygen deficiency as a result of valence spin states changes, which depend on whether the oxygen octahedral of the respective local B-site cations are complete or not. On the other hand, a finite electric polarization appears as a result of a non-centrosymmetric distribution of different resulting local charges and such a polarization increases when the oxygen vacancies increase. Increasing of both order parameters, magnetic and ferroelectric, are analyzed respect to all possible Co-sites and O-vacancies distributions, showing that these results suggest a class of multiferroic materials with properties controlled by their oxygen stoichiometry. Agreement and discrepancies between experiments and modeling are discussed.

<sup>1</sup>J M Florez and P Vargas thank Fondecyt 1130950 and 11130128, all authors thank the MISTI MIT-Chile, and CAR thanks the (S3TEC) and DoE under DE-SC0001299

### 3:54PM C19.00006 Transport and Raman signatures of electron-doped $\text{SmNiO}_3$ thin films ,

KOUSHIK RAMADOSS, School of Materials Engineering, Purdue University, West Lafayette, IN 47907, NIRAJAN MANDAL<sup>1</sup>, Department of Physics, Purdue University, West Lafayette, IN 47907, YOU ZHOU, School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, YONG CHEN<sup>2</sup>, Department of Physics, Purdue University, West Lafayette, IN 47907, SHRIRAM RAMANATHAN, School of Materials Engineering, Purdue University, West Lafayette, IN 47907 — We report low temperature transport and Raman spectroscopy measurements of electron-doped  $\text{SmNiO}_3$  (SNO) thin films. It has been shown that pristine SNO films can be doped with electrons using hydrogen. Our transport measurements indicate a Coulomb interaction dominated variable range hopping (VRH) for electron-doped samples whereas the pristine films show a Mott type VRH mechanism at low temperatures. The electron-doped samples display a strong localization which can be correlated with the high spin state of  $\text{Ni}^{2+}$  ions. The spatial Raman map shows a remarkable shift of about  $167\text{ cm}^{-1}$  with electron doping thus serving as a spectroscopic tool to investigate hydrogen in our films. **References**

1. J. Shi, Y. Zhou and S. Ramanathan, Nat. Commun **5**, 4860 (2014)
2. Jikun Chen *et al.*, Appl. Phys. Lett. **107**, 031905 (2015)

<sup>1</sup>Birck Nanotechnology Center, Purdue University

<sup>2</sup>School of Electrical and Computer Engineering, Purdue University

### 4:06PM C19.00007 Temperature dependent near field infrared microscopy of $\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$ thin films<sup>1</sup> ,

PENG XU, TJ HUFFMAN, MM QAZILBASH, Department of Physics, College of William and Mary, INHAE KWAK, AMLAN BISWAS, Department of Physics, University of Florida —  $\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$  thin films are studied with apertureless, scattering-type near field microscopy at mid-infrared wavelength and varied temperatures. Spatial resolution of about 20 nm is achieved with our technique. The temperature-dependent resistivity shows a continuous second order phase transition between insulating and metallic phases. At most temperatures, near-field infrared microscopy reveals local persistent phase separation that is independent of temperature. It is possible that the local persistent phase separation is induced by strain inhomogeneity in the thin films. Remarkably, we also observe global time-dependent changes in the infrared near-field signal upon repeated scanning of the same microscopic area at a fixed temperature. This observation is consistent with time-dependent, fluctuating conductivity in the vicinity of a second order phase transition.

<sup>1</sup>This work was supported by the National Science Foundation

### 4:18PM C19.00008 Step-induced magnetic phase separation in $\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3/\text{SrTiO}_3$ (100) thin films.<sup>1</sup> ,

IN HAE KWAK, AMLAN BISWAS, University of Florida, Department of Physics — We investigated thickness dependent magnetic anisotropy in  $\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3/\text{SrTiO}_3$  (100) (LSMO/STO) thin films using a combination of magnetic force microscopy (MFM) and magnetization measurements. Atomically smooth thin films of LSMO were grown on STO using pulsed laser deposition. The thin films showed step flow growth with unit cell step heights. MFM images of a 40 unit cell (u.c.)-thick film showed out-of-plane magnetic domain structure indicating bulk-like rhombohedral crystalline anisotropy. As the film thickness was decreased to 20 u.c., the MFM images showed signatures of step-induced uniaxial anisotropy. Hence, the magnetic domain structure shows that tensile strain from lattice mismatch weakens the rhombohedral crystalline anisotropy in LSMO. Magnetization vs. field,  $M(H)$  measurements for the 20 u.c. thick LSMO film revealed a clear in-plane uniaxial anisotropy with the direction along the steps being the easy axis and the coercive fields along the steps were consistently smaller than across the steps for a broad temperature range. Our combination of bulk and local magnetic measurements suggest that the microscopic origin of magnetic anisotropy is step-induced phase separation in the thinner films which are under higher tensile strain.

<sup>1</sup>Thank you for support from NSF-DMR 1410237

### 4:30PM C19.00009 Electronic and magnetic properties of quadruple manganite $\text{Ca}_{1-x}\text{Sr}_x\text{Mn}_7\text{O}_{12}$ films ,

AMANDA HUON, STEVEN MAY, Drexel University — We investigate the functional properties of epitaxial  $\text{Ca}_{1-x}\text{Sr}_x\text{Mn}_7\text{O}_{12}$  films to better understand the underlying physical phenomenon in this perovskite system. We utilize oxide molecular beam epitaxy to fabricate  $\text{Ca}_{1-x}\text{Sr}_x\text{Mn}_7\text{O}_{12}$  thin films. The epitaxial films were achieved through a two-step oxygen/ozone post-growth anneal. In parent  $x=0$  films, we find bulk-like electronic and magnetic properties including an abrupt increase in resistivity at 425 K due to a nominal charge ordering transition and a net magnetization below 43 K likely arising from helical magnetic order. Finally, we will present on how tuning the Sr concentration alters the electronic and magnetic properties, providing a means to control the phase transition temperatures. The results highlight the scientific opportunities in heterostructures based on quadruple manganites.

### 4:42PM C19.00010 Observation of a huge polaron gyrotropic response near room temperature in manganite thin films. ,

GERVASI HERRANZ, BLAI CASALS, RAFAEL CICHELERO, DAVID PESQUERA, MARIANO CAMPOY, FLORENCIO SANCHEZ, JOSEP FONTCUBERTA, Institut de Ciència de Materials de Barcelona ICMAB-CSIC, Campus UAB, 08193 Bellaterra, Spain, PABLO GARCIA FERNANDEZ, JAVIER JUNQUERA, Dept. Ciencias de la Tierra y Fs. de la Materia Condensada, U.de Cantabria, Av. de los Castros s/n, 39005 Santander, Spain — Magnetic materials induce rotation and ellipticity in the polarization of light. This phenomenon is exploited, e.g., to control the flux of light along optical fibers. In the pursuit for increased magneto-optic responses, strategies so far have been based on photonic or plasmonic effects. Here we uncover a novel physical mechanism by which the gyrotropic activity is hugely enhanced around the Curie temperature in optimally doped ferromagnetic manganites. This phenomenon is observed only for a narrow range of wavelengths and temperatures and is strongly dependent on the angle of incidence and polarization. We understand such an outstanding response as the result of the interplay between Jahn-Teller distortions and spin-orbit coupling in narrow-band manganites. The showcased material is  $\text{La}_{2/3}\text{Ca}_{1/3}\text{MnO}_3$ , for which the extraordinary gyrotropic response is seen near room temperature. This raises the possibility of optimizing the stoichiometric composition to drive the effect to higher temperatures. The observed phenomenon gives an added functionality –unseen previously in any manganite or other magnetic oxides– and puts a new perspective on the use of these materials for optical data storage and retrieval.

### 4:54PM C19.00011 The Manipulation of Electronic Phase Separation in Manganites. ,

LIFENG YIN, State Key Laboratory of Surface Physics and Department of Physics, Fudan University, Shanghai 200433, China — The Electronic Phase Separation (EPS) is a common phenomenon in strongly correlated systems where two or more electronic phases coexist owing to a delicate balance of competition between these phases. A model system is  $(\text{La}_{5/8-y}\text{Pr}_y)\text{Ca}_{3/8}\text{MnO}_3$  (LPCMO), a colossal magnetoresistance (CMR) manganite that is known for its large-scale EPS. Since the transport and magnetic properties depend sensitively on EPS, it is crucial to manipulate the EPS domains, especially for the applications of CMR manganites in multifunctional electronic and spintronic devices. Through the broken symmetry induced edge states, we can control the nucleation and growth of ferromagnetic metallic domains, thus the spatial distribution of EPS domains in turn. When the Pr doping is chemical ordered, we found the size of EPS domains will be one order of magnitude smaller. Furthermore, the EPS phenomena can be fully eliminated by the spatial confinement when the sample size is smaller than 500nm. These findings could help to understand the origin of large-scale EPS in LPCMO.

**5:06PM C19.00012 Enhanced magnetization in ultrathin manganite layers via structural “delta-doping” of octahedral rotations**<sup>1</sup>, EUN JU MOON, Drexel University, BRIAN J. KIRBY, National Institute of Standards and Technology, STEVEN J. MAY, Drexel University — The design of rotations and distortions of the corner-shared  $BO_6$  octahedra has emerged as an exciting platform to control electronic or magnetic behavior in  $ABO_3$  perovskite heterostructures. Recent work has shown that purely structural effects can be used to spatially confined magnetism in oxide heterostructures and point to the design of rotational gradients as routes to realize novel electronic or ferroic states in oxide superlattices [Nat. Comm. **5**, 5710 (2014)]. Here, we demonstrate a structural “delta doping” approach for controlling magnetism in ultrathin layers within isovalent manganite superlattices. Polarized neutron reflectivity and temperature dependent magnetization measurements are used to correlate enhanced magnetization with local regions of suppressed octahedral rotations in the heterostructures.

<sup>1</sup>This work was supported by the U. S. Army Research Office under grant No. W911NF-15-1-0133.

**5:18PM C19.00013 Ultrafast structural dynamics of  $LaVO_3$  thin films grown by hybrid molecular beam epitaxy**, MATTHEW BRAHLEK, JASON LAPANO, VLADIMIR STOICA, LEI ZHANG, HAI-TIAN ZHANG, HIROFUMI AKAMATSU, CRAIG EATON, VENKATRAMAN GOPALAN, Pennsylvania State University, JOHN FREELAND, HAIDAN WEN, Argonne National Lab, ROMAN ENGEL-HERBERT, Pennsylvania State University —  $LaVO_3$ , with a partially full d-shell is expected to be metallic, but due to electron-electron interactions a gap emerges and the ground state is a Mott insulator. Such effects are a strong function of the bonding geometry, and particularly the V-O-V bond angle. Controlling these structural effects on the ultrafast time scale can lead to control over the underlying electronic ground state. Here we report the ultrafast structural dynamics of 25 and 50 nm thick  $LaVO_3$  thin films grown by the hybrid molecular beam epitaxy technique on  $SrTiO_3$  when excited across the bandgap by 800 nm light. Using time-resolved x-ray diffraction on the 100 ps time scale at Sector 7 of the Advanced Photon Source, we directly measured the structural changes with atomic accuracy by monitoring integer Bragg diffraction peaks and find a large out-of-plane strain of 0.18% upon optical excitation; the recovery time is ~1 ns for the 25 nm film and ~2 ns for the 50 nm film, consistent with the thermal transport from the film to the substrate. Further, we will discuss the response of the oxygen octahedral rotation patterns indicated by changes of the half-order diffraction peaks. Understanding such ultrafast structural deformation is important for optimizing optical excitations to create new metastable phases starting from a Mott insulator. This work was supported by the Department of Energy under Grant DE-SC0012375, and DE-AC02-06CH11357.

**Monday, March 14, 2016 2:30PM - 5:30PM –**  
**Session C20 DCOMP: Electronic Structure Methods II** 319 - Lucas Wagner, University of Illinois at Urbana-Champaign

**2:30PM C20.00001 A DMC study on FePc electronic state**, TOM ICHIBHA, KENTA HONGO, RYO MAEZONO, Japan Adv Inst of Sci and Tech — We performed fixed-node DMC calculations on an isolated FePc [Iron(II) Phthalocyanine] using CASSCF nodal surfaces, getting its ground state,  $^3A_{2g} [d_{z^2}^2 d_{xz, yz}^2 d_{xy}^2]$ . Virial ratios for each state are achieved to be within 0.042% around 2.0. Recent studies [1] are proposing a mixed state with  $^3E_g(b)$  and  $^3B_{2g}$  as the ground state, while past ab-initio calculations [2] are predicting  $^3A_{2g}$  or  $^3E_g(a)$ , giving still controversial arguments even within isolated/no-LS coupling model. Under  $D_{4h}$  ligand field parameter space, ( $10Dq$ ,  $D_t$ ,  $D_s$ ), the state,  $^3A_{2g}$ , is reported to be possible as a ground state [3], while it is not when we restrict the space into 2-dim sub-space corresponding to more specified symmetry as in FePc with plane square alignment of neighboring N to Fe ('superposition model' [4]). Our optimized geometry also satisfies the same symmetry, and hence appears to be contradicting to the ligand theory[4]. [1] J. Fernández-Rodríguez *et al.*, Phys. Rev. B **91**, 214427 (2015). [2] K. Nakamura *et al.*, Phys. Rev. B **85**, 235129 (2012). [3] P.S. Miedema *et al.*, J. Phys.: Conf. Ser. **190**, 012143 (2009). [4] M.D. Kuzmin *et al.*, J. Chem. Phys. **138**, 244308 (2013).

**2:42PM C20.00002 An effective model for  $LaTiO_3$  using first principles quantum Monte Carlo**, KIEL WILLIAMS, LUCAS WAGNER, Univ of Illinois - Urbana — The rare earth perovskites have long been of interest due in part to the interplay of their geometries and electronic properties. The perovskite  $LaTiO_3$  in particular is an antiferromagnetic insulator with a small 0.2 eV band gap that displays the GdFeO<sub>3</sub> distortion at ambient pressure. We apply a new technique[1] to derive an effective model for  $LaTiO_3$  as a function of the distortion. Since this technique treats one and two-body degrees of freedom on an equal footing, we use it to evaluate the evolution of effective model parameters with changes in the lattice. We will report on the progress in assessing whether the insulating nature is due to the distortion, or vice versa. [1] Changlani, Zheng, and Wagner J. Chem. Phys. **143**, 102814 (2015).

**2:54PM C20.00003 A new constraint DFT technique for self-consistent determination of  $U$  values**, TOMOYUKI HAMADA<sup>1</sup>, Hitachi, Ltd. Research and Development Group, TAKAHISA OHNO<sup>2</sup>, National Institute of Materials Science — A new constraint density functional (DFT) technique workable in combination with the projector augmented wave (PAW) and pseudopotential (PP) methods was developed. This technique calculates the effective on-site-interaction parameter,  $U_{eff}$ , of correlated electrons of materials, self-consistently, by using the DFT+U method. The  $U_{eff}$  determined by this technique has a clear physical meaning in that it determines the electronic structures of strongly correlated electronic systems (SCESs) and *vice versa*. The technique was used to determine the  $U_{eff}$  of correlated electrons of hexagonal neodymium sesquioxide ( $h-Nd_2O_3$ ) and orthorhombic iron oxide ( $\alpha-FeO$ ) in the antiferromagnetic states, and it was shown to be effective for this purpose. The newly developed constraint DFT technique enables first principles DFT+U PAW and PP calculations of SCESs free from any empirical parameters, which are more reliable than the DFT+U PAW and PP calculations of them using empirical  $U_{eff}$ s.

<sup>1</sup>Hatoyama, Saitama, 350-0395, Japan

<sup>2</sup>1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

**3:06PM C20.00004 Electronic and structural properties of  $M_3(HITP)_2$  ( $M = Ni, Cu$  and  $Co$ ) metal-organic frameworks**, ORLANDO SILVEIRA, HELIO CHACHAM, SIMONE ALEXANDRE, Federal University of Minas Gerais — Theoretical and experimental works have demonstrated that electrical and structural properties of metal-organic frameworks (MOF) can be significantly changed by the identity of the metal center, leading to a potential strategy for tuning the selectivity of the material toward different types of technological applications. In this work, we use first principle calculations to investigate the electronic properties of 2D MOF  $M_3(HITP)_2$  ( $M$  is Ni, Cu and Co and HITP = 2,3,6,7,10,11 hexaiminotriphenylene). Our results show that for  $M=Ni$  and  $Co$ , the structures are perfect planar and there is a full charge delocalization in the 2D plane of stacking due to the predominance of  $\pi - \pi$  bonding. The band structure for  $M = Ni$  shows that this material is a semiconductor with an indirect band gap of 132 meV, whilst for  $M = Co$  the band structure shows that this material is a ferromagnetic semiconductor with a direct band gap of 386 meV for spin down and an indirect band gap of 246 meV for spin up. For  $M=Cu$ , the material is a metal and adopts a distorted structure due to a different hybridization of the metal atom in comparison with its counterparts. We also propose a tight binding model that can represent the electronic structure near the Fermi level of this family of MOF.

**3:18PM C20.00005 Band structure of correlated  $\text{Sr}_2\text{RuO}_4$  using DFT+DMFT**, OLIVIER GINGRAS, MICHEL CT, Univ of Montreal, ANDR-MARIE TREMBLAY, Univ of Sherbrooke — The discovery of superconductivity in the cuprates stimulated investigations on materials sharing similar structural properties. Ruthenates, including  $\text{Sr}_2\text{RuO}_4$  became of great interest since they were found to be unconventional superconductors, possibly *p*-wave, at sufficiently low temperature. A lot of experimental data was acquired and analyzed over the past decade. Of particular interest is the discrepancy between the calculated and measured effective masses. In this presentation, we will present DFT+DMFT calculations as implemented in the ABINIT program to compute the electronic structure of  $\text{Sr}_2\text{RuO}_4$ .

**3:30PM C20.00006 A general optimization method applied to a vdW-DF functional for water**, MICHELLE FRITZ, JOSE M. SOLER, Universidad Autnoma de Madrid, MARIVI FERNÁNDEZ-SERRA, Stony Brook University — In particularly delicate systems, like liquid water, ab initio exchange and correlation functionals are simply not accurate enough for many practical applications. In these cases, fitting the functional to reference data is a sensible alternative to empirical interatomic potentials. However, a global optimization requires functional forms that depend on many parameters and the usual trial and error strategy becomes cumbersome and suboptimal. We have developed a general and powerful optimization scheme called data projection onto parameter space (DPPS) and applied it to the optimization of a van der Waals density functional (vdW-DF) for water. In an arbitrarily large parameter space, DPPS solves for vector of unknown parameters for a given set of known data, and poorly sampled subspaces are determined by the physically-motivated functional shape of ab initio functionals using Bayes' theory. We present a new GGA exchange functional that has been optimized with the DPPS method for 1-body, 2-body, and 3-body energies of water systems and results from testing the performance of the optimized functional when applied to the calculation of ice cohesion energies and ab initio liquid water simulations. We found that our optimized functional improves the description of both liquid water and ice when compared to other versions of GGA exchange.

**3:42PM C20.00007 Solvated ions as defects in liquid water: A first-principles perspective<sup>1</sup>**, ERIC SCHWEGLER, TUAN ANH PHAM, Lawrence Livermore Natl Lab, MARCO GOVONI, GIULIA GALLI, Institute for Molecular Engineering-The University of Chicago, and Argonne National Laboratory — Understanding the electronic properties of solvated ions is crucial in order to control and engineer aqueous electrolytes for a wide variety of emerging energy and environmental technologies, including photocatalytic water splitting. In this talk, we present a strategy to evaluate electronic energy levels of simple solvated ions in aqueous solutions, using a combination of first-principles molecular dynamics simulations and many-body perturbation theory within the GW approximation. We considered  $\text{CO}_3^{2-}$ ,  $\text{HCO}_3^-$ ,  $\text{NO}_3^-$ ,  $\text{NO}_2^-$  ions and we show that by analogy to defects in semiconductors, these solvated ions may be classified as deep or shallow defects in liquid water. In particular  $\text{CO}_3^{2-}$  and  $\text{NO}_2^-$  ions behave as shallow defects, while  $\text{HCO}_3^-$  and  $\text{NO}_3^-$  as deep ones. We also show that the inclusion of many-body corrections constitutes significant improvement over conventional density functional theory calculations, yielding satisfactory agreement with photoemission experiments.

<sup>1</sup>Part of this work was supported by the U.S. Department of Energy at the LLNL under Contract DE-AC52-07NA27344. T.A.P acknowledge the support from the Lawrence Fellowship. Part of this work was supported by LDRD at ANL.

**3:54PM C20.00008 Evaluation of Hamaker coefficients using Diffusion Monte Carlo method**, RYO MAEZONO, KENTA HONGO, School of Information Science, JAIST, Japan — We evaluated the Hamaker's constant for Cyclohexasilane to investigate its wettability, which is used as an ink of 'liquid silicon' in 'printed electronics'. Taking three representative geometries of the dimer coalescence (parallel, lined, and T-shaped), we evaluated these binding curves using diffusion Monte Carlo method. The parallel geometry gave the most long-ranged exponent,  $\sim 1/r^6$ , in its asymptotic behavior. Evaluated binding lengths are fairly consistent with the experimental density of the molecule. The fitting of the asymptotic curve gave an estimation of Hamaker's constant being around 100 [zJ]. We also performed a CCSD(T) evaluation and got almost similar result. To check its justification, we applied the same scheme to Benzene and compared the estimation with those by other established methods, Lifshitz theory and SAPT (Symmetry-adopted perturbation theory). The result by the fitting scheme turned to be twice larger than those by Lifshitz and SAPT, both of which coincide with each other. It is hence implied that the present evaluation for Cyclohexasilane would be overestimated.

**4:06PM C20.00009 Exploring Reaction Mechanism on Generalized Force Modified Potential Energy Surfaces (G-FMPES) for Diels-Alder Reaction**, SANJIV JHA, Univ of Southern Mississippi, KATIE BROWN, Auburn University, GOPINATH SUBRAMANIAN, Univ of Southern Mississippi — We apply a recent formulation for searching minimum energy reaction path (MERP) and saddle point to atomic systems subjected to an external force. We demonstrate the effect of a loading modality resembling hydrostatic pressure on the trans to cis conformational change of 1,3-butadiene, and the simplest Diels-Alder reaction between ethylene and 1,3-butadiene. The calculated MERP and saddle points on the generalized force modified potential energy surface (G-FMPES) are compared with the corresponding quantities on an unmodified potential energy surface. Our study is performed using electronic structure calculations at the HF/6-31G\*\* level as implemented in the AIMS-MOLPRO code. Our calculations suggest that the added compressive pressure lowers the energy of cis butadiene. The activation energy barrier for the concerted Diels-Alder reaction is found to decrease progressively with increasing compressive pressure.

**4:18PM C20.00010 Fast molecular dynamics simulations using high-order forces and nonlocal operators in real space<sup>1</sup>**, GRADY SCHOFIELD, N. SCOTT BOBBITT, JAMES R. CHELIKOWSKY, Univ of Texas, Austin — We present a new modification to the finite-difference based real space pseudopotential density functional theory method as implemented in the code PARSEC. By using a high-order treatment of the nonlocal pseudopotential terms in the Hamiltonian, as well as integration performed during post-processing the wave functions, we improve the accuracy of total energy and interatomic forces. We perform molecular dynamics simulations for several systems, including organic molecules and small clusters. We demonstrate significant reduction in energy drift owing to the accuracy of our improved force calculations. Furthermore, the reduction in numerical noise as atoms move over the grid permits a larger grid spacing than would be possible with a conventional discretization.

<sup>1</sup>This work is supported by the DOE through the SciDAC program funded by ASCR and BES under award number DE-SC0008877. Computations were performed on machines at TACC.

**4:30PM C20.00011 Real-space pseudopotential methods for calculating the vibrational Stark tuning rate<sup>1</sup>**, BENJAMIN GARRETT, JAMES CHELIKOWSKY, University of Texas at Austin — We introduce a real-space method based on pseudopotentials constructed within density functional theory for computing the vibrational Stark effect. With wave functions defined in real space and cluster boundary conditions, convergence is controlled solely by the grid spacing. Moreover, charged systems can be incorporated without a compensating background charge. Real space methods also have the advantage that neither polarization functions nor supercells are required to simulate external electric fields. We illustrate this method by calculating the Stark tuning rates of small carbonyls and nitriles. The use of high-order integration techniques allow for a coarser (less expensive) grid spacing. Perturbative methods for determining the tuning rate will also be discussed.

<sup>1</sup>We acknowledge support from the U.S. Department of Energy from grant DE-FG02-06ER46286.

**4:42PM C20.00012 Unbiased QM/MM approach using accurate multipoles from a linear scaling DFT calculation with a systematic basis set**, STEPHAN MOHR, Barcelona Supercomputing Center, CEA Grenoble, LUIGI GENOVESE, CEA Grenoble, LAURA RATCLIFF, Argonne Leadership Computing Facility, MICHEL MASELLA, CEA Saclay — The quantum mechanics/molecular mechanics (QM/MM) method is a popular approach that allows to perform atomistic simulations using different levels of accuracy. Since only the essential part of the simulation domain is treated using a highly precise (but also expensive) QM method, whereas the remaining parts are handled using a less accurate level of theory, this approach allows to considerably extend the total system size that can be simulated without a notable loss of accuracy. In order to couple the QM and MM regions we use an approximation of the electrostatic potential based on a multipole expansion. The multipoles of the QM region are determined based on the results of a linear scaling Density Functional Theory (DFT) calculation using a set of adaptive, localized basis functions, as implemented within the BigDFT software package. As this determination comes at virtually no extra cost compared to the QM calculation, the coupling between QM and MM region can be done very efficiently. In this presentation I will demonstrate the accuracy of both the linear scaling DFT approach itself as well as of the approximation of the electrostatic potential based on the multipole expansion, and show some first QM/MM applications using the aforementioned approach.

**4:54PM C20.00013 Large-scale All-electron Density Functional Theory Calculations using Enriched Finite Element Method<sup>1</sup>**, BIKASH KANUNGO, VIKRAM GAVINI, Univ of Michigan - Ann Arbor — We present a computationally efficient method to perform large-scale all-electron density functional theory calculations by enriching the Lagrange polynomial basis in classical finite element (FE) discretization with atom-centered numerical basis functions, which are obtained from the solutions of the Kohn-Sham (KS) problem for single atoms. We term these atom-centered numerical basis functions as enrichment functions. The integrals involved in the construction of the discrete KS Hamiltonian and overlap matrix are computed using an adaptive quadrature grid based on gradients in the enrichment functions. Further, we propose an efficient scheme to invert the overlap matrix by exploiting its *LDL* factorization and employing spectral finite elements along with Gauss-Lobatto quadrature rules. Finally, we use a Chebyshev polynomial based acceleration technique to compute the occupied eigenspace in each self-consistent iteration. We demonstrate the accuracy, efficiency and scalability of the proposed method on various metallic and insulating benchmark systems, with systems ranging in the order of 10,000 electrons. We observe a 50-100 fold reduction in the overall computational time when compared to classical FE calculations while being commensurate with the desired chemical accuracy.

<sup>1</sup>We acknowledge the support of NSF (Grant No. 1053145) and ARO (Grant No. W911NF-15-1-0158) in conducting this work.

**5:06PM C20.00014 Ultrafast Response of the Hubbard Model: Non-adiabatic TDDFT+DMFT versus Non-equilibrium DMFT Solution<sup>1</sup>**, SHREE RAM ACHARYA, University of Central Florida, VOLODYMYR TURKOWSKI, TALAT S. RAHMAN, Department of Physics, University of Central Florida — We study the ultrafast response of electrons in the one-band Hubbard model to an external laser-pulse perturbation by using the Non-adiabatic Time-Dependent Density Functional Theory + Dynamical Mean-Field Theory (TDDFT+DMFT) approach. The corresponding exchange-correlation kernel (XC) is obtained from the DMFT charge susceptibility by using the Quantum Monte Carlo solver for the impurity problem. Detailed analysis of the time-dependent excited charge density, the Fermi distribution function, and the spatially nonhomogeneous response (metallic domain growth), is performed for different values for the carrier density and local Coulomb repulsion. We compare the results with the corresponding non-equilibrium DMFT solutions, and demonstrate that non-adiabaticity (frequency-dependence) of the XC kernel is important in order to reproduce the non-equilibrium DMFT solution. Also, from the numerical results for the charge susceptibility, we obtain an approximate analytical expression for the XC kernel. Using this kernel, we reveal possible types of "elementary" excitations and the dynamics of metallic domain growth in the case of the one-band Hubbard model. Possible generalization of the approach to the multi-orbital case is discussed.

<sup>1</sup>Work supported in part by DOE Grant No. DOE-DE-FG02-07ER46354

**5:18PM C20.00015 Improving Boundary Conditions for Electronic Structure Calculations**, G. A. BENESH, Baylor University, ROGER HAYDOCK, University of Oregon — Boundary conditions imposed on a local system joined to a much larger substrate system routinely introduce unphysical reflections that affect the calculation of electronic properties such as energies, charge densities, and densities of states. These problems persist in atomic cluster, slab, and supercell calculations alike. However, wave functions in real, physical systems do not reflect at artificial boundaries. Instead, they carry current smoothly across the surface separating the local system from the underlying medium. Haydock and Nex have derived a non-reflecting boundary condition that works well for discrete systems [Phys. Rev. B 75, 205121 (2006)]. Solutions satisfying their maximal breaking of time-reversal symmetry (MBTS) boundary condition carry current away from the boundary at a maximal rate—in much the same way as exact wave functions in physical systems. The MBTS approach has now been extended to studies employing continuous basis functions. In model systems, MBTS boundary conditions work well for calculating wave functions, eigenenergies, and densities of states. Results are reported for an Al(001) surface. Comparisons are made with slab calculations, embedding calculations, and experiment.

## Monday, March 14, 2016 2:30PM - 5:30PM –

Session C21 GMAG DMP: Magnetic Chains and Kondo Effects 320 - Christopher Landee, Clark University

**2:30PM C21.00001 Magnetic Behavior of quasi-1D-Ferromagnetic Fe Chains in Metallo-Organic Superlattices<sup>1</sup>**, C. MONTON, Univ of Texas, San Antonio, A. C. BASARAN, I. VALMIANSKI, Univ California, San Diego, T. GREDIG, California State University, Long Beach, D. ALTBIR, V. L. CARVALHO-SANTOS, Universidad de Santiago de Chile, IVAN K. SCHULLER, Univ California, San Diego — We report structural and magnetic properties of metallo-organic iron-phthalocyanine (FePc) / metal-free-phthalocyanine (H2Pc) superlattices. H2Pc is a weak diamagnetic molecule in which, instead of a metal ion, two hydrogen atoms occupy the center of the molecule. Due to molecular stacking, the divalent Fe(II) ion of FePc forms quasi one-dimensional (1D) chains. These Fe chains can be oriented either parallel or perpendicular to the substrate based on the choice of the substrate. These quasi-1D chains exhibit two magnetic regimes: ferromagnetic-like order below 5K, and nontraditional paramagnetic order (nonlinear behavior with decreasing saturation intensity with temperature) between 5 and 40 K. We have found that reducing the average Fe chains length from 70 to 7 Fe ions substantially increases the coercive field. We discuss the magnetic behavior of quasi-1D Fe chains as a function of the chains length and we correlate the observed magnetic behavior with structural information obtained from x-ray diffraction and Monte Carlo based micromagnetic simulations.

<sup>1</sup>Work supported by DEFG02-87ER-45332, DMR 0847552, FONDECYT 1120356, FB0807, and FA9550-11-1-0347

**2:42PM C21.00002 Spin Liquid Ground State in the Frustrated  $J_1$ - $J_2$  Zigzag Chain System  $\text{BaTb}_2\text{O}_4$** , A.A. ACZEL, Oak Ridge National Laboratory, L. LI, University of Tennessee, V.O. GARLEA, Oak Ridge National Laboratory, J.-Q. YAN, University of Tennessee and Oak Ridge National Laboratory, F. WEICKERT, V.S. ZAPF, R. MOVSHOVICH, M. JAIME, Los Alamos National Laboratory, P.J. BAKER, Rutherford Appleton Laboratory, V. KEPPENS, D. MANDRUS, University of Tennessee — We have investigated polycrystalline samples of the zigzag chain system  $\text{BaTb}_2\text{O}_4$  with magnetic susceptibility, heat capacity, neutron powder diffraction, and muon spin relaxation ( $\mu\text{SR}$ ). No magnetic transitions are observed in the bulk measurements, while neutron diffraction reveals the presence of low-temperature, short-range, intrachain magnetic correlations between  $\text{Tb}^{3+}$  ions.  $\mu\text{SR}$  indicates that these correlations are dynamic, as no signatures of static magnetism are detected by the technique down to 0.095 K. These combined findings provide strong evidence for a spin liquid ground state in  $\text{BaTb}_2\text{O}_4$ .

**2:54PM C21.00003 Study of magnetic and magnetocaloric properties of monoclinic and triclinic spin chain  $\text{CoV}_2\text{O}_6$** , MOUMITA NANDI, PRABHAT MANDAL, Saha Institute of Nuclear Physics, 1/AF Bidhannagar Kolkata, India — We have investigated magnetic and magnetocaloric properties of both monoclinic and triclinic phases of  $\text{CoV}_2\text{O}_6$  from magnetization and heat capacity measurements. Conventional and inverse magnetocaloric effects have been observed in both phases of  $\text{CoV}_2\text{O}_6$ . For a field change from 0 to 7 T, maximum values of magnetic entropy change and adiabatic temperature change reach  $11.8 \text{ J kg}^{-1} \text{ K}^{-1}$  and 9.5 K respectively for monoclinic  $\text{CoV}_2\text{O}_6$  while the corresponding values reach  $12.1 \text{ J kg}^{-1} \text{ K}^{-1}$  and 13.1 K for triclinic  $\text{CoV}_2\text{O}_6$ . Particularly for triclinic  $\text{CoV}_2\text{O}_6$ , the magnetocaloric parameters are quite large in low or moderate field range. Apart from this, we have constructed magnetic phase diagram of monoclinic  $\text{CoV}_2\text{O}_6$  where field-induced complex magnetic phases appear below a certain critical temperature 6 K when external magnetic field is applied along crystallographic easy axis.

**3:06PM C21.00004 Entanglement properties of the bond alternating Heisenberg chain with general integer spins**, SHOHEI MIYAKOSHI, Chiba Univ, SATOSHI NISHIMOTO, IFW Dresden, TU Dresden, YUKINORI OTHA, Chiba Univ — Symmetry protected topological (SPT) phases are a gapped phase under a given symmetry. Unless any symmetries that protect the SPT phases are broken, the SPT phases can be distinguished from each other. Recently, it was pointed out that the entanglement spectrum of the many-body state characterizes such SPT phases. In particular, the degeneracy of the entanglement spectrum reflects the corresponding symmetries and edge states of the system. Motivated by recent studies of the SPT phases, we study the bond-alternating Heisenberg model with general integer spins and clarify the entanglement properties of the ground state using the density matrix renormalization group method. In particular, this model has the intermediate phase at  $S > 1$  due to the bond alternation. The entanglement properties of this phase in the case of  $S > 2$  have not been studied sufficiently because of the numerical difficulties under an extremely small spin-gap situation. We studied the case of  $S = 1, 2, 3$  using the antiperiodic boundary condition. Under the antiperiodic boundary condition, we found that the doubly degenerate spectra which characterize the intermediate phase can be observed in the entanglement spectrum. We will also discuss the effect of the single-ion uniaxial anisotropy.

**3:18PM C21.00005 Finite temperature dynamics of spin-1/2 chains with symmetry breaking interactions<sup>1</sup>**, SALVATORE R. MANMANA, ALEXANDER C. TIEGEL, THOMAS PRUSCHKE, Institute for Theoretical Physics, University of Goettingen, ANDREAS HONECKER, LPTM, Université de Cergy-Pontoise — I will discuss recent developments for flexible matrix product state (MPS) approaches to calculate finite-temperature spectral functions of low-dimensional strongly correlated quantum systems. The main focus will be on a Liouvilian formulation. The resulting algorithm does not specifically depend on the MPS formulation, but is applicable for any wave function based approach which can provide a purification of the density matrix, opening the way for further developments of numerical methods. Based on MPS results for various spin chains, in particular systems with Dzyaloshinskii-Moriya interactions caused by spin-orbit coupling and dimerized chains, I will discuss how symmetry breaking interactions change the nature of the finite-temperature dynamic spin structure factor obtained in ESR and neutron scattering experiments.

<sup>1</sup>We acknowledge funding by the Helmholtz Virtual Institute "New States of Matter and Their Excitations".

**3:30PM C21.00006 Magnetic Spin Relaxation Probed with Sweep Speed Dependent Coercivity<sup>1</sup>**, THOMAS GREDIG, MATTHEW BYRNE, Department of Physics and Astronomy, California State University Long Beach — The magnetic spin relaxation of finite-length iron chains has been investigated in iron phthalocyanine thin films by means of sweep speed dependence on magnetic coercivity. The  $\text{Fe(II)}$  ions are embedded in a carbon matrix and molecules self-assemble during vacuum sublimation, so that the  $\text{Fe(II)}$  cores form well-separated chains of 1.3 nm and tunable chain lengths within the polycrystalline thin film. The average length of the chains is controlled through deposition variables and ranges from 30 nm to 300 nm. The coercivity strongly increases with chain length in this regime. This may be an interesting experimental realization of a low-dimensional finite-sized Ising model. The coercivity dependence on chain length and sweep speed is described with an Ising model based on Glauber dynamics.

<sup>1</sup>Research support from NSF under grant DMR 0847552.

**3:42PM C21.00007 ANISOTROPIC PHASE DIAGRAM OF THE FRUSTRATED SPIN CHAIN  $\beta\text{-TeVO}_4$** , F. WEICKERT, M JAIME, N HARRISON, B. L. SCOTT, Los Alamos Natl Lab, A. LEITMAE, L. HEINMAA, R STERN, O JANSON, NICPB Tallinn, Estonia, H. BERGER, EPFL, Lausanne, Switzerland, H ROSNER, MPI CPfS, Dresden, Germany, A. A. TSIRLIN, Augsburg University, Germany — We will present experimental as well as theoretical data on  $\beta\text{-TeVO}_4$  a candidate for the  $J_1$ - $J_2$  chain model with ferromagnetic  $J_1 \sim 18 \text{ K}$  and antiferromagnetic  $J_2 \sim 48 \text{ K}$  coupling constants. The  $T - H$  magnetic phase diagram is revealed by measurements of the magnetization, specific heat, magnetostriction, and thermal expansion on oriented single crystals at temperatures between 0.5 K and 50 K and in magnetic fields up to 50 T. The high field data were taken in a capacitor bank-driven pulsed magnet at NHMFL – LANL and complemented with measurements in a superconducting magnet. Our comprehensive study allows for the first time a detailed mapping of the phase diagram in both directions,  $H \parallel ab$  and  $H \parallel c$ . We find clear evidence for 5 different phases including full polarization of the magnetic moments above 23 T that is only weakly dependent on the crystal orientation. Surprisingly, the phase boundary at the saturation field splits into two distinct lines below 5 K. The magnetic phases occurring at fields below 10 T show significant magnetic anisotropy between  $H \parallel ab$  and  $H \parallel c$ . The nature of the different phases and regions in  $\beta\text{-TeVO}_4$  is still far from being understood, but our results will stimulate further research on this interesting model compound.

**3:54PM C21.00008 Unusual features of magnetism in transition-metal-doped phthalocyanines**  $C_{32}H_{16}N_8TM$  (TM = Mn, Fe, Co, Ni, Cu), ZHENGJUN WANG, MOHINDAR S. SEEHRA, Department of Physics and Astronomy, West Virginia University — Transition-metal-doped phthalocyanines (TMPc), semiconductors with potential optoelectronic applications [1], are planar molecules with the TM atom at the center bound to four N atoms and forming a linear chain along the monoclinic b-axis. Because of this symmetry, the ground states of TMPc often violate the Hund's rules; e.g. the  $S = 3/2$  state for  $d^5$  Mn(II) in  $\beta$ -MnPc,  $S = 1/2$  state for the  $d^7$  Co(II) in  $\beta$ -CoPc, and  $S=0$  for Ni(II) in NiPc. The magnetic properties of TMPc are also affected by the stack angle  $\delta$  between the orientation of the molecular plane and the b-axis,  $\delta$  being 65(45) for  $\alpha$  ( $\beta$ ) phase [2]. For  $\beta$ -CoPc, our M vs. T data fits well with the Bonner-Fisher model for  $S = 1/2$  AFM Heisenberg linear chain [3] yielding the  $Co^{2+}$ - $Co^{2+}$  exchange constant  $J/k_B = -1.5$  K. For  $\beta$ -MnPc, a long-presumed ferromagnet with  $T_C \approx 9$  K [4], our magnetic studies show it to be an Ising chain magnet with Arrhenius magnetic relaxation governed by  $J/k_B = 2.6$  K and the zero-field splitting  $D/k_B = 8.3$  K. In  $\beta$ -MnPc, the absence of  $\lambda$ -type peak in specific heat and no peaks in ac susceptibilities near the quoted  $T_C \approx 9$  K confirms the absence of long range order (LRO). Instead we argue that LRO is absent in  $\beta$ -MnPc as  $D > J$  makes the spins in a chain parallel but canted with respect to spins in neighboring chains. [1]G. Mattioli et al, Phys. Rev. Lett. 101, 126805 (2008); [2]Z. Wang et al, IEEE Trans. Mag. 51, 2700104(2015); [3]J. Bonner & M. Fisher, Phys. Rev. 135, A640 (1964); [4]Y. Taguchi et al, J. Magn. Magn. Mater. 301, 1229 (2007).

**4:06PM C21.00009 Heat transport in spin chains with weak spin-phonon coupling<sup>1</sup>**, ALEXANDER CHERNYSHEV, University of California, Irvine, ALEXANDER ROZHKOV, Institute for Theoretical and Applied Electrodynamics, Russian Academy of Sciences, Russia — We propose that the heat conductivity by 1D spin excitations in  $S = 1/2$  Heisenberg spin chains can be quantitatively described within the bosonization framework, in which large-momentum scattering of spin excitations is due to optical phonons with the spin-phonon couplings that are well within the physical bounds. Our theory provides an excellent fit to the data from the systematic experimental thermal conductivity studies in the high-quality single-crystalline large- $J$  spin-chain cuprates that have recently become available. Our description of the spin-phonon scattering is also in accord with a physically intuitive picture of phonons playing the role of thermally-populated weak impurities for the fast spin excitations. Our approach stands out from previous considerations that require large coupling constants to explain the data and thus imply a spin-Peierls transition, absent in real materials.

<sup>1</sup>Supported by the DoE

**4:18PM C21.00010 Spin dynamics in critical regime of the spin-1/2 XXZ chain**, WANG YANG, JIANDA WU, CONGJUN WU, University of California San Diego — The spin-1/2 Heisenberg XXZ chain is one of the most well-studied quantum integrable models. Although its eigenstates and spectrum are solvable through Bethe ansatz, even understanding its zero temperature spin dynamics remains a challenge. In the axial anisotropic regime, by tuning longitudinal magnetic field, the system undergoes a quantum phase transition, entering into the critical regime. Recent experiments provided some evidences for understanding spin dynamics in the critical regime. Here we investigate the spin dynamics in this regime by form factor methods. Our results can be directly compared with experiments on relevant materials.

**4:30PM C21.00011 First principles electron transport simulations in the Kondo regime**, IVAN RUNGGER, National Physical Laboratory, MIŁOS RADONJIC, WILHELM APPELT, LIVIU CHIONCEL, University of Augsburg, ANDREA DROGHETTI, Universidad del País Vasco — When magnetic atoms, molecules or thin films are brought into contact with metals the electron-electron interaction leads to the appearance of the correlated Kondo state at low temperatures. In this talk we will present results for the electronic structure and conductance in the Kondo regime of recent STM and break junction experiments for stable radical molecules<sup>1</sup>, which correspond to spin half molecular magnets. We will outline the methodological approach to evaluate the conductance of such systems from first principles, as implemented in the Smeagol electron transport code<sup>2</sup>. The method combines the density functional theory (DFT) with Anderson impurity solvers within the continuum time quantum Monte Carlo (CTQMC) and numerical renormalization group (NRG) approaches.

<sup>1</sup>J. Liu et al., J. Am. Chem. Soc. **135**, 651 (2013); R. Frisenda et al., Nano Lett. **15**, 3109 (2015).

<sup>2</sup>A. Rocha et al., Nature Mater. **4**, 335 (2005); A. Rocha et al., Phys. Rev. B **73**, 085414 (2006); I. Rungger et al., Phys. Rev. B **78**, 035407 (2008)

**4:42PM C21.00012 Cobalt on silicene/ZrB<sub>2</sub>: an intriguing Kondo system**, TOBIAS GILL, BEN WARNER, HENNING PRSER, UCL, UK, ANTOINE FLEURENCE, YUKIKO YAMADA-TAKAMURA, JAIST, Japan, CYRUS HIRJIBEHEDIN, UCL, UK — Magnetic atoms placed upon metallic substrates have been used as prototypical systems for the investigation of the fundamentals of atomic-scale magnetism. Often these magnetic impurities undergo the Kondo effect, in which the magnetic moment of the impurity is collectively screened by a cloud of conduction electrons forming a many-body singlet ground state. Here we present results for individual Co adatoms on the silicene/ZrB<sub>2</sub> surface. Unlike on metallic surfaces, Co atoms exhibit a distinct energy-dependent change in the spatial distribution of their electronic states when imaged with scanning tunneling microscopy. At low biases around the Fermi level, the Co atoms exhibit a two-lobe structure that is oriented along one of three equivalent directions in the plane and that is revealed by scanning tunneling spectroscopy to result from a Kondo resonance centered upon each lobe. This spatially anisotropic Kondo resonance is reminiscent of the orbital states of magnetic atoms on semiconductor surfaces or of the spatially distributed Kondo resonances seen for magnetic molecules on metallic surfaces, and is a result of the interaction between a magnetic impurity and the unusual electronic structure of the silicene/ZrB<sub>2</sub> surface.

**4:54PM C21.00013 ABSTRACT WITHDRAWN —**

**5:06PM C21.00014 Sub-molecular modulation of a 4f driven Kondo resonance by surface-induced asymmetry**, BEN WARNER, FADI EL HALLAK, UCL, NICOLAE ATODIRESEI, Forschungszentrum Juelich, PHILIPP SEIBT, HENNING PRUSER, UCL, VASILE CACIUC, Forschungszentrum Juelich, MICHAEL WATERS, U. of Nottingham, ANDREW J. FISHER, UCL, STEFAN BLUGEL, Forschungszentrum Juelich, JORIS VAN SLAGEREN, U. of Stuttgart, CYRUS F. HIRJIBEHEDIN, UCL — Coupling between a magnetic impurity and an external bath can give rise to many-body quantum phenomena, including Kondo and Hund's Impurity states in metals, and Yu-Shiba-Rusinov states in superconductors. While advances have been made in probing the magnetic properties of d-shell impurities on surfaces, the confinement of f orbitals makes them much more difficult to access directly. Here we show that a 4f driven Kondo resonance can be modulated spatially by asymmetric coupling between a metallic surface and a molecule containing a 4f-like moment. Strong hybridisation of dysprosium double-decker phthalocyanine (DyPc<sub>2</sub>) with Cu(001) induces Kondo screening of the central magnetic moment. Misalignment between the symmetry axes of the molecule and the surface induces asymmetry in the molecule's electronic structure, spatially mediating electronic access to the magnetic moment through the Kondo resonance. This work demonstrates the important role that molecular ligands play in mediating electronic and magnetic coupling and in accessing many-body quantum states.

**5:18PM C21.00015 Revealing the Atomic Site-Dependent g Factor within a Single Magnetic Molecule via the Extended Kondo Effect<sup>1</sup>**, SHIXUAN DU, Institute of Physics, Chinese Academy of Sciences — Control over charge and spin states at the single molecule level is crucial not only for a fundamental understanding of charge and spin interactions but also represents a prerequisite for development of molecular electronics and spintronics. In this talk, I will talk about the extended spin distribution in space beyond the central Mn ion, and onto the non-magnetic constituent atoms of the MnPc molecule. This extended spin distribution results in an extended Kondo effect, which can be explained by spin polarization induced by symmetry breaking of the molecular framework, as confirmed by DFT calculations. Measuring the evolution of the Kondo splitting with applied magnetic fields at different atomic sites, we find a spatial variation of the g-factor within a single molecule for the first time. The existence of atomic site-dependent g-factors can be attributed to specific molecular orbitals distributed over the entire molecule. This work not only open up a new opportunity for quantum information recording, but also provide a new route to explore the internal electronic and spin structure of complex molecules, hard to achieve otherwise. (L.W. Liu et al., Phys. Rev. Lett. 2015, 114, 126601. In collaboration with Liwei Liu, Kai Yang, Yuhang Jiang, Li Gao, Qi Liu, Boqun Song, Wende Xiao, Haitao Zhou, Hongjun Gao in CAS, Min Ouyang in MU, and A.H. Castro Neto in SNU.)

<sup>1</sup>Revealing the Atomic Site-Dependent g Factor within a Single Magnetic Molecule via the Extended Kondo Effect

**Monday, March 14, 2016 2:30PM - 5:30PM –**  
**Session C22 DCOMP: Electrons, Phonons, and Electron-Phonon Scattering II** 321 - David Broido, Boston College

**2:30PM C22.00001 Controlling electron-phonon scattering with metamaterial plasmonic structures**, KRZYSZTOF KEMPA, XUEYUAN WU, JIANTAO KONG, DAVID BROIDO, Boston College — Electron-plasmon scattering can be faster than electron-phonon scattering. While in metals plasmons occur in the UV range, phonons dominate behavior at much lower frequencies (far IR range), and this typically decouples these phenomena. In metamaterial plasmonic structures, however, plasma effects can be tuned down to the far IR range, allowing for their interference with phonons. It was recently shown, that such interference can protect hot electron energy induced in a solar cell, from dissipation into heat [1]. In this work we explore the possibility of using such an effect to control the electron-phonon interaction and transport in semiconductors. We demonstrate, that this could lead to a novel path to enhancing the electrical and thermal conductivities and the thermoelectric figure of merit. [1] Hot electron plasmon-protected solar cell, J. Kong, A.H. Rose, C. Yang, J. M. Merlo, M.J. Burns, M. Naughton, and K. Kempa, Opt. Express 23, A1087-A1095 (2015) doi:10.1364/OE.23.0A1087

**2:42PM C22.00002 Temperature-dependence of electron bands in wurtzite GaN, including non-adiabatic (Polaron) contributions<sup>1</sup>**, JEAN PAUL NERY, JIAN LIU, P. B. ALLEN, Stony Brook University — We study the temperature dependence of the band gap of wurtzite structure GaN [1]. Virtual interband electron-phonon scattering is accounted properly by adiabatic (Allen-Heine-Cardona) theory. The correct way to avoid an unphysical divergence, is to use a non-adiabatic treatment for intraband scattering by small  $q$  polar optical phonons [2,3]. This is equivalent to including Fröhlich polaron effects. The  $T = 0$  zero-point weak-coupling polaron shift ( $-\alpha\hbar\omega$ ) is well known, but finite  $T$  effects are less studied. We also calculate the  $T$  dependence of the band mass (both polaron and adiabatic contributions). We compare results from an *ab-initio* density-functional approach with those obtained starting from the traditional Fröhlich Hamiltonian approach. [1] M. Cardona and Kremer, Thin Solid Films 571, 680 (2014). [2] S. Poncé *et al.*, The Journal of Chemical Physics 143, 102813 (2015) [3] C. Verdi and F. Giustino, Phys. Rev. Lett. 115, 176401 (2015)

<sup>1</sup>Supported in part by DOE grant No. DE-FG02-08ER46550.

**2:54PM C22.00003 Anti-ferromagnetism enables electron-phonon coupling in iron-based superconductors**, SINISA COH, MARVIN L. COHEN, STEVEN G. LOUIE, UC Berkeley and Lawrence Berkeley National Laboratory — We show that a generic form of an anti-ferromagnetic wavefunction opens strong electron-phonon coupling channels in the iron-based superconductors. In the non-magnetic state these channels exist locally on a single iron atom, but are cancelled out between two iron atoms in the primitive unit cell. Our findings are mostly based on symmetry and are relevant for any iron-based superconductor. This work was supported by NSF Grant No. DMR15-1508412 and the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by the DOE at Lawrence Berkeley National Laboratory's NERSC facility.

**3:06PM C22.00004 Acoustic Faraday rotation in Weyl semimetals**, DONGHAO LIU, JUNREN SHI, Peking Univ — We investigate the phonon problems in Weyl semimetals, from which both the phonon Berry curvature and the phonon Damping could be obtained. We show that even without a magnetic field, the degenerate transverse acoustic modes could also be split due to the adiabatic curvature. In three dimensional case, acoustic Faraday rotation shows up. And furthermore, since the attenuation procedure could distinguish the polarized mode, single circularly polarized acoustic wave could be realized. We study the mechanism in the novel time reversal symmetry broken Weyl semimetal. New effects rise because of the linear dispersion, which give enlightenment in the measurement of this new kind of three-dimensional material.

**3:18PM C22.00005 Strong enhancement of s-wave superconductivity near a quantum critical point of  $(\text{Ca}_{1-x}\text{Sr}_x)_3\text{Ir}_4\text{Sn}_{13}$  and  $(\text{Ca}_{1-x}\text{Sr}_x)_3\text{Rh}_4\text{Sn}_{13}$ <sup>1</sup>**, ELVEZIO MORENZONI, PABITRA BISWAS, ZURAB GUGUCHIA, RUSTEM KHASANOV, MANUEL CHINOTTI, JONAS KRIEGER, Paul Scherrer Institut, L LI, KEFENG WANG, CEDOMIR PETROVIC, Brookhaven National Laboratory, EKATERINA POMJAKUSHINA, Paul Scherrer Institut — We report microscopic studies by muon spin rotation as a function of pressure of the  $(\text{Ca}_{1-x}\text{Sr}_x)_3\text{Ir}_4\text{Sn}_{13}$  and  $(\text{Ca}_{1-x}\text{Sr}_x)_3\text{Rh}_4\text{Sn}_{13}$  cubic compounds, which display superconductivity and a structural phase transition associated with the formation of a charge density wave (CDW)[1]. In  $\text{Ca}_3\text{Ir}_4\text{Sn}_{13}$  we find a strong enhancement of the superfluid density and a dramatic increase of the pairing strength above a pressure of  $\approx 1.6$  GPa giving direct evidence of the presence of a quantum critical point separating a superconducting phase coexisting with CDW from a pure superconducting phase [2]. The superconducting order parameter in both phases has the same s-wave symmetry. Similar behavior is found in the other family. In spite of the conventional phonon-mediated BCS character of these weakly correlated 3-4-13 systems, the dependence of the effective superfluid density on the critical temperature put these compounds in the “Uemura” plot close to unconventional superconductors. These systems exemplify that conventional BCS superconductors can also display characteristics of unconventional superconductors. [1] S.K. Goh et al. Phys. Rev. Lett. 114, 097002 (2015). [2] P.K. Biswas et al., Phys. Rev. B (2015).

<sup>1</sup>Supported by the Swiss National Science Foundation and by the U.S. DOE under Contract No. DE-SC00112704

**3:30PM C22.00006 Ambient Pressure Structural Quantum Critical Point in the Phase Diagram of  $(\text{Ca}_x\text{Sr}_{1-x})_3\text{Rh}_4\text{Sn}_{13}$** <sup>1</sup>, SWEE K. GOH, Department of Physics, The Chinese University of Hong Kong, D. A. TOMPSETT, Imperial College London, P. J. SAINES, University of Oxford, H. C. CHANG, University of Cambridge, T. MATSUMOTO, M. IMAI, K. YOSHIMURA, Kyoto University, F. M. GROSCHE, University of Cambridge — The quasiskutterudite superconductor  $\text{Sr}_3\text{Rh}_4\text{Sn}_{13}$  features a pronounced anomaly in electrical resistivity at  $T^* \sim 138$  K. The anomaly is caused by a second-order structural transition, which can be tuned to 0 K by applying physical pressure and chemical pressure via the substitution of Ca for Sr. A broad superconducting dome is centered around the structural quantum critical point. Detailed analysis of the tuning parameter dependence of  $T^*$  as well as insights from lattice dynamics calculations strongly support the existence of a structural quantum critical point at ambient pressure when the fraction of Ca is 0.9 ( $x_c=0.9$ ). This establishes the  $(\text{Ca}_x\text{Sr}_{1-x})_3\text{Rh}_4\text{Sn}_{13}$  series as an important system for exploring the physics of structural quantum criticality and its interplay with the superconductivity, without the need of applying high pressures. Refs: Swee K. Goh *et al.*, Phys. Rev. Lett. 114, 097002 (2015); Wing Chi Yu *et al.*, Phys. Rev. Lett. (in press, 2015)

<sup>1</sup>This work was supported by CUHK (Startup Grant, Direct Grant No. 4053071), UGC Hong Kong (ECS/24300214), Trinity College (Cambridge), Grants-in-Aid from MEXT (No. 22350029 and 23550152) and Glasstone Bequest (Oxford).

**3:42PM C22.00007 Pressure-enhanced superconductivity in A15-type Nb<sub>3</sub>Ge via increased Fermi surface nesting**<sup>1</sup>, RYAN STILLWELL, JASON JEFFRIES, SCOTT MCCALL, ZSOLT JENEI, SAM WEIR, Lawrence Livermore Natl Lab, YOGESH VOHRA, University of Alabama at Birmingham — The A15-type superconductors are the most widely used superconductors in industrial applications yet the physics behind maximizing the superconducting transition temperature is still not completely understood. The highest transition temperatures found to date have recently been reported for high-pressure hydride materials and it is believed that they too are BCS-type phonon-mediated superconductors, just like the A15-type superconductors. Understanding the electron-phonon coupling has therefore been brought front stage in the search to understand the mechanisms for optimizing high-temperature superconductors. Using a multi-faceted suite of high-pressure techniques we found that Nb<sub>3</sub>Ge has an isostructural phase transition at high pressure that correlates directly with a bandstructure change seen in high-pressure magnetotransport measurements. Our results suggest that A15-type superconductivity is not only phonon-mediated but that the degree of Fermi surface nesting is a controlling parameter for maximizing the superconducting transition temperature.

<sup>1</sup>Lawrence Livermore National Laboratory is operated by Lawrence Livermore National Security, LLC, for the U.S. Department of Energy, National Nuclear Security Administration under contract DE-AC52-07NA27344

**3:54PM C22.00008 Strong Coupling Superconductivity in the Vicinity of the Structural Quantum Critical Point in  $(\text{Ca}_x\text{Sr}_{1-x})_3\text{Rh}_4\text{Sn}_{13}$** <sup>1</sup>, WING CHI YU, YIU WING CHEUNG, Department of Physics, The Chinese University of Hong Kong, PAUL J. SAINES, Department of Chemistry, University of Oxford, MASAKI IMAI, TAKUYA MATSUMOTO, CHISHIRO MICHIOKA, KAZUYOSHI YOSHIMURA, Department of Chemistry, Kyoto University, SWEE K. GOH, Department of Physics, The Chinese University of Hong Kong — The family of the superconducting quasiskutterudites  $(\text{Ca}_x\text{Sr}_{1-x})_3\text{Rh}_4\text{Sn}_{13}$  features a structural quantum critical point at  $x_c = 0.9$ , around which a dome-shaped variation of the superconducting transition temperature  $T_c$  is found. In this talk, we present the specific heat data for the normal and the superconducting states of the entire series straddling the quantum critical point. Our analysis indicates a significant lowering of the effective Debye temperature on approaching  $x_c$ , which we interpret as a result of phonon softening accompanying the structural instability. Furthermore, a remarkably large enhancement of  $2\Delta/k_B T_c$  and  $\Delta C/\gamma T_c$  beyond the Bardeen-Cooper-Schrieffer values is found in the vicinity of the structural quantum critical point. Reference: Wing Chi Yu *et al.* Phys. Rev. Lett. (in press, 2015)

<sup>1</sup>This work was supported by the CUHK (Startup Grant, Direct Grant No. 4053071), UGC Hong Kong (ECS/24300214), Grants-in-Aid from MEXT (22350029 and 23550152), and Glasstone Bequest, Oxford

**4:06PM C22.00009 Investigation of the superconducting and normal state properties of the filled-skutterudite system  $\text{PrPt}_4\text{Ge}_{12}$  via chemical substitution.**<sup>1</sup>, INHO JEON, KEVIN HUANG, DUYGU YAZICI, NORAVEE KANCHANAVATEE, BENJAMIN D. WHITE, SOOYOUNG JANG, NAVEEN POUSE, M. BRIAN MAPLE, University of California, San Diego, PEI-CHUN HO, California State University Fresno — We report a systematic chemical substitution study on the unconventional superconductor system  $\text{PrPt}_4\text{Ge}_{12}$ , which Sb ions are substituted for Ge. Polycrystalline samples of  $\text{PrPt}_4\text{Ge}_{12-x}\text{Sb}_x$  up to  $x = 5$  were synthesized and investigated by means of x-ray diffraction, electrical resistivity, magnetic susceptibility, and specific heat measurements. We observed a suppression of superconductivity with increasing Sb substitutions and evidence for a weak “rattling” mode associated with the Pr ions, characterized by a value of  $\Theta_E \sim 60$  K. As part of a systematic study of the effect of various elemental substitutions on the properties of  $\text{PrPt}_4\text{Ge}_{12}$ , measurements of the superconducting and normal state properties of the  $\text{Pr}_{1-x}\text{Eu}_x\text{Pt}_4\text{Ge}_{12}$  system are currently being performed. This work was supported by the U. S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Grant No. DE-FG02-04-ER46105 (characterization and physical properties measurements), and the National Science Foundation under Grant No. DMR 1206553 (low-temperature measurements).

**4:18PM C22.00010 First principles study of the electron-phonon coupling on the light-actinides Ac-Th alloy: effect of spin-orbit coupling**<sup>1</sup>, OMAR DE LA PEÑA SEAMAN, ROMEO DE COSS-MARTINEZ, PAOLA GONZALEZ-CASTELAZO, Institute of Physics (IFUAP), Benemerita Universidad Autonoma de Puebla (BUAP), ROLF HEID, KLAUS-PETER BOHNEN, Institute of Solid State Physics (IFP), Karlsruher Institute of Technology (KIT) — We have studied the electronic, lattice dynamics, and electron-phonon (e-ph) properties of the  $\text{Ac}_{1-x}\text{Th}_x$  actinide alloy. This system have been studied within the framework of density functional perturbation theory, using a mixed-basis pseudopotential method and the virtual crystal approximation (VCA) for modeling the alloy. The electronic density of states (DOS), the full-phonon dispersion as well as the Eliashberg spectral function ( $\alpha^2 F(\omega)$ ) and the electron-phonon coupling ( $\lambda$ ) parameter have been calculated with and without the inclusion of spin-orbit coupling (SOC). For Ac the observed effects of SOC on  $\alpha^2 F(\omega)$  are very minor. However, as Th-content increases on the alloy the SOC influence is more important. Such evolution has its roots on a continuous increase of density of states at the Fermi level ( $N(E_F)$ ) difference between schemes, as well as a steady hardening of the SOC full phonon dispersion. The evolution of  $\lambda$  as a function of Th-content for both schemes is presented and discussed on the light of SOC effects on the electronic and vibrational properties.

<sup>1</sup>This research was supported by Conacyt-México under project No. 221807

**4:30PM C22.00011 Truncated phase-space approach to polaron response**<sup>1</sup>, DRIES SELS, Boston Univ — A method is presented to obtain the linear response coefficients of a system coupled to a bath. The method is based on a systematic truncation of the Liouville equation for the reduced distribution function in the Weyl representation. Explicit expressions for the conductivity of the Frhlich polaron are obtained, and the discrepancy between the Kadanoff and the Feynman-Hellwarth-Iddings-Platzman mobility is elucidated. We argue why both approaches require a correction. Finally, we show how due to the system-bath coupling, the external perturbation induces a retarded internal field which dynamically screens the external force. Whereas the effect on the dc-mobility is of second order, dynamical properties such as the effective mass and the optical absorption are modified in first order.

**4:42PM C22.00012 First-Principles Calculation of forces and phonons in solid**, ZHENHUA NING, WILLIAM SHELTON, Louisiana State University — We have developed a multiple scattering theory approach to calculate Hellmann-Feynman forces and phonons via the calculation of the force constant and dynamical matrix. To demonstrate the accuracy and validity of our approach we compare with the ELK code, which is a full potential Linear Augmented Plane Wave (FLAPW) based method. As we will show our forces and phonon dispersion curves are in good agreement with the FLAPW code. This work lays the foundation for developing a first principles approach for calculation of phonons in substitutionally disordered materials.

**4:54PM C22.00013 Phonon and magnon dispersions of incommensurate spin ladder compound  $\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$** <sup>1</sup>, XI CHEN, Univ of Texas, Austin, DIPANSHU BANSAL, Oak Ridge National Lab, SEAN SULLIVAN, JIANSHI ZHOU, Univ of Texas, Austin, OLIVIER DELAIRE, Oak Ridge National Lab, LI SHI, Univ of Texas, Austin — There are a variety of compounds consisting of two or more interpenetrating sublattices with lattice periods incommensurate at least along one crystal axis. One example is spin ladder compound  $\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$  consisting of incommensurate spin ladder and spin chain sublattices. It has been predicted that unique phonon modes occur in these compounds due to the relative motion of the sublattices. In the low-wavelength limit, there is only one longitudinal acoustic mode due to the rigid translation of both sublattices. In addition, one extra pseudo-acoustic mode is present due to relative sliding motions of the two sublattices. Although the theoretical aspects of the lattice dynamics of incommensurate compounds have been studied, there have been few experimental investigations on their phonon dynamics. In this work, single crystals of  $\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$  are grown by the traveling solvent floating zone method. The phonon dispersion of  $\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$  is studied through inelastic neutron scattering measurements in order to better understand its phonon dynamics. In addition, its magnon dispersion is investigated and correlated to the large directional magnon thermal conductivity. The measurements reveal a wealth of intriguing features on phonons and magnons in the spin ladder compound.

<sup>1</sup>This work is supported by ARO MURI program under Award W911NF-14-1-0016.

**5:06PM C22.00014 High Temperature Superconductivity at High Pressures for  $\text{H}_3\text{SixP}(1-x)$ ,  $\text{H}_3\text{PxS}(1-x)$  and  $\text{H}_3\text{ClxS}(1-x)$** <sup>1</sup>, DIMITRIOS PAPACONSTANTOPOULOS, FUDONG FAN, George Mason Univ, MICHAEL MEHL, Naval Research Lab — Recent experimental and computational works have established the occurrence of superconducting temperatures,  $T_c$ , around 200K at corresponding 200GPa pressures in hydrogen-based sulfur compounds. In this work we have investigated the effects of phosphorus and chlorine substitutions of sulfur on  $T_c$ , as well as the effect of hydrogen vacancies. In addition, we have explored the superconductivity-relevant parameters in the  $\text{H}_3\text{SixP}(1-x)$  system. In executing this work we have used the virtual-crystal-approximation and performed a systematic set of LAPW calculations for many different concentrations of the sulfur component. From the densities of states and the scattering phase-shifts at the Fermi level, we calculated electron-ion matrix elements and estimated the electron-phonon coupling constants for different concentrations as well as  $T_c$ . We find that the high values of  $T_c$  correlate with the position of the Fermi level with respect to peaks (van Hove singularities) in the density of electronic states of these materials.

<sup>1</sup>US Department of Energy

**5:18PM C22.00015 Effect of van Hove singularities on high- $T_c$  superconductivity in H3S**, WATARU SANO, Department of applied physics, University of Tokyo, TAKASHI KORETSUNE, RIKEN Center of Emergent Matter Science, TERUMASA TADANO, Department of applied physics, University of Tokyo, RYOSUKE AKASHI, Department of physics, University of Tokyo, RYOTARO ARITA, RIKEN Center of Emergent Matter Science — One of interesting open questions for the high- $T_c$  superconductivity in sulfur hydrides is why some of the H3S phases under high pressures are so special. Recently, it has been pointed out that the presence of the van Hove singularities (vHs) around the Fermi level is crucial. Interestingly, such vHs are always absent in H2S, for which  $T_c$  is estimated to be much lower. Although there have been quantitative calculations of  $T_c$  based on the Migdal-Eliashberg theory, the effect of the vHs on the superconductivity is yet to be fully understood. This is because the energy dependence of the density of states (DOS) has been neglected to simplify the Eliashberg equation. In this study, we perform a calculation beyond the constant DOS approximation. In contrast with the conventional calculations, this approach with a sufficiently large number of Matsubara frequencies enables us to calculate  $T_c$  self-consistently without introducing the empirical pseudo Coulomb potential. We show that the constant DOS approximation seriously overestimates (underestimates)  $T_c$  by ~60 K (~10 K) for H3S (H2S). We then consider the effect of the anharmonicity of the phonon and the energy shift due to the zero-point motion. Eventually,  $T_c$  is estimated to be 180 K for H3S and 35 K for H2S, which successfully explains the pressure dependence of  $T_c$  observed in the experiment.

## Monday, March 14, 2016 2:30PM - 5:42PM –

Session C23 DMP: Acoustic, Thermal, and Photonic Metamaterial Concepts 322 - Matthew Sheldon, Texas AM University

**2:30PM C23.00001 Photonic hypercrystals**, EVGENII NARIMANOV, Purdue University — We introduce a new universality class of artificial optical media - the photonic hypercrystals. These hyperbolic metamaterials with a periodic spatial variation of dielectric permittivity on a subwavelength scale, combine the features of optical metamaterials and photonics crystals within the same medium.

**3:06PM C23.00002 A Metasurface Anti-reflection Coating for Enhancing Surface Plasmon-Polariton of Metallic Hole Array.**, KHAGENDRA BHATTARAI, Department of Physics, University of South Florida, Tampa, FL 33620, USA, JIYEON JEON, JUN KIM, Korea Research Institute of Standards and Science, Daejeon, 305-340, Korea, ZAHYUN KU, Air Force Research Laboratory, Dayton, OH 45433, USA, SANG JUN LEE, Korea Research Institute of Standards and Science, Daejeon, 305-340, Korea, JIANGFENG ZHOU, Department of Physics, University of South Florida, Tampa, FL 33620, USA, USA COLLABORATION, KRISS, KOREA COLLABORATION, AFRL, USA COLLABORATION — We demonstrate a metasurface made of metallic disk resonator array as an anti-reflection (AR) coating to enhance (reduce) the transmission (reflection) through metal hole array (MHA). Our result show that the simulated (measured) transmission at the first order surface plasmon-polariton (SPP) resonance is increased up to 82 % ( 88%) compared to uncoated MHA. The electric field of the surface wave is also enhanced by 33%. Using an effective medium theory, we show that the metasurface operates at off-resonance wavelengths and can be understood as a thin film that exhibits high effective permittivity (~30) with very low loss (loss tangent ~0.005). Thus we reveal the mechanism of the metasurface AR coating as the traditional thin film AR coating. With tunable effective permittivity, our structure provides great flexibility to achieve AR coating for general substance at any wavelength.

**3:18PM C23.00003 Hybrid graphene/dielectric metasurfaces for enhanced transmission modulation**, CHRISTOS ARGYROPOULOS, University of Nebraska-Lincoln — All-dielectric silicon based metasurfaces are powerful platforms to enhance light-matter interactions at nanoscale regions. Their low-loss nature, CMOS processing compatibility and increased damage threshold promise to outperform the functionalities of the recently established plasmonic metallic metasurfaces. In our talk, we will demonstrate ways to hybridize all-dielectric metasurfaces with graphene in order to obtain new electro-optical devices. In particular, a hybrid graphene/dielectric metasurface design will be presented to achieve tunable and modulated transmission at near-infrared (near-IR) frequencies (C. Argyropoulos, *Optics Express*, vol. 23, No. 18, pp. 23787-23797, 2015). The proposed all-dielectric metasurface is composed of periodically arranged pairs of asymmetric silicon nanobars, which can sustain trapped magnetic resonances with a sharp Fano-type transmission signature. One-atom-thick graphene is placed over this dielectric metasurface and strong transmission modulation is obtained at near-IR telecom wavelengths as the doping level of graphene is increased. The enhanced in-plane fields along the all-dielectric metasurface strongly interact with the tunable properties of graphene. This leads to strong coupling between the incoming radiation and graphene. Several new integrated nanophotonic components are envisioned based on the proposed device, such as efficient electro-optical transmission modulators.

**3:30PM C23.00004 Nonlinear light-matter interactions in engineered optical media<sup>1</sup>**, NATALIA LITCHINITSER, University at Buffalo, The State University of New York — In this talk, we consider fundamental optical phenomena at the interface of nonlinear and singular optics in artificial media, including theoretical and experimental studies of linear and nonlinear light-matter interactions of vector and singular optical beams in metamaterials. We show that unique optical properties of metamaterials open unlimited prospects to “engineer” light itself. Thanks to their ability to manipulate both electric and magnetic field components, metamaterials open new degrees of freedom for tailoring complex polarization states and orbital angular momentum (OAM) of light. We will discuss several approaches to structured light manipulation on the nanoscale using metal-dielectric, all-dielectric and hyperbolic metamaterials. These new functionalities, including polarization and OAM conversion, beam magnification and de-magnification, and sub-wavelength imaging using novel non-resonant hyperlens are likely to enable a new generation of on-chip or all-fiber structured light applications. The emergence of metamaterials also has a strong potential to enable a plethora of novel nonlinear light-matter interactions and even new nonlinear materials. In particular, nonlinear focusing and defocusing effects are of paramount importance for manipulation of the minimum focusing spot size of structured light beams necessary for nanoscale trapping, manipulation, and fundamental spectroscopic studies. Colloidal suspensions offer as a promising platform for engineering polarizabilities and realization of large and tunable nonlinearities. We will present our recent studies of the phenomenon of spatial modulational instability leading to laser beam filamentation in an engineered soft-matter nonlinear medium. Finally, we introduce so-called virtual hyperbolic metamaterials formed by an array of plasma channels in air as a result of self-focusing of an intense laser pulse, and show that such structure can be used to manipulate microwave beams in a free space.

<sup>1</sup>This work was supported by the Army Research Office Awards (W911NF-15-1-0146, W911NF-11-1-0297).

**4:06PM C23.00005 Broadband non-unity magnetic permeability in planar hyperbolic metamaterials**, GEORGIA THEANO PAPADAKIS, DAGNY FLEISCHMAN, ARTUR R. DAVOYAN, KRISHNAN THYAGARAJAN, HARRY A. ATWATER, Caltech — Metal/dielectric heterostructures with extreme anisotropy and topologically nontrivial dispersion are of fundamental and applied interest due to unique optical and opto-electronic properties. Here we demonstrate that, surprisingly, such systems exhibit a broadband non-unity magnetic response. Typically the electromagnetic properties of such metal-dielectric stacks are deduced from effective medium theories for unbounded, i.e., infinite in size periodic arrangements (c.f., Maxwell-Garnett approximation). In this talk, we show that this description is incomplete for metamaterials with finite number of layers. We demonstrate that a few-layer metal-dielectric metamaterial exhibits a non-unity magnetic permeability across the whole visible spectrum. The response can be diamagnetic or paramagnetic depending on the type of the terminating layers: metallic or dielectric, with non-resonant magnetic permeability that can be engineered to attain values as low as -2 or as high as 2. We have developed a theoretical model that explains the underlying mechanism. We further experimentally validate non-unity effective permeability in the optical range of frequencies. Ag/SiO<sub>2</sub> and Ge-based metamaterials fabricated with electron beam evaporation are characterized by ellipsometric measurements and also phase and amplitude of transmittance/reflectance. These results open pathways for creating broadband subwavelength magnetic structures in the visible regime.

**4:18PM C23.00006 Microscopic model of the nonlocal response of metamaterial plasmonic structures**, JIANTAO KONG, KRZYSZTOF KEMPA, Boston College — Nonlocal effects are generally omitted in typical approaches to calculating the electromagnetic response of the metamaterial plasmonic structures. In some situations, however, where the electron momenta far exceed those of photons, nonlocal corrections are essential. In this work, we investigate simple models of the nonlocal dielectric functions, based on the d-function formalism of Feibelman [1,2], and assess their validity by comparing with experiments. We show, that the applicability of the commonly used hydrodynamic approximation is very limited, since it often strongly overestimates the nonlocal response. [1] Feibelman, *Prog. Surf. Sci.* 12, 287 (1982); *Phys. Rev. B* 40, 2752 (1989) [2] Liebsch, *Phys. Rev. B* 48, 15 (1993)

**4:30PM C23.00007 Semiconductor Hyperbolic Metamaterials for the Mid-Infrared**, DONGXIA WEI, University of Delaware, CHRISTIAN HARRIS, Lincoln University, CORY BOMBERGER, JING ZHANG, JOSHUA ZIDE, STEPHANIE LAW, University of Delaware — Hyperbolic metamaterials have shown great promise for controlling light in the visible spectral range. However, moving metamaterials to the infrared is not just a matter of scaling geometries, but also of choosing new materials with appropriate optical properties. We demonstrate infrared hyperbolic metamaterials with optical properties tunable across the mid-infrared created from semiconductor superlattices grown by molecular beam epitaxy. The metamaterials are made of alternating subwavelength layers of metal (doped semiconductor) and dielectric (undoped semiconductor). By tuning the doping density, layer thicknesses, and metal:dielectric thickness ratio, we can control the onset and bandwidth of metamaterial behavior across the infrared. Our materials exhibit low optical losses as well as high sample uniformity and sharp interfaces. Transmission and reflection properties of the samples are studied by Fourier transform infrared spectroscopy and modeled with effective medium theory. We will also show the results from a beam optics experiment which demonstrates that our materials exhibit negative refraction.

**4:42PM C23.00008 Semiconductor-based mid-IR metamaterials: experimental and theoretical studies**, ANDREY SEMICHAEVSKY, CHRISTIAN HARRIS, Lincoln University (PA), DONGXIA WEI, STEPHANIE LAW, University of Delaware — All-semiconductor (III-V) metamaterials (MTM) for the infrared (IR) can be applied to superlensing and optical cloaking [1]. 1-D metallic-semiconductor superlattices can be designed to have hyperbolic dispersion due to the choice of their effective permittivity tensor components. In this paper we go beyond the effective-medium theories and provide a detailed analysis of how the choice of doping levels and layer thicknesses in the InAs - InAs:Si will affect the reflectance of the MTM superlattice in the IR. In order to do that, four metamaterial samples with various doping profiles were grown by MBE and characterized using FTIR. For the same samples we performed full-wave calculations of the wavelength- and angle-resolved reflectance. Our numerical model is suitable for 1-D inhomogeneous lossy dispersive media and is capable of accounting for an arbitrary doping profile and the quantum mechanical tunneling of electrons in the heterostructure. Experimental and theoretical results for the reflectance of IR metamaterial structures are compared. [1] S. Law, C. Roberts, T. Kilpatrick, L. Yu, T. Ribaud, E. A. Shaner, V. Podolskiy, and D. Wasserman, *Phys. Rev. Letters*, **112**, 017401, 2014.

**4:54PM C23.00009 Broadband enhanced transmission of acoustic waves through serrated metal gratings**, DONG-XIANG QI, REN-HAO FAN, YU-QIANG DENG, RU-WEN PENG, MU WANG, Nanjing Univ, JIANGNAN UNIVERSITY COLLABORATION — In this talk, we present our studies on broadband properties of acoustic waves through metal gratings. We have demonstrated that serrated metal gratings, which introduce gradient coatings, can give rise to broadband transmission enhancement of acoustic waves. Here, we have experimentally and theoretically studied the acoustic transmission properties of metal gratings with or without serrated boundaries. The average transmission is obviously enhanced for serrated metal gratings within a wide frequency range, while the Fabry-Perot resonance is significantly suppressed. An effective medium hypothesis with varying acoustic impedance is proposed to analyze the mechanism, which was verified through comparison with finite-element simulation. The serrated boundary supplies gradient mass distribution and gradient normal acoustic impedance, which could efficiently reduce the boundary reflection. Further, by increasing the region of the serrated boundary, we present a broadband high-transmission grating for wide range of incident angle. Our results may have potential applications to broadband acoustic imaging, acoustic sensing and new acoustic devices. References: [1] Dong-Xiang Qi, Yu-Qiang Deng, Di-Hu Xu, Ren-Hao Fan, Ru-Wen Peng, Ze-Guo Chen, Ming-Hui Lu, X. R. Huang and Mu Wang, Appl. Phys. Lett. 106, 011906 (2015); [2] Dong-Xiang Qi, Ren-Hao Fan, Ru-Wen Peng, Xian-Rong Huang, Ming-Hui Lu, Xu Ni, Qing Hu, and Mu Wang, Applied Physics Letters 101, 061912 (2012).

**5:06PM C23.00010 Manipulate acoustic waves by impedance matched acoustic metasurfaces<sup>1</sup>**, YING WU, King Abdullah Univ of Sci & Tech (KAUST), JUN MEI, South China University of Technology, RASHA ALJAHDALI, King Abdullah Univ of Sci & Tech (KAUST) — We design a type of acoustic metasurface, which is composed of carefully designed slits in a rigid thin plate. The effective refractive indices of different slits are different but the impedances are kept the same as that of the host medium. Numerical simulations show that such a metasurface can redirect or reflect a normally incident wave at different frequencies, even though it is impedance matched to the host medium. We show that the underlying mechanisms can be understood by using the generalized Snell's law, and a unified analytic model based on mode-coupling theory. We demonstrate some simple realization of such acoustic metasurface with real materials. The principle is also extended to the design of planar acoustic lens which can focus acoustic waves.

<sup>1</sup>Manipulate acoustic waves by impedance matched acoustic metasurfaces

**5:18PM C23.00011 Simulation and Experimental Realization of a Nano-scale Thermal Cloak.**, XUE BAI, NUS Graduate School for Integrative Sciences and Engineering, National University of Singapore, Kent Ridge 119620, Republic of Singapore., XIANGFAN XU, Center for Phononics and Thermal Energy Science, School of Physical Science and Engineering, Tongji University, 200092, Shanghai, China., BAOWEN LI, Department of Mechanical Engineering, University of Colorado, Boulder, Colorado 80309, USA, XUDONG CHEN, JOHN T. L. THONG, Department of Electrical and Computer Engineering, National University of Singapore, 4 Engineering Drive 3, Republic of Singapore — Manipulation of heat flow at microstructures plays an important role in modern industry, especially for electronic and optoelectronic devices, for their performance and reliability are highly temperature dependent. Analogous to the invisible cloak in transformation optics, the thermal cloak can hide objects from heat and realize isothermal region in transformation thermodynamics. However, due to the macro-scale thermal properties may not be suitable for nano-materials, the realization of the nano-scale thermal cloak highly relies on the thermal transport in nanostructures. Here, we report our recent work of the realization of nano-scale thermal cloak based on the thermal property study of nano-materials via a spatially resolved thermal resistance measurement technique. The simulation and experiment verified its maintenance of isothermal region and heat protection capabilities. This work may provide a new way to manipulate heat transport in nano-scale devices..

**5:30PM C23.00012 Microscopic Model of the Nonlocal Response of Metamaterial Plasmonic Structures II**, ALEXANDER SHVONSKI, KRZYSZTOF KEMPA, Boston College — Nonlocal effects are generally omitted in typical approaches to calculating the electromagnetic response of metamaterial plasmonic structures. In some situations, however, where the electron momenta far exceed those of photons, nonlocal corrections are essential. In this work, we calculate the nonlocal plasmonic response of a microscopic model of a metamaterial plasmonic structure by employing the random phase approximation, and the self-consistent ground Lang-Kohn states. We compare our results with experiment, and various simple models, including the hydrodynamic approximation.

**Monday, March 14, 2016 2:30PM - 5:30PM –**

**Session C24 DMP: Time-resolved Energy Transfer and Exciton Transport in Nanostructures**  
323 - Maxim Sukharev, Arizona State University

**2:30PM C24.00001 Ultrafast Single and Multiexciton Energy Transfer in Semiconductor Nanoplatelets<sup>1</sup>**, RICHARD SCHALLER, Argonne National Laboratory & Northwestern University — Photophysical processes such as fluorescence resonance energy transfer (FRET) enable optical antennas, wavelength down-conversion in light-emitting diodes (LEDs), and optical bio-sensing schemes. The rate and efficiency of this donor to acceptor transfer of excitation between chromophores dictates the utility of FRET and can unlock new device operation motifs including quantum-funnel solar cells and reduced gain thresholds. However, the fastest reported FRET time constants involving spherical quantum dots (QDs) (0.12-1 ns), do not outpace biexciton Auger recombination (0.01-0.1 ns), which impedes multiexciton-driven applications including electrically-pumped lasers and carrier-multiplication-enhanced photovoltaics. Precisely controlled, few-monolayer thick semiconductor nano-platelets with tens-of-nanometer diameters exhibit intense optical transitions and hundreds-of-picosecond Auger recombination, but heretofore lack FRET characterizations. We examine binary CdSe NPL solids and show that inter-plate FRET (~6-23 ps, presumably for co-facial arrangements) can occur 15-50 times faster than Auger recombination and demonstrate multiexcitonic FRET, making such materials ideal candidates for advanced technologies.

<sup>1</sup>This work was performed at the Center for Nanoscale Materials, a U.S. Department of Energy Office of Science User Facility under Contract No. DE-AC02-06CH11357.

**3:06PM C24.00002 Spontaneous emission enhancement of colloidal CdSe nanoplatelets.**, ZHILI YANG, University of Maryland, College Park, MATTHEW PELTON, University of Maryland, Baltimore, EDO WAKS, University of Maryland, College Park — Colloidal CdS /CdSe/CdS nanoplatelets synthesized recently are high efficient nano-emitters and gain media for nanoscale lasers and other nonlinear optical devices. They are characterized as quantum well structure due to energy gap difference between core CdSe and shell CdS, of which the luminescent wavelength could be tuned precisely by their thickness of growth. However, the influence of environment on the material's optical properties and further enhancement of the emission to implement nanoscale systems remains to be investigated. Here we demonstrate spontaneous emission rate enhancement of these CdSe nanoplatelets coupled to a photonic crystal cavity. We show clearly the photoluminescent spectrum modification of the nanoplatelets emission and an averaged Purcell enhancement factor of 3.1 is achieved when they are coupled to carefully-designed nanobeam photonic crystal cavities compared to the ones on unpatterned surface in our experiment of lifetime measurement. Also the phenomenon of cavity quality factor increasing is observed when increasing intensity of pumping, which attributes to saturable absorption of the nanoplatelets. Our success in enhancement of emission from these nanoplatelets here paves the road to realize actual nanoscale integrated systems such as ultra-low threshold micro-cavity lasers.

### 3:18PM C24.00003 Interfacial charge separation and trapping in composite photocatalysts<sup>1</sup>

DINKO CHAKAROV, Chalmers Univ of Tech — We explore the phenomena of interfacial charge separation and trapping in composite metal-semiconductor systems and the interaction (energy and charge exchange) between optically excited nanoparticles and the surrounding medium. Disc-shaped copper nanoparticles (Cu NPs) were fabricated by hole-mask colloidal lithography on bare and thin titania film covered fused silica substrates. The dynamics of Cu oxide formation around the NPs were studied in water by localized surface plasmon resonance (LSPR) spectroscopy. We found that the oxidation rate is strongly enhanced under UV irradiation when the NPs are on the surface of the titania film, in comparison to NPs deposited on an inert fused silica substrate. The reason is sought in the ability of TiO<sub>2</sub> to create hydroxyl radicals with strong oxidative potential in water under UV irradiation and the charge transfer at the interface between the Cu NPs and the TiO<sub>2</sub>. The results demonstrate the potential of using LSPR spectroscopy to monitor the oxidation of Cu NPs in situ and in different environments.

<sup>1</sup>The work was financially supported by The Nordic Energy Research Council through project N-I-S-F-D.

### 3:30PM C24.00004 Fluorescence of semiconductor nanocrystals coupled to optical Tamm

**cavities**<sup>1</sup>, FU FENG, Institut Des Nanosciences de Paris, PASCALE SENELLART TEAM<sup>2</sup>, BENOIT DUBERTRET TEAM<sup>3</sup>, AGNES MAITRE TEAM<sup>4</sup> — We describe here the photoluminescence properties of a layer of colloidal CdSe/CdS fluorescent nanocrystals embedded in such a Tamm cavity. Spectral and angular analysis of fluorescence shows that the nanocrystals emission is into the Tamm states; the emission dispersion relation for disks of various diameters shows the effect of the Tamm states lateral confinement. We also combined spatial and angular emission analysis and showed that the direction of emission is not the same for different points on a disk: emission from the left (resp. right) portion of the cavity is directed mostly in the left (resp. right) direction, in agreement with our numerical simulations. Our measurement scheme constitutes a probe of the Tamm state electric field phase gradient inside the cavity.

<sup>1</sup>Spatial and K space resolved spectroscopy

<sup>2</sup>Team of Pascale Senellart at Laboratoire de Photonique et de Nanostructures(LPN)

<sup>3</sup>Team of Benoit Dubertret at Laboratoire de Physique et d'Etude des Matériaux(ESPCI)

<sup>4</sup>Team of Agnes Maitre at Institut Des Nanosciences de Paris

### 3:42PM C24.00005 Measuring Exciton Migration in Conjugated Polymer Films with Ultrafast Time Resolved Stimulated Emission Depletion Microscopy

, SAMUEL PENWELL, UC Berkeley — Conjugated polymers are highly tunable organic semiconductors, which can be solution processed to form thin films, making them prime candidates for organic photovoltaic devices. One of the most important parameters in a conjugated polymer solar cell is the exciton diffusion length, which depends on intermolecular couplings, and is typically on the order of 10 nm. This mean exciton migration can vary dramatically between films and within a single film due to heterogeneities in morphology on length scales of 10's to 100's nm. To study the variability of exciton diffusion and morphology within individual conjugated polymer films, we are adapting stimulated emission depletion (STED) microscopy. STED is typically used in biology with sparse well-engineered fluorescent labels or on NV-centers in diamond. I will, however, describe how we have demonstrated the extension of STED to conjugated polymer films and nanoparticles of MEH-PPV and CN-PPV, despite the presence of two photon absorption, by taking care to first understand the material's photophysical properties. We then further adapt this approach, by introducing a second ultrafast STED pulse at a variable delay. Excitons that migrate away from the initial subdiffraction excitation volume during the ps-ns time delay, are preferentially quenched by the second STED pulse, while those that remain in the initial volume survive. The resulting effect of the second STED pulse is modulated by the degree of migration over the ultrafast time delay, thus providing a new method to study exciton migration. Since this technique utilizes subdiffraction optical excitation and detection volumes with ultrafast time resolution, it provides a means of spatially and temporally resolving measurements of exciton migration on the native length and time scales. In this way, we will obtain a spatiotemporal map of exciton distributions and migration that will help to correlate the energetic landscape to film morphology at the nanoscale.

### 4:18PM C24.00006 How Microstructure Defines Function in Organic Conjugated Materials:

**Insights from Modelling**, YOANN OLIVIER, University of Mons, Laboratory for Chemistry of Novel Materials, Place du Parc 20, Mons, Belgium — Organic conjugated materials have attracted an increasing interest over the years for their use in organic opto- electronic devices such as light-emitting diodes, solar cells, or field- effect transistors as a result of their low cost, light weight and ease of processing from solution. The improvement of the device performances requires a deep understanding of the electronic processes taking place in these devices down to the molecular scale. Especially, the way organic conjugated molecules or polymer chains organize in the solid state appears as a critical parameter to control in order to fine tune the materials electronic and photophysical properties. In our laboratory, we have developed a multi-faceted modeling scheme that encompasses classical molecular dynamics, quantum-chemistry, non-adiabatic quantum dynamics and kinetic Monte Carlo simulations to assess multiple fundamental opto- electronic processes occurring in conjugated materials used in devices. Here, we will more specifically review work dealing with the modeling of charge transport in conjugated polymers as well as singlet fission and exciton transport in small molecules. In all cases, we will highlight how these processes are sensitive to the relative arrangement of the materials at the nanoscale.

### 4:54PM C24.00007 Probing surface recombination velocities in semiconductors using two-photon microscopy

, BENOIT GAURY, Maryland Nanocenter, University of Maryland, College Park. CNST, National Institute of Standards and Technology, PAUL HANEY, National Institute of Standards and Technology — We propose an analysis of the diffusion problem related to the two-photon time-resolved photoluminescence microscopy technique. We are considering a model of excess carrier diffusion in three dimensions, with recombination that is first order in carrier density (ie valid in low injection regime) and various boundary conditions that will apply to different use of the technique. First, we study a single planar boundary with enhanced recombination (parameterized with a recombination velocity). This planar boundary may represent the exposed sample surface, or any deep subsurface structure, such as a grain boundary or materials interface. Next, we assume the diffusion to be bounded by two parallel planes parameterized with different recombination velocities. This may apply to thin films where the diffusion length is higher than the sample thickness, or when the carrier generation volume axially spans the entire film. Finally, we investigate diffusion in a sphere where the spherical surface plays the role of a closed grain boundary. For all these cases we give analytical solutions for the three-dimensional diffusion problem for an excitation of arbitrary spatial or time dependence. We believe the solutions and scalings to be simple enough to enable convenient data fitting.

### 5:06PM C24.00008 Direct measurement of non-equilibrium phonon occupations in femtosecond laser heated Au films

, TYLER CHASE, MARIANO TRIGO, ALEXANDER REID, RENKAI LI, THEODORE VECCHIONE, XIAOZHE SHEN, STEPHEN WEATHERSBY, RYAN COFFEE, NICK HARTMANN, DAVID REIS, XIJIE WANG, HERMANN DÜRR, SLAC - Natl Accelerator Lab — We use ultrafast electron diffraction to detect the temporal evolution of phonon populations in femtosecond laser-excited ultrathin single-crystalline gold films. From the time-dependence of the Debye-Waller factor we extract a 4.7 ps time-constant for the increase in mean-square atomic displacements. We show from the increase of the diffuse scattering intensity that the population of phonon modes near the X and K points in the Au fcc Brillouin zone grows with timescales of 2.3 and 2.9 ps, respectively, faster than the Debye-Waller average. We find that thermalization continues within the initially non-equilibrium phonon distribution after 10 ps. The observed momentum dependent timescale of phonon populations is in contrast to what is usually predicted in a two-temperature model.

**5:18PM C24.00009 Time-resolved spectroscopy at surfaces and adsorbate dynamics: insights from a model-system approach**, EMIL BOSTRÖM, ANDERS MIKKELSEN, CLAUDIO VERDOZZI, Lund University — We introduce a finite-system, model description of the initial stages of femtosecond laser induced desorption at surfaces. Using the exact many-body time evolution and also results from a novel time-dependent DFT description for electron-nuclear systems, we analyse the competition between several surface-response mechanisms and electronic correlations in the transient and longer time dynamics under the influence of dipole-coupled fields. Our model allows us to explore how coherent multiple-pulse protocols impact desorption in a variety of prototypical experiments.

**Monday, March 14, 2016 2:30PM - 5:30PM –**  
**Session C25 DCMP: Optical Spectroscopy of Superconductors** 324 - Peter Armitage, Johns Hopkins University

**2:30PM C25.00001 Ultrafast studies of coexisting electronic order in cuprate superconductors**, JAMES HINTON, UC San Diego, ERIC THEWALT, UC Berkeley, LBNL, ZHANYBEK ALPICHSEV, MIT, AARON STERNBACH, ALEX MCLEOD, UC San Diego, L. JI, MIKE VEIT, CHELSEY DORROW, University of Minnesota, JAKE KORALEK, SLAC, LBNL, XUDONG XHAO, Jilin University, NEVEN BARISIC, CEA Saclay, ALEXANDER KEMPER, North Carolina State University, LBNL, NUH GEDIK, MIT, MARTIN GREVEN, University of Minnesota, DIMITRI BASOV, UC San Diego, JOE ORENSTEIN, UC Berkeley, LBNL — The cuprate family of high temperature superconductors displays a variety of electronic phases which emerge when charge carriers are added to the antiferromagnetic parent compound. These electronic phases are characterized by subtle differences in the low energy electronic excitations. Ultrafast time-resolved reflectivity (TRR) provides an ideal tool for investigating the cuprate phase diagram, as small changes in the electronic structure can produce significant contrast in the non-equilibrium reflectivity. Here we present TRR measurements of cuprate superconductors, focusing on the model single-layer cuprate  $\text{HgBa}_2\text{CuO}_{4+\delta}$ . We observe a cusp-like feature in the quasiparticle lifetime near the superconducting transition temperature  $T_c$ . This feature can be understood using a model of coherently-mixed charge-density wave and superconducting pairing. We propose extending this technique to the nanoscale using ultrafast scattering scanning near-field microscopy (u-SNOM). This will allow us to explore how these electronic phases coexist and compete in real-space.

**2:42PM C25.00002 Probing broken symmetry states in cuprate superconductors with polarization-sensitive infrared spectroscopy**<sup>1</sup>, ALOK MUKHERJEE, MUMTAZ MURAT ARIK, JUNGRYEOL SEO, JOHN CERNE, University at Buffalo, HAO ZHANG, KE JUN XU, JOHN Y. T. WEI, University of Toronto, N.P. ARMITAGE, Johns Hopkins University, T. KIRZHNER, G. KOREN, Technion-Israel Institute of Technology — The nature of the pseudogap state in high-temperature superconducting (HTS) cuprates has drawn a lot of attention in the past two decades. A fundamental question is whether the pseudogap is a distinct phase with its own broken symmetries. Recent optical studies in the near-IR (800 meV) [1] and THz (2-6 meV) [2] ranges have observed symmetry breaking in the pseudogap state of HTS cuprates, suggesting that the pseudogap is a distinct phase. To probe the spectral character of this broken symmetry, we have performed infrared/visible Faraday and Kerr effect measurements at zero magnetic field and various temperatures on a series of HTS cuprate thin films, grown epitaxially by pulsed laser-ablated deposition. We will present and discuss our data, primarily complex Faraday/Kerr angle as a function of energy (0.1-3 eV), temperature (10-300K) and sample orientation with respect to the incident light polarization. 1. Xia, J et.al PRL 100, 127002 (2008). 2. Lubashevsky, Y et.al PRL 112, 147001 (2014) .

<sup>1</sup>This work supported by NSF- DMR1410599, NSERC, CFI-OIT and the Canadian Institute for Advanced Research

**2:54PM C25.00003 Optical anisotropy of a cuprate high  $T_c$  superconductor**<sup>1</sup>, LIUYAN ZHAO, California Institute of Technology, CARINA BELVIN, Wellesley College, RUIXING LIANG, WALTER HARDY, DOUG BONN, University of British Columbia, PETER ARMITAGE, Johns Hopkins University, DAVID HSIEH, California Institute of Technology — Evidence for a symmetry breaking phase transition across the pseudogap temperature  $T^*$  of cuprate high- $T_c$  superconductors has been reported in several experiments. For example, resonant ultrasound spectroscopy reveals a discontinuous change in the normal mode frequencies of the lattice across  $T^*$  while spin-flip neutron scattering shows time reversal symmetry breaking across  $T^*$ . Recent THz spectroscopy measurements also suggest the loss of mirror symmetries in the vicinity of  $T^*$ . Optical anisotropy is in principle sensitive to the point group symmetries of a crystal and is highly complementary to the aforementioned techniques. I will present our progress in measuring and understanding the optical anisotropy of  $\text{YBa}_2\text{Cu}_3\text{O}_y$  in the vicinity of its pseudogap transition temperature.

<sup>1</sup>Optical anisotropy of a cuprate high  $T_c$  superconductor

**3:06PM C25.00004 Elucidating the driving force of superconductivity increase in compressed optimally doped  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$** , XIAO-JIA CHEN, Center for High Pressure Science and Technology Advanced Research, Shanghai 201203, China, VIKTOR STRUZHNIKIN, Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20015, JIAN-BO ZHANG, Center for High Pressure Science and Technology Advanced Research, Shanghai 201203, China, ALEXANDER GAVRILIUK, Institute of Crystallography, Russian Academy of Sciences, Moscow 119333, Russia, ALEXANDER GONCHAROV, HO-KWANG MAO, Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20015, HAI-QING LIN, Beijing Computational Science Research Center, Beijing 100089, China, GENDA GU, Brookhaven National Laboratory, NY 11973 — An optimally doped cuprate  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$  is as a perfect model system to explore the mechanism of superconductivity by applying pressure as one can avoid complicated competing orders in the underdoped regime and explore pure intrinsic effects rather than secondary effects related to change in the carrier concentration. Here, by carefully examining the collected high-pressure Raman spectra at low temperatures, we have observed an enhanced two-magnon mode and connected this to the observed 10 K increase in  $T_c$  (reaching more than 100 K for the first time) in the optimally doped  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$  upon compression clearly delineating the effect of pressure-induced charge transfer that must suppress  $T_c$  for this optimally doped sample. Our finely designed experiments offer the direct and convincing evidence for identifying the magnetic fluctuations as the pairing interaction in cuprate superconductors.

**3:18PM C25.00005 Time domain THz studies of thin film spinel superconductor  $\text{LiTi}_2\text{O}_4$** <sup>1</sup>, EVAN JASPER, M.T. WARREN, T.T. MAI, J. BRANGHAM, R. VALDÉS AGUILAR, Department of Physics, The Ohio State University. Columbus OH 43210, J. M. SHIN, I. TAKEUCHI, R.L. GREENE, University of Maryland — Recent advances in growth of high-quality crystalline thin films of the only known spinel superconductor (SC)  $\text{LiTi}_2\text{O}_4$  have allowed the discovery of an anomalous anisotropic magnetoresistance in its normal state [1]. We have used time domain terahertz spectroscopy, a contactless transport measurement, to determine the ac conductivity of  $\text{LiTi}_2\text{O}_4$  and to examine the BCS nature of the superconducting state. We obtained the temperature dependence of the SC gap as well as the London penetration depth, and also found a hint of a second gap. We will discuss and compare these results in terms of the known dc transport properties [1]. [1] K. Jin, et al. Nature Communications, 6, 7183, 2015.

<sup>1</sup>Work at OSU supported by start-up funds to RVA. Work at UMD supported by UMDAFOSR FA95501410332, and NSF DMR 1410665.

**3:30PM C25.00006 Superconductivity-induced changes in density-density correlation function enabled by Umklapp processes**, WEI-CHENG LEE, Binghamton Univ — Motivated by the midinfrared scenario for high-temperature superconductivity proposed by Leggett, the effects of Umklapp processes on the density-density correlation function in the presence of long-range Coulomb interaction have been investigated. We show that because Umklapp processes enable scatterings that conserve total momentum only up to an integer times the reciprocal wave vector, significant amounts of spectral weight in the plasmonic excitations at long wavelength are transferred into lower frequency around the midinfrared regime. We further find that regardless of the gap symmetry, superconductivity generally suppresses the Umklapp scatterings due to the nature of Cooper pairs. This suppression is unique for the superconductivity due to the interplay between electron pairing and the odd parity of the matrix elements associated with Umklapp channels, which usually does not occur in other known competing orders. Specific predictions for the experimental signatures in optical conductivity and electron energy loss spectroscopy will be discussed.

**3:42PM C25.00007 New Method for Imaging Gap Nodal Structure of Unconventional Superconductors through the Anisotropic Nonlinear Meissner Effect<sup>1</sup>**, SEOKJIN BAE, YUEWEN TAN, RAHUL GOGNA, NATHAN MENDELSON, Univ of Maryland-College Park, STEVEN REMILLARD, Hope College, STEVEN ANLAGE, Univ of Maryland-College Park — We present a new measurement method which can be used to image gap nodal structure of superconductors whose pairing symmetry is unknown. This method utilizes photoresponse from a microwave resonance of the superconducting sample perturbed by a scanned laser spot. For an epitaxial or single crystal sample, the anisotropy of this photoresponse is directly related to that of gap function via the non-linear Meissner coefficient, so the gap nodal directions can be inferred from the photoresponse image. The significant advantage of the presented method over previous spiral or lumped circuit resonator methods is that it does not require a complicated lithographic patterning process which often degrades superconductivity or introduces defect-dominant photoresponse and hence limits one from testing various kinds of materials. The validity of the method is confirmed both by HFSS simulation and experiments on unpatterned superconducting thin films. Photoresponse images from example unconventional superconductors will be also presented and discussed.

<sup>1</sup>This work is supported by the NSF Grants DMR-1410712.

Lognumber: MAR16-2015-004026

Title: New Method for Imaging Gap Nodal Structure of Unconventional Superconductors through the Anisotropic Non-

**3:54PM C25.00008 Imaging the Anisotropic Non-linear Meissner Effect Range<sup>1</sup>**, YUEWEN TAN, SEOKJIN BAE, STEVEN ANLAGE, Univ of Maryland, College Park — The anisotropic non-linear superconductors, which gives information about gap nodal structure, has been observed by measurements of anisotropic photoresponse to about 3 Kelvin.[1] Since the anisotropy of photoresponse originates from the non-linear Meissner effect coefficient, and the dependence for the photoresponse at temperatures below  $0.1T_c$ , [2] it will be interesting to measure photoresponse in that range. We will use a scanning laser microscope around a dilution refrigerator, and plan to measure photoresponse of unconventional superconductors in the millikelvin range. Reference: [1] A. P. Zhuravel, B. G. Ghamsari, C. Kurter, P. Jung, S. Remillard, J. Abrahams, A. V. Lukashenko, "Imaging the Anisotropic Nonlinear Meissner Effect in Nodal  $YBa_2Cu_3O_{7-\delta}$  Thin-Film Superconductors" Phys. Rev. B, 88, 020501 (2013). [2] D. J. Dahm and D. J. Scalapino, "Theory of Intermodulation in a Superconducting Microstrip Resonator", Journal of Applied Physics, 77, 1045 (1994).

linear Meissner Effect

<sup>1</sup>This work is supported by the NSF Grants DMR-1410712.

**4:06PM C25.00009 Examining the low energy electrodynamics of the superconductor-insulator transition in the potential topological superconductor  $Tl_4(Tl_{1-x}Sn_x)Te_3$ <sup>1</sup>**, N. J. LAURITA, K. A. ARPINO, S. M. KOOPAYEH, T. M. MCQUEEN, N. P. ARMITAGE, Institute for Quantum Matter, Johns Hopkins University — The search for an intrinsic single crystal topological superconductor is one of the most dynamic areas of modern condensed matter physics. One of the best candidates of such a material is  $Tl_5Te_3$  ( $T_c = 2.3K$ ), which previous ARPES measurements have shown possesses a Dirac cone within its superconducting gap. However, the fundamental nature of superconductivity, i.e. the superconducting order parameter, in  $Tl_5Te_3$  remains unknown. Additionally, it has been shown that  $Tl_5Te_3$  undergoes a superconducting-insulator transition upon doping with Sn. With no band parity inversion expected in the fully Sn doped compound one expects a topological superconductor - trivial insulator transition, the nature of which is also unknown. In this work we use highly sensitive microwave cavity perturbation measurements, a direct probe of the superfluid density, to study the low energy electrodynamics of superconductivity in  $Tl_5Te_3$  and its corresponding superconductor-insulator transition upon Sn doping.

<sup>1</sup>Work at Johns Hopkins was supported by the Gordon and Betty Moore Foundation through Grant GBMF2628, the DOE-BES through DE-FG02-08ER46544, and the ARCS Foundation.

**4:18PM C25.00010 Characterizing phase transitions in known materials with Magnetic Field Modulated Microwave Spectroscopy (MFMMS)<sup>1</sup>**, JAMES WAMPLER, Dept. of Physics, Center for Advanced Nanoscience, Univ. of California, JUAN GABRIEL RAMIREZ, Dept. of Physics, Universidad de los Andes, Bogot, Colombia, ALI BASARAN, Dept. of Physics, Gebze Technical Univ, IVAN SCHULLER, Dept. of Physics, Center for Advanced Nanoscience, Univ. of California — We have previously introduced Magnetic Field Modulated Microwave Spectroscopy (MFMMS), a sensitive and selective technique used to identify electromagnetic phase transitions in homogenous and inhomogeneous materials. By scanning the temperature, we can detect the phase transitions of a material. In standard operation, samples are placed in a microwave cavity with a resonance frequency of 9.4 GHz. A 100 kHz modulation field with 15 Oe amplitude and an optional DC field are applied while temperature is scanned. [1,2,3]. Here we will discuss different methods to further characterize phase transitions by scanning DC field while temperature is fixed. Since the response of different phase transitions to the applied field is varied, DC field scans can help to distinguish and reveal the origin of the transition. We have investigated many known superconducting and other reference materials and will compare the results in these different materials. 1. J. G. Ramirez, A. C. Basaran *et al.*, *Rep. Prog. Phys.* **77**, 093902 (2014). 2. S. Guénon *et al.*, *Scientific Reports* **4**, 7333 (2014). 3. S. Guénon *et al.*, *arxiv:1509.04452*, manuscript submitted.

<sup>1</sup>This work is supported by AFOSR: FA9550-14-1-0202

**4:30PM C25.00011 Progress towards a Hybrid Superconducting Microwave Cavity for Axion Searches<sup>1</sup>**, GIANPAOLO CAROSI, Lawrence Livermore National Laboratory, ADMX COLLABORATION, ADMX-HF COLLABORATION — Axions are a well motivated dark matter candidate and can be detected by their resonant conversion into photons using a microwave resonant cavity in an axial magnetic field. This is the basis of both the ADMX and ADMX-HF experiments. The predicted axion-photon conversion power is extremely small ( $< 10^{-22}$  W) and is directly related to the quality factor ( $Q$  = resonant frequency over bandwidth) of the microwave cavity. To date copper cavities have been used with  $Q \sim 10^5$  at frequencies of 1 GHz. As one scales to higher frequencies this  $Q$  degrades substantially. Superconducting cavities can regularly be made with  $Q > 10^9$  but would in general be driven normal in the high magnetic field of ADMX and ADMX-HF ( $> 8$  T). Here we describe progress of R&D efforts to make and test hybrid cavities with regular copper endcaps and thin-film superconducting barrels, produced with NbTiN RF sputtering, which are designed to maintain RF superconducting properties in the presence of a strong axial magnetic field at low temperatures ( $< 1$  K).

<sup>1</sup>Supported by DOE Grants DE-FG02-97ER41029, DE-FG02-96ER40956, DE-AC52-07NA27344, DE-AC03-76SF00098, NSF Grant 1067242, and the Livermore LDRD program.

**4:42PM C25.00012 Anomalous gap edge dissipation in disordered superconductors at the brink of localization**, BING CHENG, LIANG WU, NICHOLAS LAURITA, Johns Hopkins Univ, HARKIRAT SINGH, PRATAP RAYCHAUDHURI, Tata Institute of Fundamental Research, NORMAN ARMITAGE, Johns Hopkins Univ — In highly disordered conventional superconductors, it is frequently found that the optical conductivity presents an anomalous additional conductivity below the superconducting gap  $2\Delta$  even as  $T$  approaches zero. According to Bardeen-Cooper-Schrieffer theory and Matthis-Bardeen (MB) formula, no dissipation state should exist below  $2\Delta$  at  $T=0$  K. To resolve this problem, we studied a number of NbN superconducting films by time-domain terahertz spectroscopy. We found an extra conductivity beyond the predictions of MB theory begin to show up even at medium disorder level. With increasing disorder level, more and more optical spectral weights are moved to in-gap region ( $\omega < 2\Delta$ ). By using a self-consistent Abrikosov-Gorkov model, we found, disorder acts as a pairing breaking factor, which blurs the region around the gap edge and introduces dissipative states into the original gap region ( $\omega < 2\Delta$ ) in the optical conductivity. Our results show that the collective modes of superconductivity are not necessary to explain the extra dissipative states in disordered superconductors.

**4:54PM C25.00013 Extreme and Local 3rd Harmonic Response of Niobium (Nb) Superconductor<sup>1</sup>**, BAKHROM ORIPOV, Univ of Maryland-College Park, TAMIN TAI, Oak Ridge National Laboratory, STEVEN ANLAGE, Univ of Maryland-College Park — Superconducting Radio Frequency (SRF) cavities are being widely used in new generation particle accelerators. These SRF cavities are based on bulk Nb. Based on the needs of the SRF community to identify defects on Nb surfaces, a novel near-field magnetic microwave microscope was successfully built using a magnetic writer from a conventional magnetic recording hard-disk drive<sup>1</sup>. This magnetic writer can create an RF magnetic field, localized and strong enough to drive Nb into the vortex state. This probe enables us to locate defects through scanning and mapping of the local electrodynamic response in the multi-GHz frequency range. Recent measurements have shown that 3rd harmonic nonlinear response is far more sensitive to variations in input power and temperature than linear response, thus we mainly study the 3rd harmonic response. Moreover, the superconductor is usually the only source for nonlinear response in our setup, thus there is less chance of having noise or background signal. Understanding the mechanism responsible for this non-linear response is important for improving the performance of SRF cavities. Besides Nb we also study various other superconductors such as MgB2 and the cuprate Bi-Sr-Ca-Cu-O (BSCCO) for potential applications in SRF cavities.

<sup>1</sup>This work is funded by US Department of Energy through grant DE-SC0012036T and CNAM.

**5:06PM C25.00014 Observation of Raman active phonon with Fano lineshape in quasi-one-dimensional superconductor  $K_2Cr_3As_3$** , W.-L. ZHANG, H. LI, X. DAI, H.W. L, Y.-G. SHI, J.L. LUO, JIANGPING HU, P. RICHARD, H. DING, Chinese Academy of Sci (CAS), EXTREME CONDITION TEAM, CONDENSED MATTER THEORY TEAM — We study the polarization-resolved phononic Raman scattering in the recent discovered quasi-one-dimensional superconductor  $K_2Cr_3As_3$ . With support from first-principles calculations, we characterize several phonons, among which one mode has a Fano lineshape, indicative of an electron-phonon coupling. While the common expectation of an electron-phonon coupling is the conventional superconducting mechanism, we show that this mode is related to the in-plane Cr vibration, which modulates the exchange coupling between the first nearest Cr neighbors. Our result support the presence of magnetic fluctuations coupled to the electrons *via* the lattice. We acknowledge MOST (2010CB923000, 2011CBA001000, 2011CBA00102, 2012CB821403 and 2013CB921703), NSFC (11004232, 11034011/A0402, 11234014, 11274362 and 11474330) of China and by the Strategic Priority Research Program (B) of the Chinese Academy of Sciences, Grant No. XDB07020100.

**5:18PM C25.00015 Superconducting pairing in resonant inelastic X-ray scattering**, YIFEI SHI, University of Virginia, DAVID BENJAMIN, EUGENE DEMLER, Harvard University, ISRAEL KLICH, University of Virginia — We develop a method to study the effect of the superconducting transition on resonant inelastic X-ray scattering (RIXS) signal in superconductors with an order parameter with an arbitrary symmetry within a quasiparticle approach. As an example, we compare the direct RIXS signal below and above the superconducting transition for  $p$ -wave type order parameters. For a  $p$ -wave order parameter with a nodal line, we show that, counterintuitively, the effect of the gap is most noticeable for momentum transfers in the nodal direction. This phenomenon may be naturally explained as a type of nesting effect.

## Monday, March 14, 2016 2:30PM - 5:30PM —

Session C26 DMP: 2D Devices: Low-dimensional Properties and Contacts 325 - Doug Strachan, University of Kentucky

**2:30PM C26.00001 Electron Transport Simulations of 4-Terminal Crossed Graphene Nanoribbons Devices<sup>1</sup>**, PEDRO BRANDIMARTE, CFM CSIC-UPV/EHU and DIPC, Spain, NICK R. PAPIOR, DTU Nanotech, Denmark, MADS ENGELUND, CFM CSIC-UPV/EHU and DIPC, Spain, ARAN GARCIA-LEKUE, THOMAS FREDERIKSEN, DIPC and IKERBASQUE, Spain, DANIEL SÁNCHEZ-PORTAL, CFM CSIC-UPV/EHU and DIPC, Spain — Recently, it has been reported theoretically a current switching mechanism by voltage control in a system made by two perpendicular 14-armchair graphene nanoribbons (GNRs) [1]. In order to investigate the possibilities of using crossed GNRs as ON/OFF devices, we have studied their electronic and transport properties as function structural parameters determining the crossing. Our calculations were performed with TranSIESTA code [2], which has been recently generalized to consider  $N \geq 1$  arbitrarily distributed electrodes at finite bias. We find that the transmission along each individual GNR and among them strongly depends on the stacking. For a  $60^\circ$  rotation angle, the lattice matching in the crossing region provokes a strong scattering effect that translates into an increased interlayer transmission. [1] K. Masum Habib and R. Lake, Phys. Rev. B 86, 045418 (2012); [2] M. Brandbyge et al, Phys. Rev. B 65, 165401 (2002).

<sup>1</sup>FP7 FET-ICT PAMS-project (European Commission, contract 610446), MINECO (grant MAT2013-46593-C6-2-P) and Basque Dep. de Educación, UPV/EHU (grant IT-756-13).

**2:42PM C26.00002 Spatially Mapping Dirac Fermions in a Graphene Quantum Dot**, JUWON LEE, DILLON WONG, JAIRO VELASCO JR, Univ of California - Berkeley, JOAQUIN RODRIGUEZ-NIEVA, MIT, SALMAN KAHN, Univ of California - Berkeley, PHONG VO, MIT, HSIN-ZON TSAI, Univ of California - Berkeley, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, ALEX ZETTL, FENG WANG, Univ of California - Berkeley, LEONID LEVITOV, MIT, MICHAEL CROMMIE, Univ of California - Berkeley — Quantum confinement in graphene is important for tuning and exploiting graphene's electronic, spin, and optical properties. Here we present a novel technique for creating gate-tunable graphene quantum dots that are fully exposed and compatible with surface characterization tools. Using scanning tunneling microscopy (STM), we are able to spatially visualize and characterize the electronic structure of these gate-tunable graphene quantum dots. The quantum interference patterns observed in this way can be compared to the predictions of the Dirac equation, thus providing new insight into the behavior of confined ultra-relativistic Dirac fermions.

**2:54PM C26.00003 Imaging Quantum Confinement in Multiple Graphene Quantum Dots**, DILLON WONG, JAIRO VELASCO, JUWON LEE, Univ of California - Berkeley, JOAQUIN RODRIGUEZ-NIEVA, Massachusetts Institute of Technology, SALMAN KAHN, Univ of California - Berkeley, PHONG VO, Massachusetts Institute of Technology, HSINZON TSAI, Univ of California - Berkeley, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, ALEX ZETTL, FENG WANG, Univ of California - Berkeley, LEONID LEVITOV, Massachusetts Institute of Technology, MICHAEL CROMMIE, Univ of California - Berkeley — Quantum dots provide a useful means for controlling the electronic and spin degrees of freedom of mesoscale and nanoscale materials. Here we demonstrate a new method for fabricating interacting graphene quantum dots that is compatible with electrostatic gating and visualization by way of scanning tunneling microscopy (STM). Using this new technique we have created and spatially characterized systems of two or more interacting quantum dots. Our results show that it is possible to engineer electronic wave functions in graphene with a high degree of spatial control.

**3:06PM C26.00004 Probing electric properties at the boundary of planar 2D heterostructure**, JEWOOK PARK, Oak Ridge National Laboratory — The quest for novel two-dimensional (2D) materials has led to the discovery of hybridized 2D atomic crystals. Especially, planar 2D heterostructure provides opportunities to explore fascinating electric properties at abrupt one-dimensional (1D) boundaries reminiscent to those seen in the 2D interfaces of complex oxides. By implementing the concept of epitaxy to 2D space, we developed a new growth technique to epitaxially grow hexagonal boron nitride (hBN) from the edges of graphene, forming a coherent planar heterostructure [1]. At the interface of hBN and graphene, a polar-on-nonpolar 1D boundary can be formed which is expected to possess peculiar electronic states associated with the polarity of hBN and edge states of graphene. Scanning tunneling microscopy and spectroscopy (STM/S) measurements revealed an abrupt 1D zigzag oriented boundary, with boundary states about 0.6 eV below or above the Fermi level depending on the termination of the hBN at the boundary [2]. The boundary states are extended along the boundary and exponentially decay into the bulk of graphene and hBN. Combined STM/S and first-principles theory study not only disclose spatial and energetic distribution of interfacial state but also reveal the origin of boundary states and the effect of the polarity discontinuity at the interface. By probing electric properties at the boundary in the atomic scale, planar 2D heterostructure is demonstrated as a promising platform for discovering emergent phenomena at the 1D interface in 2D materials. This research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility. 1 L. Liu and J. Park et al., *Science* **343**, 163 (2014). 2 J. Park and J. K. Lee et al., *Nature Commun.* **5**, 5403 (2014).

**3:42PM C26.00005 Electronic Transport of Encapsulated WSe<sub>2</sub> Fabricated by Pick-up of Pre-patterned hBN**, YAFANG YANG, Massachusetts Institute of Technology, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Japan, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology, MIT TEAM — We report high quality WSe<sub>2</sub> devices encapsulated between two hexagonal boron nitride (hBN) flakes using a pick-up method with etched hBN flakes. Previous work on graphene has shown that sample disorder can be greatly reduced via isolation from charge impurities in the substrate by means of encapsulation. However, the effect of encapsulation still remains unknown for dichalcogenides devices. Besides, the quality of contact to TMDs is also a critical factor limiting the transport performance of such devices. To measure the transport properties of dichalcogenide devices as a function of temperature, low resistance electrical contacts must be made to the material. To achieve this, we encapsulate few-layer WSe<sub>2</sub> in hexagonal boron nitride that has been patterned to allow ionic liquid doping of the contact region. This technique simultaneously protects the WSe<sub>2</sub> surface above and below, resulting in the highest mobility few-layer WSe<sub>2</sub> devices reported to date.

**3:54PM C26.00006 Influence of Metal Contacts on Graphene Transport Characteristics and Its Removal with Nano-carbon Interfacial Layer**, AKINOBU KANDA, YU ITO, KENTA KATAKURA, HIROKI SONODA, SHOMA HIGUCHI, University of Tsukuba, HIKARI TOMORI, PRESTO-JST and University of Tsukuba, YOUTI OOTUKA, University of Tsukuba — Graphene is a promising candidate for the next-generation electronic material. While considerable effort has been devoted to achieve higher mobility in graphene films, relatively little attention has been paid to the effect of metal contacts, which are indispensable to the electric devices. At a graphene/metal interface, mainly due to the difference in work functions, carriers are injected from the metal to graphene. The resulting shift of local Dirac point is not limited at the graphene/metal interface but extends into the graphene channel. This carrier doping affects more significantly the performance of graphene field effect devices with shorter channel, as well as may conceal Dirac physics at the graphene/metal interface. Here, we experimentally investigate the channel length dependence of graphene transport properties in a wide gate-voltage range and extract the effect of metal contact. Several metal species are investigated. We reveal the origin of electron-hole asymmetry and the effect of the chemical interaction between graphene and metal, and derive the effective work function of graphene (4.93 eV). Furthermore, we succeed in reducing the influence of metal contact by inserting a thin nano-carbon layer (amorphous carbon or multilayer graphene (MLG)) at the interface.

**4:06PM C26.00007 Atomically Thin One-Dimensional Contacts to Two-Dimensional Semiconductors**, MARCOS GUIMARAES, Kavli Institute at Cornell, Cornell University, Ithaca, New York 14853, USA, HUI GAO, KIBUM KANG, Department of Chemistry and Chemical Biology, Cornell University, Ithaca, New York 14853, USA, DANIEL RALPH, Department of Physics, Cornell University, Ithaca, New York 14853, USA, JIWOONG PARK, Department of Chemistry and Chemical Biology, Cornell University, Ithaca, New York 14853, USA — Two dimensional van der Waals materials, including graphene and transition metal dichalcogenides (TMDs), are promising candidates for atomically thin circuitry. However, electrical contacts to semiconducting TMDs made using metal electrodes (e.g. Ti, Au) show high contact resistances ( $\geq 50 \text{ k}\Omega\cdot\mu\text{m}$ ). This makes it difficult to study and utilize the intrinsic properties of TMD materials, and the 3D metal contacts add significant thickness to the final devices. Here we report one-dimensional, atomically-thin, lateral contacts between graphene and monolayer TMDs with low contact resistance. The graphene/TMD lateral heterostructures are mechanically strong, and the structural and electronic properties of each individual material are well preserved after the growth processes. The interface between graphene and MoS<sub>2</sub> shows a much lower resistance (below  $20 \text{ k}\Omega\cdot\mu\text{m}$ ) than conventional metal contacts despite its atomic thickness and one dimensionality. Our devices exhibit linear I-V characteristics and very weak temperature dependence down to 77 K, confirming the ohmic properties of our contacts. By studying graphene/WS<sub>2</sub> devices fabricated in a similar way we show that our method is universal and can be expanded to other two-dimensional semiconducting TMDs.

**4:18PM C26.00008 High-Performance WSe<sub>2</sub>, MoS<sub>2</sub>, and MoSe<sub>2</sub> Transistors Enabled by a New Contact Strategy**, HSUN JEN CHUANG, BHIM CHAMLAGAIN, Wayne State University, MICHAEL KOEHLER, The University of Tennessee, MEEGHAGE MADUSANKA PERERA<sup>1</sup>, Wayne State University, JIAQIANG YAN, Oak Ridge National Laboratory, DAVID MANDRUS, The University of Tennessee, DAVID TOMNEK, Michigan State University, ZHIXIAN ZHOU, Wayne State University — Fabrication of high-performance transistors of transition metal dichalcogenides (TMDs) including WSe<sub>2</sub>, MoS<sub>2</sub>, and MoSe<sub>2</sub> has been a major challenge in 2D electronics. The performance of current metal-contacted TMDs is limited by the presence of a significant Schottky barrier in most cases. Here we introduce a new strategy for fabricating low-resistance ohmic contacts to a variety of TMDs. We demonstrate low contact resistance  $\approx 0.3 \text{ k}\Omega\mu\text{m}$ , high on/off ratios up to  $>10^9$ , and high drive currents exceeding  $320 \mu\text{A } \mu\text{m}^{-1}$  in few-layer WSe<sub>2</sub> field-effect transistors (FETs). These favorable characteristics are combined with a two-terminal field-effect hole mobility  $\mu_{\text{FE}} \approx 2 \times 10^2 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  at room temperature, which increases to  $>2 \times 10^3 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  at cryogenic temperatures. We observe a similar performance also in MoS<sub>2</sub> and MoSe<sub>2</sub> FETs. \*We acknowledge the partial support by NSF grant number DMR-1308436 and the WSU Presidential Research Enhancement Award.

**4:30PM C26.00009 Niobium disulfide as a edge-contact electrode of transition metal dichalcogenides(TMDC) semiconductor.**, HUNYOUNG BARK, JINHWAN LEE, JAEHYUCK JUNG, Sungkyunkwan Univ, CHANGGU LEE, peterlee@skku.edu, GRAPHENE ENGINEERING LAB TEAM — Two dimensional ultrathin transition metal dichalcogenides(TMDC) semiconductor is considered as a promising candidate for future flexible and transparent electronic devices. However, direct metal contact to two dimensional ultrathin transition metal dichalcogenides(TMDC) semiconductor forms a schottky contact, which suppress electrical performance like electron mobility. Here, we suggest edge contact method using niobium disulfide for low contact resistance. Niobium disulfide is a two dimensional transition metal dichalcogenides(TMDC) conductor and has a similar atomic structure with other two dimensional transition metal dichalcogenides(TMDC) semiconductors. Niobium disulfide forms a covalent bonding with transition metal dichalcogenides(TMDC) semiconductor instead of van der Waals bonding which occurred in conventional metal contact methods. Covalent bonding between transition metal dichalcogenides(TMDC) semiconductor and niobium disulfide decrease a contact resistance. Therefore, niobium disulfide electrode device shows improved device performance compared with conventional metal electrode device due to low contact resistance.

**4:42PM C26.00010 One-Dimensional Electrical Contact to Molybdenum Disulfide**, ZHENG YANG, CHANGHO RA, SKKU Advanced Institute of Nano Technology, FAISAL AHMED, SKKU Mechanical Engineering Department, DAEYEONG LEE, MINSUP CHOI, XIAOCHI LIU, DESHUN QU, WON JONG YOO, SKKU Advanced Institute of Nano Technology, NANO DEVICE PROCESSING LAB TEAM — Molybdenum disulfide (MoS<sub>2</sub>) is one of the promising two-dimensional materials for future application in nano electronics, which has high carrier mobility, very good stability under atmosphere, proper band gap, etc. However, its application to electronic switching devices is hindered by Fermi level pinning at metal-MoS<sub>2</sub> interfaces. Here, we experimentally demonstrate one-dimensional electrical contact to MoS<sub>2</sub> formed via controllable plasma etching. We fabricated Al/MoS<sub>2</sub> FET (n-type), Mo/MoS<sub>2</sub> FET (n-type), and Pd/MoS<sub>2</sub> FET (ambipolar). For Mo/MoS<sub>2</sub> FET (n-type), on/off current ratio is around  $10^8$  and mobility is around  $104 \text{ cm}^2/(\text{Vs})$ . By contrast, for Pd/MoS<sub>2</sub> FET (ambipolar), on/off current ratio is around  $10^8$ , hole mobility is ranged from 350 to  $650 \text{ cm}^2/(\text{Vs})$ , and the mean free path of holes at 9K is around 23 nm. All the measured mobilities are evaluated by using two-terminal field-effect configuration. We can also achieve complementary logic gates with intrinsic MoS<sub>2</sub>/metal one-dimensional electrical contact.

**4:54PM C26.00011 Engineering MoS<sub>2</sub> contact with graphene electrodes under electrostatic doping**, EN-MIN SHIH, REBECA RIBEIRO-PALAU, GHIDEWON AREFE, YOUNG-DUCK KIM, JIA LI, JAMES HONE, CORY DEAN, Columbia University — Semiconductor transition metal dichalcogenides (TMDs) are 2D semiconductors that host attractive transport properties such as unconventional quantum Hall effect and spin-valley physics. However, metal contacts typically result in a Schottky barrier, making it difficult to access fundamental properties of the intrinsic charge transport. In this report, we utilize graphene electrodes to achieve ohmic contact to MoS<sub>2</sub> monolayer and bilayer. Our devices are fully encapsulated by boron-nitride, which reduces the disorders from Si/SiO<sub>2</sub> substrate, and benefit from a dual-gate geometry, which allow us to independently dope the MoS<sub>2</sub> channel and graphene contact regions. The transition from non-ohmic to ohmic contacts is studied as a function of graphene doping and the MoS<sub>2</sub> carrier density. Our results reveal the operational range of these new devices, and provide new insight into future device design.

**5:06PM C26.00012 WSe<sub>2</sub> heterostructures with p-type multi-layer graphene contacts**, GHIDEWON AREFE, NATHAN FINNEY, Columbia University, DONGJEA SEO, Yonsei University, YOUNG DUCK KIM, DAMIEN CHANG, XU CUI, Columbia University, KYUNG NAM KANG, Stevens Institute of Technology, SAHNG-KYOON JERNG, SEUNG HYUN CHUN, Sejong University, EUI-HYEOK YANG, Stevens Institute of Technology, JAMES HONE, Columbia University — Recent advances in 2D material research have opened up new opportunities to study fundamental physics and to imagine new applications for this advanced class of materials. 2D tungsten diselenide (WSe<sub>2</sub>) is a transition metal dichalcogenide (TMDC) semiconductor that is intrinsically p-type with great potential for advanced opto-electronic applications. WSe<sub>2</sub> monolayers grown by CVD and highly p-doped PECVD multilayer graphene are used to construct 2D heterostructure p-type field effect transistors as a platform to study the potential for applications and novel physical phenomena. P-type graphene is being used to overcome the challenge of making good electrical contact to WSe<sub>2</sub> that is Ohmic at low temperatures and to allow for the construction of an entirely 2D heterostructure. Electrical transport and novel optical effects will be studied in these WSe<sub>2</sub> heterostructures that are fully encapsulated in hexagonal boron nitride (h-BN) in order to show greatly improved environmental stability and high mobility at low temperature due to the suppression of extrinsic scattering effects such as charge impurities, surface polar optical phonons, and absorbents from air.

**5:18PM C26.00013 Doping, strain engineering, and interlayer interaction in bilayer hexagonal boron nitride sheets<sup>1</sup>**, SUSUMU SAITO, YOSHITAKA FUJIMOTO, Tokyo Inst of Tech - Tokyo — We study electronic properties of bilayer hexagonal boron nitride (h-BN) sheets with different stacking sequences in the framework of the density-functional theory. The bulk h-BN material usually takes the so-called AA (or AA') stacking, corresponding to the "non-polar" bilayer h-BN sheet. On the other hand, the rhombohedral BN takes the ABC stacking, and the corresponding bilayer sheet has "upper" and "lower" layers which are not equivalent with each other. Interestingly, the energetics of stacking sequences for bilayer h-BN sheets is found to be different from that for bulk h-BN materials. We report that strain engineering for bilayer h-BN sheets can possess much wider possibilities than that for monolayer h-BN due to the modification of the interlayer interaction. We also study the substitutional C doping into bilayer h-BN sheets, and report the energetics and the strain effect for these C-doped sheets. Finally we discuss the similarities and differences between bilayer h-BN sheets and double-wall h-BN nanotubes.

<sup>1</sup>This work was partly supported by the MEXT Elements Strategy Initiative to Form Core Research Center, Grant in Aid for Scientific Research, MEXT Japan, Science of Atomic Layers, and JSPS KAKENHI Grant No. 26390062.

**Monday, March 14, 2016 2:30PM - 5:30PM –**

**Session C27 DCMP: Heavy Fermion Compounds: Experiment and Theory** 326 - Sheng Ran, University of California, San Diego

### 2:30PM C27.00001 Global phase diagram and single particle excitations in Kondo insulators

, QIMIAO SI, Rice University, JEDEDIAH PIXLEY, Condensed Matter Theory Center and Joint Quantum Institute, Department of Physics, University of Maryland, RONG YU, Department of Physics, Renmin University of China, SILKE PASCHEN, Institute of Solid State Physics, Vienna University of Technology — Motivated by quantum criticality in Kondo insulators [1] tuned by pressure or doping we study the effects of magnetic frustration and the properties of the single particle excitations in a Kondo lattice model [2]. Focusing on the Kondo insulating limit we study the Shastry-Sutherland Kondo lattice and determine the zero temperature phase diagram, which incorporates a valence bond solid, antiferromagnet, and Kondo insulating ground states, with metal-to-insulator quantum phase transitions. We argue that this phase diagram is generic and represents a “global” phase diagram of Kondo insulators in terms of quantum fluctuations and the Kondo interaction. We then focus on the momentum distribution of single particle excitations within the Kondo insulating ground state. We show how features of the Fermi-surface of the underlying conduction electrons appear in the Kondo insulating phase. Lastly, we discuss the implications of our results for quantum criticality in Kondo insulators [1] as well as for the recent de Haas-von Alphen measurements in the Kondo insulator SmB<sub>6</sub> [3,4]. [1] Q. Si and S. Paschen, *physica status solidi (b)* 250, 425 (2013). [2] J. H. Pixley, et. al., arXiv:1509.02907 (2015). [3] B. Tan et al, *Science* 349, 287 (2015). [4] G. Li et al, *Science* 346, 1208 (2014).

### 2:42PM C27.00002 Probing the Kondo State using Terahertz Radiation

, CHRISTOPH WETLI, Department of Materials, ETH Zurich, JOHANN KROHA, Institute of Physics, Bonn University, CORNELIUS KRELLNER, KRISTIN KLIEMT, Institute of Physics, Goethe University Frankfurt, OLIVER STOCKERT, MPI for Chemical Physics of Solids, Dresden, HILBERT V. LOEHNEISEN, Institute of Solid State Physics, Karlsruhe Institute of Technology, MANFRED FIEBIG, Department of Materials, ETH Zurich — The appearance of quantum critical phase transitions is boosting the interest in the field of Kondo-lattice systems. After intense research over the last decades, experimental insights have been mainly gained by measuring the specific heat capacity or the magnetic susceptibility and relating them to the increase of the effective mass. Lately, it has been demonstrated that ARPES experiments allow direct access to the electrons contributing to the Kondo-lattice effect, but with some experimental restrictions. We will show that THz radiation is a powerful and highly accurate alternative for investigating the approach to the coherent Kondo-state of heavy-fermion systems. Photons in the THz range directly couple to the electronic heavy quasiparticles causing the Kondo-singlet behavior. Additionally, this technique allows studying Kondo-state dynamics on the picosecond time scale. We report lifetime measurements of excited Kondo singlets for the two crystalline rare earth heavy-fermion systems CeCu<sub>6</sub> and YbRh<sub>2</sub>Si<sub>2</sub>, where the lifetimes scale inversely proportional to the Kondo-temperature. THz spectroscopy thus gives a very different perspective towards the Kondo-lattice effect, with the unique ability to combine temporal resolution and possible measurements in magnetic field.

### 2:54PM C27.00003 Quantum oscillations near a metallic quantum critical point

, ARKADY SHEKHTER, NHMFL, Tallahassee FL — Quantum criticality is a pervasive origin of new physics in metals, such as the linear-in-temperature resistivity observed in multiple classes of unconventional superconductors. One of the most direct probes of quantum critical metals is the quantum oscillation technique, which provides Fermi surface geometry information, as well as quasiparticle masses and lifetimes. Recent quantum oscillation experiments in high temperature superconductors show a suppression of the quantum oscillation amplitude with doping. This has been interpreted as an enhancement of the quasiparticle effective mass approaching a critical doping—in strong support of a quantum critical origin of their phase diagrams. We suggest that rather than a pure mass enhancement, the aforementioned quantum oscillation experiments indicate the increasing role of quantum fluctuation modes in the thermodynamics, contributing to the suppression of the quantum oscillation amplitude with temperature. We show that attempt to calculate the temperature dependent amplitude of quantum oscillations in the anomalous metals results in a violation of the third law of thermodynamics unless non-quasiparticle effects are considered.

### 3:06PM C27.00004 Emergence of anisotropic heavy fermions in antiferromagnetic Kondo lattice CeIn<sub>3</sub> revealed by photoemission

, YUN ZHANG, Department of Engineering Physics, Tsinghua University, Beijing 100084, China, HAIYAN LU, XIEGANG ZHU, SHIYONG TAN, QIYUN CHEN, WEI FENG, DONGHUA XIE, LIZHU LUO, WEN ZHANG, XINCHUN LAI, Science and Technology on Surface Physics and Chemistry Laboratory, Mianyang 621907, China, DONGLAI FENG TEAM, HUIQIU YUAN TEAM — One basic concept in heavy fermions systems is the entanglement of localized spin state and itinerant electron state. It can be tuned by two competitive intrinsic mechanisms, Kondo effect and Ruderman-Kittel-Kasuya-Yosida interaction, with external disturbances. The key issue regarding heavy fermions properties is how the two mechanisms work in the same phase region. To investigate the relation of the two mechanisms, the cubic antiferromagnetic heavy fermions compound CeIn<sub>3</sub> was investigated by soft x-ray angle resolved photoemission spectroscopy. The hybridization between f electrons and conduction bands in the paramagnetic state was observed directly, providing compelling evidence for Kondo screening scenario and coexistence of two mechanisms. The hybridization strength shows slight and regular anisotropy in K space, implying that the two mechanisms are competitive and anisotropic. This work illuminates the concomitant and competitive relation between the two mechanisms and supplies some evidences for the anisotropic superconductivity of CeIn<sub>3</sub>.

### 3:18PM C27.00005 Global phase diagram of the Ising-anisotropic Kondo lattice

, EMILIAN M NICA, Rice University, KEVIN INGERSANT, University of Florida, QIMIAO SI, Rice University — In recent years, a significant amount of work has been dedicated to understanding heavy-fermion quantum criticality. What has emerged is a proposed global phase diagram [1] meant to capture the interplay between Kondo singlet formation, magnetic ordering and intrinsic fluctuations associated with the quantum-mechanical nature of the local moments. Using an Extended Dynamical Mean-Field Theory (EDMFT) approach, we study a prototypical Ising-anisotropic Kondo lattice model in the presence of a transverse field that provides a way of controlling the quantum fluctuations of the local moments. We show that the transverse field opens up a line of continuous transitions directly from an antiferromagnetic phase with Kondo destruction (and, hence, a small Fermi surface) to a paramagnetic heavy-fermion state (with a large Fermi surface). We show that the critical scaling characteristics along this line are the same as for the previously studied zero-transverse field case, indicating the robustness of the Kondo-destruction scenario with respect to enhanced quantum fluctuations. General implications of our results for the global phase diagram and heavy-fermion quantum criticality will be discussed. [1] “Kondo Destruction and Quantum Criticality in Kondo Lattice Systems,” Q. Si, J. H. Pixley, E. Nica, S. J. Yamamoto, P. Goswami, R. Yu, and S. Kirchner, *J. Phys. Soc. Jpn.* **83**, 061005 (2014).

### 3:30PM C27.00006 Spin wave spectrum in CeRhIn<sub>5</sub> under applied magnetic fields

, DAVID FOBES, S.-Z. LIN, Los Alamos National Lab, NM, USA, N.J. GHIMIRE, Argonne National Lab, IL, USA, F. RONNING, E.D. BAUER, J.D. THOMPSON, C.D. BATISTA, Los Alamos National Lab, NM, USA, G. EHLERS, Oak Ridge National Lab, TN, USA, M. JANOSCHEK, Los Alamos National Lab, NM, USA — The phase diagram of CeRhIn<sub>5</sub> is in many ways a prototypical example of a heavy fermion superconductor; it is a heavy fermion antiferromagnet that can be tuned to a quantum critical point (QCP) via pressure, around which unconventional superconductivity emerges. Closer inspection reveals unusual behavior however; the interplay between magnetism and unconventional superconductivity is atypical, and electrical transport behavior and changes in the Fermi surface at the QCP are not in agreement with the prototypical spin-density-wave-type scenario. This is supported by our previous measurements of the spin wave spectrum at ambient pressure replicated by a simple frustrated  $J_1 - J_2$  model based on localized Ce 4f electrons. We show that the addition of magnetic anisotropy and Zeeman terms to our Anisotropic Next-Nearest Neighbor Ising (ANNNI) model Hamiltonian quantitatively describes the spin wave spectrum under the application of magnetic field as obtained by neutron scattering, and reproduces the experimental magnetic phase diagram. Finally, this model predicts that the magnetic ordering vector should change logarithmically as a function of temperature across the high-field incommensurate-to-commensurate phase boundary, in agreement with our latest neutron diffraction results.

**3:42PM C27.00007 An efficient continuous-time quantum Monte Carlo impurity solver in Kondo Regime**, CHANGMING YUE, YILIN WANG, Institute of Physics, Chinese Academy of Science, XI DAI, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — An efficient continuous-time quantum Monte Carlo impurity solver with high acceptance ratio at low temperature is developed to study the strongly correlated heavy-fermion materials. In this solver, the imaginary time evolution operator for the high energy multiplets, which decays very rapidly with time, is approximated by a  $\delta$  function, and as a result the virtual charge fluctuations of  $f^n \rightarrow f^{n\pm 1}$  are all included without applying Schrieffer-Wolff transformation explicitly. As benchmarks, our algorithm perfectly reproduces the results for both Coqblin-Schrieffer and Kondo lattice models obtained by ct- $J$  method developed by Junya Otsuki et al. Furthermore, it allows us to study low energy physics of heavy-fermion materials directly without fitting the exchange coupling  $J$  in the Kondo model. As an example, we test our solver on CeCoIn<sub>5</sub>, the famous heavy fermion material within the framework of LDA+DMFT to obtain its quasi-particle spectrum.

**3:54PM C27.00008 Investigation of quantum criticality in the new heavy fermion compound Ce<sub>2</sub>PdAl<sub>7</sub>Ge<sub>4</sub>**, ERIC BAUER, N. A. WAKEHAM, D. KIM, N. J. GHIMIRE, F. RONNING, R. MOVSHOVICH, J. D. THOMPSON, Los Alamos National Laboratory — Ce-based intermetallic compounds exhibit a variety of interesting ground states including magnetic order, heavy fermion behavior, unconventional superconductivity, and non-Fermi liquid behavior. When magnetic order is suppressed to  $T = 0$  K, or quantum critical point, by chemical substitution, pressure, or magnetic field, a dome of unconventional superconductivity is often found. Close to the quantum critical point, non-Fermi liquid temperature dependencies of the thermodynamic and transport properties are observed. Recently, a new family of tetragonal Ce<sub>2</sub>MAI<sub>7</sub>Ge<sub>4</sub> (M=Co, Ni, Pd, Ir) compounds was discovered. While the Ce<sub>2</sub>MAI<sub>7</sub>Ge<sub>4</sub> (M=Co, Ir, Ni) materials order magnetically between  $T_m = 0.8 - 1.6$  K, Ce<sub>2</sub>PdAl<sub>7</sub>Ge<sub>4</sub> exhibits non-Fermi liquid behavior at low temperature. Here, we discuss the quantum criticality in Ce<sub>2</sub>PdAl<sub>7</sub>Ge<sub>4</sub>.

**4:06PM C27.00009 Fermiology Of Ce<sub>2</sub>Rh<sub>3</sub>Ge<sub>5</sub>**, MARK WARTENBE, FSU — The competition between localized and delocalized f electrons in heavy fermion materials produces a wide variety of interesting physical phenomena. Among these compounds is Ce<sub>2</sub>Rh<sub>3</sub>Ge<sub>5</sub>. This heavy-fermion system undergoes an antiferromagnetic transition below 4K and exhibits an angle dependent magnetic phase transition around 25 tesla. In addition, RF conductivity measurements in pulsed field (65T) have revealed quantum oscillations. Temperature dependence at fixed angle indicates relatively heavy effective masses of values ranging from  $\sim 3m_e$  on up to  $\sim 10m_e$ . This indicates that the narrow f-electron density of states is partially hybridized close to the Fermi energy, but also places strict cryogenic constraints upon the measurement ( $^3\text{He}$  temperatures are required). Fermi surface calculations have produced complex figures which lend validation to such rich behavior. Presented are updated measurements including magnetization and revised theoretical calculations..

**4:18PM C27.00010 Investigation of the physical properties of the new heavy fermion compounds Ce<sub>2</sub>MAI<sub>7</sub>Ge<sub>4</sub> (M = Co, Ir, Ni, Pd)**, NIRMAL GHIMIRE<sup>1</sup>, Los Alamos National Laboratory, SAMANTHA CARY, THOMAS ALBRECHT-SCHMITT, Florida State University, CRAIG BROWN, National Institute of Standards and Technology, SERENA ELEY, NICHOLAS WAKEHAM, PRISCILA ROSA, MARC JANOSCHEK, LEONARDO CIVALE, JOE THOMPSON, FILIP RONNING, ERIC BAUER, Los Alamos National Laboratory — Ce-based intermetallic compounds provide a fascinating ground to study several exotic physical phenomena due to the presence of competing low Kondo and RKKY interactions. One widely explored entity in these compounds is the quantum phase transition that is accessed by the suppression of the magnetic order down to absolute temperature by an external parameter such as magnetic field, chemical substitution, or pressure. Exotic phenomena like unconventional superconductivity and non-Fermi liquid behavior are ubiquitous in the vicinity of the quantum critical point. Quantum criticality in these Ce-based materials is often observed in layered, tetragonal systems such as the CeM<sub>2</sub>X<sub>2</sub> (M=transition metal; X=Si, Ge) or CeMIn<sub>5</sub> (M=Co, Rh, Ir) compounds. We present the structural and physical properties of a new family of heavy fermion compounds Ce<sub>2</sub>MAI<sub>7</sub>Ge<sub>4</sub> (M = Co, Ir, Ni, Pd) that crystallize in the tetragonal space group P-42<sub>1</sub>m. Ce<sub>2</sub>MAI<sub>7</sub>Ge<sub>4</sub> (M=Co, Ir, Ni) show complex magnetic order below 2 K, while Ce<sub>2</sub>PdAl<sub>7</sub>Ge<sub>4</sub> does not order magnetically down to 400 mK, and, instead, shows quantum critical behavior at low temperature.

<sup>1</sup>Present affiliation: Argonne National Laboratory

**4:30PM C27.00011 Antiferromagnetic Kondo lattice in the layered compounds Re<sub>2</sub>NiGa<sub>9</sub>Ge<sub>2</sub> (Re=Ce, Pr, Sm)**, YANGLIN ZHU, JINYU LIU, JIN HU, Department of Physics and Engineering Physics, Tulane University, New Orleans, LA 70018, DANIEL ADAMS, LEONARD SPINU, Department of Physics and AMRI, University of New Orleans, New Orleans, LA 70148, ZHIQIANG MAO, Department of Physics and Engineering Physics, Tulane University, New Orleans, LA 70018. — Intermetallic compounds containing rare-earth/actinide elements with 4f/5f electrons have formed a special family of strongly correlated materials, i.e. heavy fermion systems. We have recently found a new layered rare earth intermetallic system showing moderate heavy fermion behavior: Re<sub>2</sub>NiGa<sub>9</sub>Ge<sub>2</sub> (Re=Ce, Sm, Pr). The Re=Ce and Sm members were previously synthesized [1], while their electronic properties have not been reported. We have recently grown single crystals of Re<sub>2</sub>NiGa<sub>9</sub>Ge<sub>2</sub> (Re=Ce, Sm, Pr) and characterized their electronic and magnetic properties. We find all these materials are antiferromagnetic, with  $T_N = 2.5$  K, 5 K, 3.4 K respectively for Re=Ce, Pr and Sm. Moreover, they also exhibit large values of electronic specific coefficient:  $\gamma \approx 101$  mJ mol-Ce<sup>-1</sup> K<sup>-2</sup> for Re=Ce, 368 mJ mol-Pr<sup>-1</sup> K<sup>-2</sup> for Re=Pr, and 196.4 mJ mol-Sm<sup>-1</sup> K<sup>-2</sup> for Re=Sm, indicating enhanced Kondo effect and the presence of AFM Kondo lattice. Our findings suggest that Re<sub>2</sub>NiGa<sub>9</sub>Ge<sub>2</sub> (Re=Ce, Pr, Sm) could be interesting candidate materials for exploring novel exotic properties of correlated electrons through external parameter tuning such as chemical substitution and pressure. Reference: [1] M. A. Zhuravleva and M. G. Kanatzidis, Inorg. Chem. 2008, 47 (20), 9471-9477.

**4:42PM C27.00012 High-resolution x-ray diffraction study of the heavy-fermion compound YbBiPt**, B. G. UELAND, S. M. SAUNDERS, S. L. BUD'KO, Ames Laboratory, Dept. of Physics and Astronomy, Iowa State University, G. M. SCHMIEDESHOFF, Department of Physics, Occidental College, P. C. CANFIELD, A. KREYSSIG, A. I. GOLDMAN, Ames Laboratory, Dept. of Physics and Astronomy, Iowa State University — YbBiPt is a heavy-fermion compound possessing significant short-range antiferromagnetic correlations below  $T^* = 0.7$  K, fragile antiferromagnetic order below  $T_N = 0.4$  K, a Kondo temperature of  $T_K \approx 1$  K, and crystalline-electric-field splitting (CEF) on the order of  $E/k_B = 1 - 10$  K. Its lattice is face-centered cubic at ambient temperature, but certain data, particularly those from studies aimed at determining the CEF level scheme, suggest that the lattice distorts at lower temperature. Here, we present results from high-energy x-ray diffraction experiments which show that, within our experimental resolution of  $\approx 6 - 10 \times 10^{-5}$  Å, no structural phase transition occurs between 1.5 and 50 K. Despite this result, we demonstrate that the compound's thermal expansion may be modeled using CEF level schemes appropriate for Yb<sup>3+</sup> residing on a site with either cubic or less than cubic point symmetry. Work at the Ames Laboratory was supported by the US DOE, BES, DMSE, under Contract No. DE-AC02-07CH11358. Work at Occidental College was supported by the NSF under DMR-1408598. This research used resources at the Advanced Photon Source a US DOE, Office of Science, User Facility.

**4:54PM C27.00013 Intermediate valence to heavy fermion through a quantum phase transition in  $\text{Yb}_3(\text{Rh}_{1-x}\text{T}_x)_4\text{Ge}_{13}$  ( $T = \text{Co, Ir}$ ) single crystals<sup>1</sup>**, BINOD RAI, EMILIA MOROSAN, Rice University, Houston TX, 77005 — Single crystals of  $\text{Yb}_3(\text{Rh}_{1-x}\text{T}_x)_4\text{Ge}_{13}$  ( $T = \text{Co, Ir}$ ) have been grown using the self-flux method. Powder X-ray diffraction data on these compounds are consistent with the cubic structure with space group  $Pm\bar{3}n$ . Intermediate valence behavior is observed in  $\text{Yb}_3(\text{Rh}_{1-x}\text{T}_x)_4\text{Ge}_{13}$  upon  $T = \text{Co}$  doping, while  $T = \text{Ir}$  doping drives the system into a heavy fermion state. Antiferromagnetic order is observed in the Ir-doped samples  $\text{Yb}_3(\text{Rh}_{1-x}\text{T}_x)_4\text{Ge}_{13}$  for  $0.5 < x \leq 1$  with  $T_N = 0.96$  K for  $\text{Yb}_3\text{Ir}_4\text{Ge}_{13}$ . With decreasing  $x$ , the magnetic order is suppressed towards a quantum critical point around  $x_c = 0.5$ , accompanied by non-Fermi liquid behavior evidenced by logarithmic divergence of the specific heat and linear temperature dependence of the resistivity. The Fermi liquid behavior is recovered with the application of large magnetic fields.

<sup>1</sup>Gordon and Betty Moore Foundation EPiQS initiative through grant GBMF4417 and Welch Foundation

**5:06PM C27.00014 Electronic and Magnetic Properties of Cd-Doped  $\text{PuRhIn}_5$ <sup>1</sup>**, JIAN-XIN ZHU, Los Alamos National Laboratory — Since their discovery nearly a decade ago, plutonium-based superconductors have attracted considerable interest, which is now heightened by the latest discovery of superconductivity in other Pu-115 compounds. Within the generalized gradient approximation (GGA) of density functional theory and its combination with the dynamical mean-field theory, we present a study of electronic structure in the paramagnetic state of Cd-doped  $\text{PuRhIn}_5$ . A doping-induced delocalization-localization transition is identified. In addition, the spin-polarized GGA-based total energy calculations are performed to determine the magnetic exchange interactions in the pristine  $\text{PuRhIn}_5$ . The implication to the nature of quantum criticality is discussed.

<sup>1</sup>This work was carried out under the auspices of the National Nuclear Security Administration of the U.S. Department of Energy at LANL under Contract No. DE-AC52-06NA25396, and was supported by the LANL ASC Program.

**5:18PM C27.00015 Phenomenological Magnetic Model in Tsai-Type Approximants**, TAKANORI SUGIMOTO, TAKAMI TOHYAMA, Department of Applied Physics, Tokyo University of Science, TAKANOBU HIROTO, Department of Advanced Material Science, University of Tokyo, RYUJI TAMURA, Department of Applied Physics, Tokyo University of Science — Recent neutron diffraction study has reported a curious ferromagnetism in Tsai-type approximants  $\text{Au-Si-RE}$  ( $\text{RE}=\text{Tb, Dy, Ho}$ ), which have the same local structure as quasi-crystals with a translational symmetry simultaneously. In these materials, magnetic moments of rare-earth atoms have a single-ion anisotropy determined locally via spin-orbit coupling around crystal fields satisfying a distorted icosahedral crystal structure. We phenomenologically propose a possible magnetic model reproducing the magnetic structure and the thermodynamical quantities. The corresponding energies of the single-ion anisotropy and RKKY exchange couplings are also estimated by comparing magnetization curves and susceptibility of our model and experiments. Moreover, simulated annealing calculations with the energies in our model coincide with the strange ferromagnetism. In conclusion, a distortion of icosahedral cluster in body-centered cubic structure plays a key role to emerge the peculiar magnetic structure. Our magnetic model does not only explain magnetic behaviors in quasi-crystal approximants, but also can approach to a coexistence of a long-ranged order and a quasi-periodicity.

**Monday, March 14, 2016 2:30PM - 5:30PM –**

**Session C28 DMP: Quantum Anomalous Hall Effect I** 327 - Nikesh Koirala, Rutgers University

**2:30PM C28.00001 Achieving High-Temperature Ferromagnetic Topological Insulator**, FERHAT KATMIS, Massachusetts Institute of Technology — Topological insulators (TIs) are insulating materials that display conducting surface states protected by time-reversal symmetry, wherein electron spins are locked to their momentum. This unique property opens new opportunities for creating next-generation electronic and spintronic devices, including TI-based quantum computation. Introducing ferromagnetic order into a TI system without compromising its distinctive quantum coherent features could lead to a realization of several predicted novel physical phenomena. In particular, achieving robust long-range magnetic order at the TI surface at specific locations without introducing spin scattering centers could open up new possibilities for devices. Here, we demonstrate topologically enhanced interface magnetism by coupling a ferromagnetic insulator (FMI) to a TI ( $\text{Bi}_2\text{Se}_3$ ); this interfacial ferromagnetism persists up to room temperature, even though the FMI ( $\text{EuS}$ ) is known to order ferromagnetically only at low temperatures ( $<17$  K). The induced magnetism at the interface resulting from the large spin-orbit interaction and spin-momentum locking feature of the TI surface is found to greatly enhance the magnetic ordering (Curie) temperature of the TI/FMI bilayer system. Due to the short range nature of the ferromagnetic exchange interaction, the time-reversal symmetry is broken only near the surface of a TI, while leaving its bulk states unaffected. The topological magneto-electric response originating in such an engineered TI could allow for an efficient manipulation of the magnetization dynamics by an electric field, providing an energy efficient topological control mechanism for future spin-based technologies. Work supported by MIT MRSEC through the MRSEC Program of NSF under award number DMR-0819762, NSF Grant DMR-1207469, the ONR Grant N00014-13-1-0301, and the STC Center for Integrated Quantum Materials under NSF grant DMR-1231319.

**3:06PM C28.00002 Probing the Spin Transfer Efficiency at Topological Insulator/Ferromagnetic Insulator Interfaces<sup>1</sup>**, HAILONG WANG, JAMES KALLY, JOON SUE LEE, ANTHONY RICHARDELLA, SUSAN KEMPINGER, YU PAN, ERIC KAMP, NITIN SAMARTH, Pennsylvania State University, TAO LIU, HOUCHEUNG CHANG, MINGZHONG WU, Colorado State University, DANIELLE REIFSNYDER-HICKEY, ANDRE MKHOYAN, University of Minnesota — The development of next-generation spintronics devices has driven extensive studies of spin-charge conversion through measurement of the inverse spin Hall effect (ISHE) and ferromagnetic resonance (FMR) driven spin pumping of pure spin currents in ferromagnet/non-magnet bilayers. Topological insulators (TIs) such as the Bi-chalcogenides are naturally relevant in this context because the inherent spin-momentum locking in their surface states promises very efficient spin-charge conversion, although the first experimental studies have involved ferromagnetic metals that provide a shunting current path [e.g. Nature, 511,449 (2014)]. To circumvent the current shunting problem, we are growing and characterizing bilayers of TIs and the ferrimagnetic insulator  $\text{Y}_3\text{Fe}_5\text{O}_{12}$  (YIG). Here, we report measurements of FMR-driven spin pumping in TI/YIG bilayers, showing robust spin pumping signals at room temperature. Analysis of the ISHE voltages and FMR linewidth broadening show that, as in other studies of spin pumping into TIs [Nano Lett., 15 (10) (2015)], the interface condition presents a critical challenge for enhancing the spin conversion efficiency in these devices.

<sup>1</sup>Funded by C-SPIN/SRC/DARPA and ONR

**3:18PM C28.00003 Spin manipulation at the interface of a topological insulator/GaAs heterostructure<sup>1</sup>**, DONGXIA QU, Lawrence Livermore National Laboratory, XIAOYU CHE, XUFENG KOU, MURONG LANG, University of California, Los Angeles, JONATHAN CROWHURST, MICHAEL R. ARMSTRONG, JOSEPH ZAUG, Lawrence Livermore National Laboratory, KANG L. WANG, University of California, Los Angeles, GEORGE F. CHAPLINE, Lawrence Livermore National Laboratory, LAWRENCE LIVERMORE NATIONAL LABORATORY TEAM, UNIVERSITY OF CALIFORNIA, LOS ANGELES TEAM — One primary goal of spintronics is to discover materials and devices, which enable efficient electrical control of spins. The emerging field of topological insulator (TI) provides intriguing opportunities for spin generation and manipulation, owing to its strong spin-orbit character. Here we report that spins can be driven from a topological insulator thin film  $(\text{Bi}_{0.5}\text{Sb}_{0.5})_2\text{Te}_3$  into an adjacent semiconductor GaAs at room temperature. In a TI/GaAs heterostructure, a photo-induced spin current flows across the interface and induces an electrical current via the inverse spin Hall effect, which converts the spin current into a charge current. We find that the magnitude and direction of the helicity-dependent photocurrent can be controlled by gate-voltage, indicative of electric tuning of the spin configuration.

<sup>1</sup>This work is supported by grants 15-LW-018 and 16-SI-004 from the Department of Energy, Laboratory Directed Research and Development (LDRD) funding.

**3:30PM C28.00004 Spin Pumping into Topological Insulator  $\text{Bi}_2\text{Te}_3$** , FARIS BASHEER ABDULAHAD, JIN-HAN LIN, YUNG LIOU, WEN-KAI CHIU, Academia Sinica, JUN-ZHI LIANG, Fu Jen Catholic University, SHANG-FAN LEE, Academia Sinica — A spin chemical potential bias can induce a spin polarized current by the exchange interaction of a ferromagnet with the spin-momentum locking surface states of the topological insulators. We carried out our ferromagnetic resonance experiment in a  $\text{NiFe}/\text{Bi}_2\text{Te}_3$  heterostructure. Apart from the enhanced Gilbert damping constant, we observed strong enhancement of the effective magnetic field at low temperatures. The enhanced field decreased exponentially with increasing temperature at an energy scale of 2.5 meV, representing the strength of the exchange coupling. We attribute the enhanced field to the induced spin polarized current in the surface states of  $\text{Bi}_2\text{Te}_3$ .

**3:42PM C28.00005 Magnetic proximity effect in a topological insulator-magnetic insulator heterostructure**, WENMIN YANG, SHUO YANG, KEHUI WU, JIANWANG CAI, YONGQING LI, Institute of Physics Chinese Academy of Sciences — Ferromagnetic topological insulators (TIs) have become one of the most actively pursued materials in condensed matter physics due to their unique properties, where several exotic phenomena have been predicted and observed, such as the quantum anomalous Hall effect and the topological magneto-electric effect. In this talk, I will introduce the fabrication and characterization of a heterostructure consisting of a thin film of the topological insulator  $\text{Bi}_2\text{Se}_3$  and the magnetic insulator  $\text{Y}_3\text{Fe}_5\text{O}_{12}$  (YIG), and study the low temperature transport properties. Compared to non-magnetic  $\text{Bi}_2\text{Se}_3$ , the magnetoresistance (MR) of  $\text{Bi}_2\text{Se}_3$ -YIG deviates from the typical weak antilocalization behavior in low perpendicular magnetic fields. In parallel fields, we observe unusual negative MR and sharp MR jumps when single domains nucleate and annihilate. Furthermore, magnetization measurements reveal that this unusual MR correlates to domain wall configurations of the YIG layer. These results can be explained due to the appearance of a perpendicular magnetic exchange field at the interface. The understanding of the interfacial interaction is valuable to further reveal unique physics in TI based magnetic heterostructures.

**3:54PM C28.00006 Epitaxial Growth and Characterization of Iron Chalcogenide/Bismuth Chalcogenide Heterostructures**, THOMAS FLANAGAN, ABHINAV KANDALA, JOON SUE LEE, SUSAN E. KEMPINGER, ANTHONY RICHARDELLA, NITIN SAMARTH, Pennsylvania State University — Heterostructures consisting of topological insulators (TIs) interfaced with superconductors and with ferromagnets have been predicted to give rise to phenomena of both fundamental and applied interest. With superconductors, the region of proximity-induced superconductivity should have  $p_x + ip_y$  symmetry, and vortices in this region have been predicted to host Majorana modes, which may be useful as quantum bits. With ferromagnets, such phenomena as the topological magnetoelectric effect have been predicted. Iron chalcogenides, such as iron selenide and iron telluride, are ideal candidates for combining with TIs, since, with only minor changes to growth conditions, they can be superconducting, ferromagnetic, or antiferromagnetic. We describe the growth and characterization of heterostructures that combine thin films of the iron and bismuth chalcogenides, focusing on low temperature magnetoresistance measurements. Our measurements reveal a transient hysteretic magnetoresistance with surprisingly long relaxation times (minutes). This phenomenon appears to be a generic characteristic of all heterostructures that interface TIs with magnetic spins, albeit with structure-specific relaxation times. We discuss possible origins of this unusual phenomenon. Funded by ARO/MURI.

**4:06PM C28.00007 Epitaxial Growth of Two-Dimensional Stanene**, JINFENG JIA<sup>1</sup>, Shanghai Jiao Tong University — Ultrathin semiconductors present various novel electronic properties. The first experimental realized two-dimensional (2D) material is graphene. Searching 2D materials with heavy elements bring the attention to Si, Ge and Sn. 2D buckled Si-based silicene was realized by molecular beam epitaxy (MBE) growth. Ge-based germanene was realized by mechanical exfoliation. Sn-based stanene has its unique properties. Stanene and its derivatives can be 2D topological insulators (TI) with a very large band gap as proposed by first-principles calculations, or can support enhanced thermoelectric performance, topological superconductivity and the near-room-temperature quantum anomalous Hall (QAH) effect. For the first time, in this work, we report a successful fabrication of 2D stanene by MBE. The atomic and electronic structures were determined by scanning tunneling microscopy (STM) and angle-resolved photoemission spectroscopy (ARPES) in combination with first-principles calculations. This work will stimulate the experimental study and exploring the future application of stanene.

<sup>1</sup>In cooperation with Fengfeng Zhu, Wei-jiong Chen, Yong Xu, Chun-lei Gao, Dan-dan Guan, Canhua Liu, Dong Qian, Shou-Cheng Zhang

**4:18PM C28.00008 Topological Surface States in Sb Quantum Wells on GaSb(111)A Substrates<sup>1</sup>**, KAUSHINI WICKRAMASINGHE, CHOMANI GASPE, SHAYNE CAIRNS, NOLAN TEASDALE, TETSUYA MISHIMA, JOEL KEAY, METTHEW JOHNSON, SHEENA MURPHY, MICHAEL SANTOS, University of Oklahoma — A topoelectronic transition is predicted as a function of Sb quantum-well (QW) thickness. Bulk Sb is a semimetal with a negative bandgap, with neither the conduction band minimum nor the valence band maximum at the  $\Gamma$  point. Our goal is to measure the topological surface states by suppression of the bulk conductivity through quantum confinement and enhancement of the surface conductivity through remote n-type doping at the  $\Gamma$  point. Conductivity measurements on undoped QWs (0.7 to 6 nm thick) show a suppression of the bulk states, such that the surface conductivity is about 15% for a 3.6 nm QW. Hall-effect measurements, which nominally indicate p-type conduction, are complicated by the presence of both electrons and holes. We have begun experiments to populate the topological electron states by doping the GaSb barrier with Te atoms, creating donor states at the  $\Gamma$  point. At the  $\Gamma$  point of the QW, the topological electron states have a lower energy than the bulk conduction band minimum. We observe n-type conduction for a remotely-doped Sb QW with a 94 nm spacer between the doped GaSb layer and the Sb QW. We plan to make high-field magneto-transport measurements to verify that the Sb surface states are populated.

<sup>1</sup>This material is based upon work supported by the NSF under Grant No. DMR-1207537

**4:30PM C28.00009 First-principles study of topological surface states in  $\text{Bi}_2\text{Se}_3/\text{ZnSe}$  superlattices<sup>1</sup>**, KYUNGWHA PARK, Virginia Tech, Blacksburg, ZHIYI CHEN, LUKAS ZHAO, THOR AXTMANN GARCIA, MARIA TAMARGO, LIA KRUSIN-ELBAUM, The City College of New York, CUNY — Topological insulators (TIs) are interesting due to robustness of surface states within a bulk band gap in the presence of time reversal symmetry. Various TI heterostructures are based on the robustness of the topological surface states. Thus, it is crucial to understand how the topological surface states are influenced by interfaces. Recently  $\text{Bi}_2\text{Se}_3/\text{Zn}_x\text{Cd}_{1-x}\text{Se}$  superlattices grown by molecular beam epitaxy showed interesting magneto-transport properties such as a single two-dimensional conducting channel per TI layer with the Berry phase of  $\pi$ . Intrigued by this experiment, we investigate topological surface states of the  $\text{Bi}_2\text{Se}_3/\text{ZnSe}$  superlattice by using density-functional theory. Based on the stoichiometry and the charge balance of the ZnSe layer, when one side of the ZnSe layer is terminated with Zn in the superlattice, the other side must be terminated with Se. Using the superlattice model and two slab models with either a Zn-terminated or Se-terminated interface, we calculate the effect of the inherent asymmetry of the ZnSe layer on the topological surface states of  $\text{Bi}_2\text{Se}_3$ , and compare our result to the experiment.

<sup>1</sup>Funding from NSF DMR-1206354, DMR-1312483, DMR-1420634, HRD-0833180, and DOD-W911NF-13-1-0159, and Computer resources from SDSC Trestles under DMR060009N and VT ARC.

**4:42PM C28.00010 Experimental preparation of lateral Heterojunction  $\text{Sb}_2\text{Te}_3/\text{Bi}_2\text{Te}_3$  Nanoplates**, FUCONG FEI, FENGQI SONG, Nanjing Univ — For the first time, lateral heterojunction of  $\text{Sb}_2\text{Te}_3\text{-Bi}_2\text{Te}_3$  was successfully realized using a two-step solvothermal method. The two crystalline components were separated well by a sharp lattice-matched interface when the optimized procedure was used. Inspecting the heterojunction using high-resolution transmission electron microscopy showed that epitaxial growth occurred along the horizontal plane. The semiconducting temperature-resistance curve and crossjunction rectification were observed, which reveal a staggered-gap lateral heterojunction with a small junction voltage. Quantum correction from the weak antilocalization reveals the well-maintained transport of the topological surface state. This is appealing for a platform for spin filters and one-dimensional topological interface states. The relevant works on materials optimization and fabrication of spin devices are already under way. (Nanoletters 2015, 15, 5905–5911))

**4:54PM C28.00011 Nonlinear optical probe of interface ferromagnetism of  $\text{EuS-Bi}_2\text{Se}_3$  heterostructures**, CHANGMIN LEE, Department of Physics, MIT, FERHAT KATMIS, Francis Bitter Magnet Lab and Department of Physics, MIT, PABLO JARILLO-HERRERO, Department of Physics, MIT, JAGADEESH S. MOODERA, Francis Bitter Magnet Lab and Department of Physics, MIT, NUH GEDIK, Department of Physics, MIT —  $\text{EuS-Bi}_2\text{Se}_3$  heterostructure is a novel magnetic topological insulator system with canted ferromagnetism induced at the interface between  $\text{EuS}$  and  $\text{Bi}_2\text{Se}_3$ . Here we use magnetic second harmonic generation (MSHG) to probe interface ferromagnetism of  $\text{EuS-Bi}_2\text{Se}_3$  heterostructures. MSHG is a powerful nonlinear optical technique that selectively probes magnetism at the surfaces and interfaces of a centrosymmetric material. In order to study how the thickness of the magnetic  $\text{EuS}$  layer affects interface ferromagnetism, we have grown  $\text{EuS-Bi}_2\text{Se}_3$  heterostructures with varying  $\text{EuS}$  thicknesses. We have also grown heterostructures in which the  $\text{EuS}$  thickness increases linearly across a single sample. We discuss how the magnetic layer thickness affects the strength and canting angle of interface magnetism.

**5:06PM C28.00012 Van Vleck Nature of Carrier-Free Ferromagnetic Order in Vanadium-Doped Three-Dimensional Topological Insulators**, MINGDA LI, CUI-ZU CHANG, MIT, LIJUN WU, JING TAO, Brookhaven National Lab, WEIWEI ZHAO, MOSES H W CHAN, Pennsylvania State University, JAGADEESH MOODERA, JU LI, MIT, YIMEI ZHU, Brookhaven National Lab, MIT TEAM, BROOKHAVEN NATIONAL LAB TEAM, PENNSYLVANIA STATE UNIVERSITY COLLABORATION — We experimentally demonstrate that the long-range ferromagnetic (FM) order in vanadium (V)-doped topological insulator  $\text{Sb}_2\text{Te}_3$  has the nature of van Vleck-type ferromagnetism, using the state-of-art low-temperature Electron Energy Loss Spectroscopy (EELS). Contrary to the temperature-independent  $\text{Te M}_{4,5}$  peak, there is an unusual redshift of the  $\text{V L}_3$  and  $\text{L}_2$  peak positions and unambiguous change of the  $\text{L}_3\text{:L}_2$  peak ratio at  $T=10\text{K}$ . Further high-order Green's function's EELS simulation and magnetotransport show that the shift of the peak position and change of the  $\text{L}_3\text{:L}_2$  ratio are originated from the development of the core-level FM order, indicating that in V-doped  $\text{Sb}_2\text{Te}_3$ , partially filled core states will also contribute to FM order. Since van Vleck magnetism is a result of summing over all states, this magnetization of core level verifies the van Vleck-type ferromagnetism in a direct manner.

**5:18PM C28.00013 Imaging Spatially Varying Magnetic Order in Proximity Induced Magnetic Topological Insulator**, AARON J. ROSENBERG, Stanford University, FERHAT KATMIS, MIT, YIHUA H. WANG, JOHN R. KIRTLEY, Stanford University, JAGADEESH S. MOODERA, MIT, KATHRYN A. MOLER, Stanford Institute for Materials and Energy Sciences, SLAC National Laboratories — Broken time-reversal symmetry on the surface states of a three dimensional topological insulator, such as  $\text{Bi}_2\text{Se}_3$ , results in quantized anomalous Hall conductance and is predicted to exhibit topological magneto-electric effects. We plan investigate how Dirac fermions interact with magnetism by imaging the magnetization of a topological insulator ( $\text{Bi}_2\text{Se}_3$ ) sandwiched between two ferromagnetic insulator layers ( $\text{EuS}$ ) with a scanning SQUID microscope. Cooling in an in-plane field leads to a magnetization that varies spatially on a micron scale, with 6-fold rotational symmetry. Understanding the origin of this magnetism may shed light on the exchange interaction and electronic properties of topological insulators.

**Monday, March 14, 2016 2:30PM - 5:30PM –**

**Session C29 DCMP DMP: Bi-based Topological Insulators** 328 - Seongshik Oh, Rutgers University

**2:30PM C29.00001 Nanoscale Andreev Reflection Spectroscopy on Bismuth-Chalcogenide Topological Insulators<sup>1</sup>**, C. R. GRANSTROM, I. FRIDMAN, University of Toronto, R. X. LIANG, University of British Columbia, H. LEI, C. PETROVIC, Brookhaven National Laboratory, SHUO YANG, K. H. WU, Chinese Academy of Sciences, J. Y. T. WEI, University of Toronto & Canadian Institute for Advanced Research — Andreev reflection (AR) is the basic mechanism underlying the superconducting proximity effect which, at the interface between a topological insulator (TI) and a spin-singlet superconductor, can induce chiral  $p$ -wave pairing in the TI. Despite this novel importance, it is not well understood how AR is affected by the unique attributes of a three-dimensional TI, namely the Dirac dispersion and helical spin-polarization of its surface states. In this work, we use both  $s$ -wave and  $d$ -wave<sup>2</sup> superconducting tips to perform AR spectroscopy at 4.2 K on flux-grown  $\text{Bi}_2\text{Se}_3$  and  $\text{Bi}_2\text{Te}_3$  single crystals, as well as epitaxial  $\text{Bi}_2\text{Se}_3$  thin films grown on  $\text{SrTiO}_3$  substrates by molecular beam epitaxy. These AR measurements are complemented by scanning tunneling spectroscopy, in order to characterize the superconducting tip as well as the doping level and surface condition of the TI sample. Our data are analyzed using BTK theory, in light of the characteristic band structure of bismuth chalcogenides, to elucidate how the band structure affects the AR process.

<sup>1</sup>Work supported by: NSERC, CFI-OIT, the Canadian Institute for Advanced Research, and the Department of Energy.

<sup>2</sup>C. S. Turel et al., **Appl. Phys. Lett.** 99, 192508 (2011)

**2:42PM C29.00002 Pressure-induced Lifshitz and Weyl Semi-metallic Phase Transitions in BiSb**, SOBHIT SINGH, Department of Physics and Astronomy, West Virginia University, Morgantown, WV-26505, IRAIS VALENCIA-JAIME, ANDRES GARCIA-CASTRO, Cinvestav-Unidad Querétaro, Querétaro-76230, México, FRANCISCO MUNÓZ, Departamento de Física, Facultad de Ciencias, Universidad de Chile, Casilla 653, Santiago 7800024, Chile, ALDO ROMERO, Department of Physics and Astronomy, West Virginia University, Morgantown, WV-26505 — By means of first-principle calculations, we report a non-magnetic stoichiometric crystal structure of BiSb with broken space-inversion symmetry. This structure belongs to the  $R\bar{3}m$  space group and it was obtained after a systematic study of the low-energy phases of  $\text{Bi}_{1-x}\text{Sb}_x$  ( $0 < x < 1$ ) compounds found by using minima hopping structure search method [1]. This structure is insulating in bulk and has non-trivial band topology. We observe pressure-induced Lifshitz and Weyl semi-metallic phases as electronic phase transitions in this system. The obtained Weyl semi-metallic phase exist in the 4.0 – 6.0 GPa pressure range. We find that a total 12 pairs of Weyl points, 12 monopoles and 12 antimonopoles, exist in the bulk Brillouin zone. The Weyl points with opposite chirality are located at different energy values yielding separate electron and hole Fermi-surfaces, which drives novel topological transport properties in this system. The surface state calculations reveal reminiscence of the Fermi-arcs at (001) surface of the BiSb slab, which further confirm the existence of Weyl semi-metallic phase in BiSb [2-4]. [1] J. Chem. Phys. 120, 9911 (2004) [2] Science 349, 622 (2015) [3] Nat Phys 11, 748 (2015) [4] Phys. Rev. X 5, 031013 (2015)

**2:54PM C29.00003 Ab initio study of the adsorption, diffusion, and intercalation of alkali metal atoms on the (0001) surface of the topological insulator  $\text{Bi}_2\text{Se}_3$** , MIKHAIL OTROKOV, Donostia International Physics Center, San Sebastian, Spain, ANASTASIA RYABISHCHENKOVA, Tomsk State University, Tomsk, Russia, MIGUEL ANGEL GOSALVEZ, Donostia International Physics Center, San Sebastian, Spain, VLADIMIR KUZNETSOV, Tomsk State University, Tomsk, Russia, EVGUENI CHULKOV, Donostia International Physics Center, San Sebastian, Spain — We present the results of an *ab initio* study of the adsorption, diffusion, and intercalation of alkali metal adatoms on the (0001) stepped surface of the topological insulator  $\text{Bi}_2\text{Se}_3$  for the case of low coverage. The calculations of the activation energies of the adatoms diffusion on the surface and in the van der Waals gaps near the steps, as well as the estimation of diffusion lengths, show that efficient intercalation through the steps is possible only for Li and Na. Data obtained for K, Rb, and Cs atoms indicate that their thermal desorption at high temperatures can start before intercalation. These results are discussed in the context of the experimental data available [?, ?].

## References

- [1] Z.-H. Zhu, et al. Phys. Rev. Lett. **107**, 186405 (2011).
- [2] M. Bianchi, et al. ACS Nano **6**, 7009 (2012).

**3:06PM C29.00004 Topological insulators are tunable waveguides for hyperbolic polaritons**, JIHI-SHENG WU, DIMITRI BASOV, MICHAEL FOGLER, University of California San Diego — We present a theoretical analysis showing that layered topological insulators, for example,  $\text{Bi}_2\text{Se}_3$  are optically hyperbolic materials in a range of THz frequencies. As such, these topological insulators possess deeply subdiffractive, highly directional collective modes: hyperbolic phonon-polaritons. We predict that in thin crystals the dispersion of these modes is split into discrete subbands and is strongly influenced by electron surface states. If the surface states are doped, then hybrid collective modes result from coupling of the phonon-polaritons with surface plasmons. The strength of the hybridization can be controlled by an external gate that varies the chemical potential of the surface states. We also show that momentum-dependence of the plasmon-phonon coupling leads to a polaritonic analog of the Goos-Hänchen effect. Directionality of the polaritonic rays and their tunable Goos-Hänchen shift are observable via THz nanoimaging.

**3:18PM C29.00005 ARPES study of the surface states and their aging in a topological insulator,  $\text{Bi}_2\text{Se}_3$** , KALOBARAN MAITI, Tata Institute of Fundamental Research — Topological insulators possess time reversal symmetry protected metallic surface states over the insulating bulk, where these surface states are expected to be immune to weak disorder, chemical passivation of the surface or temperature change. However, significant discrepancy from such behavior has been found experimentally in various materials. We studied the detailed electronic structure and its aging of a topological insulator,  $\text{Bi}_2\text{Se}_3$  employing high resolution photoemission spectroscopy. Both the band structure results and high resolution angle resolved photoemission data reveal significantly different surface electronic structure for different surface terminations. Furthermore, oxygen impurity on Se terminated surface exhibits an electron doping scenario, while oxygen on Bi terminated surface corresponds to a hole doping scenario. The intensity of the Dirac states reduces with aging indicating fragility of the topological order due to surface impurities. References

1. D. Biswas, S. Thakur, K. Ali, G. Balakrishnan, and K. Maiti, Sci. Rep. (Nature) **5**, 10260 (2015).
2. D. Biswas and K. Maiti, EPL **110**, 17001 (2015).
3. D. Biswas, S. Thakur, G. Balakrishnan, and K. Maiti, Sci. Rep. (Nature) (2015) (to be published).

**3:30PM C29.00006 Interband Spin-Orbit Coupling in Topological Surface States Explored by Photoemission Spectroscopies**, ANDREW WEBER, STEFAN MUFF, MAURO FANCIULLI, J. HUGO DIL, (1) Ecole Polytechnique Federale de Lausanne (2) Swiss Light Source, Paul Scherrer Institute, QUINN GIBSON, HUIWEN JI, IVO PLETIKOSIC, ROBERT CAVA, Department of Chemistry, Princeton University, ALEXEI FEDOROV, Advanced Light Source, Lawrence Berkeley National Laboratory, ANTHONY CARUSO, Department of Physics, University of Missouri-Kansas City, JUREK SADOWSKI, Center for Functional Nanomaterials, Brookhaven National Laboratory, ELIO VESCOVO, National Synchrotron Light Source, Brookhaven National Laboratory, TONICA VALLA, Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory — Three-dimensional crystals with a topologically non-trivial band gap in the bulk Brillouin zone are typically classified by either Z2 topological invariants or by Chern number topological invariants. The Z2 topological band insulators are said to possess surface states protected by time-reversal-symmetry and topological crystalline insulators possess surface states protected by mirror-symmetry. Here we provide evidence, through spin- and angle-resolved photoemission spectroscopy and first-principles calculations of layered  $(\text{Bi}_2)_m(\text{Bi}_2\text{X}_3)_n$  ( $\text{X} = \text{Se, Te}$ ) materials, that surfaces of Z2 strong topological insulators can possess states protected by mirror-symmetry alone. The role of interband coupling in producing mirror-protected surface states with novel Fermi contours and spin-textures will be discussed, and an argument for the unification of Z2 and Chern number invariant classifications will be made.

**3:42PM C29.00007 Strong Zeeman effects in the Landau level spectrum of  $(\text{In}_x\text{Bi}_{1-x})_2\text{Se}_3$** , DANIEL WALKUP, WENWEN ZHOU, ILIJA ZELJKOVIC, Boston College, YOSHINORI OKADA, Boston College and Tohoku University, ZHENSONG REN, Boston College, KANE SCIPIONI, Boston College and University of Illinois at Urbana-Champaign, STEPHEN WILSON, Boston College and University of California Santa Barbara, VIDYA MADHAVAN, Boston College and University of Illinois at Urbana-Champaign — We investigate the surface states of  $(\text{In}_x\text{Bi}_{1-x})_2\text{Se}_3$  by scanning tunneling spectroscopy (STS) in the range  $0 \leq x \leq 3\%$ . We carefully examine the low-lying Landau levels of the topological surface states in attempt to extract the parameters of the surface-state Hamiltonian as a function of doping. Close examination of the data oblige us to index the Landau levels in a manner different to precedent on pristine  $\text{Bi}_2\text{Se}_3$ , and fits to the Landau level spectra yield large g-factors on the order of 40, which decrease with increasing x. The Landau levels of pristine  $\text{Bi}_2\text{Se}_3$  are also reexamined, yielding high g-factors roughly consistent with results obtained from magnetic oscillations, and suggesting a decrease in the surface-state Zeeman coupling with increasing In as the topological phase transition is approached.

**3:54PM C29.00008 Nonequilibrium spin texture within a thin layer below the surface of current-carrying topological insulator Bi<sub>2</sub>Se<sub>3</sub>: A first-principles quantum transport study<sup>1</sup>**, PO-HAO CHANG, BRANISLAV NIKOLIC, Univ of Delaware, TROELS MARKUSSEN, SREN SMIDSTRUP, KURT STOKBRO, QuantumWise — Using extension of nonequilibrium Green function combined with density functional theory (NEGF+DFT) formalism to situations involving noncollinear spins and spin-orbit coupling, we investigate microscopic details (on the 1 Å scale) of nonequilibrium spin density  $S(r)$  driven by unpolarized charge current injection into a ballistic thin film of Bi<sub>2</sub>Se<sub>3</sub> as prototypical topological insulator (TI) material. We find large nonzero component of  $S(r)$  in the direction transverse to current flow on the metallic surfaces of TI, as well as within few bulk atomic layers near the surfaces because of penetration of evanescent wavefunctions from the metallic surfaces into the bulk. In addition, an order of magnitude smaller components emerge in the perpendicular (within surfaces and nearly bulk regions of TI) and longitudinal (within bulk region of TI near its surface) directions, thereby creating a complex nonequilibrium spin texture. We also demonstrate how DFT calculations with properly optimized local orbital basis set can precisely match putatively more accurate calculations with plane wave basis set for the supercell of Bi<sub>2</sub>Se<sub>3</sub>.

<sup>1</sup>P.-H.C. and B.K.N. were supported by NSF Grant No. 281 FQ ECCS 1509094. The supercomputing time was provided by 282 XSEDE, which is supported by NSF Grant No. ACI-1053575. 283 QuantumWise acknowledges support from the Danish Innovation Fund Grant No

**4:06PM C29.00009 Tunneling spectroscopy of a magnetic adatoms on topological insulator surfaces<sup>1</sup>**, M. MISIORNY, Chalmers Univ. of Technology, Göteborg, Sweden and Adam Mickiewicz Univ., Poznań, Poland, M. BJERNGAARD, Johns Hopkins Univ., Baltimore, USA and Univ. of Amsterdam, Amsterdam, The Netherlands, J. PAASKE, Univ. of Copenhagen, Copenhagen, Denmark — In this communication, we address the question of how the presence of a magnetic impurity on a topological insulator (TI) surface manifests in the inelastic electron tunneling spectroscopy (IETS) when such a system is probed by a STM. For this purpose, we consider a single magnetic adatom with arbitrary spin, whose dynamics is governed by the local magnetic anisotropy. The spin is exchange-coupled to two-dimensional helical surface electrons, corresponding to the surface of a three-dimensional TI like Bi<sub>2</sub>Se<sub>3</sub>, with its characteristic hexagonally warped Dirac cone band structure. Employing an effective exchange-tunneling model, we calculate the non-linear differential conductance from a spin-polarized STM tip to the helical substrate, valid in the perturbative regime of weak exchange-tunneling and including the nonequilibrium pumping of the adatom spin states. The interplay between the magnetic anisotropy and the spin-momentum locked surface electrons is shown to give a number of specific imprints in the IETS, which could be investigated by spin-resolved scanning tunneling spectroscopy. M. Misiorny, M. Bjerngaard and J. Paaske, manuscript in preparation

<sup>1</sup>Work supported by the Polish Ministry of Science and Education as Iuventus Plus project (IP2014 030973) in years 2015-2016.

**4:18PM C29.00010 Laser-driven parametric instability and generation of entangled photon-plasmon states in graphene and topological insulators<sup>1</sup>**, ALEXEY BELYANIN, YONGRUI WANG, Texas AM University, IVAN OLADYSHKIN, MIKHAIL TOKMAN, Institute of Applied Physics, Russian Academy of Sciences — Massless Dirac electrons in graphene and on the surface of topological insulators such as Bi<sub>2</sub>Se<sub>3</sub> demonstrate strong nonlinear optical response and support tightly confined surface plasmon modes. Although both systems constitute an isotropic medium for low-energy in-plane electron excitations, their second-order nonlinear susceptibility becomes non-zero when its spatial dispersion is taken into account. In this case the anisotropy is induced by in-plane wave vectors of obliquely incident or in-plane propagating electromagnetic waves. In this work we show that a strong (0.1-1 MW/cm<sup>2</sup>) near-infrared or mid-infrared laser beam obliquely incident on graphene can experience a parametric instability with respect to decay into lower-frequency (idler) photons and THz surface plasmons. The parametric gain leads to efficient generation of THz plasmons. Furthermore, the parametric decay process gives rise to quantum entanglement of idler photon and surface plasmon states. This enables diagnostics and control of surface plasmons by detecting idler photons. A similar parametric process can be implemented in topological insulator thin films.

<sup>1</sup>This work has been supported in part by the Air Force Office for Scientific Research through grant FA9550-15-1-0153

**4:30PM C29.00011 Electronic structures of topological insulators with non-conventional terminations<sup>1</sup>**, XIEGANG ZHU, YUN ZHANG, WEI FENG, BINGKAI YUAN, XINCHUN LAI, Science and Technology on Surface Physics and Chemistry Laboratory, Mianyang 621700, Sichuan, P. R. China — Until now, most works on topological insulators focus on the natural cleaving surfaces, *i.e.*, conventional terminations. However, researches on the non-conventional surfaces of TIs are hindered due to the difficulties in preparation of those surfaces and the existence of large number of dangling bonds on those surfaces. What is more, due to the complications in the surface lattice structures, DFT calculations on the non-conventional surfaces are not favorable. In this work, by adopting the tight binding method based Green's Function, we systematically studied the surface states of non-conventional terminations of topological insulator Bi<sub>2</sub>Te<sub>3</sub> and Bi<sub>2</sub>Se<sub>3</sub>. By using MBE, we manage to prepare topological insulator Bi<sub>2</sub>Te<sub>3</sub> thin films with fractional quintuple layer (FQL) termination. Scanning tunneling microscopy (STM) reveals that the as-grown Bi<sub>2</sub>Te<sub>3</sub> thin films may not necessarily terminate at the Van der Waals gap between two adjacent quintuple layers. The electronic structures of the FQL surfaces are studied in combination with quasi-particle interference (QPI) by scanning tunneling spectroscopy (STS). Our results suggest that the topological nature of SSs be preserved on non-conventional terminations. The robustness of the topological SSs is also demonstrated.

<sup>1</sup>Work supported by grants from NSFC11404298, CAEP2014B0302045

**4:42PM C29.00012 Role of spin-orbit scattering in quasiparticle interference**, YUHKI KOHSAKA, RIKEN CEMS, MANABU KANOU, Materials and Structures Laboratory, Tokyo Institute of Technology, TADASHI MACHIDA, KATSUYA IWAYA, TETSUO HANAGURI, RIKEN CEMS, TAKAO SASAGAWA, Materials and Structures Laboratory, Tokyo Institute of Technology — Quasiparticle interference measured by scanning tunneling spectroscopy is profoundly affected by spin textures in momentum space. In this spin effect, used to study spin-polarized electronic states with scanning tunneling spectroscopy, spin of electrons are usually supposed to be preserved unless magnetic impurities are doped. We report that electron spin is indeed not preserved but rotated by nonmagnetic impurities in the process of quasiparticle interference of a spin-polarized two-dimensional electron gas formed on the surface of a polar semiconductor BiTeI. The results imply that spin-orbit scattering plays a significant role in quasiparticle interference of materials where spin-orbit interaction is strong.

**4:54PM C29.00013 Considering a Topological Insulator as a Viscous Electronic Fluid**, THEODORE REBER, JONATHAN RAMEAU, JOHN SCHNEELOCH, RUIDAN ZHONG, GENDA GU, PETER JOHNSON, Brookhaven National Lab — Certain topological insulators' protected surface states may be better treated as hydrodynamic fluids than as collections of quasiparticles. We will present data showing that Bi<sub>0.5</sub>Sb<sub>1.5</sub>Se<sub>1.6</sub>Te<sub>1.4</sub> natively exists in the hydrodynamic regime at room temperature. A calculation of the viscosity finds that Bi<sub>0.5</sub>Sb<sub>1.5</sub>Se<sub>1.6</sub>Te<sub>1.4</sub> is surprisingly comparable to that of standard fluids such as water and helium, when normalized to the entropy of each system. This finite viscosity implies an unexpected method for current dissipation via turbulence.

**5:06PM C29.00014 Modification of the electronic band structure of the topological insulator  $\text{Bi}_2\text{Te}_3$  by the adsorption of the organic molecule Manganese Phthalocyanine**, ANDREW HEWITT, JONATHON BOLTERSDORF, PAUL MAGGARD, DANIEL DOUGHERTY, North Carolina State University — Topological insulators (TIs) have a spin-textured surface state protected by time-reversal symmetry within a bulk insulating gap. Typical approaches to breaking time-reversal symmetry have been to introduce dilute magnetic impurities into a solid-solution synthesis. Organic molecules offer another route for magnetic-doping of TIs. It has been shown that a coupling may exist, along with a new hybrid-interface state, between the magnetic molecule Manganese Phthalocyanine (MnPc) and the TI  $\text{Bi}_2\text{Te}_3$ . We report the modification of the electronic band structure by the adsorption of MnPc molecules as measured by ultraviolet photoelectron spectroscopy. We show a new state emerging below the Fermi level at less than a monolayer coverage of MnPc molecules. We also observe an *n*-doping effect as charge is transferred from the molecule to the TI substrate in agreement with recent work. We suggest that this interface system may have important implications for understanding the role of local time reversal symmetry breaking in TIs and in controlling spin injection into these novel materials.

**5:18PM C29.00015 Electrical Detection of Spin-to-Charge Conversion in a Topological Insulator  $\text{Bi}_2\text{Te}_3$** ,<sup>1</sup>, CONNIE H. LI, OLAF M.J. VAN 'T ERVE, Naval Research Laboratory, YAOYI LI, LIAN LI, University of Wisconsin, Milwaukee, BERRY T. JONKER, Naval Research Laboratory — Spin-momentum locking in topological insulators (TIs) dictates that an unpolarized charge current creates a net spin polarization. We recently demonstrated the first electrical detection of this spontaneous polarization in a transport geometry, using a ferromagnetic (FM) / tunnel barrier contact, where the projection of the TI surface state spin on the magnetization of detector is measured as a voltage [1]. Alternatively, if spins are injected into the TI surface state system, it is distinctively associated with a unique carrier momentum, and hence should generate a charge accumulation, similar to that of inverse spin Hall effect. Here we experimentally demonstrate both effects in the same device fabricated in  $\text{Bi}_2\text{Te}_3$ : the electrical detection of the spin accumulation generated by an unpolarized current flowing through the surface states, and that of the charge accumulation generated by spins injected into the surface states system. This reverse measurement is an independent confirmation of spin-momentum locking in the TI surface states, and offers additional avenue for spin manipulation. It further demonstrates the robustness and versatility of electrical access to the TI surface state spin system, an important step towards its utilization in TI-based spintronics devices.

<sup>1</sup> [1] C. H. Li, et. al., Nat. Nanotech. 9, 218 (2014). Supported by NRL core funds and Nanoscience Institute.

## Monday, March 14, 2016 2:30PM - 5:30PM – Session C30 DMP DCMP: Novel Ferroic Systems 329 - R Ramesh, UC Berkeley

**2:30PM C30.00001 Moving Towards Domain Wall Devices in Ferroics**<sup>1</sup>, MARTY GREGG, Queens University Belfast — Domain walls in ferroelectric, ferroelastic and multiferroic oxides are distinct functional materials in their own right. They can be conducting, or even superconducting, when surrounding domains are insulating [1, 2]; they can demonstrate magnetism when the surrounding bulk is non-magnetic [3] and they can contain ordered electrical dipoles when the matrix containing them is non-polar [4]. Since domain walls can also be created, destroyed, and controllably moved from place to place, there is an amazing opportunity for us to design new forms of devices in which functionality is actively and dynamically deployed (now you see it; now you don't). This is the essence of the emerging field known as “domain wall nanoelectronics” [5]. In time, this arena of research could change the way we think of nanoscale functional devices, moving increasingly towards agile circuitry and neuromorphic device architectures. While the control of domain wall injection, movement and annihilation has been developed rather well in the nanomagnetism community (in race-track [6] and domain wall logic [7] research), similar research has not been widely performed in nanoscale ferroelectrics, ferroelastics and multiferroics. This talk will discuss progress that has been made to date and the way in which nanomagnetism research can be used as a source of inspiration. Site-specific domain wall injection and motion control in both proper and improper ferroelectrics using inhomogeneous electric and elastic fields, as well as dielectric patterning in uniaxial ferroelectrics, will be specifically considered [8]. As will be shown, sufficient control has been developed to allow the creation of a diode for domain wall motion in ferroelectrics, for example. [1] J. Seidel *et al.* Nat. Mater., **8**, 229 (2009); J. Guyonnet *et al.* Adv. Mater., **23**, 5377 (2011); P. Maksymovych, *et al.* Nano Lett., **11**, 1906 (2011); T. Sluka *et al.* Nat. Commun., **4**, 1808 (2013); [2] A. Aird, E. K. H. Salje, J.Phys.:Condens. Matter, **10**, L377 (1998); [3] S. Farokhipoor *et al.*, Nature **515**, 379 (2014); [4] S. Van Aert *et al.* Adv. Mater., **24**, 523 (2012); [5] G. Catalan *et al.* Rev Mod Phys **84**, 119 (2012); [6] S. S. P. Parkin, M. Hayashi & L. Thomas, Science **320**, 190–194 (2008); [7] D. A. Allwood *et al.* Science **309**, 1688–1692 (2005). [8] J. R. Whyte *et al.*, Adv Mat, **26**, 293 (2014); J. R. Whyte *et al.*, J. Appl. Phys. **116**, 066813 (2014); J. R. Whyte *et al.*, Nat. Commun. **6**, 7361 (2015); R. G. P. McQuaid *et al.* Nat. Commun. (under review 2015).

<sup>1</sup>The author acknowledges support from the Engineering and Physical Sciences Research Council (EPSRC)

**3:06PM C30.00002 Epitaxial Thin Films of Y doped  $\text{HfO}_2$** , CLAUDY SERRAO, ASIF KHAN, RAMESH RAMAMOORTHY, SAYEEF SALAHUDDIN, UC Berkeley — Hafnium oxide ( $\text{HfO}_2$ ) is one of a few metal oxides that is thermodynamically stable on silicon and silicon oxide. There has been renewed interest in  $\text{HfO}_2$  due to the recent discovery of ferroelectricity and antiferroelectricity in doped  $\text{HfO}_2$ . Typical ferroelectrics – such as strontium bismuth tantalate (SBT) and lead zirconium titanate (PZT) – contain elements that easily react with silicon and silicon oxide at elevated temperatures; therefore, such ferroelectrics are not suited for device applications. Meanwhile, ferroelectric  $\text{HfO}_2$  offers promise regarding integration with silicon. The stable phase of  $\text{HfO}_2$  at room temperature is monoclinic, but  $\text{HfO}_2$  can be stabilized in the tetragonal, orthorhombic or even cubic phase by suitable doping. We stabilized Y-doped  $\text{HfO}_2$  thin films using pulsed laser deposition. The strain state can be controlled using various perovskite substrates and controlled growth conditions. We report on Y-doped  $\text{HfO}_2$  domain structures from piezo-response force microscopy (PFM) and structural parameters via X-ray reciprocal space maps (RSM). We hope this work spurs further interest in strain-tuned ferroelectricity in doped  $\text{HfO}_2$ .

**3:18PM C30.00003 Ab initio study of  $\text{ZrO}_2$  monolayers epitaxial on Si**<sup>1</sup>, MEHMET DOGAN, DIVINE KUMAR, CHARLES AHN, FREDERICK WALKER, SOHRAB ISMAIL-BEIGI, Yale University — Growing thin films of crystalline metal oxides on semiconductors has been of much scientific interest because of their applications in electronic devices. One research goal is to achieve ferroelectricity in a crystalline and thin oxide film that is epitaxial on a semiconductor. This would enable the realization of non-volatile field-effect transistors where the state is encoded in the polarization direction of the oxide. We study oxides that are not ferroelectric in the bulk but become ferroelectric as an ultra-thin film on a semiconductor. Recent advances in epitaxial growth methods permit fabrication of such systems. We use density functional theory to study the interface between  $\text{ZrO}_2$  monolayers and Si (001). These monolayers have multiple metastable states. We present an analysis of these configurations and energy barriers between them. We consider the likely experimental situation where different configurations coexist to form a multi-domain system, and investigate domain dynamics. Furthermore, we demonstrate that the  $\text{ZrO}_2$  monolayers can be used as a buffer layer to induce ferroelectricity in perovskite oxides such as  $\text{SrTiO}_3$  on Si. We also show that these monolayers modify the transport properties of Si which would allow for the desired device applications.

<sup>1</sup>This work is supported by the National Science Foundation through grant MRSEC NSF DMR-1119826.

**3:30PM C30.00004 Ferroelectric to paraelectric transition in  $\text{YCrO}_3$  revisited**, RAJEEV GUPTA, Department of Physics and Materials Science Programme, IIT Kanpur, Kanpur 208016, India, ASHISH MALL, Materials Science Programme, IIT Kanpur, Kanpur 208016, India, ASHISH GARG, Department of Materials Science and Engineering, IIT Kanpur, Kanpur 208016, India — X-ray diffraction (XRD) and Raman spectroscopy measurements are used to explore the origin of ferroelectricity in the orthorhombic ferroelectric oxide  $\text{YCrO}_3$ . Temperature dependent XRD studies carried out up to 900K and subsequent Reitveld refinement of the data shows that there is no evidence of any structural phase transition in  $\text{YCrO}_3$  across the ferroelectric to paraelectric phase transition at  $T_c = 470\text{K}$ . Temperature dependent unpolarized Raman spectroscopy measurements, from 300 K to 600 K, were carried out to investigate structural changes near  $T_c$  locally within the material. All Raman modes below  $600\text{ cm}^{-1}$  were assigned to phonon modes of Pnma structure and for further analysis of the Raman data, the line shape parameters were obtained by fitting a Lorentzian function to each peak. Surprisingly, despite absence of observation of any structural change in XRD measurements,  $\text{YCrO}_3$  shows a strong anomalous temperature variation near  $T_c$  in the peak positions and line widths for selected modes as a function of temperature. It is believed that  $\text{YCrO}_3$  is an improper ferroelectric and ferroelectricity arises due to local rotations of  $\text{CrO}_6$  octahedra leading to non-centrosymmetry. Our results seem to suggest that  $\text{YCrO}_3$  undergoes an iso-structural transition across  $T_c$ .

**3:42PM C30.00005 Phase Transitions in Nanoscale  $\text{SrTiO}_3$** , TIAN YU, HAN ZHANG, New Jersey Institute of Technology, MARK CROFT, Rutgers University, MEGAN SCOFIELD, DARA BOBB-SEMPLE, State University of New York at Stony Brook, JING TAO, Brookhaven National Laboratory, CHERNO JAYE, DANIEL FISHER, National Institute of Standards and Technology, STANISLAUS WONG, State University of New York at Stony Brook, TREVOR TYSON, New Jersey Institute of Technology — Free standing  $\text{SrTiO}_3$  has recently been shown to be polar for  $\sim 10\text{ nm}$  particles (APL 105, 091901 (2014)). We have conducted pressure dependent x-ray diffraction on monodispersed nanoscale samples with varying particle size. Distinctly different behavior is found in the diffraction patterns for sample with reduced size. The nature of the low temperature polar state under pressure will be discussed. The results are compared with reported work on bulk  $\text{SrTiO}_3$ . This work is supported by DOE Grant DE-FG02-07ER46402.

**3:54PM C30.00006 High-pressure synthesis of predicted oxynitride perovskite: Yttrium Silicon Oxynitride ( $\text{YSiO}_2\text{N}$ )**<sup>1</sup>, MUHTAR AHART, M. SOMAYAZULU, RAJASEKARAKUMAR VADAPPOO, Extreme Materials Initiative, Geophysical laboratory, Carnegie institution for Science, R. E. COHEN, Extreme Materials Initiative, Carnegie institution for Science; Department für Geo und Umweltwissenschaften, Ludwig-Maximilians-Universität, Germany — We synthesized the previously predicted [1] polar oxynitride perovskite in a diamond anvil cell with laser heating.  $\text{YSiO}_2\text{N}$  was predicted to have the polar  $P4mm$  structure with an effective spontaneous polarization of  $130\text{ }\mu\text{C}/\text{cm}^2$ . A mixture of Yttrium nitride (YN) and amorphous Silicon dioxide ( $\text{SiO}_2$ ) were loaded into a diamond anvil cell and laser heated at or above  $1200\text{ }^\circ\text{C}$  at  $12\text{ GPa}$ . The run products were investigated by x-ray diffraction, Raman spectroscopy, and second harmonic generation, for their phase and structural properties. The x-ray diffraction pattern ( $a = 3.235\text{ }\text{\AA}$ ,  $c = 4.485\text{ }\text{\AA}$ ) shows the phase formation of  $\text{YSiO}_2\text{N}$  and matches with the diffraction pattern derived from the first-principle predicted lattice parameters. However, minor unknown peaks are on the diffraction pattern indicating of the co-existence of other unknown phases. Further study of Raman spectroscopy observes the theoretically predicted modes, and second harmonic generation shows strong non-linear optical signal, which confirms the polar properties of  $\text{YSiO}_2\text{N}$ . [1] R. Caracas and R. E. Cohen, Appl. Phys. Lett. 91, 092902 (2007).

<sup>1</sup>This work is supported by ONR grants N00014-12-1-1038 and N00014-14-1-0561, by the ERC Advanced grant ToMCaT.

**4:06PM C30.00007 Ferroelectricity in corundum derivatives**<sup>1</sup>, MENG YE, DAVID VANDERBILT, Rutgers Univ — The search for new ferroelectric (FE) materials holds promise for broadening our understanding of FE mechanisms and extending the range of application of FE materials. The known FE materials  $\text{LiNbO}_3$  can be regarded as derived from the  $\text{Al}_2\text{O}_3$  corundum structure with cation ordering. Here we consider more general binary ( $\text{ABO}_3$ ) and ternary ( $\text{A}_2\text{BB}'\text{O}_6$ ) corundum derivatives as an extended class of potential FE materials, motivated by the fact that some members of this class have recently been synthesized. There are four structure types for these corundum derivatives, and the number of cation combinations is enormous, but in many cases the energy barriers for polarization reversal may be too large to allow FE behavior. Here we present a first-principles study of the polar structure, coherent FE barrier, and domain-wall switching barrier for a representative set of polar corundum derivatives, allowing us to identify several potentially new FE materials. We also discuss the conditions under which ferroelectricity is compatible with magnetic ordering. Finally, we identify several empirical measures that can provide a rule of thumb for estimating the barrier energies. Our results should assist in the experimental search for new FE materials in the corundum derivative family.

<sup>1</sup>This work is supported by ONR grant No. N-00014-12-1-1035

**4:18PM C30.00008 The origin of hyper-ferroelectricity in  $\text{LiBO}_3$  ( $B=\text{V, Nb, Ta, Os}$ )**, LIXIN HE, PENGFEI LI, XINGUO REN, G-C GUO, University of Science and Technology of China — The electronic and structural properties of  $\text{LiBO}_3$  ( $B=\text{V, Nb, Ta, Os}$ ) are investigated via first-principles methods. We show that  $\text{LiBO}_3$  are belong to the recently proposed hyperferroelectrics, i.e., they all have unstable longitudinal optical phonon modes. Especially, the ferroelectric-like instability in the metal  $\text{LiOsO}_3$  is a limiting case of a hyperferroelectrics, whose optical dielectric constant goes to infinity. We further show via an effective Hamiltonian that in contrast to normal proper ferroelectricity, in which the ferroelectric instability usually comes from long range coulomb interactions, the hyperferroelectric instability is due to the structure instability driven by the short range interactions. This could happen in systems with large ion size mismatches, which therefore provides a useful guidance in searching for novel hyperferroelectrics.

**4:30PM C30.00009 Ferroelectric switching pathways in  $\text{Ca}_3\text{Ti}_2\text{O}_7$  from first principles**, ELIZABETH NOWADNICK, ANDREW MULDER, CRAIG FENNIE, Cornell University — Hybrid improper ferroelectricity, where polarization can be induced via a trilinear coupling to two non-polar order parameters (in this case octahedral rotations), has recently been experimentally demonstrated in the  $n=2$  Ruddlesden-Popper compound  $\text{Ca}_3\text{Ti}_2\text{O}_7$ . The observation of an unexpectedly low ferroelectric switching barrier and abundant structural domains suggests that these domains may be critical to the switching process. Key issues that remain to be understood include what are the specific structural properties of  $\text{Ca}_3\text{Ti}_2\text{O}_7$  that enable this low-energy switching, and how these properties could be further optimized. To address these questions, we analyze the possible ferroelectric switching pathways that can be facilitated by the presence of orthorhombic twin domains and vertical stacking faults in the  $n=2$  Ruddlesden-Popper structure of  $\text{Ca}_3\text{Ti}_2\text{O}_7$ . Utilizing first principles methods, we calculate the energy barriers of the various switching pathways and study the evolution of the octahedral rotation and polar order parameters during these switching processes. These results offer insight into what is the likely switching mechanism in  $\text{Ca}_3\text{Ti}_2\text{O}_7$ , and which order parameter is primarily responsible for controlling the energy barriers.

**4:42PM C30.00010 An efficient ab-initio approach for the anharmonic properties of structurally complex ceramics<sup>1</sup>**, LIANG-FENG HUANG, JAMES M. RONDINELLI, Department of Materials Science and Engineering, Northwestern University — In the conventional quasiharmonic method for the simulation of crystal anharmonic properties (e.g., thermal expansion and thermomechanics), the phonon spectra of about ten (or more) volumes have to be calculated, which is often computationally prohibitive for complex ceramics with large unit cells. In this work, we describe an efficient alternative method, i.e., a self-consistent quasiharmonic approximation (SC-QHA) method, where the phonon modes of only two or three volumes are necessary. At the same time, it provides a convenient framework to analyze the microscopic origins underlying the anharmonic properties. We successfully apply the SC-QHA method to the hybrid improper ferroelectric  $\text{Ca}_3\text{Ti}_2\text{O}_7$  to explain the recent experimentally measured thermal expansion data [Senn, Phys. Rev. Lett., 114, 0(2015)], and related lattice dynamical properties in an efficient manner.

<sup>1</sup>Supported by the ONR MURI Understanding Atomic Scale Structure in Four Dimensions to Design and Control Corrosion Resistant Alloys under Grant No. N00014-14-1-0675.

**4:54PM C30.00011 Polarization Domain Switching of Improper Hybrid Ferroelectric  $(\text{Ca},\text{Sr})_3\text{Ti}_2\text{O}_7$  Crystals<sup>1</sup>**, SEONG JOON LIM, BIN GAO, JAEWOOK KIM, FEI-TING HUANG, SANG-WOOK CHEONG, Rutgers Center for Emergent Materials, Rutgers University, Piscataway, New Jersey, 08854, RCEM TEAM — The observation of switchable polarization loops at room temperature in  $(\text{Ca},\text{Sr})_3\text{Ti}_2\text{O}_7$ , induced by improper hybrid ferroelectricity, has drawn much attention. Since the ferroelectric polarization directly couples with structural distortions (oxygen octahedral tilting and rotation) in hybrid improper ferroelectrics, the energy barrier for polarization switching is predicted to be large, and the observation of ferroelectric polarization loops was a surprise. Furthermore, the observed complexity of the domain wall configuration in  $(\text{Ca},\text{Sr})_3\text{Ti}_2\text{O}_7$  may complicate the domain wall motion or the domain nucleation for polarization switching. Thus, it is imperative to understand the mechanism and dynamics of polarization domain switching. Particularly, it has to be clarified if polarization switching occurs through  $90^\circ$  or  $180^\circ$  switching. Comparing piezoresponse force microscope and polarized optical microscope images before and after applying electric fields consecutively, we explored the mechanism and dynamics of polarization domain switching.

<sup>1</sup>This work is funded by the Gordon and Betty Moore Foundations EPIQS Initiative through Grant GBMF4413 to the Rutgers Center for Emergent Materials.

**5:06PM C30.00012 Conducting Ferroelectric Walls, Domain Topology, and Domain Switching Kinetics in a Hybrid Improper Ferroelectric**, SANG-WOOK CHEONG, Rutgers Univ, RUTGERS CENTER FOR EMERGENT MATERIALS TEAM<sup>1</sup> — Charged polar interfaces such as charged ferroelectric domain walls or heterostructured interfaces of  $\text{ZnO}/(\text{Zn},\text{Mg})\text{O}$  and  $\text{LaAlO}_3/\text{SrTiO}_3$ , across which the normal component of electric polarization changes suddenly, can host large two-dimensional conduction. Charged ferroelectric domain walls can be highly conducting but energetically unfavored; however, they were found to be mysteriously abundant in hybrid improper ferroelectric  $(\text{Ca},\text{Sr})_3\text{Ti}_2\text{O}_7$  single crystals. From the exploration of antiphase domain boundaries, which are hidden in piezoresponse force microscopy, using dark-field electron microscopy, we have explored the macroscopic topology of polarization domains and antiphase domains. We found that the macroscopic domain topology is directly responsible for the presence of charged domain walls, and is closely related with the polarization domain switching mechanism in  $(\text{Ca},\text{Sr})_3\text{Ti}_2\text{O}_7$ .

<sup>1</sup>Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA,

**5:18PM C30.00013 Exploration of the ferroelectric properties of a new Titanium-based compound**, REMI FEDERICCI, ESPCI - UPMC - CNRS, FLORIN POPA, LUC BROHAN, Institut des matériaux Jean Rouxel (IMN) - Université de Nantes - CNRS - 2 rue de la Houssinière, B.P. 32229 44322 Nantes Cedex 03, France, BENOIT BAPTISTE, KEEVIN BENEUT, POALA GIURA, Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC), Sorbonne Université UPMC Univ. Paris 06, UMR CNRS 7590, MNHN, IRD UMR, FABIO FINOCCHI, INSP - UPMC - CNRS, ABHAY SHUKLA, Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC), Sorbonne Université UPMC Univ. Paris 06, UMR CNRS 7590, MNHN, IRD UMR, BRIGITTE LERIDON, ESPCI - UPMC - CNRS — Even though ferroelectric materials are well known and widely used in many applied fields, the families of compounds exhibiting ferroelectricity are just a few. Among them,  $\text{BaTiO}_3$  and its substitution-related compounds play a major role and have been widely investigated. We present here an experimental study on a new titanium-based perovskite structure. The synthesis and structural characterization (through XRD and Raman spectroscopy) of this material will be exposed, in excellent agreement with DFT calculations. We will demonstrate possible ferroelectricity at room temperature and discuss the probable microscopic mechanisms at play in this material.

**Monday, March 14, 2016 2:30PM - 5:30PM –**

**Session C31 DCP: Journal of Chemical Physics Editor's Choice** 331 - David Nesbitt, JILA, University of Colorado

**2:30PM C31.00001 JCP Editors Choice Award - Theoretical Methods and Algorithms<sup>1</sup>**, TODD GINGIRCH, University of California, Berkeley —

<sup>1</sup>Philip Geissler, Award Winner is not able to attend

**3:06PM C31.00002 Elucidation of Chemical Reactions by Two-Dimensional Resonance Raman Spectroscopy**, ANDREW MORAN, University of North Carolina — Two-dimensional (2D) Raman spectroscopies were proposed by Mukamel and Loring in 1985 as a method for resolving line broadening mechanisms of vibrational motions in liquids. Significant technical issues challenged the development of both five- and seven-pulse 2D Raman spectroscopies. For this reason, 2D Raman experiments were largely abandoned in 2002 following the first demonstrations of 2D infrared spectroscopies (i.e., an alternate approach for obtaining similar information). We have recently shown that 2D Raman experiments conducted under electronically resonant conditions are much less susceptible to the problems encountered in the earlier 2D Raman work, which was carried out off-resonance. In effect, Franck-Condon activity obviates the problematic selection rules encountered under electronically off-resonant conditions. In this presentation, I will discuss applications of 2D resonance Raman spectroscopies to photodissociation reactions of triiodide and myoglobin. It will be shown that vibrational resonances of the reactants and products can be displayed in separate dimensions of a 2D resonance Raman spectrum when the photo-dissociation reaction is fast compared to the vibrational period. Such 2D spectra expose correlations between the nonequilibrium geometry of the reactant and the distribution of vibrational quanta in the product, thereby yielding insight in the photo-dissociation mechanism. Our results suggest that the ability of 2D resonance Raman spectroscopy to detect correlations between reactants and products will generalize to other ultrafast processes such as electron transfer and energy transfer.

**3:42PM C31.00003 Photoexcited Nuclear Dynamics with Ab Initio Electronic Structure Theory: Is TD-DFT Ready For the Challenge?** , JOSEPH SUBOTNIK, University of Pennsylvania — In this talk, I will give a broad overview of our work in nonadiabatic dynamics, i.e. the dynamics of strongly coupled nuclear-electronic motion whereby the relaxation of a photo-excited electron leads to the heating up of phonons. I will briefly discuss how to model such nuclear motion beyond mean field theory. Armed with the proper framework, I will then focus on how to calculate one flavor of electron-phonon couplings, known as derivative couplings in the chemical literature. Derivative couplings are the matrix elements that couple adiabatic electronic states within the Born-Oppenheimer treatment, and I will show that these matrix elements show spurious poles using formal (frequency-independent) time-dependent density functional theory. To correct this TD-DFT failure, a simple approximation will be proposed and evaluated. Finally, time permitting, I will show some ab initio calculations whereby one can use TD-DFT derivative couplings to study electronic relaxation through a conical intersection.

**4:18PM C31.00004 Simulations of mean ionic activity coefficients and solubilities in aqueous electrolyte solutions<sup>1</sup>** , ATHANASSIOS PANAGIOTOPOULOS, Princeton University — Aqueous electrolyte solutions play an important role in industrial, geochemical and biological applications. The mean ionic activity coefficients quantify the deviation of salt chemical potential from ideal solution behavior; experimental measurements are available for many salts over broad ranges of concentration and temperature, but there have been practically no prior simulation results, because of sampling difficulties for explicit-solvent electrolyte solutions. We have developed a new approach for determination of activity coefficients of aqueous electrolytes [1]. Common fixed-point-charge models for water and ions are unable to reproduce simultaneously activity coefficients and solubilities. Polarizable models perform better, but still predict an incorrect temperature dependence of these properties [2]. [1] Z. Mester and A. Z. Panagiotopoulos "Mean ionic activity coefficients in aqueous NaCl solutions from molecular dynamics simulations," *J. Chem. Phys.* **142**: 044507, 10 pp (2015). <http://dx.doi.org/10.1063/1.4906320> [2] H. Jiang, Z. Mester, O. A. Moulton, I. G. Economou, and A. Z. Panagiotopoulos, "Thermodynamic and Transport Properties of H<sub>2</sub>O+NaCl from Polarizable Force Fields," *J. Chem. Theory Comput.* **11**: 3802-3810 (2015). <http://pubs.acs.org/doi/abs/10.1021/acs.jctc.5b00421>

<sup>1</sup>Work supported by the U.S. Department of Energy, Office of Basic Energy Science

**4:54PM C31.00005 Chirality-sensitive microwave spectroscopy - application to terpene molecules** , MELANIE SCHNELL, Max Planck Institute for the Structure and Dynamics of Matter — Most molecules of biochemical relevance are chiral. Even though the physical properties of two enantiomers are nearly identical, they might exhibit completely different biochemical effects, such as different odor in the case of carvone. In nature and as products of chemical syntheses, chiral molecules often exist in mixtures with other chiral molecules. The analysis of these complex mixtures to identify the molecular components, to determine which enantiomers are present, and to measure the enantiomeric excesses (ee) is still one of the challenging and very important tasks of analytical chemistry. We recently experimentally demonstrated a new method of differentiating enantiomeric pairs of chiral molecules in the gas phase. It is based on broadband rotational spectroscopy and is a three-wave mixing process that involves a closed cycle of three rotational transitions. The phase of the acquired signal bares the signature of the enantiomer, as it depends upon the product of the transition dipole moments. Furthermore, because the signal amplitude is proportional to the ee, this technique allows not only for determining which enantiomer is in excess, but also by how much. A unique advantage of our technique is that it can also be applied to mixtures of chiral molecules, even when the molecules are very similar. In my lecture, I will introduce the technique and give an update on the recent developments.

**Monday, March 14, 2016 2:30PM - 5:06PM –**

**Session C32 DCP: Device Characterization of Nanostructured Devices and Heterostructures**

332 - Matt Law, UC-Irvine

**2:30PM C32.00001 Designer Nanocrystal Materials for Photovoltaics** , CHERIE KAGAN, University of Pennsylvania — Advances in synthetic methods allow a wide range of semiconductor nanocrystals (NCs) to be tailored in size and shape and to be used as building blocks in the design of NC solids. However, the long, insulating ligands commonly employed in the synthesis of colloidal NCs inhibit strong interparticle coupling and charge transport once NCs are assembled into the solids state as NC arrays. We will describe the range of short, compact ligand chemistries we employ to exchange the long, insulating ligands used in synthesis and to increase interparticle coupling. These ligand exchange processes can have a dramatic influence on NC surface chemistry as well as NC organization in the solids, showing examples of short-range order. Synergistically, we use 1) thermal evaporation and diffusion and 2) wet-chemical methods to introduce extrinsic impurities and non-stoichiometry to passivate surface traps and dope NC solids. NC coupling and doping provide control over the density of states and the carrier type, concentration, mobility, and lifetime, which we characterize by a range of electronic and spectroscopic techniques. We will describe the importance of engineering device interfaces to design NC materials for solar photovoltaics.

**3:06PM C32.00002 Towards a Dithiocarbamate Ligand for CdS Nanoparticle-based Photocatalysis** , ANDREW O'HARA, Department of Physics and Astronomy, Vanderbilt University, ANDREW D. LACROIX, Department of Chemistry, Vanderbilt University, SOKRATES T. PANTELIDES, Department of Physics and Astronomy, Vanderbilt University, JANET E. MACDONALD, Department of Chemistry, Vanderbilt University — Photocatalysis of water into H<sub>2</sub> and O<sub>2</sub> presents a clean, renewable route for energy storage and production. Traditionally, most semiconducting nanoparticle research on photocatalysis has focused on the ability to reduce chemical systems using the photoexcited electron. Here we employ a combination of theory and experiments to develop a possible route towards the oxidation of chemical systems via the hole from photoexcitation using an asymmetric bipyridine ligand with conjugated dithiocarbamate ligand bound to the surface of cadmium sulfide nanorods. In particular, we use density functional theory to calculate the electronic levels and optical absorption of the designer ligand, free from the cadmium sulfide surface as well as attached to the surface, with and without the copper center. These calculations are compared with experimental UV/VIS absorption and fluorescence spectroscopy measurements to understand the role of copper chelation. Furthermore, theoretical comparisons are made with a related ligand known to oxidize water under an applied potential bias. Finally, we discuss whether we expect photocatalysis from the ligand and possible improvements to its design.

**3:18PM C32.00003 Influence of Defect States on Charge Transport in CuInSe<sub>2-x</sub>S<sub>x</sub> Quantum Dot Films** , HYEONG JIN YUN, ANDREW FIDLER, JAEHOON LIM, ADDIS FUHR, JEFFREY PIETRYGA, Los Alamos National Laboratory, SAM KEENE, MATT LAW, University of California, Irvine, VICTOR KLIMOV, Los Alamos National Laboratory, CENTER FOR ADVANCED SOLAR PHOTO-PHYSICS TEAM — CuInSe<sub>2-x</sub>S<sub>x</sub> quantum dots (QDs) are environmental-friendly alternatives to Cd- or Pb-based QDs for solar energy applications. The key to using QD thin films in opto-electronic devices like solar cells is understanding their charge-transport properties, which are known to be influenced by defects that can serve as carrier traps. Here, we combine field effect transistor (FET) and ultrafast transient photocurrent (u-TPC) measurements to obtain a more complete picture of the nature and role of trap states in CuInSe<sub>2-x</sub>S<sub>x</sub> QD thin films. FET devices employing indium contacts exhibit *n*-type transport with electron mobility of 5.34 10<sup>-4</sup> cm<sup>2</sup>/Vs, but they also indicate high concentrations of electrons in the films. Early-time dynamical signatures revealed in u-TPC suggest that this high carrier density arises from the presence of trap states in CuInSe<sub>2-x</sub>S<sub>x</sub> QDs. In order to reduce the density of trap states, atomic layer deposition was used to infill the CuInSe<sub>2-x</sub>S<sub>x</sub>-based devices with amorphous alumina, which results in both higher FET mobilities, and a reduction in trap-related decay signatures in u-TPC measurements.

**3:30PM C32.00004 Probing the interface between semiconducting nanocrystals and molecular metal chalcogenide surface ligands: insights from first principles<sup>1</sup>**, EMILIO SCALISE, STEFAN WIPPERMANN, Max Planck Institute fuer Eisenforschung GmbH, GIULIA GALLI, Institute for Molecular Engineering University of Chicago, DMITRI TALAPIN, Chemistry Department University of Chicago — Colloidal nanocrystals (NCs) are emerging as cost-effective materials offering exciting prospects for solar energy conversion, light emission and electronic applications. Recent experimental advances demonstrate the synthesis of fully inorganic nanocrystal solids from chemical solution processing. The properties of the NC-solids are heavily determined by the NCs surface and their interactions with the host matrix. However, information on the atomistic structure of such composites is hard to obtain, due to the complexity of the synthesis conditions and the unavailability of robust experimental techniques to probe nanointerfaces at the microscopic level. Here we present a systematic theoretical study of the interaction between InAs and InP NCs with  $\text{Sn}_2\text{S}_6^{4-}$  ligands. Employing a grand canonical ab initio thermodynamic approach we investigate the relative stability of a multitude of configurations possibly realized at the NC-ligand interface. Our study highlights the importance of different structural details and their strong impact on the resulting composite's properties. We show that to obtain a detailed understanding of experimental data it is necessary to take into account complex interfacial structures beyond simplified NC-ligand model interfaces.

<sup>1</sup>S. W. acknowledges BMBF NanoMatFutur Grant No. 13N12972. G.G. acknowledges DOE-BES for funding part of this work.

**3:42PM C32.00005 Lifetime, Mobility, and Diffusion of Photoexcited Carriers in Ligand-Exchanged PbSe Nanocrystal Films Measured by Time-Resolved Terahertz Spectroscopy<sup>1</sup>**, SIMING LI, GLENN GUGLIETTA, Drexel University, YAOTING WU, NATALIE GOGOTSI, CHRISTOPHER MURRAY, University of Pennsylvania, JASON BAXTER, Drexel University — Colloidal semiconductor nanocrystals have been used as building blocks for electronic and optoelectronic devices ranging from field effect transistors to solar cells. Properties of the nanocrystal films depend sensitively on the choice of capping ligand to replace the insulating synthesis ligands. Thus far, ligands leading to the best performance in transistors result in poor solar cell performance, and vice versa. To understand this dichotomy, we used time-resolved terahertz spectroscopy to study the mobility and lifetime of PbSe nanocrystal films with five common ligand-exchange reagents. The films treated with different displacing ligands show more than an order of magnitude difference in the peak conductivities and a bifurcation of time-dynamics. Inorganic chalcogenide ligand-exchanges with  $\text{Na}_2\text{S}$  or  $\text{NH}_4\text{SCN}$  show high mobilities but nearly complete decay of transient photocurrent in 1.4 ns. In contrast, ligand exchanges with EDA, EDT, and TBAI show lower mobilities but longer lifetimes, resulting in longer diffusion lengths. This bifurcated behavior may explain the divergent performance of field-effect transistors and photovoltaics constructed from nanocrystal building blocks with different ligand exchanges. Ref: Guglietta et al., ACS Nano, 2015.

<sup>1</sup>NSF

**3:54PM C32.00006 Biexciton Dissociation Efficiency at Quantum Dot-Oxide Interfaces**, MISCHA BONN, HAI WANG, ENRIQUE CANOVAS, Max Planck for Polymer Research — Harvesting multiexcitons populating semiconductor quantum dots (generated by carrier multiplication, CM) has been proposed as a path towards higher efficiencies in photovoltaic devices. Although CM efficiency has been widely interrogated in colloidal QD solutions, less focus has been placed on the physics regarding biexciton collection at electrodes. We investigate interfacial biexciton transfer dynamics from PbS quantum dots directly nucleated onto mesoporous  $\text{SnO}_2$  films as a function of impinging photon flux and photon energy. A priori, this system seems very well-suited for achieving efficient biexciton dissociation, as the ultrafast QD-to-oxide transfer rate for 800nm excitation is substantially faster than Auger relaxation. Remarkably, the biexciton dissociation efficiency is below the detection efficiency, i.e. essentially zero. This seemingly counterintuitive result can be understood by noting that efficient hot electron transfer at the QD-oxide interface can compete with CM within the QDs. Hot electron transfer is observed to occur on sub-100 fs timescales, nulling the CM efficiency. Implications of these results for solar energy conversion are discussed.

**4:06PM C32.00007 Matrix engineering, state filling, and charge transport in PbSe quantum dot solids**, MATT LAW, University of California, Irvine — Colloidal semiconductor quantum dots (QDs) are attractive building blocks for solar photovoltaics (PV). In this talk, I will highlight our recent progress in designing PbX (X = S, Se, Te) QD thin film absorbers for next-generation PV. Basic requirements for QD absorber layers include efficient light absorption, charge separation, charge transport, and long-term stability. I begin by discussing QD film fabrication, charge transport physics, insights from theory, and evidence that the carrier diffusion length is short and limited by electronic states in the QD band gap. Studies of carrier mobility as a function of basic film parameters such as inter-QD spacing, QD size, and QD size distribution have led to a better understanding of charge transport within highly disordered QD films. Efforts to improve carrier mobility by enhancing inter-dot electronic coupling, passivating surface states, and implementing surface doping will be highlighted. Engineering the inter-QD matrix to produce QD/inorganic or QD/organic nanocomposites is presented as a powerful way to optimize coupling, remove surface states, eliminate hysteretic charge trapping and ion motion, and achieve long-term environmental stability for high-performance, robust QD films that feature good carrier multiplication efficiency. New results on the use of atomic layer deposition infilling of QD films to yield all-inorganic QD transistors free of the bias-stress effect will be presented, and the likely role of ion transport in QD optoelectronics discussed. The use of infrared transmission spectroscopy to understand state filling and study charge transport in QD thin film transistors will be presented.

**4:42PM C32.00008 "Flash" synthesis of "giant" Mn-doped CdS/ZnSe/ZnS nanocrystals with ZnSe layer as hole quantum-well**, RUILIN XU, JIAYU ZHANG, Advanced Photonics Center, Southeast University — Usually, exciton-Mn energy transfer in Mn-doped CdS/ZnS nanocrystals (NCs) can readily outcompete the exciton trapping by an order of magnitude. However, with the accumulation of non-radiative defects in the giant shell during the rapid growth of the thick shell (up to ~20 monolayers in no more than 10 minutes), the photoluminescence (PL) quantum yield of this kind of giant NCs is significantly reduced by the accumulation of non-radiative defects during the rapid growth of thick shell. That is because the exciton-Mn energy transfer in Mn-doped CdS/ZnS NCs is significantly inhibited by the hole trapping as the major competing process, resulting from the insufficient hole-confinement in CdS/ZnS NCs. Accordingly flash synthesis of giant Mn-doped CdS/ZnSe/ZnS NCs with ZnSe layer as hole quantum-well is developed to suppress the inhibition. Meanwhile  $\text{Mn}^{2+}$  PL peak changes profoundly from ~620 nm to ~540 nm after addition of ZnSe layer. Studies are under the way to explore the relevant mechanisms.

**4:54PM C32.00009 Development of an improved molecular dynamics force field for surface-adsorption simulations of molybdenum disulfide**, GARY LEUTY, National Research Council/Air Force Research Lab, RAJIV BERRY, Air Force Research Laboratory, CHRISTOPHER MURATORE, University of Dayton, VIKAS VARSHNEY, Air Force Research Laboratory, HEATH TURNER, University of Alabama — Transition metal dichalcogenides (TMDs) such as molybdenum disulfide ( $\text{MoS}_2$ ) have garnered significant interest in recent years. With a layered structure similar to graphene, TMDs also have an intrinsic band gap. This band gap makes them an attractive alternative to graphene in many applications.  $\text{MoS}_2$  in particular has received attention due to the placement and tenability of its band gap, via functionalization, mechanical manipulation or physisorption. The latter of these is of interest in biosensor devices. Such applications are dependent on understanding physisorption on the  $\text{MoS}_2$  surface at the molecular level. This can be difficult experimentally but is possible via computer simulation techniques such as molecular dynamics (MD) simulations. MD simulations, however, require a force field accurate to the process modeled. Such a force field must correctly describe non-bonded interactions between substrate layers and between the surface and adsorbates. The force fields we are aware of have focused on intra-layer covalent bonding for structural and vibrational analysis. This work seeks to develop, through DFT and MD simulations with experimental characterization of surface adsorption, a more accurate parameterization for non-bonded interactions for  $\text{MoS}_2$ .

# Monday, March 14, 2016 2:30PM - 5:30PM –

Session C33 DPOLY: Polymers in Batteries and Electrochemical Capacitors 336 - David Hallinan, Florida State University

**2:30PM C33.00001 Exploring Strategies for High Dielectric Constant and Low Loss Polymer Dielectrics<sup>1</sup>**, LEI ZHU, Department of Macromolecular Science and Engineering, Case Western Reserve University, Cleveland, OH 44106 — Polymer dielectrics having high dielectric constant, high temperature capability, and low loss are attractive for a broad range of applications such as film capacitors, gate dielectrics, artificial muscles, and electrocaloric cooling. Unfortunately, it is generally observed that higher polarization or dielectric constant tends to cause significantly enhanced dielectric loss. It is therefore highly desired that the fundamental physics of all types of polarization and loss mechanisms be thoroughly understood for dielectric polymers. In this presentation, we intend to explore advantages and disadvantages for different types of polarization. Among a number of approaches, dipolar polarization is promising for high dielectric constant and low loss polymer dielectrics, if the dipolar relaxation peak can be pushed to above the gigahertz range. In particular, dipolar glass, paraelectric, and relaxor ferroelectric polymers are discussed for the dipolar polarization approach.

<sup>1</sup>This work is supported by NSF Polymers Program (DMR-1402733).

**2:42PM C33.00002 Energy conversion in polyelectrolyte hydrogels<sup>1</sup>**, MONICA OLVERA DE LA CRUZ, AYKUT ERBAS, Northwestern University, OLVERA DE LA CRUZ TEAM — Energy conversion and storage have been an active field of research in nanotechnology parallel to recent interests towards renewable energy. Polyelectrolyte (PE) hydrogels have attracted considerable attention in this field due to their mechanical flexibility and stimuli-responsive properties. Ideally, when a hydrogel is deformed, applied mechanical work can be converted into electrostatic, elastic and steric-interaction energies. In this talk, we discuss the results of our extensive molecular dynamics simulations of PE hydrogels. We demonstrate that, on deformation, hydrogels adjust their deformed state predominantly by altering electrostatic interactions between their charged groups rather than excluded-volume and bond energies. This is due to the hydrogel's inherent tendency to preserve electro-neutrality in its interior, in combination with correlations imposed by backbone charges. Our findings are valid for a wide range of compression ratios and ionic strengths. The electrostatic-energy alterations that we observe in our MD simulations may induce pH or redox-potential changes inside the hydrogels. The resulting energetic difference can be harvested, for instance, analogously to a Carnot engine, or facilitated for sensor applications.

<sup>1</sup>Center for Bio-inspired Energy Science (CBES)

**2:54PM C33.00003 Sulfone-Containing Dipolar Glass Polymers with High Dielectric Constant and Low Loss Property<sup>1</sup>**, YUFENG ZHU, ZHONGBO ZHANG, MORTON LITT, LEI ZHU, Department of Macromolecular Science and Engineering, Case Western Reserve University, Cleveland, Ohio 44106 — Sulfone-containing polyoxetanes are designed and synthesized for high dielectric constant and low loss dipolar glasses. The precursor polymer, poly(3,3-bis(chloromethyl)oxetane) (PBCMO) is synthesized by bulk cationic polymerization with boron trifluoride diethyl etherate as initiator. The number-average molecular weight of PBCMO is 73 kDa, with a polydispersity of 1.53 as obtained from size-exclusion chromatography results. Post-modification of PBCMO yields the dipolar glass polymer, poly(3,3-bis(methylsulfonylmethyl)oxetane) (MST). Nuclear magnetic resonance result shows 100% conversion. Differential scanning calorimetry result indicates that MST has a glass transition temperature of ca. 120 C. Due to the large dipole moment (4.25 D) and small size of the side-chain sulfone groups, MST exhibits a high dielectric constant of 8.7 and a low dissipation factor of 0.01 at 25 C and 1 Hz. This study suggests that dipolar glass polymers with large dipole moments and small-sized dipoles in the side chains are promising candidates for high energy density and low loss dielectric applications.

<sup>1</sup>This work is supported by NSF Polymers Program (DMR-1402733).

**3:06PM C33.00004 Generalized Ferroelectricity in the Mesomorphic Phase of Nylon Polymers**, ZHONGBO ZHANG, LEI ZHU, MORTON LITT, Case Western Reserve Univ — Novel ferroelectric polymers, featured by narrow electric displacement-electric (D-E) hysteresis loop, are attractive for electric energy storage applications due to their high dielectric constant and low loss property. Currently, only poly(vinylidene fluoride) (PVDF)-based copolymers (e-beamed) and terpolymers show novel ferroelectric behavior. It is desired to achieve novel ferroelectricity in other polymers such as nylons by carefully modifying the chemical and crystal structures. In this presentation, isomorphic crystals are successfully achieved by copolymerization of nylon 11 and nylon 12 with different compositions. In this way, both chemical and structural defects (i.e., dangling amide groups and kinked bonds) are introduced into the mesomorphic phase. As a consequence, hydrogen bonding interaction is successfully weakened and thus enhanced ferroelectricity with higher maximum polarization and better polarizability is obtained. In addition, for the purpose of further disturbing the mesomorphic phase and pinning effect, partially methylated nylon copolymers are synthesized. With the help of N-methylation of amide groups, the methylated nylon copolymers show relatively narrow hysteresis loops, suggesting the pinning effect from the N-methylated amide moieties.

**3:18PM C33.00005 Nanostructure and free volume effects in enhancing the dielectric response of strongly dipolar polymers**, RUI DONG, North Carolina State Univ, YASH THAKUR, Penn State Univ, VIVEK RANJAN, North Carolina State Univ, MARCO BUONGIORNO NARDELLI, North Texas Univ, QIMING ZHANG, Penn State Univ, JERRY BERNHOLC, North Carolina State Univ — Materials for capacitive energy storage with high energy density and low loss are desired in many fields. We perform multiscale simulations to investigate several members of the aromatic polyurea family. We find that the disordered structures with misaligned chains have considerably larger dielectric constants, due to significant increase in the free volume, which leads to easier reorientation of dipolar groups in the presence of an electric field. Large segment motion is still not allowed below the glass transition temperature, upholding the very low loss at high field and elevated temperature that we observe experimentally. Optimization of the nanostructure and free volume effects thus provides a new, very promising pathway for the design of high-performance dielectrics for capacitive energy storage.

**3:30PM C33.00006 Azobenzene Modified Polymer Electrolyte Membrane for Ion Gating<sup>1</sup>**, CAMILO PIEDRAHITA, Univ of Akron, MIREILLE MBALLA, The Pennsylvania State University, RUIXUAN HE, THEIN KYU, Univ of Akron — By virtue of ion concentration gradient across cell membranes, neuron cells are highly polarized driving electrical potential difference (e.g., Gibbs law). To regulate and control ion movement, living cells have specific channels with gates that are permeable to cations, enabling or excluding them via charge polarity and size. This mechanism for generating and transmitting signals from one neuron to another controls body movement via brain function. By virtue of trans-cis isomerization, azobenzene derivative (AZO) has been heavily sought for ion-gating in biological cells as a means of signal generation and transmission through nervous systems. In this work, PEM consisted of PEGDA/SCN/LiTFSI was modified with AZO derivatives for gating of lithium ions. At low concentrations of azobenzene of 3 wt

<sup>1</sup>Supported by NSF-DMR 1502543

**3:42PM C33.00007 Molecular Dynamics Simulation of Ion Solvation in Polymer Melts: Effects of Dielectric Inhomogeneity and Chain Connectivity on Solvation Energy of Ions<sup>1</sup>**, LIJUN LIU<sup>2</sup>, ISSEI NAKAMURA, State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences — We study the ion solvation in block copolymer melts and polymer blends using molecular dynamics simulations. In our simulations, polymers are formed through the connection of beads that provide the dielectric response. Thus, we highlight the effect of the dielectric contrast between different species on the solvation energy of ions. We demonstrate the local enrichment of higher-dielectric components near ions, which corresponds well with the result of mean-field theories. Moreover, the chain connectivity significantly affects the reorientation of molecular dipoles in response to the electrostatic field from ions. Thus, we illustrate the marked difference in the solvation energy between the block copolymer and polymer blend. Importantly, the solvation energy substantially depends on the chain length of the polymers, in stark contrast to the Born solvation energy. We also show that our simulation results exhibit striking similarity to the result of the recent self-consistent mean field theories. However, for strongly correlated dipoles and ions, our simulations provide qualitatively opposite behaviors to these results, suggesting further development of the theoretical frameworks.

<sup>1</sup>This work was supported by the National Natural Science Foundation of China (21474112 and 21404103). We are grateful to the Computing Center of Jilin Province for essential support.

<sup>2</sup>I use my CPS ID in this submission.

**3:54PM C33.00008 A new lattice Monte Carlo method for simulating dielectric inhomogeneity<sup>1</sup>**, XIAOZHENG DUAN, State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, ZHEN-GANG WANG, Division of Chemistry and Chemical Engineering, California Institute of Technology, ISSEI NAKAMURA, State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences — We present a new lattice Monte Carlo method for simulating systems involving dielectric contrast between different species by modifying an algorithm originally proposed by Maggs et al. The original algorithm is known to generate attractive interactions between particles that have different dielectric constant than the solvent. Here we show that such attractive force is spurious, arising from incorrectly biased statistical weight caused by the particle motion during the Monte Carlo moves. We propose a new, simple algorithm to resolve this erroneous sampling. We demonstrate the application of our algorithm by simulating an uncharged polymer in a solvent with different dielectric constant. Further, we show that the electrostatic fields in ionic crystals obtained from our simulations with a relatively small simulation box correspond well with results from the analytical solution. Thus, our Monte Carlo method avoids the need for the Ewald summation in conventional simulation methods for charged systems.

<sup>1</sup>This work was supported by the National Natural Science Foundation of China (21474112 and 21404103). We are grateful to Computing Center of Jilin Province for essential support.

**4:06PM C33.00009 Effect of Eutectic Concentration on Conductivity in PEO:LiX Based Solid Polymer Electrolytes**, PENGFEI ZHAN, LALITHA GANAPATIBHOTLA<sup>1</sup>, JANNA MARANAS, The Pennsylvania State University — Polyethylene oxide (PEO) and lithium salt based solid polymer electrolytes (SPEs) have been widely proposed as a substitution for the liquid electrolyte in Li-ion batteries. As salt concentration varies, these systems demonstrate rich phase behavior. Conductivity as a function of salt concentration has been measured for decades and various concentration dependences have been observed. A PEO:LiX mixture can have one or two conductivity maximums, while some mixtures with salt of high ionic strength will have higher conductivity as the salt concentration decrease. The factors that affect the conductivity are specific for each sample. The universal factor that affects conductivity is still not clear. In this work, we measured the conductivity of a series of PEO:LiX mixtures and statistical analysis shows conductivity is affected by the concentration difference from the eutectic concentration ( $\Delta c$ ). The correlation with  $\Delta c$  is stronger than the correlation with glass transition temperature. We believe that at the eutectic concentration, during the solidification process, unique structures can form which aid conduction.

<sup>1</sup>Currently at Dow Chemical.

**4:18PM C33.00010 Status of Li-polymer batteries for vehicle applications**, VENKAT SRINIVASAN, Lawrence Berkeley National Lab — Polymer-based batteries have the potential to revolutionize energy storage because of their ability to allow lithium metal anodes to be used, thereby promising higher energy densities. In addition, there have been vast strides in tuning polymers specific to battery applications, including the use of mixed conductors that provide both electronic and ionic conduction, and multifunctional polymers that serve as, for example, conductors and binders. There has been renewed interest in this topic recently, in the context of solid-state batteries. However, it is still not clear if the properties of presently available solid electrolytes are sufficient to meet the targets for electric vehicle applications. In this talk, we will present a material-to-cell level analysis of solid electrolytes to access the status of presently available materials. Continuum scale models will be used with experiments to understand the underlying processes in the battery and to project energy and power capabilities of solid-state cells based on their material properties. The models use appropriate material properties, where available, and are compared to experimental data to ensure validity. The validated model is then used to estimate the cell-level energy and power capability following the testing protocols specific to electric vehicle application. This analysis helps to identify existing challenges and provides guidelines for research at both material and cell levels for this promising class of next-generation batteries.

**4:54PM C33.00011 Pendant Dynamics of Ethylene-Oxide Containing Polymers with Diverse Backbones<sup>1</sup>**, JOSHUA BARTELS, JING-HAN HELEN WANG, QUAN CHEN, JAMES RUNT, RALPH COLBY, Penn State University — In the last twenty years, a wide variety of ion conducting polymers have used ether oxygens to facilitate ion conduction, and it is therefore important to understand the dynamics of ether oxygens (EOs) when attached to different polymer backbones. Four different EO-containing polymer architectures are studied by dielectric spectroscopy to understand the backbone effect on the EO dipoles. Polysiloxanes, polyphosphazenes, polymethylmethacrylates, and a polyester ether are compared, with different EO pendant lengths for the siloxane and methylmethacrylate backbones. The flexible polysiloxanes and polyphosphazene backbones impart superior segmental mobility with a glass transition temperature 15 K lower than that of the organic backbone polymers. Short EO pendants are found to impart a lower static dielectric constant at comparable EO content as compared to longer EO pendants of either inorganic or organic backbones. The long-pendant polymethylmethacrylate polymers show two relaxations corresponding to fast EOs near the pendant tail end and slow EOs close to the slower backbone, whereas the long-pendant polysiloxane shows a single relaxation due to the siloxane backbone relaxing faster than the EO pendant.

<sup>1</sup>Supported by the NSF Division of Materials Research Polymers Program through grants DMR-1404586 (RHC) and DMR-1505953 (JR)

**5:06PM C33.00012 Understanding self-assembly of charged–neutral block copolymer (BCP) and surfactant complexes using molecular dynamics (MD) simulation<sup>1</sup>**, MONOJOY GOSWAMI<sup>2</sup>, BOBBY SUMPTER<sup>3</sup>, Oak Ridge National Laboratory, MICHAEL KILBEY<sup>4</sup>, University of Tennessee, Knoxville — Here we report the formation of phase separated BCP-surfactant complexes resulting from the electrostatic self-assembly of charge-neutral block copolymers with oppositely charged surfactants. Complexation behaviors of oppositely charged polyelectrolytes has gained considerable attention in the field of soft condensed matter physics due to their potential application as functional nanomaterials for batteries, wastewater treatment and drug delivery systems. Numerous experiments have examined the self-assembled structures resulting from complexation of charge-neutral BCP and surfactants, however, there is a lack of comprehensive understanding at the fundamental level. To help bridge this gap, we use, MD simulations to study self-assembly and dynamics of the BCP-surfactant complex at the molecular level. Our results show an overcharging effect in BCPs with hydrophobic neutral blocks and a formation of core-shell colloidal structure. Hydrophilic neutral blocks, on the other hand, show stable, hairy colloidal structures with neutral blocks forming a loosely-bound, fuzzy outer layer. Our results qualitatively agree with previous SANS and SAXS experiments.

<sup>1</sup>This work was supported by the U.S. Department of Energy (DOE), Office of Basic Energy Sciences, Materials Science and Engineering Division.

<sup>2</sup>Presenting Author

<sup>3</sup>Collaborating author

<sup>4</sup>Collaborating author

**5:18PM C33.00013 Charge transport and structural dynamics in nanoscale confined ionic liquids: role of the dimensionality of confinement<sup>1</sup>**, JOSHUA SANGORO, MAXIMILIAN HERES, TYLER COSBY, Univ of Tennessee, Knoxville — Charge transport and structural dynamics in systematic series of low molecular weight and polymerized ionic liquids (ILs) confined in nanopores and as thin films are investigated by broadband dielectric spectroscopy. Detailed analysis of the dielectric spectra of ILs confined in unidirectional nanopores with mean diameters down to 3 nm and ultra thin polymer films with thicknesses down to 5 nm reveal that the dimensionality of confinement plays a crucial role in determining the resultant ion transport properties in confined ionic liquids. In this talk, the impact of the dimensionality of confinement on ion transport and dynamics will be discussed within the framework of current theories of charge transport and glassy dynamics.

<sup>1</sup>Support from National Science Foundation, DMR Polymers is gratefully acknowledged

## **Monday, March 14, 2016 2:30PM - 5:30PM – Session C34 DPOLY: The Physics of Confined Structured Fluids I** 337 - Jaroslaw Majewski, LANL

**2:30PM C34.00001 Pattern Formation in Polymer Blend Thin Films**, NIGEL CLARKE, SAM COVENEY, University of Sheffield — We introduce a model for thin films of multicomponent fluids which includes lateral and vertical phase separation, preferential component attraction at both surfaces, and surface roughening. We apply our model to thin films of binary polymer blends, and use simulations of different surface-blend interaction regimes to investigate pattern formation. We demonstrate that surface roughening couples to phase separation. For films undergoing lateral phase separation via a transient wetting layer, this results in distinct stages of roughening as the film evolves between different phase equilibria.

**2:42PM C34.00002 Intricacies of Polymer Dewetting: Nanoscaled Architectures for the Tailored Control of Polystyrene Thin Film Stability<sup>1</sup>**, JUSTIN CHEUNG, MANI SEN, ZHIZHAO CHEN, NAISHENG JIANG, MAYA ENDOH, TADANORI KOGA, Stony Brook University, SUSHIL SATIJA, National Institute of Standards and Technology — Recently, structural properties of polymer thin films have garnered attention for their relevance in the fields of organic photovoltaics and biosensors. The dewetting of polymer films poses an obstacle in the face of widespread implementation. For this study, we show that adsorbed polymer chains on a substrate surface play crucial roles in film stability. Polystyrene (PS) thin films (20 nm in thickness) with different molecular weights (Mw) on silicon (Si) substrates were used as a model. The PS films were annealed at high temperatures for several days, and Mw dependence on film stability was evidenced. At the same time, the annealed PS films were leached with a good solvent and the residue films (i.e., irreversibly adsorbed layers) were characterized by x-ray reflectivity (XR). We reveal strong correlation between film stability and two different interfacial structures of the adsorbed polymer chains: their opposing wettability against chemically identical free polymer chains results in a wetting-dewetting transition at the adsorbed polymer-free polymer interface. This is a unique aspect of polymer thin film stability and may be generalizable to other polymer systems regardless of the magnitude of solid-polymer attractive interactions.

<sup>1</sup>We acknowledge the financial support of NSF Grant (CMMI-1332499)

**2:54PM C34.00003 Two-dimensional directed polymers anchored at curved edges**, BENJAMIN LOEWE, PAUL M. GOLDBART, Georgia Institute of Technology — It is well known that the equilibrium statistical mechanics of a liquid of mutually avoiding directed polymers in two dimensions can be analyzed by means of an analogy with the imaginary-time many-body quantum mechanics of a system of particles moving in one dimension <sup>1</sup>. In this approach, the polymers have commonly been considered to be anchored to a straight-edge boundary. It has recently been shown that topological obstacles that constrain the polymer configurations, such as point-like pins, can induce voids in which the polymer density profile is heavily suppressed <sup>2</sup>. Here, we extend this approach to the study of the equilibrium statistical mechanics of liquids of mutually avoiding directed polymers that are anchored at boundaries that form closed curves, either circular or (low-eccentricity) elliptic. Specifically, we study how the curvature and eccentricity of these boundaries modifies the free energy of the system. For the case of elliptic boundaries, we show that the eccentricity alters the ground state of the quantum system, and thereby influences the structure of any constraint-induced voids in the density profile.

<sup>1</sup>P. G. de Gennes, J. Chem. Phys. 48, 2257 (1968).

<sup>2</sup>D. Z. Rocklin, S. Tan, and P. M. Goldbart, Phys. Rev. B 86, 165421 (2012)

**3:06PM C34.00004 Role of Corners in Fracture of Polymeric Adhesives**, MARK STEVENS, Sandia Natl Labs — Understanding the molecular mechanisms of deformation and failure in structural polymer adhesives is a challenging problem. About a decade ago, we performed MD simulations on coarse-grained models of epoxies or highly crosslinked polymer networks between solid adherends finding very large failure strains in contrast to experimental data. We now have performed similar tensile simulations except with open ends between two solid adherends. The open boundary and the presence of corners dramatically alters the fracture behavior. In contrast to systems with periodic boundaries, the failure strain decreases with increasing system size. This decrease greatly reduces the difference between simulation and experiment. In the open geometry, the sides of the polymer network contract inward forming wedge shaped corners where the crack initiation occurs. The deformation of the open ends is constrained by the minimal paths in the network connecting the two adherends, but the initiation of fracture is not related to the minimal paths. The crack initiation in the corners is consistent with a diverging stress in the corners according to fracture mechanics. The local stress in the corners becomes large well before failure, but in the direction parallel to the interface due to the deformation of the corners into the wedge shape.

**3:42PM C34.00005 Confinement Effects on Polymer Morphology and Properties<sup>1</sup>**, SPIROS H. ANASTASIADIS, KIRIAKI CHRISOPOULOU, ELENA PERIVOLARI, HELLEN PAPANANOU, Foundation for Research and Technology-Hellas and Univ. of Crete, Heraklion Crete, Greece — The behavior of polymers restricted in space or to surfaces/interfaces can be very different from that in the bulk. In this work, we investigate the morphology and thermal properties of poly(ethylene oxide), PEO, in nanohybrids containing two kinds of silica nanoparticles of largely different sizes in an attempt to bridge the case of severely confined polymers within the galleries of layered silicates with that of polymer-single nanoparticle nanocomposites. Hybrids with different ratio between the two silica nanoparticles were prepared in order to increase the level of confinement. The good dispersion of the nanoparticles was verified by transmission electron microscopy whereas the morphology and crystallization behavior were investigated with X-ray diffraction, Fourier transform infrared spectroscopy, differential scanning calorimetry and polarised optical microscopy. The polymer behavior in the three component systems is found indeed intermediate between that of PEO/montmorillonite and that of PEO/silica with a single-size particles. Moreover, the behavior can be tuned by varying the ratio of the large to the small nanoparticles.

<sup>1</sup>This research has been partially supported by the European Unions Horizon 2020 research and innovation programme (NFFA Europe -grant agreement No. 654360).

**3:54PM C34.00006 Conjugated polyelectrolyte assembly at water-oil interfaces.**, FENG LIU, CAILI HUANG, RUSSELL THOMAS, University of Massachusetts-Amherst, RUSSELL TEAM — Conjugated polyelectrolytes featured with conjugated backbone and functional side chains are interesting optoelectronic materials and widely used to modify electrodes in electronic devices such as light emitting diodes and solar cells to enhance device performance. Conjugated polyelectrolyte can be designed to have alternating hydrophilic and hydrophobic side chains, and thus inducing interesting surface and interface properties. In this work, we using polyfluorene based material, to study its behavior at water-toluene interface. The aliphatic side-chains will favorably interact with toluene, and amine side-chains will interact with water, making this material a good surfactant. At interface the polymer chain is stretched to a Janus type of geometry. Flattened molecules will assemble into ultra thin films via pi-pi intermolecular stacking, and thus creating barriers between liquids. When liquid volume is reduced, jamming at interface will show up. These properties are strongly affected by the environment of the liquids, such as temperature and PH values, and polyelectrolyte diffusion to interfaces. This study leads to new methods to structure liquids using single component, which can be extended to applications such as electro-spinning or fabricate flow devices.

**4:06PM C34.00007 Neutron reflectivity as a tool to study the interdigitation of grafted polymer chains and its dynamics.**, LILIANE LEGER, FRDRIK RESTAGNO, Laboratoire de Physique des Solides, CNRS, Univ. Paris-Sud, Universit Paris-Saclay, 91405 Orsay Cedex, France, FABRICE COUSIN, FRANOIS BOUE, Laboratoire Lon-Brillouin, CEA, CNRS, 91191 Gif-sur-Yvette CEDEX FRANCE, ALEXIS CHENNEVIERE, Laboratoire de Physique des Solides, CNRS, Univ. Paris-Sud, Universit Paris-Saclay, 91405 Orsay Cedex, France — Three series of experiments aimed at characterizing the interdigitation between a brush and a melt, and based on neutron reflectivity, are presented and discussed. The density profile of brush chains has been analysed for series of annealing times, on h-PS brushes in contact with d-PS melts, as a function of molecular weights and grafting densities. We show that the relaxation dynamics of the brush chains can be modelled taking into account the long relaxation time of end tethered chains along with the reptation of the melt chains which accelerates the arm retraction process. Using a non-grafted layer with a thickness smaller than the equilibrium size of the brush when immersed into a thick melt allows one to apply chosen degrees of confinement to the brush. We show that the interdigitation dynamics is affected by such confinements, in a way reminiscent of the change of the glass transition temperature in nanometric PS films. Finally, when the upper d-PS layer is sheared above  $T_g$ , flow with large slip at the wall has been observed and interpreted in terms of stretching and expulsion of the grafted chains from the melt. We show how neutron reflectivity directly evidence this expulsion.

**4:18PM C34.00008 Controlling Valence of DNA-Coated Emulsion Droplets with Multiple Flavors of DNA**, ANGUS MCMULLEN, DYLAN BARGTEIL, DAVID PINE, JASNA BRUJIC, New York University — We explore the control of valence of DNA-coated emulsion droplets as a first step in developing DNA-directed self-assembly of emulsions. Emulsion droplets differ from solid colloids in that they are deformable and the DNA strands attached to them are free to move along the emulsion surface. The balance of binding energy and droplet deformation provides control over a droplet's valence via its ligand density. After binding, some DNA often remains unbound due to the entropic cost of DNA recruitment. In practice, therefore, the assembly kinetics yield a distribution in valence. Our goal is to control valence by altering the binding kinetics with multiple flavors of DNA. We coat one set of droplets with two DNA types,  $A$  and  $B$ , and two other sets with one complementary strand,  $A'$  or  $B'$ . When an  $AB$  droplet binds to an  $A'$  droplet, the adhesion patch depletes  $A$  strands, leaving the rest of the droplet coated with more  $B$  than  $A$  strands. This increases the chance that the next droplet to bind will be a  $B'$  rather than an  $A'$ . Controlling valence will allow us to build a wide array of soft structures, such as emulsion polymers or networks with a determined coordination number. This work was supported by the NSF MRSEC Program (DMR-0820341).

**4:30PM C34.00009 Unraveling the dynamics of aminopolymer/silica composites**, JAN-MICHAEL CARRILLO, Oak Ridge National Laboratory, MILES SAKWA-NOVAK, Georgia Institute of Technology, ADAM HOLEWINSKI, University of Colorado Boulder, MATTHEW POTTER, Georgia Institute of Technology, GERNOT ROTHER, Oak Ridge National Laboratory, CHRISTOPHER JONES, Georgia Institute of Technology, BOBBY SUMPTER, Oak Ridge National Laboratory — The structure and dynamics of a model branched polymer, representing poly(ethylenimine), was investigated through coarse-grained molecular dynamics simulations and neutron scattering experiments. The monomer concentration and solvent quality were varied in the simulations and detailed comparisons between the calculated structural and dynamical properties of the unconfined polymer and those confined within an adsorbing and non-adsorbing cylindrical pore, representing the silica based structural support of the composite, were made. The simulations show a direct relationship in the structure of the polymer and the non-monotonic dynamics of the polymers as a function of monomer concentration within an adsorbing cylindrical pore. However, the non-monotonic behavior disappears for the case of the branched polymer within a non-adsorbing cylindrical pore. Overall the simulation results are in good agreement with quasi-elastic neutron scattering (QENS) studies of branched poly(ethylenimine) in mesoporous silica (SBA-15) of comparable size, suggesting an approach that can be a useful guide for understanding how to tune porous polymer composites for enhancing desired dynamical and structural behavior targeting carbon dioxide adsorption.

**4:42PM C34.00010 A new, non-destructive, real-time measurement technique of the surface area of aerogel during synthesis**, YANG SHEN, Tongji University, Shanghai, China, JEONGSEOP A. LEE, W. P. HALPERIN, Northwestern University — We have developed a new method of measuring surface area of silica aerogel during the synthesis stage using a standard pulsed NMR setup. The applicability of this method can be extended to a much broader type of chemical reactions yielding a rigid porous condensate whose surface relaxation rate differs substantially from its surrounding liquids. The number of various chemical species involved in the reaction poses little to no limitation to its applicability owing to the physics in the fast exchange limit. This is the main distinguishing feature from a conventional NMR or infrared spectroscopy method in which individual chemical bondings from various reaction intermediaries are tracked in time which is often difficult if not impossible due to complex reactions. The result from this technique yields a surface area that is analogous to the result from a well-established BET (Brunauer-Emmett-Teller) technique, but without the need for extraction or supercritical extraction of the porous medium. This work was supported by the DOE BES under grants No. DE-FG02-05ER46248. J. Lee, *et al.*, Phys Rev B., **90**, 174501 (2014). E. Collin, *et al.*, Phys Rev B., **80**, 094422 (2009).

**4:54PM C34.00011 PEE-PEO block copolymer exchange rate between micelles is detergent and temperature activated**, ALLEN SCHANTZ, PATRICK SABOE, Penn State University, HEE-YOUNG LEE, Kumoh National Institute of Technology, IAN SINES, Saint Gobain, PAUL BUTLER, NIST Center for Neutron Research, KYLE BISHOP, JANNA MARANAS, MANISH KUMAR, Penn State University — We examine the kinetics of polymer chain exchange between polymer/detergent micelles, a system relevant to the synthesis of protein-containing biomimetic membranes. Although chain exchange between polymer aggregates in water is too slow to observe, adding detergent allows us to determine chain exchange rates using time-resolved small-angle neutron scattering (TR-SANS). We examine a membrane-protein-relevant, vesicle-forming ultra-short polymer, Poly(ethyl ethylene)20-Poly(ethylene oxide)18 (PEE20-PEO18). PEE20-PEO18 is solubilized in mixed micelles with the membrane-protein-compatible non-ionic detergent octyl- $\beta$ -D-glucoside (OG). We show that OG activates block copolymer exchange, and obtain rate constants at two detergent concentrations above the CMC (critical micellar concentration) of OG. We find that chain exchange increases two orders of magnitude when temperature increases from 308 to 338 K, and that even a 1 mg/mL increase in OG concentration leads to a noticeable increase in exchange rate. We also calculate the activation energy for chain exchange and find that it is much higher than for lipid exchange. These findings explain the need for high detergent concentration and/or temperature to synthesize densely packed polymer/protein membranes.

**5:06PM C34.00012 Electrically Responsive Soft Photonic BCP Films**, ATSUSHI NORO, MAHO OHNO, YUSHU MATSUSHITA, Nagoya University — We report electro-responsive soft photonic films composed of lamellar-forming block copolymer/nonvolatile protic solvent/metal salt. Thin films of polystyrene-*b*-poly(2-vinylpyridine) (SP,  $M_n=153k$ ,  $\phi_S=0.57$ ,  $PDI=1.18$ ) were prepared by spin-coating of the solutions on ITO glass substrates, then mixture of glycol-based solvent and lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) was added to the thin films, producing soft photonic films. If needed, the spin-coated SP thin films were ionized by iodomethane before addition of the mixture of glycol-based solvent and LiTFSI. TEM observations and U-SAXS measurements revealed that these photonic films kept lamellar structures after addition of the solvent, that is, the P phase was swollen selectively with the solvent. Systematic electro-responsiveness of photonic properties of the films was also confirmed by applying voltages to the films.

**5:18PM C34.00013 Face-on and Edge-on Orientation Transition and Self-epitaxial Crystallization of All-conjugated Diblock Copolymer<sup>1</sup>**, HUA YANG, YANCHUN HAN, Chinese Academy of Sci (CAS) — The orientation transition and self-epitaxial crystallization of all-conjugated diblock copolymers poly(*p*-phenylene)-block-(3-hexylthiophene) (PPP-*b*-P3HT, BmTn) were systematically investigated by in-situ temperature-resolved two-dimensional grazing incidence X-ray diffraction (2D GIXD) in step-by-step heating and cooling process. B39T18 was selected, the results of 2D GIXD showed that the PPP block crystal adopted a face-on orientation while the crystallization of P3HT block was hindered in as-casted films. Three different molecular orientations transition were obtained in self-epitaxial crystallization circles. First, P3HT crystallize with edge-on during the heating process and induced the PPP blocks crystallized with edge-on during the cooling process. Then, the as-casted film was heated in the melting temperature region of PPP blocks and isothermally crystallized. The partial melting of PPP blocks promoted the P3HT blocks crystallize in a face-on due to the steric limitation effect, PPP blocks crystallized with a face-on via the self-epitaxy during cooling. Furthermore, the face-on transformed to thermodynamically stable edge-on in the melt annealing process.

<sup>1</sup>The financial support from the National Basic Research Program of China (973 Program, 2012CB821500) is gratefully acknowledged.

**Monday, March 14, 2016 2:30PM - 5:06PM —**

**Session C35 DBIO GSOF GSNP: Active Matter: Collective Phenomena in Living Systems II**

338 - Yuhai Tu, IBM Research

**2:30PM C35.00001 Using a stochastic field theory to understand group behavior in microswimmer suspensions**, PATRICK UNDERHILL, YUZHOU QIAN, PETER KRAMER, Rensselaer Polytech Inst — Active suspensions of microswimmers appear both in natural biological systems (e.g. bacteria or algae) and in synthetic systems. Even without external forcing they are out of equilibrium, which gives rise to interesting properties in both small and large concentrations of the particles. These properties have been observed in experiments as well as simulation/modeling approaches. It is important to understand how hydrodynamic interactions between active swimmers cause and/or alter the suspension properties including enhanced transport and mixing. One of the most successful approaches has been a mean field theory. However, in some situations the mean field theory makes predictions that differ significantly from experiments and direct (agent or particle based) simulations. There are also some quantities that cannot be calculated by the mean field theory. In this talk, we will describe our new approach which uses a stochastic field to overcome the limitations of the mean field assumption. It allows us to calculate how interactions between organisms alter the correlations and mixing in conditions where the mean field theory cannot.

**2:42PM C35.00002 ABSTRACT WITHDRAWN —**

**2:54PM C35.00003 Geometry and mechanics of growing bacterial colonies.**, ZHIHONG YOU, DANIEL PEARCE, Univ of Leiden, ANUPAM SENGUPTA, ETH Zurich, LUCA GIOMI, Univ of Leiden — Bacterial colonies are abundant on living and non-living surfaces, and are known to mediate a broad range of processes in ecology, medicine and industry. Although extensively researched from single cells up to the population levels a comprehensive biophysical picture, highlighting the cell-to-colony dynamics, is still lacking. Here, using numerical and analytical models, we study the mechanics of self-organization leading to the colony morphology of cells growing on a substrate with free boundary. We consider hard rods to mimic the growth of rod-shaped non-motile cells, and show that the colony, as a whole, does not form an ordered nematic phase, nor does it result in a purely disordered (isotropic) phase. Instead, different sizes of domains, in which cells are highly aligned at specific orientations, are found. The distribution of the domain sizes follows an exponential relation indicating the existence of a characteristic length scale that determines the domain size relative to that of the colony. A continuum theory, based on the hydrodynamics of liquid crystals, is built to account for these phenomena, and is applied to describe the buckling transition from a planar to three-dimensional (3D) colony. The theory supports preliminary experiments conducted with different strains of rod shaped bacterial cells, and reveals that the buckling transition can be regulated by varying the cell stiffness and aspect ratio. This work proposes that, in addition to biochemical pathways, the spatio-temporal organization in microbial colonies is significantly tuned by the biomechanical and geometric properties of the microbes in consideration.

**3:06PM C35.00004 Cell-cell interactions impacts on the rate of swarm expansion and the edge shape of a colony swarming *Pseudomonas aeruginosa*** , ABOUTALEB AMIRI, University of Notre Dame, Physics Deptment, GIORDANO TIERRA, Charles University in Prague, Mathematical Institute, ZHILIANG XU, University of Notre Dame, Applied computational Mathematics and Statistics , JOSHUA SHROUT, University of Notre Dame, Department of Civil and Environmental Engineering , MARK ALBER, University of Notre Dame, Physics Department, Department of Applied Computational Mathematics and Statistics — Collective motion has been observed by several bacterial species including the pathogenic bacterium *P. aeruginosa*. A flagellum at the pole is known to generate a self-propulsion motion. However, the role of type IV pili (TFP), distributed on the cell membrane, during swarming needs to be investigated in more details. In this work we introduce a model that combines the hydrodynamic and biophysical interactions in order to study the impact of the TFP interactions on swarming behavior of the colony. The model describes the motion and interactions of rod-shaped self propelled bacteria inside a thin liquid film. It also includes the equations describing the production and diffusion of surfactant rhamnolipids that is responsible for extraction of water from substrate, and Marangoni driven expansion of the thin liquid film by altering the surface tension. We show that TFP interactions are responsible for slower expansion rate of colonies of TFP deficient mutants compared to wild type. Experimental observations were used to calibrate the model and verify the model assumptions and predictions.

**3:18PM C35.00005 The 3-D spatial structure of multicellular aggregates can give them a competition-dependent growth advantage in early biofilm development** , VERNITA GORDON, U. Texas, Austin, KASPER KRAGH, U. Copenhagen, JAIME HUTCHISON, U. Texas, Austin, GAVIN MELAUGH, U. Edinburgh, CHRIS RODESNEY, U. Texas, Austin, ALED ROBERTS, U. Nottingham, YASUHIKO IRIE, U. Bath, PETER JENSEN, U. Copenhagen, STEPHEN DIGGLE, U. Nottingham, ROSALIND ALLEN, U. Edinburgh, THOMAS BJARNSHOLT, U. Copenhagen — Biofilms are structured communities of sessile microbes. Traditional models of biofilm development begin with single bacteria seeding a surface. However, biofilms can also be seeded by multicellular aggregates. How the three-dimensional structure of aggregates impacts the initiation and development of biofilms is not known. Here we use a combination of experiments and simulations to determine the impact of the seeding structure. We find that whether aggregates or single cells grow better depends on the density of single cells initially seeded. The density of single cells, which we take as our measure of the level of competition, impacts per-cell access to growth resource. The overall biomass accumulation arising from an aggregate is a combination of slow growth in the resource-limited interior, and faster growth on the sides and top. When competition is low, aggregates are disadvantaged, compared with single cells. However, when competition is high, aggregates are fitter than single cells, because the cells at the top of the aggregates have better access to growth resources than do high-density single cells on the surface.

**3:30PM C35.00006 Mechanical signaling coordinates the embryonic heart** , KEVIN CHIOU, JASON ROCKS, Department of Physics and Astronomy, University of Pennsylvania, BENJAMIN PROSSER, Department of Physiology, Penn Muscle Institute, University of Pennsylvania Perelman School of Medicine, DENNIS DISCHER, Molecular & Cell Biophysics Lab, University of Pennsylvania, ANDREA LIU, Department of Physics and Astronomy, University of Pennsylvania — The heart is an active material which relies on robust signaling mechanisms between cells in order to produce well-timed, coordinated beats. Heart tissue is composed primarily of active heart muscle cells (cardiomyocytes) embedded in a passive extracellular matrix. During a heartbeat, cardiomyocyte contractions are coordinated across the heart to form a wavefront that propagates through the tissue to pump blood. In the adult heart, this contractile wave is coordinated via intercellular electrical signaling. Here we present theoretical and experimental evidence for mechanical coordination of embryonic heartbeats. We model cardiomyocytes as mechanically excitable Eshelby inclusions embedded in an overdamped elastic-fluid biphasic medium. For physiological parameters, this model replicates recent experimental measurements of the contractile wavefront which are not captured by electrical signaling models. We additionally challenge our model by pharmacologically blocking gap junctions, inhibiting electrical signaling between myocytes. We find that while adult hearts stop beating almost immediately after gap junctions are blocked, embryonic hearts continue beating even at significantly higher concentrations, providing strong support for a mechanical signaling mechanism.

**3:42PM C35.00007 Jamming and Localization of Interacting Run-and-Tumble Particles** , RICHARD BLYTHE, MARTIN EVANS, ALEXANDER SLOWMAN, University of Edinburgh — Certain species of bacteria, notably *Escherichia coli*, exhibit a characteristic run-and-tumble motion comprising a sequence of straight-line runs at constant velocity interspersed with tumble events that randomize the direction of motion. In a many-body setting, this nonequilibrium dynamics can generate the phenomenon of motility-induced phase separation, which is also seen for a wide variety of self-propelled particles more generally. Whilst the propensity of self-propelled particles to phase separate is understood at a mesoscopic level, the origin of this behaviour in the inelastic collisions between particles implied by the microscopic dynamics is not. Here we present exact results for run-and-tumble particles in one dimension that reveal a richly-structured stationary state that comprises a superposition of three distinct physical states whose relative weights vary with the run and tumble rates, namely a jammed state, a localized state and a delocalized state.

**3:54PM C35.00008 Wing attachment position of fruit fly minimizes flight cost** , ROBERT NOEST, JANE WANG, Cornell University — Flight is energetically costly which means insects need to find ways to reduce their energy expenditure during sustained flight. Previous work has shown that insect muscles can recover some of the energy used for producing flapping motion. Moreover the form of flapping motions are efficient for generating the required force to balance the weight. In this talk, we show that one of the morphological parameters, the wing attachment point on a fly, is suitably located to further reduce the cost for flight, while allowing the fly to be close to stable. We investigate why this is the case and attempt to find a general rule for the optimal location of the wing hinge. Our analysis is based on computations of flapping free flight together with the Floquet stability analysis of periodic flight for descending, hovering and ascending cases.

**4:06PM C35.00009 Noise regulation and symmetry breaking during vertebrate body elongation.** , THIERRY EMONET, DIPJYOTI DAS, SCOTT A. HOLLEY, Yale University — Elongation of the vertebrate body axis is driven by collective cell migration and cell proliferation at the posteriorly advancing embryonic tailbud. Within the Zebrafish tailbud an ordered stream of cells symmetrically bifurcates to form the left and right halves of the presomitic mesoderm. Maintaining bilateral symmetry during this process is critical to avoid catastrophic spine deformation. Using direct comparison between experimental data and a simple model of cell migration we identified the dynamic regulation of the noise in the direction of motion of individual cells as a critical factor in maintaining symmetric cell flow. Genetic perturbations that reduced noise led to body axis deformation whereas an increase in noise led to retarded elongation as predicted by our model.

**4:18PM C35.00010 Spontaneous Planar Chiral Symmetry Breaking in Cells** , JEREMY HADIDJOJO, DAVID LUBENSKY, Univ of Michigan - Ann Arbor — Recent progress in animal development has highlighted the central role played by planar cell polarity (PCP) in epithelial tissue morphogenesis. Through PCP, cells have the ability to collectively polarize in the plane of the epithelium by localizing morphogenetic proteins along a certain axis. This allows direction-dependent modulation of tissue mechanical properties that can translate into the formation of complex, non-rotationally invariant shapes. Recent experimental observations<sup>[1]</sup> show that cells, in addition to being planar-polarized, can also spontaneously develop planar chirality, perhaps in the effort of making yet more complex shapes that are reflection non-invariant. In this talk we will present our work in characterizing general mechanisms that can lead to spontaneous chiral symmetry breaking in cells. We decompose interfacial concentration of polarity proteins in a hexagonal cell packing into irreducible representations. We find that in the case of polar concentration distributions, a chiral state can only be reached from a secondary instability after the cells are polarized. However in the case of nematic distributions, we show that a finite-amplitude (subcritical, or “first-order”) nematic transition can send the system from disorder directly to a chiral state. In addition, we find that perturbing the system by stretching the hexagonal packing enables direct (supercritical, or “second-order”) chiral transition in the nematic case. Finally, we do a Landau expansion to study competition between stretch-induced chirality and the tendency towards a non-chiral state in packings that have retained the full 6-fold symmetry. [1] K. Taniguchi *et al.*, Science (2011)

**4:30PM C35.00011 Epithelial Proliferation on Curved Toroidal Surfaces.** , YA-WEN CHANG, RICARDO CRUZ, ALEXANDROS FRAGKOPOULOS, Georgia Institute of Technology, SAMANTHA MARQUEZ, Yale University, ANDRES GARCIA, ALBERTO FERNANDEZ-NIEVES, Georgia Institute of Technology — Cellular environment influences a multitude of cellular functions by providing chemical and physical signals that modulate cell behavior, dynamics, development, and eventually survival. In strongly interacting epithelial cells, cells coordinate their behavior to respond to mechanical constraints in 2D. Local differences in tissue tension has also been shown to impact cell reproduction within an epithelial-cell sheet. Much less is known about how cells respond to out-of-plane curvatures. Here, we describe the proliferation of MDCK on toroidal hydrogel substrates, which unlike spheres or planes, have regions of both positive and negative Gaussian curvature. Additionally, the range of curvatures can be controlled by varying the size and aspect ratio of the torus, allowing us to quantify the relation between substrate curvature and cell proliferation.

**4:42PM C35.00012 Brownian microswimmer in a Poiseuille Flow** , LEONARDO APAZA-PILCO, Universidad Mayor de San Andres, MARIO SANDOVAL, Metropolitan Autonomous University — We study the two and three dimensional dynamics of a microswimmer at low-Reynolds-number in a Poiseuille flow and subject to thermal fluctuations. A deterministic analysis is also performed, and we find that under certain conditions the swimmer becomes hydrodynamically trapped thus performing periodic orbits. We provide an analytical expression where this trapping occur. A numerical solution for the coupled system of stochastic differential equations based on two parameters, the Peclet number and the ratio of the swimming velocity and the flow velocity, is also obtained. Based on this parameter space, it is found that the mean-square displacement (MSD) along the longitudinal axis (flow direction) is always quadratic in time, whereas along the transversal direction the mean-square displacement achieves a constant value due to the presence of physical boundaries. A comparison among the 2D and 3D MSD results are also discussed. Finally, the effect of the Poiseuille flow on the angular probability distribution for the two-dimensional motion is also computationally shown.

**4:54PM C35.00013 Synthetic electrophysiology: optically controlled oscillators in an engineered bioelectric tissue** , HAROLD MCNAMARA, HONGKANG ZHANG, CHRISTOPHER WERLEY, Harvard University, ADAM COHEN, Harvard University and HHMI — Multicellular electrical dynamics underlie crucial physiological functions, but the complexity of natural bioelectricity can obscure the relation of individual components (proteins, cells) to emergent system-level dynamics. Here we introduce optopatch-spiking HEK(OS-HEK) tissue, a minimal synthetic bioelectric tissue with 4 transgenic components that supports optical initiation of propagating electrical waves as well direct optical voltage readout. In conjunction with a home-built inverted microscope capable of patterned illumination, we use this tissue to probe the biophysical attributes of this excitable bioelectric medium, including dispersion relations, curvature-dependent wavefront propagation, electrotonic coupling, and effects of boundaries. We then used chemical patterning to define cellular circuits that support controllable oscillations and which retain memory for more than 2 hours (corresponding to  $10^4$  oscillations), constituting a substrate for binary bioelectric data storage. Finally, we use optical patterning of boundary conditions in a physically homogeneous tissue to design dynamically reconfigurable oscillators.

## Monday, March 14, 2016 2:30PM - 5:30PM –

Session C36 GSOFT DPOLY: Soft Colloids: From Single Particle Properties to Bulk Phase Behavior and Dynamics 339 - Alberto Fernandez-Nieves, Georgia Institute of Technology

**2:30PM C36.00001 Superresolution Microscopy of the Volume Phase Transition of pNIPAM Microgels** , GAURASUNDAR MARC CONLEY, University of Fribourg, SOFI NJD, Lund University, MARCO BRAIBANTI, University of Fribourg, PETER SCHURTENBERGER, Lund University, FRANK SCHEFFOLD, University of Fribourg — Hierarchical polymer structures such as pNIPAM microgels have been extensively studied for their ability to undergo significant structural and physical transformations that can be controlled by external stimuli such as temperature, pH or solvent composition. Here we discuss in-situ three-dimensional superresolution microscopy of dye-labeled submicron sized PNIPAM microgels [1]. We use direct Stochastic Optical Reconstruction Microscopy (dSTORM) to study the internal density distribution and the particle-to-particle variability of the volume phase transition. Moreover we discuss the potential of this technique towards future applications to more complex architectures for example microgel with anisotropic shape or ones that are doped or decorated with nanoparticles. [1] G. M. Conley, S. Nojd, M. Braibanti, P. Schurtenberger, and F. Scheffold, submitted.

**2:42PM C36.00002 Swelling of Superabsorbent Poly(Sodium-Acrylate Acrylamide) Hydrogels and Influence of Chemical Structure on Internally Cured Mortar** , MATTHEW J. KRAFCIK, KENDRA A. ERK, Purdue University School of Materials Engineering — Superabsorbent hydrogel particles show promise as internal curing agents for high performance concrete (HPC). These gels can absorb and release large volumes of water and offer a solution to the problem of self-desiccation in HPC. However, the gels are sensitive to ions naturally present in concrete. This research connects swelling behavior with gel-ion interactions to optimize hydrogel performance for internal curing, reducing the chance of early-age cracking and increasing the durability of HPC. Four different hydrogels of poly(sodium-acrylate acrylamide) are synthesized and characterized with swelling tests in different salt solutions. Depending on solution pH, ionic character, and gel composition, different swelling behaviors are observed. As weight percent of acrylic acid increases, gels demonstrate higher swelling ratios in reverse osmosis water, but showed substantially decreased swelling when aqueous cations are present. Additionally, in multivalent cation solutions, overshoot peaks are present, whereby the gels have a peak swelling ratio but then deswell. Multivalent cations interact with deprotonated carboxylic acid groups, constricting the gel and expelling water. Mortar containing hydrogels showed reduced autogenous shrinkage and increased relative humidity.

**2:54PM C36.00003 Dynamics and filtration of microgel suspensions** , GERHARD NAEGELE, RAFAEL ROA, JONAS RIEST, Institute of Complex Systems, ICS-3, Forschungszentrum Juelich GmbH, 52425 Juelich, Germany — Microgel suspensions exhibit interesting transport properties determined by direct and hydrodynamic interactions. Using an annulus model to account for solvent permeability, we calculate the diffusion function and sedimentation coefficient of PNIPAM microgel suspensions, in excellent agreement with experimental results [1]. Moreover, an extension of our precise analytic methods to long-time properties including viscosity and self-diffusion coefficient is presented, with results compared to simulation and experimental data. The predicted transport properties are an important ingredient to the modeling of convective-diffusive transport in membrane ultrafiltration of permeable particles. The efficiency of the separation process depends on hydrodynamic boundary conditions, membrane properties and particle interactions. We calculate the concentration polarization layer and permeate flux at different operating conditions for cross-flow ultrafiltration of non-ionic [2] and ionic [3] microgels. Small microgel permeability already affects the filtration significantly [2].

1. J. Riest, T. Eckert, W. Richtering, G. Nägele, *Soft Matter* **11**, 2821 (2015)
2. R. Roa, E.K. Zholkovskiy, G. Nägele, *Soft Matter* **11**, 4016 (2015)
3. R. Roa, J. Riest, G. Nägele *et al.*, to be submitted (2015)

### 3:06PM C36.00004 Soft particles with anisotropic interactions<sup>1</sup>, PETER SCHURTENBERGER, Lund University

— Responsive colloids such as thermo- or pH-sensitive microgels are ideal model systems to investigate the relationship between the nature of interparticle interactions and the plethora of self-assembled structures that can form in colloidal suspensions. They allow for a variation of the form, strength and range of the interaction potential almost at will. While microgels have extensively been used as model systems to investigate various condensed matter problems such as glass formation, jamming or crystallization, they can also be used to study systems with anisotropic interactions. Here we show results from a systematic investigation of the influence of softness and anisotropy on the structural and dynamic properties of strongly interacting suspensions. We focus first on ionic microgels.<sup>2 3</sup> Due to their large number of internal counterions they possess very large polarisabilities, and we can thus use external electrical ac fields to generate large dipolar contributions to the interparticle interaction potential. This leads to a number of new crystal phases, and we can trigger crystal-crystal phase transitions through the appropriate choice of the field strength.<sup>4 5</sup> We then show that this approach can be extended to more complex particle shapes<sup>6</sup> in an attempt to copy nature's well documented success in fabricating complex nanostructures such as virus shells via self assembly.<sup>8</sup>

<sup>1</sup>European Research Council (ERC-339678-COMPASS)

<sup>2</sup>P. Holmqvist, P.S. Mohanty, G. Ngele, P. Schurtenberger, and M. Heinen, Phys. Rev. Lett. 109, 048302 (2012)

<sup>3</sup>J. Riest, P. Mohanti, P. Schurtenberger, and C. N. Likos, Z. Phys. Chem. 226, 711 (2012)

<sup>4</sup>S. Njd, P. S. Mohanty, P. Bagheri, A. Yethiraj and P. Schurtenberger, Soft Matter 9, 9199 (2013)

<sup>5</sup>P. S. Mohanty, P. Bagheri, S. Njd, A. Yethiraj and P. Schurtenberger, Phys. Rev. X 5, 011030 (2015)

<sup>6</sup>J. J. Crassous, A. M. Mihut, L. K. Mnsson, and P. Schurtenberger, Nanoscale 7, 15971-15982 (2015).

<sup>7</sup>Linda K. Mnsson, Jasper N. Immink, Adriana M. Mihut, Peter Schurtenberger, and Jrme J. Crassous, Faraday Discussions 181, 49 (2015).

<sup>8</sup>J. J. Crassous, A. M. Mihut, E. Wernersson, P. Pfliderer, J. Vermant, P. Linse, and P. Schurtenberger, Nature Communications 5:5516 doi: 10.1038/ncomms6516 (2014)

### 3:42PM C36.00005 Glass transition and jamming in soft microgel suspensions: Relationship between alpha relaxation times and elastic energy scales

, JOHN HYATT, Georgia Inst of Tech, XIAOBO HU, University of North Carolina, L. ANDREW LYON, Chapman University, ALBERTO FERNANDEZ-NIEVES, Georgia Inst of Tech — Glassy and jammed states of soft colloidal matter combine several open questions — how are glassy and jammed states differentiated from one another and from equilibrium states of dense suspensions, and how should particle “softness” be quantified? We combine light scattering and rheological measurements of well-characterized soft microgel particles at various packing fractions and degrees of swelling to answer these questions. We identify several regimes of liquid, supercooled, glassy, and jammed behavior that correlate with an increasing elastic energy scale due to interparticle interactions. When this energy scale increases above  $k_B T$ , the entropically-driven glassy state gives way to a jammed state dominated by elastic interactions.

### 3:54PM C36.00006 Swelling, Compressibility, and Phase Behavior of Soft Ionic Microgels<sup>1</sup>

ALAN DENTON, Dept. of Physics, North Dakota State University — Soft colloids have inspired great attention recently for their rich and tunable materials properties. Particular interest has focused on microgels — microscopic cross-linked polymer gel particles that, when dispersed in water, become swollen and can acquire charge through dissociation of counterions. Electrostatic interparticle interactions strongly influence the structure and thermodynamics of ionic microgel suspensions\*. Permeability to solvent molecules and small ions creates a competition between elastic and electrostatic forces that determines equilibrium particle sizes. Swelling can be controlled by adjusting temperature, pH, and salt concentration, with applications to chemical/biosensing and targeted drug delivery. By combining molecular dynamics and Monte Carlo simulation with Poisson-Boltzmann theory of electrostatics and Flory-Rehner theory of swollen polymer networks, we investigate swelling and compressibility of ionic microgel particles and implications for thermodynamic phase behavior of bulk suspensions at concentrations approaching and exceeding hard-sphere close packing. Predictions for particle size and osmotic pressure are compared with available experimental data.

\*M. M. Hedrick, J. K. Chung, and A. R. Denton, J. Chem. Phys. 142, 034904 (2015).

<sup>1</sup>This work was supported by the National Science Foundation under Grant No. DMR-1106331.

### 4:06PM C36.00007 Structure and Hydration of Highly Branched, Monodisperse Phytoglycogen Nanoparticles

, JOHN ATKINSON, University of Guelph, JONATHAN NICKELS, CHRISTOPHER STANLEY, SOULEYMANE DIALLO, JOHN KATSARAS, Oak Ridge National Laboratory, JOHN DUTCHER, University of Guelph — Monodisperse phytoglycogen nanoparticles are a promising, new soft colloidal nanomaterial with many applications in the personal care, food, nutraceutical and pharmaceutical industries. These applications rely on exceptional properties that emerge from the highly branched structure of phytoglycogen and its interaction with water, such as extraordinarily high water retention, and low viscosity and exceptional stability in water. The structure and hydration of the nanoparticles was characterized using small angle neutron scattering (SANS) and quasielastic neutron scattering (QENS). SANS allowed us to determine the size of the nanoparticles, evaluate their radial density profile, quantify the particle-to-particle spacing, and determine their water content. The results show clearly that the nanoparticles are highly hydrated, with each nanoparticle containing 250% of its mass in water, and that aqueous dispersions approach a jamming transition at  $\sim 25\%$  (w/w). QENS experiments provided an independent and consistent measure of the high level of hydration of the particles.

### 4:18PM C36.00008 High Deformability and Particle Size Distribution of Monodisperse Phytoglycogen Nanoparticles Revealed By Atomic Force Microscopy Imaging

, BENJAMIN BAYLIS, JOHN DUTCHER, University of Guelph — We have used atomic force microscopy (AFM) imaging in water to determine the volume of hydrated monodisperse phytoglycogen nanoparticles adsorbed onto mica surfaces. By significantly reducing the interaction between the AFM tip and the “sticky” nanoparticles, we were able to obtain high quality images. We found that the adsorbed particles are highly deformed, forming pancake-like objects on the hydrophilic mica surface. By measuring the distribution of particle volumes, we calculated the average effective spherical radius of the hydrated particles, and compared this value with that measured in solution using small angle neutron scattering. These measurements illustrate the distinct advantages of AFM imaging over other imaging techniques, namely the ability to measure the height of objects in a liquid environment.

### 4:30PM C36.00009 Rheology of Dilute Aqueous Dispersions of Monodisperse Phytoglycogen Nanoparticles

, HURMIZ SHAMANA, JOHN DUTCHER, University of Guelph — The viscosity of dilute colloidal dispersions is well described by the Einstein relation, which is linear in the volume fraction of the particles. For hard spheres, this allows the calculation of the specific volume of the spheres [1]. For soft colloidal particles, the analysis of the data can be complicated by the uptake of the solvent by the particles. We have measured the concentration dependence of the zero shear viscosity of dilute aqueous dispersions of monodisperse phytoglycogen nanoparticles, which absorb a large amount of water (each nanoparticle contains about 250% of its mass in water). By using values of the particle size and the hydrated and dehydrated molecular weights determined using neutron scattering, we can interpret the measured viscosity-concentration data in terms of the Einstein relation to obtain the particle density and corresponding volume fraction of the dispersions. [1] J.C. van der Werff et al., Phys. Rev. A 39, 795 (1989).

**4:42PM C36.00010 Ligand-Driven Phase Separation in Binary Particle Brush Materials<sup>1</sup>**, MICHAEL BOCKSTALLER, MICHAEL SCHMITT, JIANAN ZHANG, JIAJUN YAN, KRZYSZTOF MATYJASZEWSKI, Carnegie Mellon University — The tethering of polymer chains to the surface of nanoparticles (to form so-called 'particle brush materials') has emerged as an effective means to enable the bottom-up assembly of one-component hybrid materials with controlled microstructure and improved mechanical stability as well as novel optical or acoustic properties. The polymer-like interactions and response of these particle-brush materials suggest intriguing new opportunities to control structure formation in multicomponent particle mixtures. This contribution will demonstrate that polymer-ligand interactions can drive phase separation processes in mixed particle systems that share analogies to those of regular binary polymer blends. The role of particle size, density and degree of polymerization of tethered chains as well as the interaction parameter between the distinct tethered chains on the mechanism and kinetics of phase separation processes in mixed particle brush systems will be discussed. Ligand-driven phase separation will be shown to enable the efficient fabrication of monochromatic domain structured in mixed quantum dot systems that might find application in next generation quantum dot-enabled LEDs.

<sup>1</sup>Support by the National Science Foundation (via grant DMR-1410845) is gratefully acknowledged.

**4:54PM C36.00011 Colloidal models for anisotropic particles**, MARTIN GIRARD, MONICA OLVERA DE LA CRUZ, Northwestern Univ — Nanoparticles (NP) self-assembly is often thought as an equivalent to crystallization of atoms, where NP pairs exhibits effective potentials similar to atomic interactions. For the usual spherical NPs, this potential is only dependent on the distance between the particles due to symmetry. Use of anisotropic NPs provide an analog to atomic orbitals, leading to anisotropic effective potentials, which can be used to obtain new crystal lattices.

We express the effective potential of anisotropic NPs as the overlap between two functions, each of which is only dependent on the position and orientation of a single particle. Using a Fourier method, this contribution is expended into spherical harmonics and directly calculated in molecular dynamics simulations, reminiscent of energy calculations in quantum mechanics.

Using the effective potential of two spherical DNA-grafted NPs, we show an approximate method to obtain the Fourier components of an anisotropic shape, as well as the resulting simulations.

**5:06PM C36.00012 Mesoscale simulation of asphaltene aggregation<sup>1</sup>**, JIANG WANG, ANDREW FERGUSON, University of Illinois Urbana-Champaign — Asphaltenes constitute a heavy aromatic crude oil fraction that can aggregate and precipitate out of solution. Association is thought to proceed hierarchically according to the Yen-Mullins model, but the molecular mechanisms and pathways remain poorly understood. In this study, we perform molecular dynamics simulations of the aggregation of hundreds of asphaltenes over microseconds using the coarse-grained Martini force field. We identified a hierarchical self-assembly mechanism consistent with Yen-Mullins model, but the details of which are strongly dependent on asphaltene molecular structure. Monomeric asphaltenes first self-assemble into 1-D rod-like nanoaggregates, followed by the formation of clusters of nanoaggregates. At high concentrations, asphaltenes with short aliphatic side chains assemble into a percolating network with the binding of 1-D rods. Conversely, molecules with more and longer side chains cannot efficiently stack, producing a fractal network of 1-D rods suspended in a sea of interpenetrating aliphatic side chains. Our results provide the first molecularly-detailed validation of the full Yen-Mullins hierarchy, and are in good agreement with recent computational and experimental studies.

<sup>1</sup>ACS Petroleum Research Fund

**5:18PM C36.00013 Optical Characterization of Temperature- and Composition-Dependent Microstructure in Asphalt Binders**, ADAM RAMM, Department of Physics, The University of Texas at Austin, SAKIB NAZMUS, AMIT BHASIN, Department of Civil Engineering, The University of Texas at Austin, MICHAEL DOWNER, Department of Physics, The University of Texas at Austin — We introduce noncontact optical microscopy and optical scattering to characterize asphalt binder microstructure at temperatures ranging from 15 to 85°C for two compositionally different asphalt binders. We benchmark optical measurements against rheometric measurements of the magnitude of the temperature-dependent bulk complex shear modulus  $|G^*(T)|$ . The main findings are: (1) Elongated ( $5 \times 1 \mu\text{m}$ ), striped microstructures (known from AFM studies as "bees" because they resemble bumble-bees) are resolved optically, found to reside primarily at the surface, and do not reappear immediately after a single heating-cooling cycle. (2) Smaller ( $1 \mu\text{m}^2$ ) microstructures with no observable internal structure (hereafter dubbed ants), are found to reside primarily in the bulk, to persist after multiple thermal cycles and to scatter light strongly. Optical scattering from "ants" decreases to zero with heating from 15 to 65°C, but recovers completely upon cooling back to 15°C, albeit with distinct hysteresis. (3) Rheometric measurements of  $|G^*(T)|$  reveal hysteresis that closely resembles that observed by optical scatter, suggesting that thermally-driven changes in microstructure volume fraction cause corresponding changes in  $|G^*(T)|$ .

**Monday, March 14, 2016 2:30PM - 5:30PM –**  
**Session C37 GSOFT DBIO DPOLY: Physics of Bioinspired Materials I** 340 - Qiming Wang, University of Southern California

**2:30PM C37.00001 Condensation on Slippery Asymmetric Bumps**, KYOO-CHUL PARK, Harvard University, PHILSEOK KIM, SLIPS Technologies, Inc., JOANNA AIZENBERG, Harvard University — Controlling dropwise condensation by designing surfaces that enable droplets to grow rapidly and be shed as quickly as possible is fundamental to water harvesting systems, thermal power generation, distillation towers, etc. However, cutting-edge approaches based on micro/nanoscale textures suffer from intrinsic trade-offs that make it difficult to optimize both growth and transport at once. Here we present a conceptually different design approach based on principles derived from Namib desert beetles, cacti, and pitcher plants that synergistically couples both aspects of condensation and outperforms other synthetic surfaces. Inspired by an unconventional interpretation of the role of the beetle's bump geometry in promoting condensation, we show how to maximize vapor diffusion flux at the apex of convex millimetric bumps by optimizing curvature and shape. Integrating this apex geometry with a widening slope analogous to cactus spines couples rapid drop growth with fast directional transport, by creating a free energy profile that drives the drop down the slope. This coupling is further enhanced by a slippery, pitcher plant-inspired coating that facilitates feedback between coalescence-driven growth and capillary-driven motion. We further observe an unprecedented six-fold higher exponent in growth rate and much faster shedding time compared to other surfaces. We envision that our fundamental understanding and rational design strategy can be applied to a wide range of phase change applications.

**2:42PM C37.00002 Long-lived Multifunctional Superhydrophobic Heterostructure via Molecular Self-supply**, YONGFENG HUANG, SHENG MENG, Institute of Physics, Chinese Academy of Sciences, INSTITUTE OF PHYSICS, CHINESE ACADEMY OF SCIENCES TEAM — Superhydrophobic (SHO) surfaces with a large contact angle ( $\geq 150^\circ$ ) and low sliding angle ( $< 10^\circ$ ) are highly desirable in both fundamental science and myriad applications. Current approaches to fabricate such surfaces require calcinating at high temperatures, tedious and time-consuming treatments, toxic chemicals, and/or processing with intricate instruments. Long-duration SHO surfaces are even more challenging due to easy contamination by organic pollutants in dry conditions. To overcome these difficulties we design a simple approach via self-supplying of low surface tension chemicals to nanoparticles to fabricate multifunctional SHO heterostructures. Our method features room temperature, rapid processing, with environment-friendly raw materials. With multiple functions such as photocatalysis and transparency SHO surfaces extend their lifetime and enable self-sustaining environment maintenance.

**2:54PM C37.00003 Biphilic Surfaces for Enhanced Water Collection from Humid Air<sup>1</sup>**, JASON BENKOSKI, KONSTANTINOS GERASOPOULOS, WILLIAM LUEDEMAN, Johns Hopkins University APL — Surface wettability plays an important role in water recovery, distillation, dehumidification, and heat transfer. The efficiency of each process depends on the rate of droplet nucleation, droplet growth, and mass transfer. Unfortunately, hydrophilic surfaces are good at nucleation but poor at shedding. Hydrophobic surfaces are the reverse. Many plants and animals overcome this tradeoff through biphilic surfaces with patterned wettability. For example, the *Stenocara* beetle uses hydrophilic patches on a superhydrophobic background to collect fog from air. Cribellate spiders similarly collect fog on their webs through periodic spindle-knot structures. In this study, we investigate the effects of wettability patterns on the rate of water collection from humid air. The steady state rate of water collection per unit area is measured as a function of undercooling, angle of inclination, water contact angle, hydrophilic patch size, patch spacing, area fraction, and patch height relative to the hydrophobic background. We then model each pattern by comparing the potential and kinetic energy of a droplet as it rolls downwards at a fixed angle. The results indicate that the design rules for collecting fog differ from those for condensation from humid air.

<sup>1</sup>The authors gratefully acknowledge the Office of Naval Research for financial support through grant number N00014-15-1-2107.

**3:06PM C37.00004 Transition dynamics from macro- to micro-phase separation in asymmetric lipid bilayers<sup>1</sup>**, SHUNSUKE SHIMOBAYASHI, MASATOSHI ICHIKAWA, Department of Physics, Kyoto University, TAKASHI TANIGUCHI, Department of Chemical Engineering, Kyoto University — In general, phase separation in binary liquid mixtures completes by relaxation below the transition temperature. The coarsening dynamics to complete phase separation have been extensively investigated in binary mixture systems. In contrast, the reverse dynamics from macro- to micro-phase separation remains poorly understood because no appropriate experiments and models exist for investigating this phenomenon. In this talk, we present the direct observations of morphological transitions from macro- to micro-phase separation using micrometer-sized asymmetric lipid vesicles exposed to externally added glycolipids (GM1:monosialotetrahexosylganglioside). The transition occurs via stripe morphology as a metastable state. During the transition, monodisperse micro domains emerge through repeated scission events of the stripe domains. Moreover, we numerically confirmed the transitions by the time-dependent Ginzburg-Landau model, which describes phase separation and bending elastic membrane. Numerical results suggest crucial roles of the local spontaneous curvature induced by the local asymmetric lipid composition.

<sup>1</sup>This work was supported by Grant-in-Aid for JSPS Fellows Grant (No. 25-1270) and by KAKENHI (Nos. 26707020, 25103012, 26115709 and 15H03708).

**3:18PM C37.00005 Bio-inspired design of geometrically interlocked 3D printed joints.<sup>1</sup>**, S KUMAR<sup>2</sup>, NOEL OLIVA<sup>3</sup>, Masdar Institute, Abu Dhabi, KUMAR'S LAB TEAM — The morphology of the adhesive-adherend interface significantly affects the mechanical behavior of adhesive joints. As seen in some biocomposites like human skull, or the nacre of some bivalve molluscs' shells, a geometrically interlocking architecture of interfaces creates toughening and strengthening mechanisms enhancing the mechanical properties of the joint. In an attempt to characterize this mechanical interlocking mechanism, this study is focused on computational and experimental investigation of a single-lap joint with a very simple geometrically interlocked interface design in which both adherends have a square waveform configuration of the joining surfaces. This square waveform configuration contains a positive and a negative rectangular teeth per cycle in such a way that the joint is symmetric about the mid-bondlength. Both physical tests performed on 3D printed prototypes of joints and computational results indicate that the joints with square waveform design have higher strength and damage tolerance than those of joints with flat interface. In order to identify an optimal design configuration of this interface, a systematic parametric study is conducted by varying the geometric and material properties of the non-flat interface.

<sup>1</sup>This work was supported by Lockheed Martin (Award No: 12NZZ1)

<sup>2</sup>Professor

<sup>3</sup>Graduate Student

**3:30PM C37.00006 Multiobjective topology optimization of trabecular Bone Structure in the spine and the femur: Implications for biomimicry<sup>1</sup>**, AHMED ELBANNA, DARIN PEETZ, University of Illinois Urbana Champaign — Bone is classically considered to be a self-optimizing structure in accordance with Wolff's law. However, while the structure's ability to adapt to changing stress patterns has been well documented, whether it is fully optimal for compliance is less certain (Sigmund, 2002). Given the complexity of many biological systems, it is expected that this structure serves several purposes. We present a multi-objective topology optimization formulation for trabecular bone in the human body at two locations: the vertebrae and the femur. We account for the effect of different conflicting objectives such as maximization of stiffness, maximization of surface area, and minimization of buckling susceptibility. Our formulation enables us to determine the relative role of each of these objective in optimizing the structure. Moreover, it provides an opportunity to explore what structural features have to evolve to meet a certain objective requirements that may have been absent otherwise. For example, inclusion of stability considerations introduce numerous horizontal and diagonal members in the topology in the case of human vertebrae under vertical loading. However, the stability is found to play a lesser role in the case of the femur bone optimization. Our formulation enables investigation of bone adaptation at different locations of the body as well as under different loading and boundary conditions (e.g. healthy and diseased discs for the case of the spine). We discuss the implications of our findings on developing design rules for bio-inspired and bio-mimetic architected materials.

<sup>1</sup>National Science Foundation: CMMI

**3:42PM C37.00007 Dynamics of spider glue adhesion: effect of surface energy and contact area**, GAURAV AMARPURI, YIZHOU CHEN, TODD BLACKLEDGE, ALI DHINOJWALA, University of Akron — Spider glue is a unique biological adhesive which is humidity responsive such that the adhesion continues to increase upto 100% relative humidity (RH) for some species. This is unlike synthetic adhesives that significantly drop in adhesion with an increase in humidity. However, most of adhesion data reported in literature have used clean hydrophilic glass substrate, unlike the hydrophobic, and charged insect cuticle surface that adheres to spider glue in nature. Previously, we have reported that the spider glue viscosity changes over five orders of magnitude with humidity. Here, we vary the surface energy and surface charge of the substrate to test the change in *Larinioides cornutus* spider glue adhesion with humidity. We find that an increase in both surface energy and surface charge density increases the droplet spreading and there exists an optimum droplet contact area where adhesion is maximized. Moreover, spider glue droplets act as reusable adhesive for low energy hydrophobic surface at the optimum humidity. These results explain why certain prey are caught more efficiently by spiders in their habitat. The mechanism by which spider species tune its glue adhesion for local prey capture can inspire new generation smart adhesives.

**3:54PM C37.00008 Understanding Cell Shape Phenotypes Associated with Stem Cell Differentiation Induced by Topographical Cues of Nanofiber Microenvironment.** , DESU CHEN, University of Maryland, SUMONA SARKAR, National Institute of Standards and Technology, WOLFGANG LOSERT, University of Maryland — It is increasingly important to understand cell responses to bioinspired material structures and topographies designed to guide cell functional alterations. In this study, we investigated association between early stage cell morphological response and osteogenic differentiation of human bone marrow stromal cells (hBMSCs) induced by poly( $\epsilon$ -caprolactone) (PCL) nanofiber scaffolds (PCL-NF). Accounting for both multi-parametric complexity and biological heterogeneity, we developed an analysis framework based on support vector machines and a multi-cell level averaging method (supercell) to determine the most pronounced cell shape features describing shape phenotypes of cells in PCL-NF compared to cells on flat PCL films. We found that smaller size and more dendritic shape were the major morphological responses of hBMSCs to PCL-NF on day 1 of cell culture. Further, we investigated the shape phenotypes of hBMSCs in PCL-NF of different fiber densities to monitor the transition between 2-D and 3-D topographies. We tracked the genotypic, phenotypic and morphological responses of hBMSCs to different fiber densities at multiple time points to identify correlations between hBMSCs differentiation and early stage morphology in PCL-NF scaffolds.

**4:06PM C37.00009 Exploring elasticity and energy dissipation in mussel-inspired hydrogel transient networks** , SCOTT GRINDY, ROBERT LEARSCH, NIELS HOLTEN-ANDERSEN, Massachusetts Inst of Tech-MIT — Dynamic, reversible crosslinks have been shown to specifically control the mechanical properties of a wide variety of mechanically tough and resilient biomaterials. We have shown that reversible histidine-metal ion interactions, known to contribute to the strong mechanical properties and self-healing nature of mussel byssal threads, can be used to control and engineer the temporally-hierarchical mechanical properties of model hydrogels orthogonally from the spatial structure of the material. Here, we explore the scaling relationships in our model networks to further inform our abilities to control the relative elasticity and energy dissipation on hierarchical timescales. Scaling arguments suggest that the elasticity is dominated by long-range entanglements, while the dissipation is controlled by the exchange kinetics of the transient crosslinks. Further, we show that by using UV light, we can further control the viscoelastic properties of our mussel-inspired hydrogels *in situ*. This process opens the door for creating biocompatible hydrogel materials with arbitrary spatial control over their viscoelastic mechanical properties. Overall, we show that by understanding the interplay between bio-inspired dynamic crosslinks and soft matter physics allows us to rationally design high-strength hydrogels for specific states of dynamic loading.

**4:18PM C37.00010 Toughening elastomers using mussel-inspired catechol-metal coordination complexes** , EMMANOUELA FILIPPIDI, THOMAS CHRISTIANI, MEGAN VALENTINE, J. HERBERT WAITE, JACOB ISRAELACHVILI, KOLLBE AHN, Univesity of California, Santa Barbara — Amorphous, covalently-linked elastomers possess excellent reversible extensibility and high failure strain compared to other materials. However, by nature, the large deformability compromises the Young's modulus and the toughness of the elastomer to low values ( $\sim$  2MPa) and imparts brittle fracture. We employ the mussel-inspired strategy of iron-catechol coordination bonding creating dynamic, reversible cross-links in addition to permanent chemical cross-links in an elastomer used in ambient, dry conditions. This simple additional energy dissipative mechanism results in increased modulus and toughness without affecting the network extensibility, which is based on the covalent network. Control of the chain relaxation time scales can be further tuned using the dynamic bonds, imparting mechanical rate dependent properties to the bulk material. The quantitative understanding of the time scales associated with the chain motion versus the metal coordination may provide another simple and independent control parameter in elastomeric material design.

**4:30PM C37.00011 Bacterial Flagella as a Model Rigid Rod of Tunable Shape** , WALTER SCHWENGER, Brandeis Univ, SEVIM YARDIMCI, The Francis Crick Institute, THOMAS GIBAUD, Ecole Normale Supérieure de Lyon, HENRY SNOW, Brandeis Univ, JEFF URBACH, Georgetown University, ZVONIMIR DOGIC, Brandeis Univ — In this research, we study the physical properties of suspensions of bacterial flagella from *Salmonella typhimurium* prepared in a variety of rigid polymorphic shapes. Flagella act as a rigid colloidal particle that can exhibit non-trivial geometry including helices of varying dimensions, straight rods, or a combination of the two in the same filament. By controlling the conditions in which flagella are prepared, the polymorphic shape assumed by the filament can be controlled. Utilizing different polymorphic shapes, we combine results from optical microscopy observations of single filaments with bulk rheological measurements to help understand the role that constituent colloidal geometry plays in complex bulk behavior.

**4:42PM C37.00012 Bio-Inspired Micromechanical Directional Acoustic Sensor<sup>1</sup>** , WILLIAM SWAN, Naval Postgraduate School, FABIO ALVES, Alion Science and Technology, GAMANI KARUNASIRI, Naval Postgraduate School — Conventional directional sound sensors employ an array of spatially separated microphones and the direction is determined using arrival times and amplitudes. In nature, insects such as the *Ormia ochracea* fly can determine the direction of sound using a hearing organ much smaller than the wavelength of sound it detects. The fly's eardrums are mechanically coupled, only separated by about 1 mm, and have remarkable directional sensitivity. A micromechanical sensor based on the fly's hearing system was designed and fabricated on a silicon on insulator (SOI) substrate using MEMS technology. The sensor consists of two 1 mm<sup>2</sup> wings connected using a bridge and to the substrate using two torsional legs. The dimensions of the sensor and material stiffness determine the frequency response of the sensor. The vibration of the wings in response to incident sound at the bending resonance was measured using a laser vibrometer and found to be about 1  $\mu$ m/Pa. The electronic response of the sensor to sound was measured using integrated comb finger capacitors and found to be about 25 V/Pa. The fabricated sensors showed good directional sensitivity. In this talk, the design, fabrication and characteristics of the directional sound sensor will be described.

<sup>1</sup>Supported by ONR and TDSI

**4:54PM C37.00013 Design of Catch-and-release System by Utilizing Thermo-responsive Gel-Hairpin Composites.** , YA LIU, University of Pittsburgh, OLGA KUKSENOK, clemson university, XIMIN HE, Arizona State University , ANNA BALAZS, University of Pittsburgh — Inspired by properties of aptamers that can bind (unbind) to target proteins in their specific hairpin (chain) conformation dependent on external temperature, we use computational modeling to design an effective catch-and-release device by attaching an array of thermo-responsive hairpins to the lower critical solution temperature (LCST) thermo-responsive gels. With an increase in temperature, the polymer network swells and the hairpins can catch the target nanoparticles in the upper mixture fluid. As the temperature decreases, the polymer network collapses and the hairpins unfold to a chain conformation, releasing the arrested particles into the lower fluid for collection. We pinpoint the optimal values for obtaining the robust structural changes of the hairpins and explore the effects of the shear flow on the catch-and-release process. Our approach can be utilized for the detection, separation, and sorting of the components within the multi-component mixtures.

**5:06PM C37.00014 TUNABLE ALLOSTERIC BEHAVIOR IN RANDOM SPRING NETWORKS** , JASON W. ROCKS, Dept. of Physcs and Astronomy, University of Pennsylvania, NIDHI PASHINE, IRMGARD BISCHOFBERGER, Dept. of Physics, University of Chicago, CARL P. GOODRICH, School of Engineering and Applied Sciences, Harvard University, SIDNEY R. NAGEL, Dept. of Physics, University of Chicago, ANDREA J. LIU, Dept. of Physcs and Astronomy, University of Pennsylvania — Many proteins and other macromolecules exhibit allosteric behavior in which the binding of a ligand to one site affects the activity at a second distant site. Inspired by this biological process, we present an algorithm to tune disordered spring networks to exhibit allostery-like behavior. When the positions of a pair of nodes at one site in a network are perturbed, we can precisely tune the response of nodes located at another distant site in the system by removing only a small fraction of the bonds. This algorithm can be used to create a wide variety of different response types: response nodes can be located far away from each other, a large number of response sites can be simultaneously controlled, and even multiple independent responses can be tuned into the system. In addition, this algorithm can be generalized to account for bond bending, geometric nonlinearities and nonlinear bond potentials. However, even linear calculations match surprisingly well with macroscopic experimental realizations made by laser cutting or 3D printing.

**5:18PM C37.00015 Mechanisms of branching reactions in melanin formation – Ab initio quantum engineering approach** —, RYO KISHIDA, Department of Applied Physics, Osaka University, SUSAN MEÑEZ ASPERA, HIDEAKI KASAI, National Institute of Technology, Akashi College — Melanin, a pigment found in animals, consists of two types of oligomeric unit: eumelanin and pheomelanin. The color of the skin, the hair, and the eyes is controlled by the ratio of eumelanin/pheomelanin production. Especially, dopachrome and dopaquinone are the precursor molecules of melanin which directly affect the composition of melanin through their branching reactions. Dopachrome is converted into two possible monomers of eumelanin. Dopaquinone can undergo both eumelanin and pheomelanin synthesis. To understand the mechanisms and controlling factors that govern the conversions, reactions of the two molecules are investigated using density functional theory-based first-principles calculations. Our results deepen mechanistic understanding of the reactions and open possibilities to design properties and functions of melanin. In this talk, we will discuss about the competitions of the branching reactions.

**Monday, March 14, 2016 2:30PM - 5:30PM —**

**Session C38 DPOLY GSOFT: Assembly of Soft Nanoparticles and Colloids in Solution** 341 - Du Yeol Ryu, Yonsei University

**2:30PM C38.00001 Self-assembly of Iron Oxide Nanoparticles on Liquid Surfaces by Using Miscible Solvent Pairs**, JIAYANG HU, DATONG ZHANG, KATHLEEN M. KENNEDY, IRVING P. HERMAN, Columbia University — Nanoparticle (NP) self-assembly on liquid-air interfaces by using immiscible solvent pairs is a fast and effective way to prepare two-dimensional (2D) close-packed superlattices. However, this technique is limited by the number of available solvent pairs that are immiscible with each other while being different in the dispersity of NPs. Here, we report forming 2D superlattices using toluene/dimethyl sulfoxide miscible solvent pairs. In-situ small angle X-ray scattering patterns from NP layers sitting on the meniscus agree with patterns expected from 2D tilted closed packed superlattices. Real time optical microscopy shows that after drop casting, most of NPs coagulate immediately and sink to the bottom over several days, but leave a continuous ML on the surface, without forming 3D clusters that are usually seen in the immiscible techniques generated by the coffee ring effect. TEM images show that NPs nucleate simultaneously on different parts on the liquid surface until they touch, therefore covering the whole surface.

**2:42PM C38.00002 The effects of surfactant dynamics on deposition patterns in evaporating colloidal drops**<sup>1</sup>, NARINA JUNG, HAEWON SEO, Mechanical and Nuclear Engineering, UNIST, PILWON KIM, Mathematical Science, UNIST, CHUN SANG YOO, Mechanical and Nuclear Engineering, UNIST — Evaporation of a colloidal droplet typically leaves ring-like deposit patterns on a substrate, now well-known as the coffee ring effect. We investigate the effect of surfactant dynamics on the deposition process in a drying droplet. A coarse grained model has been developed to simulate cases with Marangoni stresses, adsorption kinetics, and intermolecular interaction of surfactant particles and to examine the related deposit formation of colloidal particles. By using the two-dimensional lattice for the lateral cross-section of a droplet, we are able to capture the full dynamics of recirculating flows with surfactant and colloidal particles during drying. The roles of surfactant on droplet and colloidal particle dynamics are investigated by systematically varying parameters, such as the maximum area fraction and the initial concentration of surfactant. We further highlight important factors to generate Marangoni eddies.

<sup>1</sup> This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government(MSIP)(No.2015R1A2A2A01007378).

**2:54PM C38.00003 Non-equilibrium colloidal assembly pathways via synergistic dipolar, depletion, and hydrodynamic interactions**, ANNA COUGHLAN, MICHAEL BEVAN, Johns Hopkins University — The ability to assemble nano- and micro- colloidal particles into ordered materials and controllable devices provides the basis for emerging technologies. However, current capabilities for manipulating colloidal assembly are limited by the degree of order, time to generate/reconfigure structures, and scalability to large areas. These limitations are due to problems with designing, controlling, and optimizing the thermodynamics and kinetics of colloidal assembly. Our approach is to provide viable non-equilibrium pathways for rapid assembly of defect free colloidal crystals using combinations of magnetic field and depletion mediated assembly. Results include video microscopy experiments and Stokesian Dynamic computer simulations of superparamagnetic colloidal particles experiencing depletion attraction in time varying magnetic fields. Findings show multi-body hydrodynamic interactions and magnetic dipole relaxation mechanisms are essential to capture assembly and annealing of attractive colloidal crystals. With the ability to measure, model and tune colloidal interactions and dynamics, we demonstrate the use of time varying fields to manipulate non-equilibrium pathways for the assembly, disassembly, and repair of colloidal microstructures.

**3:06PM C38.00004 Criterion for noise-induced synchronization: application to colloidal alignment**<sup>1</sup>, JONAH EATON, New York University, THOMAS A WITTEN, BRIAN MOTHS, University of Chicago — Asymmetric, self-assembled colloidal clusters can rotate stably as they descend under gravity. One may synchronize a dispersion of copies of such a cluster using a force that randomly switches between two different directions[1]. This is an instance of “noise-induced synchronization,” demonstrated broadly in dynamical systems that have a stable, periodic motion[2]. When such a system is perturbed by a prescribed transient force, it acquires a phase angle  $\psi$  that depends on its initial phase  $\phi$ . For our colloidal dispersion the probability distribution of phases  $\psi$  long after a switch in forcing is in general not uniform; thus the entropy  $H$  of the ensemble has decreased. The phase map  $\psi(\phi)$  provides strong constraints on the change  $\Delta H$  resulting from a switch: we show that the quantity  $\langle \log |d\psi/d\phi| \rangle$  is an upper bound on  $\langle \Delta H \rangle$ . Thus whenever  $\langle \log |d\psi/d\phi| \rangle < 0$ ,  $H$  must decrease indefinitely on average. Our simulations show that this average is a good guide to the actual synchronization behavior. This bound and other properties of  $\Delta H$  apply broadly to any dynamical system with a well-defined  $\psi(\phi)$ . [1] B. Moths, T. Witten. Phys Rev Lett, **110** 028301 (2013). [2] H. Nakao et al. Phys Rev E, **72** 026220 (2005).

<sup>1</sup>US-Israel Binational Science Foundation

**3:18PM C38.00005 Characterization of hyperuniformity in colloidal suspensions through small angle static light scattering.**, COLINE BRETZ, Compass (Solvay-CNRS-University of Pennsylvania), TIM STILL, University of Pennsylvania, DENIS BARTOLO, ENS Lyon, JEAN BAUDRY, ESPCI-CNRS, ARJUN YODH, University of Pennsylvania, REMI DREYFUS, Compass (Solvay-CNRS-University of Pennsylvania) — Hyperuniform materials have attracted increasing interest over the past decade due to their potential exciting photonic properties. Our work aims at exploring novel ways of assembling hyperuniform materials from colloidal suspensions. Three-dimensional systems of micrometer-sized colloids are considered and characterized by studying their structure factor using static small angle light scattering (SLS). A SLS set-up has been constructed for this purpose. Using an index-matched suspension of colloidal particles, we are able to record the structure factors of suspensions of micrometer-sized colloids in a three-dimensional cell. We will show how our apparatus allows us to follow the spatial organization of the colloids and characterize their hyperuniformity.

**3:30PM C38.00006 Nanoparticle interactions in electrolyte solutions: A classical density functional theory and molecular dynamics study**, K. MICHAEL SALERNO, AMALIE L. FRISCHKNECHT, MARK STEVENS, Sandia National Laboratories — We know that multivalent ions can dramatically alter the interactions between macroions, and we are interested in the fundamentals of nanoparticle interactions. We performed molecular dynamics (MD) simulations at the primitive model level and classical fluids density functional theory (DFT) calculations of negatively charged interacting nanoparticles, 2 - 7 nm in diameter, in solution with 1:1, 1:2, or 1:3 salt. We found qualitative agreement between the MD simulations and DFT calculations for the ion density profiles around the nanoparticles and for the interaction free energy between two nanoparticles. As expected, the nanoparticle interaction free energies depend strongly on the cation valence, with pure repulsion for a 1:1 salt, changing to attraction for multivalent cations due to formation of charge ordered structures. Attractive free energy depths can reach 10 kT for 7 nm diameter nanoparticles, indicating that kinetic arrest and aggregation may occur. The interaction free energies depend non-monotonically on the nanoparticle charge due to layering of the counterions around the nanoparticles for large nanoparticle charges.

**3:42PM C38.00007 Self-Assembly of DNA-coated colloids<sup>1</sup>**, DAVID PINE, New York Univ NYU — DNA-coated particles have emerged as a powerful tool for programming the self-assembly of colloids and nanoparticles. The power of this approach lies in the highly specific molecular recognition properties of DNA and in the thermal reversibility of the interactions between DNA strands attached to different particles. These two properties taken together can, in principle, direct the bottom-up self-assembly of different materials into almost any desired structure. Here we discuss the self-assembly of single and multi-component crystals of DNA-coated colloids.

<sup>1</sup>This work is supported by the Army Research Office under MURI Grant Award Number W911NF-10-1-0518 and the MRSEC Program of the NSF under Award Number DMR-1420073.

**4:18PM C38.00008 Hierarchical assembly of anisotropic particles in AC electric fields.**, ISAAC TORRES DIAZ, BRADLEY RUPP, XIAOQING HUA, YUGUANG YANG, MICHAEL A. BEVAN, Johns Hopkins University — Hierarchical microstructures composed of colloids are of great interest for technological applications and advanced materials such as metamaterials and microfluidic devices. The dynamics of spherical colloidal particles has been analyzed previously for several systems, and has led to the control of the formation of perfect crystals using AC electric fields. However, spherical particles do not have a dependence on its orientation as anisotropic particles. Recently, researchers reported experiments showing the capabilities of anisotropic particles to assemble in different configurations, yet a detailed understanding of the mechanism and control is lacking. This work shows both theoretical and experimental results of the control of a colloidal system composed of anisotropic colloidal particles with a tri-axial ellipsoidal shape subjected to a non-uniform electric field close to a planar wall. We show that particles pack into different structures and orientations as a function of the applied electric field amplitude and frequency by taking into account dipole-field, dipole-dipole, and colloidal interactions. This analysis provides a theoretical framework for the equilibrium and non-equilibrium structures that can be formed via field mediated interaction, which are validated by experimental microscopy results, and can ultimately be used to engineer the hierarchical assembly of anisotropic particles.

**4:30PM C38.00009 Quantitative Characterization of Surface Self-Assembly Imaging Using Shapelets<sup>1</sup>**, NASSER MOHIEDDIN ABUKHDEIR, ROBERT SUDERMAN, University of Waterloo, DANIEL J. LIZOTTE, University of Western Ontario — Microscopy and imaging of surface self-assembly phenomena have advanced significantly over the past decade. In order to determine structure/property relationships robust automated analysis of the resulting images is required, but has not advanced at an equally rapid pace. Recently, quantitative characterization techniques have been developed and applied, such as using bond-orientational order (BOO) theory. BOO-based methods have significant limitations in that they do not provide pixel-level resolution and are not robust in the presence of measurement noise. In this work, a fundamentally different method for automated quantitative characterization of surface self-assembly imaging is presented which uses a family of localized functions called "shapelets". The method is presented and applied to quantitative characterization of stripe and hexagonal patterns which are frequently observed in surface self-assembly. The shapelet-based method is shown to be general, highly accurate, and robust in the presence of measurement noise. It is able to efficiently determine local pattern characteristics such as pattern strength and orientation for the determination of structure/property relationships.

<sup>1</sup>This work was made possible by the Natural Sciences and Engineering Research Council of Canada and Compute Ontario.

**4:42PM C38.00010 Micro-evaporators: a powerful tool to control the growth of dense organized colloidal materials<sup>1</sup>**, CELINE BUREL, CNRS/Solvay/UPenn, JACQUES LENG, LOF, UMR 5258 Solvay-CNRS-Bordeaux 1, BERTRAND DONNIO, REMI DREYFUS, CNRS-Solvay-UPenn, JEAN-BAPTISTE SALMON, LOF, UMR 5258 Solvay-CNRS-Bordeaux 1 — Latex colloids have been concentrated inside a microfluidic channel, referred to as a microevaporator, in a controlled way up to the formation of millimeter-long colloidal materials. The solvent of this colloidal dispersion is transported by pervaporation through a thin PDMS membrane sealing the channel, inducing a flow from the reservoir containing the dispersion, up to the tip of the channel. Thus, as pervaporation occurs, colloids get concentrated at the tip of the channel up to the growth of a packed bed of colloids. The frontier between the dilute dispersion and the concentrated jammed or crystalline phase is clearly delimited by a concentration front. The position of the latter was recorded by using direct videomicroscopy. We investigated the dynamics of growth of such concentrated materials by measuring the position of the concentration front as a function of time. From these data we also estimated the volume fraction of the colloids within the concentrated material using mass conservation. We found that the estimated values are much smaller than the expected volume fractions for a dense colloidal assembly. We finally propose some explanations for such a discrepancy.

<sup>1</sup>This work was supported by CNRS-SOLVAY-UPENN and ANRT.

**4:54PM C38.00011 Prediction of Binary Nanoparticle Superlattices from Soft Potentials<sup>1</sup>**, NATHAN HORST, Department of Materials Science and Engineering, Iowa State University, ALEX TRAVESSET, Department of Physics and Astronomy, Iowa State University — Driven by the hypothesis that a sufficiently continuous short-ranged potential is able to account for shell flexibility and phonon modes and therefore provides a more realistic description of nanoparticle interactions than a hard sphere model, we compute the solid phase diagram of particles of different radii interacting with an inverse power law potential. We explore 24 candidate lattices where the p-exponent, determining the short-range properties of the potential, is varied between p=12 and p=6, and optimize the free energy with respect to additional internal parameters. The phase diagrams contain the phases found in ongoing self-assembly experiments, including DNA programmable self-assembly and nanoparticles with capping ligands assembled by evaporation from an organic solvent. The resulting phase diagrams can be mapped quantitatively to existing experiments as a function of only two parameters: nanoparticle radius ratio ( $\gamma$ ) and softness asymmetry (SA).

<sup>1</sup>Supported by DOE under contract number DE-AC02-07CH11358

**5:06PM C38.00012 Meniscus height controlled convective self-assembly<sup>1</sup>**, SATYAN CHOUDHARY, ALFRED CROSBY, University of Massachusetts Amherst — Convective self-assembly techniques based on the coffee-ring effect allow for the fabrication of materials with structural hierarchy and multi-functionality across a wide range of length scales. The coffee-ring effect describes deposition of non-volatiles at the edge of droplet due to capillary flow and pattern formations due to pinning and de-pinning of meniscus with the solvent evaporation. We demonstrate a novel convective self-assembly method which uses a piezo-actuated bending motion for driving the de-pinning step. In this method, a dilute solution of nanoparticles or polymers is trapped by capillary forces between a blade and substrate. As the blade oscillates with a fixed frequency and amplitude and the substrate translates at a fixed velocity, the height of the capillary meniscus oscillates. The meniscus height controls the contact angle of three phase contact line and at a critical angle de-pinning occurs. The combination of convective flux and continuously changing contact angle drives the assembly of the solute and subsequent de-pinning step, providing a direct means for producing linear assemblies. We demonstrate a new method for convective self-assembly at an accelerated rate when compared to other techniques, with control over deposit dimensions.

<sup>1</sup>Army Research Office ( W911NF-14-1-0185)

**5:18PM C38.00013 Strain-Temperature-Transformation (STT) Diagram for Soft Solids**, SHOUBO LI, WENTAO XIONG, XIAORONG WANG, Chemical Engineering, Tongji University, Shanghai — Soft materials comprise a variety of physical states that are easily deformed by shear stains or thermal fluctuations. They include suspensions, colloids, polymers, foams, gels, liquid crystals, and a number of biological materials. In this contribution, a generalized strain-temperature-transformation (STT) diagram for many soft materials is presented in which the physical states encountered are related to the strain and temperature changes. The boundary defined for the solid-to-liquid transformation in the STT diagram displays a surprising Z-shaped curve. We discuss this feature with respect to the physical nature of materials.

## Monday, March 14, 2016 2:30PM - 5:30PM –

**Session C39 DBIO GSOF: Physics of Cancer and Development II** 342 - Kandice Tanner, National Institute of Health

**2:30PM C39.00001 Stabilization of EphA2 dimers as a novel anti-cancer strategy**, DEO SINGH, FOZIA AHMED, MATT SALLOTO, KALINA HRISTOVA, Johns Hopkins University — We have recently shown that EphA2 receptors exist in a monomer-dimer equilibrium in the absence of ligand. The monomers promote tumorigenic activity and thus a therapeutic strategy that minimizes the monomer population may be beneficial in the clinic. The YSA peptide is an EphA2-targeting peptide that effectively delivers anticancer agents to cancer tumors. The quantitative measurements of the dimerization of EphA2 receptors in the presence of these peptides using quantitative spectral Forster resonance transfer (QS-FRET) methodology in conjunction with two-photon microscopy that has been developed recently in our lab suggests that this peptide stabilizes the EphA2 dimers. Thus, such peptides that stabilize the EphA2 dimers may be used for the treatment of some cancers that overexpress EphA2.

**2:42PM C39.00002 Criticality and Cancer Dormancy**, AMY WU, NIST, DAVID LIAO, UC San Francisco, VLADIMIR KIRLIN, CORINA TAMITA, SIMON LEVIN, JAMES STURM, ROBERT AUSTIN, Princeton University — The presence of driver mutations and subsequent clonal expansion by Darwinian evolution does not explain dormancy and re-emergence of cancer from a community of cancer and stromal cells. Dormancy appears to be a collective property of multiple cell communities including non-cancerous cells. At the simplest level, we view cancer cells interacting with stromal cells via complex, non-linear population dynamics, dynamics which can lead to very non-intuitive but perhaps deterministic and understandable progression dynamics of cancer. We explore here the dynamics of stromal-cancer cell populations in the presence of a chemotherapy drug gradient to determine to what extent the time-dependence of the populations can be quantitatively understood in spite of the underlying complexity of the individual agents. The surprising result is that a basic understanding, in a quantitative and predictive manner, can be achieved. It will be intriguing to move to predictive drug dosages, the population dynamics presented here provide a model system for the clinic.

## 2:54PM C39.00003 ABSTRACT WITHDRAWN –

**3:06PM C39.00004 Development as a Factor in the Evolution of Modularity in Biological Systems**, JESSICA LOWELL, Brandeis University — Biological networks and other systems tend to be modular in structure, with reuse of motifs and the ability to be separated into semi-independent units. The evolutionary forces that produce this modularity are a topic of active research, as modular solutions rarely emerge from models of biological evolution. Through simulations combining evolution and development, I investigate the role that development plays in the emergence of modularity, using a popular metric for network modularity and representing non-network structures as networks in which building blocks are nodes and connections between them are arcs. Preliminary results show that the modularities of structures evolved by an L-systems-based evolutionary developmental algorithm are higher than those evolved by a non-developmental evolutionary algorithm that models evolution in the same way. To ensure that these results are not specific to a single algorithm, I am conducting evolutionary developmental simulations using other methods for simulating development, evolving both networks and building-block structures. This study sheds light on the role of development as a factor in the origin of modularity in biological networks and other biological systems.

**3:18PM C39.00005 Mechanoregulatory tumor-stroma crosstalk in pancreatic cancer: Measurements of the effects of extracellular matrix mechanics on tumor growth behavior, and vice-versa, to inform therapeutics<sup>1</sup>**, JONATHAN CELLI, DUSTIN JONES, HAMID EL-HAMIDI, GWENDOLYN CRAMER, WILLIAM HANNA, ANDREW CAIDE, SEYEDEHROJIN JAFARI, University of Massachusetts Boston — The rheological properties of the extracellular matrix (ECM) have been shown to play key roles in regulating tumor growth behavior through mechanotransduction pathways. The role of the mechanical microenvironment may be particularly important tumors of the pancreas, noted for an abundance of rigid fibrotic stroma, implicated in therapeutic resistance. At the same time, cancer cells and their stromal partners (e.g. tumor associated fibroblasts) continually alter the mechanical microenvironment in response to extracellular physical and biochemical cues as part of a two-way mechanoregulatory dialog. Here, we describe experimental studies using 3D pancreatic cell cultures with customized mechanical properties, combined with optical microrheology to provide insight into tumor-driven matrix remodeling. Quantitative microscopy provides measurements of phenotypic changes accompanying systematic variation of ECM composition in collagen and laminin-rich basement membrane admixtures, while analysis of the trajectories of passive tracer particles embedded in ECM report dynamic changes in heterogeneity, microstructure and local shear modulus accompanying both ECM stiffening (fibrosis) processes, and ECM degradation near invading cells.

<sup>1</sup>We gratefully acknowledge funding from the National Cancer Institute, R00CA155045 (PI: Celli)

### 3:30PM C39.00006 Exploring Kupffer's Vescicle Through Self Propelled Particle Simulations

, KASSIDY LUNDY, Syracuse Univ, AGNIK DASGUPTA, JEFF AMACK, SUNY Upstate Medical University, M. LISA MANNING, Syracuse Univ — Early development is an important stage in the formation of functional, relatively healthy organisms. In zebrafish embryos, a transient organ in the tailbud called Kupffer's Vescicle (KV) is responsible for the initial left-right (L-R) asymmetry that results in asymmetric organ and tissue placement in the adult zebrafish. Originating as a collection of symmetrically organized monociliated cells, the KV experiences a shift in cell shapes over time that leaves more cells on the anterior or top side of the KV. This arrangement helps to generate a stronger counter-clockwise fluid flow across the anterior side of the organ, which is required for L-R asymmetry. In seeking to understand the source of the shape changes occurring within the KV, we simulate a Self Propelled Particle (SPP) model that includes parameters for cell polarization and speed. We model the KV as a large particle moving in a straight line with constant velocity to mimic the physical forces of the notochord acting on this organ, and we model the surrounding tailbud cells as smaller, slower active particles with an orientation that changes over time due to rotational noise. Our goal is to calculate the forces exerted on the KV by the surrounding tissue, to see if they are sufficient to explain the shape changes we observe in the KV that lead to L-R asymmetry.

### 3:42PM C39.00007 Systems-level analysis of the regulation and function of p53 dynamics in cancer.

, ERIC BATCHELOR, Natl Inst of Health - NIH — Living cells use complex signaling pathways to detect environmental stimuli and generate appropriate responses. As methods for quantifying intracellular signaling have improved, several signaling pathways have been found to transmit information using signals that pulse in time. The transcription factor p53 is a key tumor suppressor and stress-response regulator that exhibits pulsatile dynamics. In response to DNA double-strand breaks, the concentration of p53 in the cell nucleus increases in pulses with a fixed amplitude, duration, and period; the mean number of pulses increases with DNA damage. p53 regulates the expression of over 100 target genes involved in a range of cellular stress responses including apoptosis, cell cycle arrest, and changes in metabolism. p53 pulsing directly impacts p53 function: altering p53 dynamics by pharmacologically inhibiting p53 degradation changes patterns of target gene expression and cell fate. While p53 pulsing serves an important signaling function, it is less clear what it accomplishes mechanistically. Here we will describe our recent efforts to determine the impact of p53 pulsing on the dynamics and coordination of target gene expression.

### 4:18PM C39.00008 Cell-Substrate Adhesion by Amoeboid Cells<sup>1</sup>

, BRET FLANDERS, KRISHNA PANTA, Kansas State University — Amoeboid migration is a rapid ( $10 \mu\text{m min}^{-1}$ ) mode of migration that some tumor cells exhibit. To permit such rapid movement, the adhesive contacts between the cell and the substrate must be relatively short-lived and weak. In this study, we investigate the basic adhesive character of amoeboid cells (*D. discoideum*) in contact with silanized glass substrates. We observe the initiation and spreading of the adhesive contacts that these cells establish as they settle under gravity onto the substrate and relax towards mechanical equilibrium. The use of interference reflection microscopy and cellular tethering measurements have allowed us to determine the basic adhesive properties of the cell: the membrane-medium interfacial energy; the bending modulus; the equilibrium contact angle; and the work of adhesion. We find the time scale on which settling occurs to be longer than expected. Implications of these results on adhesion and migration will be discussed.

<sup>1</sup>The authors are grateful for support from NSF (CBET-1451903) and NIH (1R21EY026392).

### 4:30PM C39.00009 Fragmentation of cancer cells<sup>1</sup>

, SIVA VANAPALLI, NABIOLLAH KAMYABI, Texas Tech University — Tumor cells have to travel through blood capillaries to be able to metastasize and colonize in distant organs. Among the numerous cells that are shed by the primary tumor, very few survive in circulation. In vivo studies have shown that tumor cells can undergo breakup at microcapillary junctions affecting their survival. It is currently unclear what hydrodynamic and biomechanical factors contribute to fragmentation and moreover how different are the breakup dynamics of highly and weakly metastatic cells. In this study, we use microfluidics to investigate flow-induced breakup of prostate and breast cancer cells. We observe several different modes of breakup of cancer cells, which have striking similarities with breakup of viscous drops. We quantify the breakup time and find that highly metastatic cancer cells take longer to breakup than lowly metastatic cells suggesting that tumor cells may dynamically modify their deformability to avoid fragmentation. We also identify the role that cytoskeleton and membrane plays in the breakup process. Our study highlights the important role that tumor cell fragmentation plays in cancer metastasis.

<sup>1</sup>Cancer Prevention and Research Institute of Texas

### 4:42PM C39.00010 Blood based cell biopsy for early detection of cancer<sup>1</sup>

, CHA-MEI TANG, DANIEL ADAMS, Creatv MicroTech, Inc., DIANE ADAMS, Rutgers, the State Univrsity of New Jersey, R. KATHERINE ALPAUGH, Fox Chase Cancer Center, MASSIMO CRISTOFANILLI, Northwestern University, STUART MARTIN, University of Maryland School of Medicine, SARANYA CHUMSRI, Mayo Clinic Cancer Center, Jacksonville, JEFFREY MARKS, Duke University Medical Center — Early detection (ED) of cancer holds the promise for less aggressive treatments and better outcome. However, there are few accepted methods for ED. We report on a previously unknown blood cell found specifically in the peripheral blood of many solid tumors. They are defined as Cancer Associated Macrophage-Like cells (CAMLs) and are characterized by large size ( $25\text{-}300 \mu\text{m}$ ) and expression of cancer markers. CAMLs were isolated on precision filters during blood filtration. We conducted prospective studies in breast cancer (BC) to ascertain CAML prevalence, specificity and sensitivity in relation to disease status at clinical presentation. We report on two related but separate studies: 1) the isolation of CAMLs from patients with known invasive BC, compared to healthy volunteers and, 2) a double blind study conducted on women undergoing core needle biopsy to evaluate suspicious breast masses. The studies show that CAMLs are found in all stages of BC and suggest that detection of CAMLs can differentiate patients with BC from those with benign breast conditions and healthy individuals. This non-invasive blood test can be potentially used for ED of BC and other malignancies after validation studies with the advantage of a minimally invasive procedure and longitudinal monitoring.

<sup>1</sup>This work was supported by grants from Maryland TEDCO MTTTCF, R01-CA154624 from NIH, KG100240 from Susan G. Komen Foundation, Era of Hope Scholar award from DoD (BC100675), and U01-CA084955 from NCI EDNRN.

### 4:54PM C39.00011 Quantifying Microtentacle Dynamics for Non-adherent Tumor Cells<sup>1</sup>

, ELEANOR ORY, DESU CHEN, University of Maryland, College Park, KRISTI CHAKRABARTI, STUART MARTIN, University of Maryland School of Medicine, WOLFGANG LOSERT, University of Maryland, College Park, UNIVERSITY OF MARYLAND, COLLEGE PARK COLLABORATION, UNIVERSITY OF MARYLAND SCHOOL OF MEDICINE COLLABORATION — In current cancer medicine, metastasis is still responsible for 90

<sup>1</sup>Era of Hope Scholar award from the Department of Defense (BC100675)

**5:06PM C39.00012 Electron holes appear to trigger cancer-implicated mutations.**<sup>1</sup>, JOHN MILLER, MARTHA VILLAGRAN, University of Houston, Dept. of Physics & Texas Ctr. for Superconductivity — Malignant tumors are caused by mutations, which also affect their subsequent growth and evolution. We use a novel approach, computational DNA hole spectroscopy [M.Y. Suarez-Villagran & J.H. Miller, *Sci. Rep.* **5**, 13571 (2015)], to compute spectra of enhanced hole probability based on actual sequence data. A hole is a mobile site of positive charge created when an electron is removed, for example by radiation or contact with a mutagenic agent. Peaks in the hole spectrum depict sites where holes tend to localize and potentially trigger a base pair mismatch during replication. Our studies of reveal a correlation between hole spectrum peaks and spikes in human mutation frequencies. Importantly, we also find that hole peak positions that do *not* coincide with large variant frequencies often coincide with cancer-implicated mutations and/or (for coding DNA) encoded conserved amino acids. This enables combining hole spectra with variant data to identify critical base pairs and potential cancer 'driver' mutations. Such integration of DNA hole and variance spectra could also prove invaluable for pinpointing critical regions, and sites of driver mutations, in the vast non-protein-coding genome.

<sup>1</sup>Supported by the State of Texas through the Texas Ctr. for Superconductivity.

**5:18PM C39.00013 Tumorigenesis and Greenhouse-Effect System Dynamics: Phenomenally Diverse, but Noumenally Similar?**, SAI PRAKASH, Johns Hopkins University — We present a physicochemical model of tumorigenesis leading to cancer invasion and metastasis. The continuum-theoretic model, congruent with recent experiments, analyzes the plausibility of oncogenic neoplasia-induced cavitation or tensile yielding (plasticity) of the tumoral basement membrane (BM) to activate stromal invasion. The model abstracts a spheroid of normal and cancer cells that grows radially via water and nutrient influx while constrained by a stiffer BM and cell adhesion molecules. It is based on coupled fluid-solid mechanics and ATP-fueled mechano-damped cell kinetics, and uses empirical data alone as parameters. The model predicts the dynamic force and exergy (ATP) fields, and tumor size among other variables, and generates the sigmoidal dynamics of far-from-equilibrium biota. Simulations show that the tumor-membrane system, on neoplastic perturbation, evolves from one homeostatic steady state to another over time. Integrated with system dynamics theory, the model renders a key, emergent tissue-level feedback control perspective of malignancy: neoplastic tumors coupled with pathologically-softened BMs appear to participate in altered autoregulatory behavior, and likely undergo BM cavitation and stress-localized ruptures to their adhesome, with or without invadopiosis, thereby, initiating invasion. Serendipitously, the results also reveal a noumenal similarity of the tumor-membrane to the earth-atmosphere open reactive system as concerns self-regulation.

**Monday, March 14, 2016 2:30PM - 5:30PM –**  
**Session C40 GSNP GSOF: Extra Mechanics: Fracking, Growing, Buckling, Defects, Stat Mech, and Bio** 343 - Dominic Vella, Oxford University

**2:30PM C40.00001 Hydraulic fracture and toughening of a brittle layer bonded to a hydrogel**, ALESSANDRO LUCANTONIO, GIOVANNI NOSELLI, SISSA - International School for Advanced Studies, XAVIER TREPAT, IBEC - Institute for Bioengineering of Catalonia, ANTONIO DESIMONE, SISSA - International School for Advanced Studies, MARINO ARROYO, UPC - Universitat Politècnica de Catalunya — Brittle materials fracture under tensile or shear stress. When stress attains a critical threshold, crack propagation becomes unstable and proceeds dynamically. In the presence of several precracks, a brittle material always propagates only the weakest crack, leading to catastrophic failure [1]. Here, we show that all these features of brittle fracture are radically modified when the material susceptible to cracking is bonded to a poroelastic medium, such as a hydrogel, a common situation in biological tissues [2]. In particular, we show that the brittle material can fracture in compression and can resist cracking in tension, thanks to the hydraulic coupling with the hydrogel. In the case of multiple cracks, we find that localized fracture occurs when the permeability of the hydrogel is high, whereas decreased permeability leads to toughening by promoting multiple cracking. Our results [3] may contribute to the understanding of fracture in biological tissues and provide inspiration for the design of tough, biomimetic materials.

[1] Noselli et al., *Int. J. Fracture*, **183**, 241-258 (2013)

[2] Casares et al., *Nat. Mater.*, **14**, 343-351 (2015)

[3] Lucantonio et al., *Phys. Rev. Lett.*, **115**, 188105 (2015)

**2:42PM C40.00002 Geometry and Mechanics of Thin Growing Bilayers**<sup>1</sup>, MATTEO PEZZULLA, GABRIEL SMITH, Boston University, PAOLA NARDINOCCHI, Sapienza Università di Roma, DOUGLAS HOLMES, Boston University — We investigate how thin sheets of arbitrary shapes morph under the isotropic in-plane expansion of their top surface, which may represent several stimuli such as nonuniform heating, local swelling and differential growth. Inspired by geometry, an analytical model is presented that rationalizes how the shape of the disk influences morphing, from the initial spherical bending to the final isometric limit. We introduce a new measure of slenderness that describes a sheet in terms of both thickness and plate shape. We find that the mean curvature of the isometric state is three fourth's the natural curvature, which we verify by numerics and experiments. We finally investigate the emergence of a preferred direction of bending in the isometric state, guided by numerical analyses. The scalability of our model suggests that it is suitable to describe the morphing of sheets spanning several orders of magnitude.

<sup>1</sup>NSF grant CMMI1300860

**2:54PM C40.00003 Buckling, driven by constrained phase separation, of toroid-shaped hydrogels**, MICHAEL S. DIMITRIYEV, YA-WEN CHANG, Georgia Institute of Technology, ANTON SOUSLOV, Universiteit Leiden, ALBERTO FERNANDEZ-NIEVES, PAUL M. GOLDBART, Georgia Institute of Technology — We investigate the buckling process observed in connection with the temperature-induced shrinking of an elastic toroid composed of hydrogel. Hydrogels are polymeric network media that become swollen when mixed with water, provided the temperature is low enough. As the temperature is increased beyond a certain point, such gels undergo a first-order de-swelling transition to a de-mixed state, in which the network segregates from the water, resulting in a shrunken phase. It is known that the rapid heating of swollen hydrogels beyond the de-swelling transition results in the formation of a shrunken-phase boundary region, or shell. This shell hinders the expulsion of fluid associated with the equilibration of the sample interior, and gives rise to a prolonged period of coexistence between shrunken and swollen domains in the interior of the sample. In contrast with the spherical case, toroidal samples have been observed to undergo a constrained phase separation that is accompanied by a global buckling (or "Pringling") deformation of the sample shape. We present a model of hydrogel toroid Pringling in which such deformations are driven by this phase separation process.

**3:06PM C40.00004 Modeling and design of the self-twisting of hydrogel bilayer strips** Authors: Jiayu Liu, Jingkai Guo, Tanvi Shroff, Changkyu Yoon, David Gracias & Thao D Nguyen, JIAYU LIU, JINGKAI GUO, TANVI SHROFF, CHANGKYU YOON, DAVID GRACIAS, THAO NGUYEN, Johns Hopkins University — Self-folding of hydrogels via heterogeneous swelling can be used to create complex, 3D structures. A bilayer structure with a thermo-responsive hydrogel layer, that swells with decreasing temperature, and a non-swelling layer can respond to a temperature change by either bending into a ring or twisting into a helix. The equilibrium structure depends on the thickness ratio of the two layers, the ratio of the width to thickness of the bilayer, as well as the stiffness of the two layers and equilibrium swelling ratio of the hydrogel. These parameters can be controlled using lithographic photopatterning and multilayer deposition techniques. To guide the design of the bilayer structures, we developed a finite element model of the bilayer structure. The constitutive model of the hydrogel is described by a free energy density that includes a quasi-incompressible Neo-Hookean component for the strain energy density of the polymer network and a Flory-Huggins component for the free-energy density of mixing of the polymer and solvent. We discussed how variations in the layer thickness, slenderness, stiffness, and equilibrium swelling ratio can be used to design self-folded rings of different curvatures and helices with different helix angle and diameters.

**3:18PM C40.00005 Mechanics of a leaf detaching from tree**, TIM ZEHNBAUER, SUNGHWAN JUNG, Virginia Tech — Deciduous trees shed their leaves through an abscission process. The abscission zone is formed at the base of the petiole, and consists of a top layer with weak walls and a bottom layer that expands and breaks the walls of the cells in the top layer. Although this process is well understood biologically, the mechanical principles underlying this shedding have received little attention. In the present study, we characterize the stress-strain relation of the petiole-branch connection failure over the seasons. The testing is done with a 1kN load cell, where the stem is pulled directly from the branch to make a stress-strain curve. The slope of the stress-strain curve, Young's modulus, is obtained using least squares linear regression of the curve. We show that Young's modulus stays constant from spring to late fall, while the maximum tensile strength falls. We are investigating the role of the shape of a leaf's petiole in this behavior.

**3:30PM C40.00006 ABSTRACT WITHDRAWN —**

**3:42PM C40.00007 The role of deformable structured surfaces on viscous forces during peeling**<sup>1</sup>, CHARLES DHONG, JOELLE FRECHETTE, Johns Hopkins University — It is known that tree frogs are able to adhere well in flooded environments, presumably due to their interconnected network of drainage channels formed by hexagonal epithelial cells in their toe pads. To investigate this effect, a patterned surface of hexagonally arranged cylindrical posts was brought close to a stationary substrate in a submerged, viscous fluid via a normal load, and then peeled off to measure a retraction force. Because these structured surfaces were made from PDMS, they are able to deform throughout the process. We find that these deformable surfaces further reduce the work required to peel apart the two surfaces, even when compared to previous studies in the same system with rigid structures, and we isolated these contributions independent of conservative forces. We then conducted experiments to compare the effect of deformation on the viscous forces and conservative forces. We find that there are several regimes where deformation either increases or decreases the retraction force since we have found that elasticity decreases retraction forces when considering viscous contributions but is also known to increase adhesion in the context of conservative forces.

<sup>1</sup>Office of Naval Research, National Science Foundation, Hopkins Extreme Materials Institute

**3:54PM C40.00008 Bio-inspired microfluidics: The case of the velvet worm**<sup>1</sup>, ANDRES CONCHA, PAULA MELLADO, Adolfo Ibanez university, BERNAL MORERA-BRENES, Laboratorio de Genetica Evolutiva, Universidad Nacional de Costa Rica, CRISTIANO SAMPAIO-COSTA, University of Sao Paulo., L. MAHADEVAN, School of Engineering and Sciences, Harvard University., JULIAN MONGE-NAJERA, Tropical Biology, Universidad de Costa Rica. — The rapid squirt of a proteinaceous slime jet endow velvet worms (Onychophora) with a unique mechanism for defense from predators and for capturing prey by entangling them in a disordered web that immobilizes their target. However, to date neither qualitative nor quantitative descriptions have been provided for this unique adaptation. We have investigated the mechanism that allows velvet worms the fast oscillatory motion of their oral papillae and the exiting liquid jet that oscillates with frequencies  $f \sim 30 - 60$  Hz. Using anatomical images and high speed videography, we show that even without fast muscular action of the papilla, a strong contraction of the slime reservoir and the geometry of the reservoir-papilla system suffices to accelerate the slime to speeds up to  $v \sim 5$  m/s in about  $\Delta t \sim 60$  ms. A theoretical analysis and a physical simulacrum allow us to infer that this fast oscillatory motion is the result of an elastohydrodynamic instability driven by the interplay between the elasticity of oral papillae and the fast unsteady flow during squirting. We propose several applications that can be implemented using this instability, ranging from high-throughput droplet production, printing, and micro-nanofiber production among others.

<sup>1</sup>A.C was partially supported by Fondecyt grant 11130075.

**4:06PM C40.00009 Nonlinear adhesion dynamics of confined lipid membranes**<sup>1</sup>, TUNG TO, THOMAS LE GOFF, OLIVIER PIERRE-LOUIS, Univ Lyon 1 UA 442 CNRS — Lipid membranes, which are ubiquitous objects in biological environments are often confined. For example, they can be sandwiched between a substrate and the cytoskeleton between cell adhesion, or between other membranes in stacks, or in the Golgi apparatus. We present a study of the nonlinear dynamics of membranes in a model system, where the membrane is confined between two flat walls. The dynamics derived from the lubrication approximation is highly nonlinear and nonlocal. The solution of this model in one dimension exhibits frozen states due to oscillatory interactions between membranes caused by the bending rigidity. We develop a kink model for these phenomena based on the historical work of Kawasaki and Otha<sup>2,3,4</sup>. In two dimensions, the dynamics is more complex, and depends strongly on the amount of excess area in the system. We discuss the relevance of our findings for experiments on model membranes, and for biological systems<sup>5</sup>.

<sup>1</sup>Supported by the grand ANR Biolub

<sup>2</sup>T. Le Goff, P. Politi and O. Pierre-Louis, PRE **90**, 032114 (2014).

<sup>3</sup>T. Le Goff, P. Politi and O. Pierre-Louis, PRE **92**, 022918 (2015).

<sup>4</sup>T. Le Goff, O. Pierre-Louis and P. Politi, J. Stat. Mech. **P08004**, 1742 (2015).

<sup>5</sup>T. B. T. To, T. Le Goff, O. Pierre-Louis, preprint.

**4:18PM C40.00010 Statistical Mechanics of Sliced Graphene Ribbons.**, MARK BOWICK, Syracuse University, EMILY RUSSELL, Google, RASTKO SKNEPNEK, University of Dundee, DAVID NELSON, Harvard University — Two-dimensional crystalline membranes have recently been realized experimentally in such systems as graphene and molybdenum disulfide, sparking a resurgence in interest in their statistical properties. Thermal fluctuations can significantly change the effective mechanical properties of these membranes, renormalizing both bending rigidity and elastic moduli so that thermal membranes are stiffer to bending than their bare bending rigidity would suggest. We use molecular dynamics simulations to examine the further effect of topology and geometry on the properties of thermal membranes, and find that the introduction of a slit suppresses the scale of thermal fluctuations.

**4:30PM C40.00011 Statistical mechanics of thin spherical shells**, ANDREJ KOSMRLJ, Princeton University, DAVID R. NELSON, Harvard University — We explore how thermal fluctuations affect the mechanics of thin amorphous spherical shells via renormalization group calculations. It is well known that for flat solid membranes thermal fluctuations effectively increase the bending rigidity and reduce the bulk and shear moduli. This is still true for spherical shells. However, the additional coupling between the shell curvature, the local in-plane stretching modes and the local out-of-plane undulations leads to novel phenomena. In spherical shells thermal fluctuations effectively produce negative surface tension, which is equivalent to applying external pressure. We find that small spherical shells are stable, but for sufficiently large shells this thermally generated pressure becomes big enough to crush spherical shells. Such shells can be reinflated by increasing internal pressure, where the effective shell size grows non-linearly as a function of internal pressure with a power law exponent characteristic for thermally fluctuating flat membranes under uniform tension.

**4:42PM C40.00012 Phyllotactic transformations as plastic deformations of tubular crystals with defects**, DANIEL BELLER, DAVID NELSON, Harvard University — Tubular crystals are 2D lattices in cylindrical topologies, which could be realized as assemblies of colloidal particles, and occur naturally in biological microtubules and in single-walled carbon nanotubes. Their geometry can be understood in the language of phyllotaxis borrowed from botany. We study the mechanics of plastic deformations in tubular crystals in response to tensile stress, as mediated by the formation and separation of dislocation pairs in a triangular lattice. Dislocation motion allows the growth of one phyllotactic arrangement at the expense of another, offering a low-energy, stepwise mode of plastic deformation in response to external stresses. Through theory and simulation, we examine how the tube's radius and helicity affects, and is in turn altered by, dislocation glide. The crystal's bending modulus is found to produce simple but important corrections to the tube's deformation mechanics.

**4:54PM C40.00013 Defect-driven shape instabilities in cohesive filament bundles<sup>1</sup>**, ISAAC BRUSS, University of Michigan, GREGORY GRASON, University of Massachusetts — When defects are incorporated into the lattice of a flexible 2D crystalline membrane, it buckles into a new configuration. Specifically, 5- and 7-fold disclinations produce conical- and saddle-like geometries respectively. For bundles composed of a crystalline array of cohesive flexible filaments, we propose a similar phenomena of defect-induced buckling. This revelation is fueled by a recently discovered mapping between the metric properties of a curved surface, and the inter-filament spacing within a deformed bundle. Using a combination of continuum elasticity theory and numerical simulations, we investigate the effects of defects in the cross section on a bundle's global structure. We find that positive disclinations promote the twisting of filaments around a central axis within the bundle, while negative disclinations promote twisting around two parallel axes simultaneously. Both instabilities are interpreted by means of their equivalent Gaussian curvature, and map appropriately to the corresponding membrane responses. Additionally, for 5-fold disclinations we uncover a new equilibria structure, torsional wrinkling, with the intriguing ability to focus gradients in filament tilt much like curvature-focusing for the analogous membrane.

<sup>1</sup>NSF (CAREER) DMR-0955760

**5:06PM C40.00014 Ring Correlations in Two-Dimensional (2D) Random Networks**, MAHDI SAD-JADI, M. F. THORPE, Arizona State Univ — Amorphous materials can be characterized by their ring structure. Recently, two experimental groups imaged bilayers of vitreous silica at atomic resolution which provides a direct access to the ring structure of a 2D glass<sup>1</sup>. It has been shown that experimental samples have various ring statistics, obey Aboav-Weaire law and have a distinct area law<sup>2</sup>. In this work, we study correlations between rings as a function of their size and topological separation. We show that correlation is medium-range and vanishes when the separation is about three rings apart. We also present a generalization of the Aboav-Weaire law.

<sup>1</sup>Lichtenstein L et al, *Angew. Chem. Int. Ed.* 51 404 (2012) and Huang P Y et al, *Nano Lett.* 12 1081 (2012)

<sup>2</sup>Kumar A et al, *Journal of Physics: Condensed Matter* 26 39 (2014): 395401.

**5:18PM C40.00015 The Effect of Loops in Connectivity Percolation**, VARDA F. HAGH, Arizona State University, M. F. THORPE, Arizona State University- Rudolf Peierls Centre for Theoretical Physics, University of Oxford — We introduce a new method that employs the concepts of redundancy and stress from rigidity theory to study the effect of loops in connectivity percolation. In the rigidity percolation redundant bonds are not necessary to maintain the rigidity of a network. These redundant bonds cause internal stress in some regions and as a result those regions carry finite forces that characterize them as over-constrained. In connectivity percolation the bonds that cause a loop correspond to redundant bonds in rigidity and all the bonds that are part of a loop are equivalent to over-constrained bonds in rigidity. To illustrate this we start with a network in 2D where all the bonds are present and remove the bonds randomly. Then using renormalization groups and numerical simulations we study the behavior of loops near percolation transition in hierarchical networks and lattices.

## Monday, March 14, 2016 2:30PM - 5:30PM –

Session C41 DBIO DPOLY DCOMP: Biopolymers in Confinement: I 344 - Kevin Dorfman, University of Minnesota - Minneapolis

**2:30PM C41.00001 Flory theory or the two state cooperativity model: What describes back-folding of DNA in nanotubes?**, KEVIN DORFMAN, ABHIRAM MURALDIHAR, Univ of Minn - Minneapolis — Currently, there are two explanations available in the literature to describe the extension of semiflexible polymers, such as DNA, confined in nanotubes whose diameter is close to the persistence length. Almost a decade ago, Odijk (Phys. Rev. E, 2008, 77, 060901) used a Flory theory to derive a scaling law for the average extension of a semiflexible polymer confined in such a tube. More recently, Dai et al. (ACS Macro Lett. 1, 1046-1050) applied a two-state cooperativity model along the lines of the Zimm-Bragg model for helix coil transitions to explain the same phenomenon. Although the two theories are fundamentally different, there are simulation results supporting both approaches. In this talk, we will present results from Pruned-Enriched Rosenbluth Method (PERM) simulations of a discrete wormlike chain model, which show strong evidence supporting Odijk's Flory theory. Moreover, we will show that Odijk's scaling theory also predicts the contour length dependence of the chain extension. In contrast, we find that the cooperativity model predicts the average extension correctly only for the molecular weights used to parameterize the model.

**2:42PM C41.00002 Pore translocation of polymer chains with physical knots**, ANTONIO SUMA, ANGELO ROSA, CRISTIAN MICHELETTI, SISSA, International School for Advanced Studies, via Bonomea 265, I-34136 Trieste, Italy — The driven translocation of knotted chains through narrow pores has important implications for single-molecule manipulation contexts. Its complex phenomenology<sup>1</sup> is, however, still largely unexplored, both as a function of knot complexity and the magnitude of the driving, translocating force. We accordingly report on a systematic theoretical and computational investigation of both aspects. In particular we consider the case of flexible chains accommodating a large repertoire of knots that are driven through pores too narrow to allow for their passage. We show that the observed rich translocation phenomenology can be rationalised in a transparent mechanical framework that can further be used for predictive purposes<sup>2</sup>.

<sup>1</sup>A. Rosa, M. Di Ventra and C. Micheletti. *Phys. Rev. Lett.*, 2012, 109, 118301

<sup>2</sup>A. Suma, A. Rosa and C. Micheletti. *Pore translocation of knotted polymer chains*, submitted, 2015

**2:54PM C41.00003 Intramolecular Fluctuation of DNA in Nanochannels via High-throughput Video Microscopy**, JULIAN SHEATS, Univ of Minn - Minneapolis, JEFFREY G. REIFENBERGER, HAN CAO, BioNano Genomics - San Diego, KEVIN D. DORFMAN, Univ of Minn - Minneapolis — Genome mapping is a promising technique that complements next generation sequencing. The distance between labels on barcoded DNA molecules is the main physical quantity employed by emerging nanochannel technologies used to construct genome maps. Here we analyze time resolved data of *E. coli* DNA in a commercial nanochannel genome mapping system to obtain the probability distribution underlying the distance between labels. Improving upon a previous study of this type<sup>1</sup>, this dynamic method avoids alignment to the reference genome, a process that is statistical in nature. The time-series analysis also allows for detection of a set of experimental artifacts present in static imaging, thereby filtering out several sources of potential systematic error. The resulting probability density remains left-skewed, supporting previous evidence. However, filtering out the artifacts resulted in a lower magnitude of skewness, which has implications for the statistical weights associated with the genome mapping algorithm.

<sup>1</sup>Reinhart, W. F. et al., *J. Chem. Phys.* **142**, 064902 (2015)

**3:06PM C41.00004 Non-Equilibrium Dynamics of Nano-channel Confined DNA: A Brownian Dynamics Simulation Study**, ANIKET BHATTACHARYA, AIQUN HUANG, University of Central Florida, WALTER REISNER, McGill University, Canada — We carry out Brownian dynamics (BD) simulation for a semi-flexible polymer chain characterized by a contour length  $Na$  and a persistence length  $\ell_p$  confined inside a rectangular nanochannel to study its compression and retraction dynamics while being pushed on one end at a constant velocity by a “nano-dozer”. We study the evolution of one dimensional concentration profile  $c(x, t)$  and the chain extension  $R$  along the channel axis ( $x$ -axis) during both the contracting as well as the retracting phases as a function of the velocity of the nano-dozer, both in steady states and in transients. Furthermore, we measure the transverse fluctuations of the chain under contraction and retraction, and the amplitude of the density profile, and compare these simulation results with those obtained from an analytical model proposed by Khorshid *et al.* Our studies are guided by recent experimental results by Khorshid *et al.* (*Phys. Rev. Lett.*, **113**, 268104 (2014)) and provide further justification to use a one dimensional PDE approach to understand the non-equilibrium dynamics of confined polymers.

**3:18PM C41.00005 Dynamics of topological events within single molecules of DNA confined in nanochannels.**<sup>1</sup>, JEFFREY REIFENBERGER, BioNano Genomics, KEVIN DORFMAN, Dept. Chemical Engineering and Materials Science, University of Minnesota - Twin Cities, HAN CAO, BioNano Genomics — Genome mapping in nanochannels offers the ability to search for large genomic rearrangements within individual molecules of DNA often missed by sequencing techniques. This method labels DNA at specific sequence motifs such as ‘GCTCTTC’ with a cy3-like fluorophore and then stains the backbone of dsDNA with an intercalating dye. DNA is electrophoretically loaded into an array of nanofluidic channels and linearized in physically confined narrow conduits fabricated on the silicon chip. The fluorescently labeled sequence motifs, unique to long genomic regions, are optically imaged and digitized reflecting structural changes that can occur within cancer. However, some molecules of DNA confined within the ~42 nm wide nanochannels contain topological structures: knots, S-folds, and end-folds that could appear as false genomic rearrangements. We present a technique in which thousands of molecules of *E. coli* DNA are sequentially imaged in the nanochannels during several minutes allowing for topological events like diffusion of knots, unfolding at the ends, and spontaneous formation of S-folds to be measured. This technology will provide insights and a solution in error correction for making more accurate measurements.

<sup>1</sup>NIH R01-HG006851

**3:30PM C41.00006 Adsorption of annealed branched polymers on curved surfaces**, JEF WAGNER, Lawrence University, GONCA ERDEMCI-TANDOĞAN, ROYA ZANDI, University of California Riverside — Annealed branched polymers play important roles in many biological and industrial systems, notable among them single stranded RNA (ssRNA) that in solution takes on a branched secondary structure. Using a mean field theory, we both perturbatively and numerically examine the adsorption of annealed branched polymers on surfaces of several different geometries in a good solvent. Independent of the geometry of the wall, we observe that as branching density increases, surface tension decreases. However, we find a coupling between the branching density and curvature in that a further lowering of surface tension occurs when the wall curves towards the polymer, but the amount of lowering of surface tension decreases when the wall curves away from the polymer. This work was inspired by the idea of using functionalized gold nano-particles to bind RNA for gene delivery. Understanding the mechanisms involved with the adsorption of annealed branched polymers onto different surfaces will play a critical role in many biomedical technologies.

**3:42PM C41.00007 Depletion forces in collapsing a flexible chain molecule in a confined or free space**, CHANIL JEON, BAE-YEUN HA, University of Waterloo — A chain molecule can be entropically collapsed in a crowded medium whether confined or not. Qualitatively, the entropic (depletion) forces between monomers can be considered as effectively reducing the solvent quality, eventually making the excluded volume  $v$  negative. Here, we characterize these forces in collapsing a flexible polymer in three distinct spaces: free, cylindrical, and (2-dimensional) slit-like. A few general features characterize flexible-chain collapse. Let  $\phi_c$  be the volume fraction of crowders of size  $a_c$  each (in units of the monomer size). In all three cases, chain compaction depends on a single parameter, i.e., the ratio  $\phi_c/a_c$ ; there also exists a general relationship between  $\phi_c/a_c$  and  $v$ . Our results suggest that the action of depletion forces is local and insensitive to the geometry of a confined space, as assumed in an effective-solvent picture. They also offer a physical sense of average crowder sizes in a poly-disperse crowded medium.

**3:54PM C41.00008 Detection of ATP hydrolysis through motion of nanoconfined DNA**, MAEDEH ROUSHAN, GIDEON LIVSHITS, ZUBAIR AZAD, HONG WANG, ROBERT RIEHN, North Carolina State University — Confinement of DNA to nanochannels with a cross-section of  $100 \times 100 \text{ nm}^2$  and hundreds of micrometer long has previously been used to investigate the equilibrium binding properties of proteins to DNA. Here we report on the observation that a range of proteins which catalyze a modification of DNA, and that do so by hydrolyzing ATP, cause a net directed motion of nanochannel-confined DNA. We present a model for this observation that does not require any motor-like action of the protein and that is purely dependent on the catalytic properties.

**4:06PM C41.00009 Stochastic resonance during a polymer translocation process**, DEBASISH MONDAL, MURUGAPPAN MUTHUKUMAR, University of Massachusetts Amherst — We study the translocation of a flexible polymer in a confined geometry subjected to a time-periodic external drive to explore stochastic resonance. We describe the equilibrium translocation process in terms of a Fokker-Planck description and use a discrete two-state model to describe the effect of the external driving force on the translocation dynamics. We observe that no stochastic resonance is possible if the associated free-energy barrier is purely entropic in nature. The polymer chain experiences a stochastic resonance effect only in presence of an energy threshold in terms of polymer-pore interaction. Once stochastic resonance is feasible, the chain entropy controls the optimal synchronization conditions significantly.

**4:18PM C41.00010 Strongly Non-equilibrium Dynamics of Nanochannel Confined DNA**, WALTER REISNER, McGill University — Nanoconfined DNA exhibits a wide-range of fascinating transient and steady-state non-equilibrium phenomena. Yet, while experiment, simulation and scaling analytics are converging on a comprehensive picture regarding the equilibrium behavior of nanochannel confined DNA, non-equilibrium behavior remains largely unexplored. In particular, while the DNA extension along the nanochannel is the key observable in equilibrium experiments, in the non-equilibrium case it is necessary to measure and model not just the extension but the molecule's full time-dependent one-dimensional concentration profile. Here, we apply controlled compressive forces to a nanochannel confined molecule via a nanodozer assay, whereby an optically trapped bead is slid down the channel at a constant speed. Upon contact with the molecule, a propagating concentration "shockwave" develops near the bead and the molecule is dynamically compressed. This experiment, a single-molecule implementation of a macroscopic cylinder-piston apparatus, can be used to observe the molecule response over a range of forcings and benchmark theoretical description of non-equilibrium behavior. We show that the dynamic concentration profiles, including both transient and steady-state response, can be modelled via a partial differential evolution equation combining nonlinear diffusion and convection. Lastly, we present preliminary results for dynamic compression of multiple confined molecules to explore regimes of segregation and mixing for multiple chains in confinement.

**4:54PM C41.00011 Role of small ion dynamics in driven translocation of polyelectrolytes through nanopores**, HARSHWARDHAN KATKAR, MURUGAPPAN MUTHUKUMAR, University of Massachusetts Amherst — Nanopores have been proposed to be used for a variety of applications such as in DNA sequencing and as molecular separation devices. In the present study, we focus on the dynamics of small ions (counterions and salt ions) while a charged polymer translocates through a finite-length nanopore under the action of an externally applied electric field. Coarse-grained molecular dynamics simulations are performed to study the translocation process, taking both the long-range hydrodynamics and the long-range electrostatics into consideration. We address the role of small ion dynamics on the properties of a DNA in a confined region.

**5:06PM C41.00012 Free Energy of a Polymer in Slit-Like Confinement across the Odijk, moderate confinement, and Bulk Regimes**, ALBERT KAMANZI, JASON S. LEITH, McGill University, DAVID SEAN, University of Ottawa, DANIEL BERARD, ANDREW C. GUTHRIE, CHRISTOPHER M.J. MCFAUL, McGill University, GARY W. SLATER, University of Ottawa, HENDRICK W. DE HAAN, University of Ontario, Institute of Technology, SABRINA R. LESLIE, McGill University, MCGILL UNIVERSITY TEAM, UNIVERSITY OF OTTAWA, UNIVERSITY OF ONTARIO COLLABORATION — We directly measure the free energy of confinement for semi-flexible polymers from the nanoscale to bulk regimes in slit-like confinement. We use Convex Lens-induced Confinement (CLiC) microscopy of DNA to load and directly count molecules at equilibrium in a single chamber of smoothly increasing height. CLiC microscopy allows for direct visualization of polymers in free solution over long periods, as a function of tunable vertical confinement - from the millimeter to the nanometer scale, and within a single device. Our direct characterization of the free energy of confinement, across several orders of magnitude of applied confinement, agree with new simulations established in this work. We compare experimental results to the "de Gennes blob model", to theory published by Casassa, as well as to simulations by Chen and Sullivan, in appropriate regimes. This work establishes a robust platform for understanding and manipulating polymers at the nanoscale, with a wide range of applications to biomedical technologies.

**5:18PM C41.00013 Do Ions Flow Freely Through Confined DNA?**, ZUBAIR AZAD, ROBERT RIEHN, North Carolina State University — Double-stranded DNA in an aqueous solution is characterized by a strongly localized counter-ion cloud. Classical experiments have shown that the mobility of large DNA coils is independent of the number of basepairs, leading to an interpretation that the molecule can be understood as a collection of segments with constant mobility whose interactions are effectively screened from each other. This "free-draining" assumption posits that DNA and other electrolytes will not influence each other's mobility. In this talk, we call this assumption into question when the local concentration of DNA is increased beyond that of a self-avoiding random walk by nanoconfinement. We present translocation of DNA and fluorescent tracer ions under established chemical gradients, pressure-driven flow, and electrophoresis in nanochannels with cross sections that are 100 nm x 100 nm. We present evidence that interactions between the DNA and ionic tracers are a non-linear function of the applied fields.

**Monday, March 14, 2016 2:30PM - 5:30PM –**

**Session C42 DPOLY: Physics of Copolymers II: Bulk and Thin Films** 345 - Steve Hudson, NIST

**2:30PM C42.00001 Fluids Density Functional Theory of Diblock Copolymers for Electrolyte Applications<sup>1</sup>**, JONATHAN R. BROWN, LISA M. HALL, Ohio State University — We use classical, fluids density functional theory (fDFT) to study microphase separation in block copolymer systems. We are motivated by systems used as battery electrolytes or in other transport applications, in which the two blocks of the system have different mechanical, dielectric, and transport properties that allow one phase to act as a charge/penetrant carrier and the other to make the film mechanically strong. We find density profiles of penetrants, showing to what degree they segregate into the A phase and their concentration near the interface, depending on the penetrant-A and penetrant-B interaction strengths as well as the A-B segregation strength. We also study the effect of tapering, or adding a gradient region (taper) between the pure A and B blocks of an AB diblock copolymer; the taper changes in composition along its length from pure A to pure B (or from B to A for an inverse taper). The effect of both penetrants and tapering on microphase domain spacing as a function of segregation strength will be discussed. Adjusting taper length allows one to tune the phase behavior of the system for easier processing or access to specific desired microphase structures.

<sup>1</sup>Based upon work supported by NSF Grant 1454343 and DOE Grant SC0014209

**2:42PM C42.00002 Unguided discovery of BCP self-assembly: challenges and outlook**, CAROL TSAI, KRIS DELANEY, GLENN FREDRICKSON, University of California, Santa Barbara — The unguided search for the stable phases of a block copolymer of a given composition and architecture is a problem of global optimization. The appeal of this pursuit arises from both a materials design perspective and also from the perspective of solving global optimization problems via heuristic algorithms. A diverse collection of such algorithms is available to employ, including evolutionary and swarm strategies. In this talk we discuss the development, successes, and challenges of a real-space genetic algorithm (GA)-SCFT method as applied to a diblock copolymer. We then consider alternative representations and algorithms for solving the forward problem in bulk block copolymer systems.

**2:54PM C42.00003 Orientational control of block copolymer microdomains by sub-tesla magnetic fields<sup>1</sup>** , MANESH GOPINADHAN, YOUNGWOON CHOO, XUNDA FENG, KOHSUKE KAWABATA, XIAOJUN DI, CHINEDUM OSUJI, Yale University — Magnetic fields offer a versatile approach to controlling the orientation of block copolymer (BCP) microdomains during self-assembly. To date however, such control has required the imposition of large magnetic fields (>3T), necessitating the use of complex magnet systems – either superconducting or very large conventional resistive magnets. Here we demonstrate the ability to direct BCP self-assembly using considerably smaller fields (<1T) which are accessible using simple rare-earth permanent magnets. The low field alignment is enabled by the presence of small quantities of mesogenic species that are blended into, and co-assemble with the liquid crystalline (LC) mesophase of the side-chain LC BCP under study. In situ SAXS experiments reveal a pronounced dependence of the critical alignment field strength on the stoichiometry of the blend, and the ability to generate aligned microdomains with orientational distribution coefficients exceeding 0.95 at sub-1 T fields for appropriate stoichiometries. The alignment response overall can be rationalized in terms of increased mobility and grain size due to the presence of the mesogenic additive. We use a permanent magnet to fabricate films with aligned nanopores, and the utility of this approach to generate complex BCP microdomain patterns in thin films by local field screening are highlighted.

<sup>1</sup>NSF DMR-1410568 and DMR-0847534

**3:06PM C42.00004 Morphology of diblock copolymers under confinement** , DAVID ACKERMAN, BASKAR GANAPATHYSUBRAMANIAN, Iowa State University — The structure adopted by polymer chains is of particular interest for materials design. In particular, a great deal of effort has been made to study diblock polymers due to the importance they have in industrial applications. The bulk structure of most systems has been the most widely studied. However, when under the effect of confinement, the polymer chains are forced to adopt structures differing from the familiar bulk phases. As many applications utilize polymers in sizes and shapes that lead to these non bulk structures, the confinement effects are important. A commonly used tool for computationally determining structures is the continuum self-consistent field theory (SCFT). We discuss our highly scalable parallel framework for SCFT using real space methods (finite element) that is especially well suited to modelling complex geometries. This framework is capable of modeling both Gaussian and worm like chains. We illustrate the use of the software framework in determining structures under varying degrees of confinement. We detail the method used and present selected results from a systematic study of confinement using arbitrary structures.

**3:18PM C42.00005 Selective Stabilization of the Fddd Diblock Copolymer Microphase in an Applied Electric Field** , JONATHAN MARTIN, WEI LI, KRIS DELANEY, GLENN FREDRICKSON, Univ of California - Santa Barbara — Using self-consistent field theory, we explore the phase behavior of AB diblock copolymer melts in a uniform applied electric field. We assign an isotropic polarizability to each monomer type, such that the electric field selectively destabilizes AB interfaces that are perpendicular to the applied field. Under the mean-field approximation of the present model, lamellar and cylindrical structures align such that their AB interfaces are parallel to the electric field, and their relative stability with respect to the disordered phase is unchanged. Sphere and network phases do not have an axis of uniformity, so the preferred orientation for each of these phases must be identified by simulation. Small distortions in morphology are induced by the electric field for these phases, such that the free energy response includes non-harmonic terms. We compute the phase diagram for a melt in an applied electric field by comparing free energies of each morphology at its preferred orientation. We find that the stability regions for the sphere and network phases shrink with increasing electric field strength. Moreover, the double gyroid phase is relatively destabilized against the Fddd phase, extending the stability region for the Fddd phase to larger segregation strengths.

**3:30PM C42.00006 Process-directed self-assembly of copolymers** , MARCUS MULLER, Georg-August University, Goettingen, Germany, JIUZHOU TANG, Institute of Chemistry, Chinese Academy of Sciences, Beijing, China — Using computer simulation and numerical self-consistent field theory of an unentangled diblock copolymer melt, we study the interplay between relaxation of molecular conformations from a highly stretched, non-equilibrium state and structure formation of the local, conserved density during self-assembly from a disordered state. In agreement with experiments, we observe that the planar elongation of molecular conformations in the initial, disordered state results in an alignment of lamella normals perpendicular to the stretch direction during the subsequent self-assembly. Although thermodynamically the parallel orientation is favored by the non-Gaussian conformations, the alignment of the lamella normal perpendicular to the stretch direction is characterized by the larger growth rate of composition fluctuations during the spinodal ordering process. Theoretical approaches to account for the transient, non-Gaussian conformations are discussed.

**3:42PM C42.00007 Morphology Control of Multicomponent Polymeric Surfactants Using Pressure<sup>1</sup>** , JUNHAN CHO, Dankook University — The development of nanoscale morphologies for a molten polymeric surfactant under pressure is investigated by using a recently formulated self-consistent field theory. A linear ABC block copolymer is taken as our model system that allows a disparity in the propensities for curved interfaces and pressure responses of ij-pairs. The interplay of those features lead the copolymer to new morphologies at a moderate segregation level and at ambient condition such as networks and pillars of 2-dimensional array. It is shown that pressure is an effective means of morphology control and identification for those new structures. The role of volume fluctuations in the development of those structures is discussed.

<sup>1</sup>J.C. acknowledges the support from Center for Photofunctional Energy Materials through Gyeonggi Regional Research Program.

**3:54PM C42.00008 Analysis of Relaxation Spectra and Influence of Molecular Weight on the Dynamics of Block Copolymers<sup>1</sup>** , VAIDYANATHAN SETHURAMAN, VENKAT GANESAN, Univ of Texas, Austin — We use molecular dynamics simulations to study both the normal mode dynamics of block copolymers and the influence of MW on the dynamics of the block copolymer. We considered two models to isolate the specific effects arising from the morphological ordering and mobility disparities between the blocks. We effected an explicit normal mode analysis of the chain dynamics in the ordered phases in the directions parallel and perpendicular to the plane of the lamella. For systems with no mobility disparity between the blocks, our analysis demonstrates that the normal modes and their relaxations in the planes parallel and perpendicular to the lamella exhibit significant deviations from the Rouse modes. For systems in which the mobility of one of the blocks was frozen in the lamellar phase, the normal modes closely resembled the Rouse modes for tethered polymers. To understand the spatial inhomogeneities in segmental dynamics of lamellar diblock copolymer systems we probed the local average relaxation times and the dynamical heterogeneities as a function of distance from the interface. Scaling of our results indicate that the interfacial width of the ordered phases serves as the length scale underlying the spatial inhomogeneities in segmental dynamics of the fast monomers.

<sup>1</sup>Funded by NSF

**4:06PM C42.00009 ABSTRACT WITHDRAWN —**

**4:18PM C42.00010 Acoustic and ultrasonic characterization constraints of self-healing (ethylene-co-methacrylic acid) copolymers**, KENNETH PESTKA II, JONATHAN BUCKLEY, Longwood University, STEPHEN KALISTA, Department of Biomedical Engineering, Rensselaer Polytechnic Institute, NICHOLAS BOWERS, Rollins College — Recent experiments indicate that small sample poly (ethylene-co-methacrylic acid) copolymers (EMAA copolymers) exhibit time dependent variation in their acoustic and ultrasonic resonant spectra after exposure to a damage event. However, due to the relatively soft nature of these thermoplastic materials, several experimental constraints affect efficacy of resonant spectral analysis. In this work we will address the effect of several characterization constraints on a self-healing EMAA ionomer (commercially known as Dupont Surlyn 8920) including the effects of transducer loading, continuous rapid resonant excitation and temporally separated long-term resonant excitation. In some circumstances, these experimental constraints can influence the time dependence of sample resonant frequency evolution, quality factor, and variation in spectral waveform. By quantifying these effects, robust characterization of post-damage self-healing EMAA samples is possible and will be presented.

**4:30PM C42.00011 The role of symmetry of chain extender in controlling the morphology of thermoplastic polyurethanes**, ONYENKACHI WAMUO, CHENG SONG, SHAW LING HSU, University of Massachusetts, Amherst — Although polyurethane is a well-studied subject, the specific role of chain extender in the alteration of segmental dynamics and morphology formation has yet to be elucidated. Relatively low molecular weight thermoplastic polyurethanes synthesized from a two-step polymerization method were utilized in this study. The effect of the symmetry of chain extenders used in the polymerization on the morphological behavior has been studied. Comparison has been made for a number of chain extenders, including a symmetric 1,4-butanediol or 1,6-hexanediol and an asymmetric 1,2-propanediol or 1,3-butanediol. Using a combination of thermal analysis, spectroscopy and mechanical properties measurements, the development of morphological features were determined as a function of time and temperature. The symmetric chain-extended polyurethanes promotes the formation of hydrogen bonding, shows two glass transition temperatures consistent with a phase separation behavior and furthermore gives a more rigid, less extensible mechanical property when compared with the asymmetric chain-extended polyurethanes. In the latter case, the reacted polymer exhibits poor chain packing thus limiting the formation of robust hydrogen bonding behavior. It showed a singular glass transition representative of a more phase mixed system and shows more extensibility in terms of its mechanical behavior.

**4:42PM C42.00012 Phase diagram of rod-coil diblock copolymer melts by self-consistent field theory**, DADONG YAN, Department of Physics, Beijing Normal University, JIUZHOU TANG, Institute of Chemistry, Chinese Academy of Sciences, YING JIANG, School of Chemistry and Environment, Beihang University, XINGHUA ZHANG, School of Science, Beijing Jiaotong University, JEFF CHEN, Department of Physics and Astronomy, University of Waterloo — A unified phase diagram is presented for rod-coil diblock copolymer melts in the isotropic phase regime as a function of the asymmetric parameter. The study is based on free-energy calculation, which incorporates three-dimensional spatial variations of the volume fraction with angular dependence. The wormlike-chain model is used in a self-consistent field treatment. Body-centered cubic, A15, hexagonal, gyroid, and lamellar structures where the rod segments are packed inside the convex rod-coil interface are found stable. As the conformational asymmetric parameter increases, the A15 phase region expands and the gyroid phase region reduces. The stability of the structures is analyzed by concepts such as packing frustration, spinodal limit, and interfacial curvature.

**4:54PM C42.00013 Temperature effects on the interfacial properties of semifluorinated diblock copolymer thin films.**<sup>1</sup>, UMESH SHRESTHA, Clemson University, STEPHEN CLARSON, University of Cincinnati, DVORA PERAHIA, Clemson University — The interfacial composition and structure of polymer films influence their response to external stimuli and their wetting behavior. Here we probe temperature effects on the interfacial morphology and surface energies of polytrifluoro propyl methyl siloxane-*b*-polystyrene (SiF-*b*-PS) films with SiF volume fraction of  $\varphi = 0.03$  to 0.46 using atomic force microscopy and surface tension measurement. Films were cast from toluene, selective for PS, and annealed at temperatures ranging from 75 to 210°C, below and above  $T_g$  of the PS block (~98°C). For  $\varphi = 0.03$  a network of small aggregates is formed and hardly changed over the temperature range studied. For  $\varphi = 0.16$  an asymmetric diblock, spherical aggregates at room temperature transformed to elongated ones at elevated temperatures whereas in the symmetric case, spherical assemblies at room temperature merged into larger structures. Independent of SiF fraction the contact angle increased with temperature which is indicative of migration of fluorine to the interface. Surprisingly, dewetting was not observed even annealing the film at much higher temperature than  $T_g$  of PS.

<sup>1</sup>NSF DMR 0907390 2009

**5:06PM C42.00014 Evaluation of the end-to-end distance of chains solubilized in a polymer Langmuir monolayer by atomic force microscopy**, JIRO KUMAKI, Yamagata Univ — Polymer chain packing in two-dimensional (2D) condensed state is still not well understood. Direct observation of the chain packing in a monolayer should be the best way to understand this, however, it is still difficult even using atomic force microscopy (AFM) except for extraordinarily thick polymers. In this study, we successfully evaluate the end-to-end distance of the chains in a Langmuir-Blodgett monolayer composed of a conventional polymer by AFM. We successfully solubilized a small amount of a polystyrene-*b*-poly(methyl methacrylate)-*b*-polystyrene (PS-*b*-PMMA-*b*-PS) triblock copolymer in a PMMA Langmuir monolayer with the PS blocks being condensed as single-PS-block particles which could be used as a probe of the position of the chain ends. The evaluated end-to-end distance was 2.5 times longer than that of the 2D ideal chain, indicating the chains in the 2D monolayer are not strongly segregated but interpenetrates into other chains.

**5:18PM C42.00015 Block copolymer adsorbed layers on solids.**<sup>1</sup>, MANI SEN, Materials Science and Engineering (MSE), Stony Brook University (SBU), NY, NAISHENG JIANG, MSE, SBU, NY, BHOJE GOWD, CSIR-NIIST, India, MAYA ENDOH, TADANORI KOGA, MSE, SBU, NY — Block copolymer thin films offer a simple and effective route to fabricate highly ordered periodic microdomain structures. The fundamental, yet unsolved question is whether these highly oriented microdomain structures persist even near an impenetrable solid wall. We here report the adsorbed structures of polystyrene-block-poly(4-vinylpyridine) (PS-*block*-P4VP,  $M_w = 41,000$ , PS (weight fraction=0.81) formed on planar silicon substrates. Perpendicularly aligned cylindrical microdomains were created by solvent vapor annealing (Gowd et al., Soft Matter, 2014, 10, 7753), and the adsorbed layer was derived by solvent leaching with chloroform, a good solvent for the polymers and thereafter characterized by using atomic force microscopy, scanning electron microscopy, grazing incidence small angle x-ray scattering, and x-ray reflectivity. The results showed that both PS and P4VP chains lie flat on the substrate, forming a microphase-separated structure (MSS) without long-range order. Moreover, a spin-coated PS-*block*-P4VP thin film annealed under vacuum at 190 °C showed similar MSS on the substrate, indicating the generality of the interfacial polymer structure. Details will be discussed in the presentation.

<sup>1</sup>Acknowledgement: NSF Grant No. CMMI-1332499

**Monday, March 14, 2016 2:30PM - 5:30PM –**

**Session C43 GSNP GSOFD DFD: Sediment Transport, Geological Flows, and Avalanches** 346  
- Mark Shattuck, CCNY

**2:30PM C43.00001 Onset of erosion and sediment transport by a fluid flow over a granular bed<sup>1</sup>**, ARSHAD KUDROLLI, Clark Univ — Erosion and deposition of grains by a fluid flowing past the surface of a granular bed occurs in many natural and industrial processes. While considerable number of empirical studies has been conducted, very little is in fact known in detail on conditions which lead to erosion and deposition of sediments and their transport coefficients. We discuss a series of laboratory experiments to develop the physics of erosion starting with a single particle resting on a surface in a fluid flow. Fluorescent fluid-particle index matching techniques allow us to visualize not only the particles at the surface of a granular bed but also the flow within the bed and the individual particles within the bed. We will discuss the conditions governing the onset of particle motion under simple shear and their transport as a function of bed and fluid flow properties.

<sup>1</sup>Supported by the U.S. DOE Office of Science and Office of BES program under DE-FG02-13ER16401, and NSF Grant No. CBET-1335928.

**3:06PM C43.00002 The cessation threshold of continuous sediment transport in Newtonian fluid<sup>1</sup>**, THOMAS PHTZ, Ocean College, Zhejiang University, ORENCIO DURAN, MARUM-Center for Marine Environmental Sciences, University of Bremen — One of the classical problems in sediment transport science is to predict the threshold Shields number below which a bed of loose sediment particles sheared by a homogeneous fluid flow ceases to move continuously. Depending on the particle-fluid density ratio ( $s$ ), it has been believed for many decades that this threshold is a consequence of either fluid forces being just strong enough to dislodge particles resting on the bed (small  $s$ , e.g., water) or of particle-bed impacts being just strong enough to eject sufficient bed particles (large  $s$ , e.g., air). However, here we find from state-of-the-art numerical simulations that particle-bed impacts play an important role in sustaining sediment transport regardless of  $s$ . Guided by these simulations, we propose a simple, unified analytical model of the cessation of continuous sediment transport, which is quantitatively consistent with measurements in water (the famous "Shields diagram") and air on Earth and Mars. This model predicts that sediment transport on Pluto (transport of nitrogen ice particles in a very thin nitrogen atmosphere) can be sustained under surface winds comparable to those on Earth and Mars. This might explain wind streaks on Pluto's surface which have puzzled the lead researchers of the New Horizons mission.

<sup>1</sup>We acknowledge support from grants National Natural Science Foundation of China (Nos. 1151101041 and 41376095) and Natural Science Foundation of Zhejiang Province (No. LR16E090001).

**3:18PM C43.00003 Rod Climbing of Suspensions**, YOUJING GUO, XIAORONG WANG, Chemical Engineering, Tongji University, Shanghai — We wish to report an unexpected effect observed for particle suspensions sucked to pass through a vertical pipe. Above a critical concentration, the suspension on the outside of the pipe may climb along the outside wall of the pipe and then display a surprising rod-climbing effect. Our study shows that the phenomenon is influenced mainly by the suspension composition, the pipe dimension and the suction speed. The effects of the pipe materials of different kinds are negligible. Increasing the suction force and the concentration increases the climbing height. Increasing the pipe diameter and wall thickness reduces the climbing effect. This behavior may be relevant to that the suspensions of the type described are all displaying markedly shear-thickening.

**3:30PM C43.00004 Laboratory investigations of granular and hydrodynamic processes in tide-water glacial fjords<sup>1</sup>**, MAC CATHLES, Michigan Society of Fellows, University of Michigan, OLUWATOYIN THOMPSON, JUSTIN BURTON, Department of Physics, Emory University — Accelerated warming in the past few decades has led to a dramatic increase in glacial activity. This is perhaps most apparent in tidewater glacial fjords, where gravitational flows from ice sheets are focused into narrow channels of thick, fast-flowing ice which terminate into the ocean. The result is a complex system involving both melting and iceberg calving which has a direct impact on the Earth's climate and sea level rise. However, there are numerous inherent difficulties in collecting field data from remote, ice-choked fjords. To address this, we use a laboratory scale model to measure aspects of tidewater glaciers which are not observable in nature. Our model has helped to uncover the source of glacial earthquakes, where floating, cubic-kilometer scaled icebergs capsize due to gravitational instability, and temporarily reverse the velocity of the glacier. In addition, we use our model to address two other important components of tidewater glaciers involving a granular ice mélange which applies stresses on the glacier, and the role of iceberg capsize in disrupting the stratified heat transport at the glacier's terminus.

<sup>1</sup>We acknowledge support from NSF DMR-1506446

**3:42PM C43.00005 A phase diagram for fluid-driven sediment transport<sup>1</sup>**, ABE CLARK, Yale University — When a fluid flows laterally over a granular bed, grains may be transported with the flow. This process shapes much of the natural world. The boundary between states with and without grain motion has been studied for decades. However, this boundary is not well understood, since the process whereby grains are transported involves the coupling of several complex phenomena: turbulent fluid flow near a rough boundary, Darcy flow through the pore structure of the granular bed, the yield strength of granular beds comprised of frictional grains with irregular shape, and inertial effects of grains that become entrained in the flow. In order to clarify the essential physics that governs the onset of granular motion, we study this process computationally by including only the minimal features and then adding complexities one by one. We start with a simple numerical model that includes only gravity, grain-grain interactions that are repulsive and frictionless, and a purely horizontal viscous fluid flow. By varying the fluid flow rate and the effective viscosity, we find behavior that is qualitatively consistent with a large collection of experimental data known as the Shields curve. Thus, our results suggest that the main features of this curve result from a competition between grain inertia and viscous damping. We find this phase diagram to be qualitatively insensitive to secondary effects, such as friction, irregular grain shape, and restitution losses.

<sup>1</sup>Funded by U.S. Army Research Office under Grant No. W911NF-14-1-0005

**4:18PM C43.00006 The drag mechanics of an intruder moving in sheared granular medium<sup>1</sup>**, HU ZHENG, Hohai University, JONATHAN BARES, DONG WANG, ROBERT BEHRINGER, Duke University — We perform an experimental study on an intruder dragged at a constant force in a quasi-statically cyclic-sheared granular medium. A Teflon disk is embedded in a layer of bidisperse photoelastic disks. The granular medium is contained in a horizontal square cell, which can be deformed into a parallelogram with the same area, to produce simple shear. To explain the mechanism of intruder motion, we analyze the evolution under cyclic shear of multiple properties: coordination number, density, affine and non-affine motion of disk-granular system. We find that the motion of the intruder is strongly dependent on the fore-and-aft jam state of the intruder. The intruder can move along the drag force or opposite to the drag force, which is determined by the value of the drag force and the packing fraction of the granular system.

<sup>1</sup>We acknowledge support from NSF Grant No. DMR1206351, NASA Grant No. NNX15AD38G and the W.M. Keck Foundation

#### 4:30PM C43.00007 Dynamics of pull out in a granular material<sup>1</sup> , YUE ZHANG, ROBERT BEHRINGER, Duke Univ

— When an object is pulled out from a granular material, some striking phenomena can be observed. To visualize the pull out process in an experiment, we use grains composed of 2D photoelastic disks, from which circular intruders of different sizes are pulled out. We apply forces that are close to the minimum to initiate intruder motion. Then we find that the velocities of intruders depend exponentially on time, and equivalently the accelerations linearly vary with displacement. To better understand this dynamic system, we compute the drag force caused by the granular disks from the acceleration of the intruder. The result shows that the drag force depends linearly on the thickness of disks above the intruder. However, the drag force is much bigger than the weight of particles above the intruder. Additionally, we visualize the force chains formed inside the photoelastic disks and calculate the space-time evolution and curvature of those force chains. It is shown that curvatures obey the same distribution for circular intruders of different sizes.

<sup>1</sup>We would like to acknowledge NSF-DMR1206351 and the W.M.Keck Foundation.

#### 4:42PM C43.00008 How does particle shape affect the near jamming properties of granular materials? Pentagons vs. disks<sup>1</sup> , YIQIU ZHAO, JONATHAN BARES, BOB BEHRINGER, Duke University

— Understanding the role of particle shape in system-scale properties is a fundamental challenge in granular physics. We investigated the difference between the response of systems made of pentagons vs. more traditional disks. We performed isotropic compression experiments on 2D photoelastic pentagons and disks near the jamming transition. These experiments show qualitative and quantitative differences in the macroscopic responses of the two systems, such as shifts in the packing fraction at jamming onset and differences in the contact number evolution. Some of these differences are due to a reduction of packing order and the appearance of side-side contacts for the pentagons. We also examined the stress relaxation and dynamical heterogeneity of pentagon particles by performing cyclic compression to allow the system explore phase diagram. We contrast disk and pentagon evolution using four-point-susceptibility and  $G^2$  techniques.

<sup>1</sup>Work supported by NSF-DMR1206351, DMS1248071, NASA NNX15AD38G, and the W.M. Keck Foundation

#### 4:54PM C43.00009 The evolution of orientational order in sheared, 2D granular media of convex and concave elongated particles<sup>1</sup> , THEODORE MARSHALL, STEPHEN TEITEL, Univ of Rochester

— We simulate granular media consisting of elongated grains in two dimensions with a uniform background shear. We study the orientational distribution and rotation over a wide range of packing fractions, and find that the distribution reaches a stable steady-state under most initial conditions. The nematic director increases with the packing fraction, but the nematic order parameter exhibits non-monotonic behavior, which occurs well below jamming. We observe the evolution of the orientational distribution starting from configurations with the director out of alignment from its steady state orientation, and the evolution of highly ordered initial states. In general, the tumbling motion caused by the background shear causes such systems to reorder into the steady-state, but some dense, highly-ordered configurations maintain their order and exhibit wagging behavior. This can occur both above and below the jamming transition. These results for smooth, convex, spherocylindrical particles are contrasted with those for concave cross-like particles.

<sup>1</sup>This work is supported by NSF grant DMRPD-09-1765

#### 5:06PM C43.00010 Stability and Structure of Star-Shape Granules<sup>1</sup> , YUCHEN ZHAO, JONATHAN BARES<sup>2</sup>, Duke Univ., Department of Physics, NC, KEVIN LIU, Julia R. Masterman Laboratory and Demonstration School, PA, MATTHEW ZHENG, North Carolina School of Science and Mathematics, NC, KAROLA DIERICH, ACHIM MENGES, Institute for Computational Design, University of Stuttgart, Stuttgart, Germany, ROBERT BEHRINGER, Duke Univ., Department of Physics, NC

— Columns made of convex noncohesive grains like sand collapse after being released from a confining container. While various architectures built by concave grains are stable. We explore why these structures are stable, and how stable they can be. We performed experiments by randomly pouring identical star-shape particles into hollow cylinders resting on glass or a roughened base, and then observed how stable these granular columns were after carefully lifting the cylinders. We used particles that are made of acrylics and have six 9 mm arms, which extend symmetrically in xyz directions. We investigated the probability of creating a stable column and other mechanical stability aspects. We define  $r$  as the weight fraction of particles that fall out of the column after the confining cylinder is removed.  $r$  gradually increases as the column height increases, or the column diameter decreases. We found high column stability when the inter-particle friction was greater. We also explored experiment conditions such as initial vibration of columns when they were confined and loading on the top. In order to understand the inner structure leading to stability, we obtained 3D CT reconstruction data of stable columns. We will discuss coordination number and orientation, etc.

<sup>1</sup>We acknowledge supports from W.M.Keck Foundation and Research Triangle MRSEC

<sup>2</sup>will be at CNRS

#### 5:18PM C43.00011 Rheology of U-Shaped Granular Particles , MATTHEW HILL, SCOTT FRANKLIN, Rochester Institute of Technology

— We study the response of cylindrical samples of U-shaped granular particles (staples) to extensional loads. Samples elongate in discrete bursts (events) corresponding to particles rearranging and re-entangling. Previous research on samples of constant cross-sectional area found a Weibullian weakest-link theory could explain the distribution of yield points. We now vary the cross-sectional area, and find that the maximum yield pressure (force/area) is a function of particle number density and independent of area. The probability distribution function of important event characteristics the stress increase before an event and stress released during an event both fall off inversely with magnitude, reminiscent of avalanche dynamics. Fourier transforms of the fluctuating force (or stress) scales inversely with frequency, suggesting dry friction plays a role in the rearrangements. Finally, there is some evidence that dynamics are sensitive to the stiffness of the tensile testing machine, although an explanation for this behavior is unknown.

## Monday, March 14, 2016 2:30PM - 5:18PM –

Session C44 GQI: Anyons, Tensor Networks and Quantum Walks 347 -

#### 2:30PM C44.00001 Universal Finite-Size Scaling around Topological Quantum Phase Transitions , TOBIAS GULDEN, MICHAEL JANAS, YUTING WANG, ALEX KAMENEV, University of Minnesota

— The critical point of a topological phase transition is described by a conformal field theory, where finite-size corrections to energy are uniquely related to its central charge. We investigate the behavior away from criticality and obtain a scaling function. In contrast to scaling functions for entanglement entropy it discriminates between phases with different topological indexes. This function appears to be universal for all five Altland-Zirnbauer symmetry classes with non-trivial topology in one spatial dimension. We obtain an analytic form of the scaling function and compare it with numerical results.

**2:42PM C44.00002 Long-range mutual information and topological uncertainty principle**, CHAO-MING JIAN, Stanford Univ, ISAAC KIM, Perimeter Institute, XIAO-LIANG QI, Stanford Univ — Ordered phases in Landau paradigm can be diagnosed by a local order parameter, whereas topologically ordered phases cannot be detected in such a way. In this paper, we propose long-range mutual information (LRMI) as a unified diagnostic for both conventional long-range order and topological order. Using the LRMI, we characterize orders in  $n+1D$  gapped systems as  $m$ -membrane condensates with  $0 \leq m \leq n-1$ . The familiar conventional order and  $2+1D$  topological orders are respectively identified as 0-membrane and 1-membrane condensates. We propose and study the topological uncertainty principle, which describes the non-commuting nature of non-local order parameters in topological orders.

**2:54PM C44.00003 Systematically Generated Two-Qubit Braids for Fibonacci Anyons**, DANIEL ZEUCH, Department of Physics and NHMFL, Florida State University, CAITLIN CARNAHAN, Department of Computer Science, Florida State University, N. E. BONESTEEL, Department of Physics and NHMFL, Florida State University — We show how two-qubit Fibonacci anyon braids can be generated using a simple iterative procedure which, in contrast to previous methods, does not require brute force search [1]. Our construction is closely related to that of [2], but with the new feature that it can be used for three-anyon qubits as well as four-anyon qubits. The iterative procedure we use, which was introduced by Reichardt [3], generates sequences of three-anyon weaves that asymptotically conserve the total charge of two of the three anyons, without control over the corresponding phase factors. The resulting two-qubit gates are independent of these factors and their length grows as  $\log 1/\epsilon$ , where  $\epsilon$  is the error, which is asymptotically better than the Solovay-Kitaev method.

[1] C. Carnahan, D. Zeuch, and N. E. Bonesteel, arXiv:1511.00719v1 (2015).

[2] H. Xu and X. Wan, Phys. Rev. A **78**, 042325 (2008).

[3] B. W. Reichardt, Quantum Information & Computation **12**, 876 (2012).

**3:06PM C44.00004 Scaling and Topological Phase Transitions: Energy vs. Entropy**, YUTING WANG, TOBIAS GULDEN, MICHAEL JANAS, ALEX KAMENEV, Univ of Minnesota - Twin Cities — The critical point of a topological phase transition is described by a conformal field theory. Finite-size corrections give rise to a scaling function away from criticality for both energy and entanglement entropy of the system. While in the past the scaling function for the usual von Neumann entropy was found to be equal for the trivial and the topological side of the transition, we find that the scaling functions for energy and Renyi entropy with  $\alpha > 1$  are different for the two sides. This provides an easy tool to distinguish between the trivial and topological phases near criticality.

**3:18PM C44.00005 Ising anyons at finite temperature**, CHRIS SELF, Imperial College London, JAMES WOOTTON, University of Basel, SOFYAN IBLISDIR, Complutense University of Madrid, University of Barcelona, JIANNIS PACHOS, University of Leeds — Topological quantum computing offers a robust approach to quantum computation using braiding and fusion of anyonic particles. A particular type of anyons called Ising anyons are known to emerge from the microscopics of a spin lattice model called the Kitaev honeycomb<sup>1,2</sup>. We study the Ising anyon phase of the Kitaev honeycomb at finite temperature using Monte Carlo methods. We find evidence of the thermal fractionalization of the spins into Majorana modes, similar to the recent results of <sup>3</sup> who studied the non-Ising anyon phases of the model. We relate these findings to the finite temperature stability of the topological characteristics of the model. In addition we probe the thermal edge currents of the Kitaev honeycomb. Analogy to conformal field theory suggests that if the system has a boundary then at very low temperatures there should be a chiral edge current along that boundary that scales with  $T^2$ . By defining a microscopic current operator and taking its finite temperature expectation value we demonstrate edge currents that obey this scaling.

<sup>1</sup>A. Kitaev Ann. Phys. 321.1 (2006): 2-111.

<sup>2</sup>V. Lahtinen et al. New J. Phys 11.9 (2009): 093027.

<sup>3</sup>J. Nasu et al. arXiv:1504.01259 (2015)

**3:30PM C44.00006 Robust Topological and Holographic Degeneracies of Classical Systems**, SEYYED MOHAMMAD SADEGH VAEZI, ZOHAR NUSSINOV, Washington University in St.Louis, GERARDO ORTIZ, Indiana University, Bloomington — We challenge the hypothesis that the ground states of a physical system whose degeneracy depends on topology must necessarily realize topological quantum order and display non-local entanglement. To this end, we introduce and study a classical rendition of the Toric Code model embedded on Riemann surfaces of different genus numbers. We find that the minimal ground state degeneracy (and those of all levels) depends on the topology of the embedding surface alone. As the ground states of this classical system may be distinguished by local measurements, a characteristic of Landau orders, this example illustrates that topological degeneracy is not a sufficient condition for topological quantum order. This conclusion is generic and, as shown, it applies to many other models. We also demonstrate that in certain lattice realizations of these models, and other theories, one can find a ground state entropy that is "holographic", i.e., extensive in the system's boundary.

**3:42PM C44.00007 Topological defects on the lattice**<sup>1</sup>, DAVID AASEN, Caltech, ROGER MONG, University of Pittsburgh, PAUL FENDLEY, Oxford — We construct defects in two-dimensional classical lattice models and one-dimensional quantum chains that are topologically invariant in the continuum limit. We show explicitly that these defect lines and their trivalent junctions commute with the transfer matrix/Hamiltonian. The resulting splitting and joining properties of the defect lines are exactly those of anyons in a topological phase. One useful consequence is an explicit definition of twisted boundary conditions that yield the precise shift in momentum quantization, and so provide a natural way of relating microscopic and macroscopic properties. Another is a generalization of Kramers-Wannier duality to a wide class of height models. Even more strikingly, we derive the modular transformation matrices explicitly and exactly from purely lattice considerations. We develop this construction for a variety of examples including the two-dimensional Ising model.

<sup>1</sup>Institute for Quantum Information and Matter, an NSF physics frontier center with support from the Moore Foundation. NSERC-PGSD

**3:54PM C44.00008 How quickly can anyons be braided?**, CHRISTINA KNAPP, Univ of California - Santa Barbara, DONG LIU, MENG CHENG, MICHAEL ZALETEL, PARSA BONDERSON, Microsoft Station Q, CHETAN NAYAK, Microsoft Station Q, Univ of California-Santa Barbara — Topological phases of matter are a potential platform for the storage and processing of quantum information with intrinsic error rates that decrease exponentially with inverse temperature. However, it is less well-understood how error rates depend on the speed with which anyons are braided. In general, adiabatic corrections to the Berry phase vanish inversely with the length of time for the braid, with faster decay occurring as the time-dependence is made smoother. Here, we show that such corrections will not affect quantum information encoded in a topological state unless topologically non-trivial quasiparticles are created. Moreover, we show how measurements that detect unintentionally created quasiparticles can be used to control this source of error.

**4:06PM C44.00009 Edge theory approach to topological entanglement entropy and other entanglement measures of (2+1) dimensional Chern-Simons theories on a general manifold** , XUEDA WEN, Physics Department, UIUC, SHUNJI MATSUURA, Niels Bohr Institute, University of Copenhagen & Yukawa Institute for Theoretical Physics, Kyoto University, SHINSEI RYU, Physics Department, UIUC — Topological entanglement entropy of (2+1) dimensional Chern-Simons gauge theories on a general manifold is usually calculated with Witten's method of surgeries and replica trick, in which the spacetime manifold under consideration is very complicated. In this work, we develop an edge theory approach, which greatly simplifies the calculation of topological entanglement entropy of a Chern-Simons theory. Our approach applies to a general manifold with arbitrary genus. The effect of braiding and fusion of Wilson lines can be straightforwardly calculated within our framework. In addition, our method can be generalized to the study of other entanglement measures such as mutual information and entanglement negativity of a topological quantum field theory on a general manifold.

**4:18PM C44.00010 Highly entangled tensor networks** , YINGFEI GU, DANIEL BULMASH, XIAO-LIANG QI, Stanford University — Tensor network states are used to represent many-body quantum state, e.g., a ground state of local Hamiltonian. In this talk, we will provide a systematic way to produce a family of highly entangled tensor network states. These states are entangled in a special way such that the entanglement entropy of a subsystem follows the Ryu-Takayanagi formula, i.e. the entropy is proportional to the minimal area geodesic surface bounding the boundary region. Our construction also provides an intuitive understanding of the Ryu-Takayanagi formula by relating it to a wave propagation process. We will present examples in various geometries.

**4:30PM C44.00011 Tensor network characterization of superconducting circuits** , GUILLAUME DUCLOS-CIANCI, Anyon Systems Inc., DAVID POULIN, Université de Sherbrooke, ALIREZA NAJAFI-YAZDI, Anyon Systems Inc. — Superconducting circuits are promising candidates in the development of reliable quantum computing devices. In principle, one can obtain the Hamiltonian of a generic superconducting circuit and solve for its eigenvalues to obtain its energy spectrum. In practice, however, the computational cost of calculating eigenvalues of a complex device with many degrees of freedom can become prohibitively expensive. In the present work, we investigate the application of tensor network algorithms to enable efficient and accurate characterization of superconducting circuits comprised of many components. Suitable validation test cases are performed to study the accuracy, computational efficiency and limitations of the proposed approach.

**4:42PM C44.00012 Direct Measurement of Topological Phases in Discrete-Time Quantum Walks: Theory<sup>1</sup>** , VINAY RAMASESH, EMMANUEL FLURIN, IRFAN SIDDIQI, NORMAN YAO, Department of Physics, UC Berkeley — Quantum walks have been intensively investigated theoretically, from initial studies motivated by their connection to classical randomized algorithms to more recent works demonstrating topological phenomena in these walks. In particular, quantum walks simulate dynamics under effective lattice Hamiltonians which feature spin-orbit coupling. Here, we demonstrate that by adding an additional coin operator which varies from step to step, one can perform a traversal of the effective Brillouin zone, analogous to a Bloch oscillation. The geometric phase picked up by the walker along the Bloch oscillation is a genuine signature of the walks topology, a quantity known in 1D as the Zak phase. Unlike previous interferometric proposals, our work requires neither spin-dependent Ramsey spectroscopy nor an external impurity with additional degrees of freedom. We develop a protocol, illustrating its use in a circuit QED system, which allows for the detection of the Zak phase.

<sup>1</sup>This research is supported by the ARO.

**4:54PM C44.00013 Direct Measurement of Topological Phases in Discrete-Time Quantum Walks - Experiment<sup>1</sup>** , EMMANUEL FLURIN, VINAY V RAMASESH, SHAY HACHOEN GOURGY, Quantum Nanoelectronics Laboratory, UC Berkeley, NORMAN Y YAO, Department of Physics, UC Berkeley, IRFAN SIDDIQI, Quantum Nanoelectronics Laboratory, UC Berkeley — We perform quantum walks in a cavity QED architecture. Here a transmon qubit plays the role of the quantum coin, while a set of coherent states in an electromagnetic cavity forms the walker's lattice. The strong dispersive coupling between the transmon and cavity naturally implements coin-dependent translations of the walker state. The walk is performed by applying qubit rotations at equally spaced intervals; interestingly, such systems simulate dynamics under effective lattice Hamiltonians which feature strong spin-orbit coupling, leading to non-trivial band topology. By adding an additional step-dependent coin operator, we perform the first direct measurement of a quantum walk Zak phase, delineating between topologically trivial and non-trivial walks. The geometric phase is detected by implementing the quantum walk with the initial state of the walker in a superposition of a coherent state and the vacuum state, which does not partake in the walk. The Zak phase acquired by the walker thus leaves an imprint in the interference fringes of the resulting Schrödinger cat state. We observe these fringes by directly measuring the cavity Wigner function.

<sup>1</sup>This research is supported by the ARO.

**5:06PM C44.00014 On the physical realizability of quantum stochastic walks** , BRUNO TAKETANI, LUKE GOVIA, PETER SCHUHMACHER, FRANK WILHELM, Saarland University — Quantum walks are a promising framework that can be used to both understand and implement quantum information processing tasks. The recently developed quantum stochastic walk combines the concepts of a quantum walk and a classical random walk through open system evolution of a quantum system, and have been shown to have applications in as far reaching fields as artificial intelligence. However, nature puts significant constraints on the kind of open system evolutions that can be realized in a physical experiment. In this work, we discuss the restrictions on the allowed open system evolution, and the physical assumptions underpinning them. We then introduce a way to circumvent some of these restrictions, and simulate a more general quantum stochastic walk on a quantum computer, using a technique we call quantum trajectories on a quantum computer. We finally describe a circuit QED approach to implement discrete time quantum stochastic walks.

**Monday, March 14, 2016 2:30PM - 5:42PM –**

**Session C45 GQI: Adiabatic Quantum Computation and Quantum Annealing: Tunneling, Speedup and Noise Effects** 348 - Davide Venturelli, NASA Ames Research Center

## 2:30PM C45.00001 Tunneling and Speedup in Permutation-Invariant Quantum Optimization

**Problem**, TAMEEM ALBASH, Univ of Southern California — Tunneling is often claimed to be the key mechanism underlying possible speedups in quantum optimization via the quantum adiabatic algorithm. Restricting ourselves to qubit-permutation invariant problems, we show that tunneling in these problems can be understood using the semi-classical potential derived from the spin-coherent path integral formalism. Using this, we show that the class of problems that fall under Reichardt's bound (1), i.e., have a constant gap and hence can be efficiently solved using the quantum adiabatic algorithm, do not exhibit tunneling in the large system-size limit. We proceed to construct problems that do not fall under Reichardt's bound but numerically have a constant gap and do exhibit tunneling. However, perhaps counter-intuitively, tunneling does not provide the most efficient mechanism for finding the solution to these problems. Instead, an evolution involving a sequence of diabatic transitions through many avoided level-crossings, involving no tunneling, is optimal and outperforms tunneling in the adiabatic regime. In yet another twist, we show that in this case, classical spin-vector dynamics is as efficient as the diabatic quantum evolution (2).

(1) B. W. Reichardt, in Proceedings of the Thirty-sixth Annual ACM Symposium on Theory of Computing, STOC 04 (ACM, New York, NY, USA, 2004) pp. 502510.

(2) S. Muthukrishnan, T. Albash, D.A. Lidar, arXiv:1505.01249.

## 3:06PM C45.00002 Understanding Quantum Tunneling through Quantum Monte Carlo Simulations

, SERGIO BOIXO, SERGEI ISAKOV, Google Inc., GUGLIELMO MAZZOLA, ETH, VADIM SMELYANSKIY, Google Inc., ZHANG JIANG, Nasa Ames, HARTMUT NEVEN, Google Inc., MATTHIAS TROYER, ETH — The tunneling between the two ground states of an Ising ferromagnet is a typical example of many-body tunneling processes between two local minima, as they occur during quantum annealing. Performing quantum Monte Carlo (QMC) simulations we find that the QMC tunneling rate displays the same scaling (in the exponent) with system size, as the rate of incoherent tunneling. The scaling in both cases is  $O(\Delta^2)$ , where  $\Delta$  is the tunneling splitting. An important consequence is that QMC simulations can be used to predict the performance of a quantum annealer for tunneling through a barrier. Furthermore, by using open instead of periodic boundary conditions in imaginary time, equivalent to a projector QMC algorithm, we obtain a quadratic speedup for QMC, and achieve linear scaling in  $\Delta$ . We provide a physical understanding of these results and their range of applicability based on an instanton picture.

## 3:18PM C45.00003 Coupled Quantum Fluctuations and Quantum Annealing

, LAYLA HORMOZI, Massachusetts Institute of Technology, JAMIE KERMAN, MIT Lincoln Laboratory — We study the relative effectiveness of coupled quantum fluctuations, compared to single spin fluctuations, in the performance of quantum annealing. We focus on problem Hamiltonians resembling the Sherrington-Kirkpatrick model of Ising spin glass and compare the effectiveness of different types of fluctuations by numerically calculating the relative success probabilities and residual energies in fully-connected spin systems. We find that for a small class of instances coupled fluctuations can provide improvement over single spin fluctuations and analyze the properties of the corresponding class. Disclaimer: This research was funded by ODNI, IARPA via MIT Lincoln Laboratory under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of ODNI, IARPA, or the US Government.

## 3:30PM C45.00004 Performance of error suppression schemes for adiabatic quantum computation in the presence of Markovian noise

, MILAD MARVIAN, DANIEL LIDAR, None — We investigate the performance of error suppression schemes for adiabatic quantum computation. Assuming a Markovian environment and using an adiabatic master equation we compare the rate of excitation from the ground subspace of the encoded Hamiltonian during the evolution to that of the unprotected Hamiltonian. For different forms of Markovian environments such as sub-Ohmic, Ohmic and super-Ohmic we identify the parameter thresholds for which encoding starts exhibiting its benefits.

## 3:42PM C45.00005 Coping with noise in programmable quantum annealers

, ALEJANDRO PERDOMO-ORTIZ, NASA/Ames Res Ctr — Solving real-world applications with quantum annealing algorithms requires overcoming several challenges, ranging from translating the computational problem at hand to the quantum-machine language, to tuning several other parameters of the quantum algorithm that have a significant impact on performance of the device. In this talk, we discuss these challenges, strategies developed to enhance performance, and also a more efficient implementation of several applications. For example, in <http://arxiv.org/abs/1503.05679> we proposed an method to measure residual systematic biases in the programmable parameters of large-scale quantum annealers. Although the method described there works from a practical point of view, a few questions were left unanswered. One of these puzzles was the observation of a broad distribution in the estimated effective qubit temperatures throughout the device. In this talk, we will present our progress in understanding these puzzles and how these new insights allow for a more effective bias correction protocol. We will present the impact of these new parameter setting and bias correction protocols in the performance of hard discrete optimization problems and in the successful implementation of quantum-assisted machine-learning algorithms.

## 3:54PM C45.00006 Does finite-temperature decoding deliver better optima for noisy Hamiltonians?

, ANDREW J. OCHOA, Department of Physics and Astronomy, Texas A&M University, KOHJI NISHIMURA, HIDETOSHI NISHIMORI, Department of Physics, Tokyo Institute of Technology, HELMUT G. KATZGRABER, Department of Physics and Astronomy, Texas A&M University — The minimization of an Ising spin-glass Hamiltonian is an NP-hard problem. Because many problems across disciplines can be mapped onto this class of Hamiltonian, novel efficient computing techniques are highly sought after. The recent development of quantum annealing machines promises to minimize these difficult problems more efficiently. However, the inherent noise found in these analog devices makes the minimization procedure difficult. While the machine might be working correctly, it might be minimizing a different Hamiltonian due to the inherent noise. This means that, in general, the ground-state configuration that correctly minimizes a noisy Hamiltonian might not minimize the noise-less Hamiltonian. Inspired by rigorous results that the energy of the noise-less ground-state configuration is equal to the expectation value of the energy of the noisy Hamiltonian at the (nonzero) Nishimori temperature [J. Phys. Soc. Jpn., 62, 40132930 (1993)], we numerically study the decoding probability of the original noise-less ground state with noisy Hamiltonians in two space dimensions, as well as the D-Wave Inc. Chimera topology. Our results suggest that thermal fluctuations might be beneficial during the optimization process in analog quantum annealing machines.

## 4:06PM C45.00007 Estimation of effective temperatures in a quantum annealer: Towards deep learning applications<sup>1</sup>

, JOHN REALPE-GÓMEZ, MARCELLO BENEDETTI, ALEJANDRO PERDOMO-ORTIZ, NASA/Ames Res Ctr — Sampling is at the core of deep learning and more general machine learning applications; an increase in its efficiency would have a significant impact across several domains. Recently, quantum annealers have been proposed as a potential candidate to speed up these tasks, but several limitations still bar them from being used effectively. One of the main limitations, and the focus of this work, is that using the device's experimentally accessible temperature as a reference for sampling purposes leads to very poor correlation with the Boltzmann distribution it is programmed to sample from. Based on quantum dynamical arguments, one can expect that if the device indeed happens to be sampling from a Boltzmann-like distribution, it will correspond to one with an instance-dependent effective temperature. Unless this unknown temperature can be unveiled, it might not be possible to effectively use a quantum annealer for Boltzmann sampling processes. In this work, we propose a strategy to overcome this challenge with a simple effective-temperature estimation algorithm. We provide a systematic study assessing the impact of the effective temperatures in the quantum-assisted training of Boltzmann machines, which can serve as a building block for deep learning architectures.

<sup>1</sup>This work was supported by NASA Ames Research Center

**4:18PM C45.00008 Hard scheduling problems for early quantum annealer**, ZHIHUI WANG, NASA Quantum Artificial Intelligence Laboratory; Univ Space Research Assn, TONY TRAN, BRYAN O'GORMAN, NASA Quantum Artificial Intelligence Laboratory, MINH DO, JEREMY FRANK, NASA Ames Research Center, ELEANOR RIEFFEL, NASA Quantum Artificial Intelligence Laboratory, NASA Ames Research Center, NASA QUANTUM ARTIFICIAL INTELLIGENCE LABORATORY TEAM, NASA PLANNING AND SCHEDULING GROUP TEAM — We present a parameterized family of single machine scheduling problem that exhibits an easy-hard-easy phase transition. As the parameter is varied, the problem goes through a fast transition from being almost trivial to find a solution to almost always has no solution, this sharp transition accompanies a peak in computational effort. While implementing realistic-sized problems on an early quantum annealing device is still a challenge in near future, using a benchmarking problem set of small size but in a well-defined hard family, one can gain insight to a how the solving time scales for the whole family.[1] We will report quantum annealing results on this and other related problems. [1] E. G. Rieffel, D. Venturelli, B. O'Gorman, M. B. Do, E. M. Prystay, and V. N. Smelyanskiy, Quantum Information Processing 14, 1 (2015).

**4:30PM C45.00009 Accurate Variational Description of Adiabatic Quantum Optimization**, GIUSEPPE CARLEO, Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland, BELA BAUER, Station Q, Microsoft Research, Santa Barbara, CA 93106-6105, USA, MATTHIAS TROYER, Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland — Adiabatic quantum optimization (AQO) is a quantum computing protocol where a system is driven by a time-dependent Hamiltonian. The initial Hamiltonian has an easily prepared ground-state and the final Hamiltonian encodes some desired optimization problem. An adiabatic time evolution then yields a solution to the optimization problem. Several challenges emerge in the theoretical description of this protocol: on one hand, the exact simulation of quantum dynamics is exponentially complex in the size of the optimization problem. On the other hand, approximate approaches such as tensor network states (TNS) are limited to small instances by the amount of entanglement that can be encoded. I will present here an extension of the time-dependent Variational Monte Carlo approach to problems in AQO. This approach is based on a general class of (Jastrow-Feenberg) entangled states, whose parameters are evolved in time according to a stochastic variational principle. We demonstrate this approach for optimization problems of the Ising spin-glass type. A very good accuracy is achieved when compared to exact time-dependent TNS on small instances. We then apply this approach to larger problems, and discuss the efficiency of the quantum annealing scheme in comparison with its classical counterpart.

**4:42PM C45.00010 Optimizing Quantum Adiabatic Algorithm**, HONGYE HU, BIAO WU, Peking Univ — In quantum adiabatic algorithm, as the adiabatic parameter  $s(t)$  changes slowly from zero to one with finite rate, a transition to excited states inevitably occurs and this induces an intrinsic computational error. We show that this computational error depends not only on the total computation time  $T$  but also on the time derivatives of the adiabatic parameter  $s(t)$  at the beginning and the end of evolution. Previous work (Phys. Rev. A 82, 052305) also suggested this result. With six typical paths, we systematically demonstrate how to optimally design an adiabatic path to reduce the computational errors. Our method has a clear physical picture and also explains the pattern of computational error. In this paper we focus on quantum adiabatic search algorithm although our results are general.

**4:54PM C45.00011 Learning quantum annealing**, ELIZABETH BEHRMAN, JAMES STECK, Wichita State University — We propose and develop a new quantum algorithm, whereby a quantum system can learn to anneal to a desired ground state. We demonstrate successful learning of entanglement for a two-qubit system, then bootstrap to larger systems. We also show that the method is robust to noise and decoherence.

**5:06PM C45.00012 Josephson Circuits as Vector Quantum Spins**, GABRIEL SAMACH, ANDREW J. KERMAN, MIT Lincoln Laboratory — While superconducting circuits based on Josephson junction technology can be engineered to represent spins in the quantum transverse-field Ising model, no circuit architecture to date has succeeded in emulating the vector quantum spin models of interest for next-generation quantum annealers and quantum simulators. Here, we present novel Josephson circuits which may provide these capabilities. We discuss our rigorous quantum-mechanical simulations of these circuits, as well as the larger architectures they may enable. This research was funded by the Office of the Director of National Intelligence (ODNI) and the Intelligence Advanced Research Projects Activity (IARPA) under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of ODNI, IARPA, or the US Government.

**5:18PM C45.00013 Distortion of a reduced equilibrium density matrix**, IRIS SCHWENK, MICHAEL MARTHALER, Karlsruhe Institute of Technology — We study a system coupled to external degrees of freedom, called bath, where we assume that the total system, consisting of system and bath is in equilibrium. An expansion in the coupling between system and bath leads to a general form of the reduced density matrix of the system as a function of the bath selfenergy. The coupling to the bath results in a renormalization of the energies of the system and in a change of the eigenbasis. We study the influence of bosonic degrees of freedom on the state of a six qubit system similar to the eight qubit unit cell of a quantum annealing processor examined by Lanting et al.<sup>1</sup>.

<sup>1</sup>T. Lanting et al., Phys. Rev. X 4, 021041 (2014).

**5:30PM C45.00014 Quantum annealing via quantum diffusion mediated by environment**, VADIM SMELYANSKIY, Google, DAVIDE VENTURELLI, University Space Research Association, ALEJANDRO PERDOMO-ORTÍZ, University of California Santa Cruz, SERGEI KNYSH, Stinger Ghaffarian Technologies, Inc, MARK DYKMAN, Department of Physics and Astronomy, Michigan State University — We show that quantum diffusion near the quantum critical point can provide an efficient mechanism of open-system quantum annealing. The analysis refers to an Ising spin chain in a slowly decreasing transverse field coupled to bosonic heat bath. The diffusion facilitates recombination of collective (multi-spin) excitations in the chain. It sharply slows down as the system moves away from the quantum critical region, leading to significant spatial fluctuations even in the absence of disorder. The excitation density reached by then non-monotonically depends on the annealing rate. We find that obtaining an approximate solution via diffusion-mediated quantum annealing can be faster than via classical Glauber dynamics or the closed-system Kibble-Zurek mechanism. We study the scaling of the excitation density with the temperature and coupling constant to environment.

## Monday, March 14, 2016 2:30PM - 4:18PM –

Session C46 GIMS: Instrumentation II: Spectroscopy 311 - Angela Hight-Walker, NIST

**2:30PM C46.00001 Temperature Controlling Digital Cameras for Time-Resolved Angle-Resolved Photoemission Spectroscopy**, ALEXANDER NGUYEN, GREGORY AFFELDT, KENNETH GOTLIEB, ALESSANDRA LANZARA, University of California, Berkeley — Angle-resolved photoemission spectroscopy experiments (ARPES) use charged couple device (CCD) detectors to measure the spectra of various material. A CCD measures the number of photons that hit it; a problem with CCDs is that thermal energy can create false photon counts. By building a temperature controller the CCD's temperature is lowered to reduce the number of false counts, similarly, the temperature controller keeps the temperature stable reducing the randomness in false counts.

**2:42PM C46.00002 Towards Laser-based Angle-Resolved Photoemission Spectroscopy at Ultralow Temperatures**, TEJAS DESHPANDE, JOHN HARTER, California Institute of Technology, ALEXEI FEDOROV, Advanced Light Source, Lawrence Berkeley National Laboratory, DAVID HSIEH, California Institute of Technology — Recent technical advances in angle-resolved photoemission spectroscopy (ARPES) have enabled electronic structures of solids to be mapped at sub-Kelvin temperatures [1] or with sub-meV energy resolution [2]. However, achieving both conditions simultaneously remains an ongoing effort in the ARPES community. To this end, we discuss our progress in employing a laser-based source to perform ARPES of novel materials at ultralow temperatures.

Borisenko. *Synchrotron Radiation News* **25**, no. 5 (2012): 6-11.

Okazaki, et al. *Science* **337**, no. 6100 (2012): 1314-1317.

**2:54PM C46.00003 Positron spectroscopy of 2D materials using an advanced high intensity positron beam<sup>1</sup>**, A MCDONALD, V CHIRAYATH, Z LIM, R GLADEN, M CHRYSLER, A FAIRCHILD, A KOYMEN, A WEISS, Univ of Texas, Arlington — An advanced high intensity variable energy positron beam (~1eV to 20keV) has been designed, tested and utilized for the first coincidence Doppler broadening (CDB) measurements on 6-8 layers graphene on polycrystalline Cu sample. The system is capable of simultaneous Positron annihilation induced Auger electron Spectroscopy (PAES) and CDB measurements giving it unparalleled sensitivity to chemical structure at external surfaces, interfaces and internal pore surfaces. The system has a 3m flight path up to a micro channel plate (MCP) for the Auger electrons emitted from the sample. This gives a superior energy resolution for PAES. A solid rare gas (Neon) moderator was used for the generation of the monoenergetic positron beam. The positrons were successfully transported to the sample chamber using axial magnetic field generated with a series of Helmholtz coils. We will discuss the PAES and coincidence Doppler broadening measurements on graphene-Cu sample and present an analysis of the gamma spectra which indicates that a fraction of the positrons implanted at energies 7-60eV can become trapped at the graphene/metal interface.

<sup>1</sup>This work was supported by NSF grant No. DMR 1508719 and DMR 1338130

**3:06PM C46.00004 Stimulated Resonant X-Ray Emission in Solids**, ZHAO CHEN, DANIEL HIGLEY, Stanford University, MARKUS HANTSCHMANN, Helmholtz-Zentrum Berlin, VIRAT MEHTA, HGST, MARTIN BEYE, Helmholtz-Zentrum Berlin, WILLIAM SCHLOTTER, JOACHIM STOHR, SLAC — We present direct evidence of resonant stimulated X-Ray emission in magnetically patterned Co/Pd multilayers. At a free electron laser, we measure X-Ray transmission through Co/Pd of ultrafast (~2fs) X-Ray pulses at the Co  $L_3$  edge for fluences of up to 2 J/cm<sup>2</sup>/fs simultaneously in the transmission and scattering geometries. With increasing fluence, we observe a nonlinear decrease in first-order scattering intensity together with a compensating increase in transmitted forward intensity for all energies within the Co resonant absorption edge. At high enough fluences (>1 J/cm<sup>2</sup>/fs), the sample absorption spectrum and scattering intensity are both suppressed by over two orders of magnitude, leaving the sample effectively transparent to X-Rays. In our geometry, these two effects are indicative of elastic stimulated scattering, which favors forward transmission at the cost of scattered intensity in all other directions. We then show that our data is well-described by stimulated emission calculations using the optical Bloch equations. Our dual measurement serves as a pioneering study of X-Ray stimulated processes, and paves the way for experiments on realizing potentially powerful X-Ray spectroscopic techniques such as stimulated RIXS.

**3:18PM C46.00005 Extreme-ultraviolet ultrafast ARPES at high repetition rates**, JAN BUSS, HE WANG, YIMING XU, SEBASTIAN STOLL, LINGKUN ZENG, STEFAN ULONSKA, JONATHAN DENLINGER, ZAHID HUSSAIN, CHRIS JOZWIAK, ALESSANDRA LANZARA, ROBERT KAINDL, Lawrence Berkeley National Laboratory — Time- and angle-resolved photoemission spectroscopy (trARPES) represents a powerful approach to resolve the electronic structure and quasiparticle dynamics in complex materials, yet is often limited in either momentum space (incident photon energy), probe sensitivity (pulse repetition rate), or energy resolution. We demonstrate a novel table-top trARPES setup that combines a bright 50-kHz source of narrowband, extreme ultraviolet (XUV) pulses at 22.3 eV with UHV photoemission instrumentation to sensitively access dynamics for a large momentum space. The output of a high-power Ti:sapphire amplifier is split to provide the XUV probe and intense photoexcitation (up to mJ/cm<sup>2</sup>). A vacuum beamline delivers spectral and flux characterization, differential pumping, as well as XUV beam steering and toroidal refocusing onto the sample with high incident flux of 3x10<sup>11</sup> ph/s. Photoemission studies are carried out in a customized UHV chamber equipped with a hemispherical analyzer (R4000), six-axis sample cryostat, and side chambers for sample loading, storage and preparation. An ARPES energy resolution down to 70 meV with the direct XUV output is demonstrated. We will discuss initial applications of this setup including Fermi surface mapping and trARPES of complex materials.

**3:30PM C46.00006 Role of Spatial Chirp in High Harmonic Extreme Ultraviolet (XUV) Absorption Spectroscopy of Thin Films**, MING-FU LIN, University of Illinois at Urbana-Champaign — XUV light from high harmonic generation is an emerging new tool for studying ultrafast dynamics. Such sources have intrinsic “spatial chirp” that can cause significant periodic artifacts in absorption spectra of inhomogeneous samples. We show that a uniform thin-film morphology is required in order to obtain harmonic-structure free absorption spectra, especially for organometallic complexes that have strong non-resonant absorption features from the organic ligands. Demonstration of several static absorption spectra of different organometallic complexes and perovskite materials reveals elemental, oxidation state, and band structure specificity in agreement with theoretical results.

**3:42PM C46.00007 High Power Terahertz Fields Generated by an Arrayed Photoconductive Antenna Structure**, BENJAMIN GRABER, DONG HO WU, US Naval Research Laboratory, CHRISTOPHER KIM, Temple University — Terahertz spectroscopy has a wide array of scientific, commercial, and industrial applications. However, to date, terahertz signal strength of available commercial systems is limited to less than 100 uW in average terahertz power. It is expected that with enhanced terahertz power one may be able to obtain better terahertz spectral information, and enable more practical terahertz applications in real environments. In order to achieve this goal we experimentally constructed an arrayed photoconductive antenna structure, in which terahertz signals from a few photoconductive antennas are combined by adjusting every terahertz signals to be in phase. The collected signals from the multiple emitters are concentrated onto a small area so that the combined terahertz signal strength is over 1mW in average power and peak electric field over 16kV/m. The terahertz frequency spectrum of combined signals is unaltered and exactly the same as that of each individual photoconductive antenna, which spans from 100GHz to 3THz. Experimental details regarding power measurement, time domain signals, and frequency spectra analysis will be discussed. This prototype array structure appears to scale linearly with the addition of photoconductive antennas.

**3:54PM C46.00008 Terahertz nano-spectroscopy and imaging of superfluid surface plasmons in conventional and anisotropic superconductors**, H. T. STINSON, J. S. WU, B. Y. JIANG, University of California, San Diego, Z. FEI, Iowa State University, A. S. RODIN, National University of Singapore, B. CHAPLER, A. S. MCLEOD, University of California, San Diego, A. CASTRO NETO, National University of Singapore, Y. S. LEE, Soongsil University, M. M. FOGLER, D. N. BASOV, University of California, San Diego — We numerically model near-field spectroscopy and superfluid polariton imaging experiments on conventional and unconventional superconductors in the infrared and terahertz regime. Our modeling shows that near-field spectroscopy can measure the magnitude of the superconducting gap in Bardeen-Cooper-Schrieffer superconductors with nanoscale spatial resolution. We demonstrate how the same technique can measure the  $c$ -axis plasma frequency, and thus the  $c$ -axis superfluid density, of layered unconventional superconductors such as cuprates and pnictides with identical spatial resolution. We discuss the development of a cryogenic terahertz near-field microscope designed to perform these proposed experiments, and recent proof of principle results at room temperature.

**4:06PM C46.00009 Inkjet Printed Wire-Grid Polarizers for the THz Frequency Range<sup>1</sup>**, A. FARID, N. J. LAURITA, Johns Hopkins Univ, B. TEHRANI, J. HESTER, M. M. TENTZERIS, Georgia Institute of Technology, N. P. ARMITAGE, Johns Hopkins Univ — We have investigated the use of inkjet printing technology for the production of THz range wire-grid polarizers using time-domain terahertz spectroscopy. Such technology affords a cheap and reproducible way of quickly manufacturing THz range metamaterial structures. Thin silver-nanoparticle ink lines were printed using a Dimatix DMP-2831 printer. We investigated the optimal printing geometry of the polarizers by looking at a number of samples with printed wires of varying thickness and spacing. We also investigate the ultimate capabilities of these polarizers by investigating their properties when stacked.

<sup>1</sup>Gordon and Betty Moore Foundation

## Monday, March 14, 2016 2:30PM - 5:30PM – Session C47 DCMP: Surface, Growth, and Morphology 312 -

**2:30PM C47.00001 Observation of heterodyne and homodyne mixing in X-ray photon correlation spectroscopy during thin film deposition<sup>1</sup>**, RANDALL HEADRICK, JEFFREY ULBRANDT, University of Vermont, MELIHA RAINVILLE, CHRISTA WAGENBACH, Boston University, SURESH NARAYANAN, ALEC SANDY, HUA ZHOU, Argonne National Laboratory, KARL LUDWIG, Boston University — The properties of artificially grown thin films are often strongly affected by the dynamic relationship between surface growth processes and subsurface structure. Coherent mixing of X-ray signals promises to provide an approach to better understand such processes. Continuously variable mixing of surface and bulk scattering signals during real-time studies of sputter deposition of a-Si and a-WiSi<sub>2</sub> films has been observed by controlling the X-ray penetration and escape depths in coherent grazing incidence small angle X-ray scattering (Co-GISAXS). Under conditions where the X-ray signal comes from both the growth surface and the thin film bulk, oscillations in temporal correlations arise from coherent interference between scattering from stationary bulk features and from the advancing surface. The absence of oscillations at larger in-plane wavevector transfer is interpreted as evidence that elongated bulk features propagate upward at the same velocity as the surface. Additionally, a highly surface sensitive mode is demonstrated that can access the surface dynamics independently of the subsurface structure.

<sup>1</sup>Acknowledgements: USDOE Office of Basic Energy Sciences under DE-FG02-07ER46380 (RH and JU), and DE-FG02-03ER46037 (MR, CW, and KL).

**2:42PM C47.00002 Unusual “Explosive” Nucleation and Superdiffusion in Pb/Si(111)-7x7<sup>1</sup>**, M. T. HERSHBERGER, Iowa State University and Ames Laboratory, M. HUPALO, Ames Laboratory, P. A. THIEL, Iowa State University and Ames Laboratory, H. HATTAB, Ames Laboratory, M. HORN VON HOEGEN, University of Duisburg-Essen, M. C. TRINGIDES, Iowa State University and Ames Laboratory — The study of the recently found “explosive” nucleation on Pb/Si(111) was further investigated to understand the origin of the sharp transition in coverage and the presence of superdiffusive motion. After small stepwise depositions of ~0.03 ML spatial correlations in the growth direction of neighboring islands are observed. The island growth rates are much higher than what is expected in classical nucleation. Islands collect material many times larger than the amount deposited in the surrounding Voronoi areas contrary to classical expectations. Their centers of mass shift by large amounts, ~10nm, again confirming the directionality in their growth and that material must be arriving over mesoscale distances. The island size distributions do not agree with the expected sharply peaked classical distributions since only fully completed islands are observed. Further depositions show additional nucleation of smaller islands and with higher densities thus conforming that when the critical coverage is reached locally the island nucleation is still active. Comparisons will be made between the diffusion length deduced in these experiments and the one extracted from earlier LEEM experiments monitoring the refilling of an initial vacant area.

<sup>1</sup>Ames Laboratory is operated by the US-DOE under Contract No. DE-AC02-07CH11358.

**2:54PM C47.00003 Submonolayer island growth with anomalous diffusion<sup>1</sup>**, JACQUES AMAR, University of Toledo, MIKHAEEL SEMAAN, California State University, Long Beach — Island nucleation and growth play an important role in the early stages of thin-film growth. Of particular interest is the exponent  $\chi$  which describes the dependence of the peak island density on deposition flux, and which also depends sensitively on the critical island-size  $i$ . While the dependence of  $\chi$  on  $i$  is known for normal diffusion, the case of anomalous monomer diffusion is also of interest, since this appears to play a role in recent experiments. Here we derive general expressions for  $\chi$  which are valid for arbitrary substrate dimension, island fractal dimension, critical island size, and monomer diffusion exponent  $\mu$ . Excellent agreement is obtained between our predictions and kinetic Monte Carlo simulations carried out for the case of irreversible growth ( $i = 1$ ), and monomer superdiffusion with  $1 < \mu \leq 2$ , although unusually large crossover effects are also observed. These results also confirm and generalize a previous prediction for the case of ballistic diffusion ( $\mu = 2$ ). We also consider the case of monomer subdiffusion corresponding to  $0 \leq \mu < 1$ . Good agreement with our predictions for  $\chi(\mu)$  is also found in this case, although the general scaling behavior is more complex due to the presence of large fluctuations.

<sup>1</sup>Supported by NSF DMR-1410840 and NSF REU Award 1262810

**3:06PM C47.00004 Interaction of Dysprosium with the Basal Plane of Graphite.**, PATRICIA THIEL, Ames Laboratory, EMMA KWOLEK, Iowa State University, HUAPING LEI, Key Laboratory of Materials Physics, Institute of Solid State Physics, CAS, YINGHUI ZHOU, Department of Physics, Xiamen University, ANN LII-ROSALES, Iowa State University, MARK WALLINGFORD, CAI-ZHUANG WANG, MICHAEL TRINGIDES, Ames Laboratory — We have studied adsorption, nucleation, growth, intercalation, and carburization of dysprosium (Dy) on graphite surfaces, and the way that these phenomena are influenced by surface defects. The experiments consist of scanning tunneling microscopy in ultrahigh vacuum. The condensation coefficient of Dy is strongly enhanced by surface defects. In the absence of defects, at room temperature, homogeneous nucleation can occur on terraces, consistent with DFT calculations of energetics. At room temperature, island shapes consist of a flat three-atom base, decorated by single-atom upper layers. Layer populations in such islands are analyzed in the context of a tailored analytic model, which provides information about interlayer mobility. At elevated temperature, Dy can intercalate with the graphite substrate and can form carbide.

**3:18PM C47.00005 Thermal evolution of Fe on  $Ge(111) - c(2 \times 8)$  surface and the effect of  $(\sqrt{3} \times \sqrt{3})$  Ag-Ge buffer layer**, TSU-YI FU, HUNG-CHANG HSU, MING-KUAN JHOU, JIA-YUAN WU, Department of Physics, National Taiwan Normal University — Using scanning tunneling microscopy, two systems of Fe deposition on a clean  $Ge(111) - c(2 \times 8)$  surface and surfaces with a  $(\sqrt{3} \times \sqrt{3})$   $R30^\circ$  Ag-Ge buffer layer were compared. Complex surface alloy structures were easily formed on Fe/Ge systems through annealing at 300-650 K. On clean  $Ge(111)$  surfaces, similar surface morphology evolution was observed when two different amounts of Fe were deposited. To reduce the complexity,  $(\sqrt{3} \times \sqrt{3})$   $R30^\circ$  Ag-Ge interface were used as buffer layers. The growth morphologies differed in the presence and absence of the buffer layers. After heat treatment to 570 K,  $(2 \times 2)$  reconstruction platform islands were formed in the Fe/Ge system, which transformed to three-dimensional (3D) islands at 640 K. With Ag buffer layer, only nanoparticle growth occurred and 3D islands were formed early at 570 K. Generally,  $\sqrt{19}$  ring clusters increased to break the order  $c(2 \times 8)$  reconstruction by increasing the temperature and disappeared at 640 K in Fe-Ge system, but only  $\sqrt{7}$  ring clusters appeared at 390 K with  $(\sqrt{3} \times \sqrt{3})$   $R30^\circ$  Ag-Ge buffer layer.

**3:30PM C47.00006 Free energy of steps using atomistic simulations<sup>1</sup>**, RODRIGO FREITAS, TIMOFEY FROLOV, MARK ASTA, Department of Materials Science and Engineering, University of California, Berkeley — The properties of solid-liquid interfaces are known to play critical roles in solidification processes. Particularly special importance is given to thermodynamic quantities that describe the equilibrium state of these surfaces. For example, on the solid-liquid-vapor heteroepitaxial growth of semiconductor nanowires the crystal nucleation process on the faceted solid-liquid interface is influenced by the solid-liquid and vapor-solid interfacial free energies, and also by the free energies of associated steps at these faceted interfaces. Crystal-growth theories and mesoscale simulation methods depend on quantitative information about these properties, which are often poorly characterized from experimental measurements. In this work we propose an extension of the capillary fluctuation method for calculation of the free energy of steps on faceted crystal surfaces. From equilibrium atomistic simulations of steps on (111) surfaces of Copper we computed accurately the step free energy for different step orientations. We show that the step free energy remains finite at all temperature up to the melting point and that the results obtained agree with the more well established method of thermodynamic integration if finite size effects are taken into account.

<sup>1</sup>The research of RF and MA at UC Berkeley were supported by the US National Science Foundation (Grant No. DMR-1105409). TF acknowledges support through a postdoctoral fellowship from the Miller Institute for Basic Research in Science.

**3:42PM C47.00007 Low temperature Silicon epitaxy on bare Si (100) and H terminated Si (100) surfaces**, XIAO DENG, PRADEEP NAMBOODIRI, KAI LI, NIST - Natl Inst of Stds & Tech, XIQIAO WANG, University of Maryland, College Park, TONGBAO LI, Tongji University, Shanghai, China, RICHARD SILVER, NIST - Natl Inst of Stds & Tech — Silicon on Silicon growth morphology is studied using an ultrahigh vacuum scanning tunneling microscopy (UHV-STM) and transmission electron microscopy (TEM). Sub-monolayer to 18 nm of silicon was evaporated using an all-silicon sublimation source (SUSI) onto a UHV prepared Si (100) sample at 250C. The results are compared with the growth characteristics on hydrogen passivated surfaces (H: Si) under identical experimental conditions. STM images indicate that growth morphology of both Si on Si and Si on H: Si is of epitaxial nature at temperatures as low as 250C. For Si on bare Si growth at 250C, there exists a stable thickness regime where Si epitaxial growth front keeps the same morphology. Although the mobility of silicon is modestly affected on the H: Si surface because of the H atoms during the initial sub-monolayer regime, the growth proceeds epitaxially with the 3D island growth mode and noticeable surface roughening.

**3:54PM C47.00008 A diffuse interface model of grain boundary faceting<sup>1</sup>**, FADI ABDELJAWAD, DOUGLAS MEDLIN, JONATHAN ZIMMERMAN, KHALID HATTAR, STEPHEN FOILES, Sandia National Laboratories — Incorporating anisotropy into thermodynamic treatments of interfaces dates back to over a century ago. For a given orientation of two abutting grains in a pure metal, depressions in the grain boundary (GB) energy may exist as a function of GB inclination, defined by the plane normal. Therefore, an initially flat GB may facet resulting in a hill-and-valley structure. Herein, we present a diffuse interface model of GB faceting that is capable of capturing anisotropic GB energies and mobilities, and accounting for the excess energy due to facet junctions and their non-local interactions. The hallmark of our approach is the ability to independently examine the role of each of the interface properties on the faceting behavior. As a demonstration, we consider the  $\Sigma 5$  (001) tilt GB in iron, where faceting along the {310} and {210} planes was experimentally observed. Linear stability analysis and numerical examples highlight the role of junction energy and associated non-local interactions on the resulting facet length scales. On the whole, our modeling approach provides a general framework to examine the spatio-temporal evolution of highly anisotropic GBs in polycrystalline metals.

<sup>1</sup>Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. DOE's National Nuclear Security Administration under Contract DE-AC04-94AL85000

**4:06PM C47.00009 External-Field-Driven Nanopatterning on Crystalline Substrate Surfaces**, ASHISH KUMAR, DWAIPAYAN DASGUPTA, DIMITRIOS MAROUDAS, Univ of Mass - Amherst — Current-driven dynamics of single-layer epitaxial islands on fcc crystalline substrates can lead to surface pattern formation with significant implications for nanofabrication. We have developed and validated a fully nonlinear model of driven island evolution on {110}, {100} and {111} substrate surfaces due to diffusional mass transport along the island edge and accounting for edge diffusional anisotropy. We find that the migration speed of a morphologically stable island is inversely proportional to the island size,  $R$ , up to a critical size that marks the onset of island morphological transition; further increase in  $R$  triggers edge fingering and/or necking or dynamical transitions. We report formation of complex nanopatterns emerging from individual larger-than-critical islands with two different types of initial configuration: a slender, high-aspect-ratio island shape and an equilibrium, rounded morphology. We have developed a linear stability theory that explains the observed morphological instabilities. We characterize the nanopatterns formed and study the dependence of the nanopattern features on the duration of application of the electric field and the misorientation angle between a fast edge diffusion direction and the electric field direction.

**4:18PM C47.00010 Progress in Application of Generalized Wigner Distribution to Growth and Other Problems<sup>1</sup>**, T.L. EINSTEIN, JOSUE MORALES-CIFUENTES, Univ. Maryland, College Park, ALBERTO PIMPINELLI, Rice Quantum Institute, DIEGO LUIS GONZALEZ, Univ. del Valle, Cali, Colombia — We recap the use of the (single-parameter) Generalized Wigner Distribution (GWD) to analyze capture-zone distributions associated with submonolayer epitaxial growth<sup>2</sup>. We discuss recent applications to physical systems, as well as key simulations. We pay particular attention to how this method compares with other methods to assess the critical nucleus size characterizing growth. The following talk discusses a particular case when special insight is needed to reconcile the various methods. We discuss improvements that can be achieved by going to a 2-parameter fragmentation approach. At a much larger scale we have applied this approach to various distributions in socio-political phenomena (areas of secondary administrative units [e.g., counties] and distributions of subway stations).

<sup>1</sup>Work at UMD supported by NSF CHE 13-05892

<sup>2</sup>TLE, AP, DLG, J. Cryst. Growth 401, 67 (2014); TLE, JRM-C, AP, DLG, J. Phys. Conf. Ser. 640, 012024 (2015).

**4:30PM C47.00011 Role of Transient Mobility on Submonolayer Island Growth: Extensions and Testing<sup>1</sup>**, JOSUE MORALES CIFUENTES, THEODORE EINSTEIN, Univ of Maryland-College Park, ALBERTO PIMPINELLI, Rice Quantum Institute — In studies of epitaxial growth a major goal is assessing the smallest stable cluster ( $i + 1$  monomers, with  $i$  the critical nucleus size), by analyzing the capture zone distribution (CZD) or the scaling of incident flux  $F$  to the density of stable islands  $N$  ( $N \propto F^\alpha$ , with  $\alpha$  the growth exponent). As noted in the previous talk, the GWD has well described the data in several experiments, including submonolayer para-hexaphenyl (6P) on amorphous mica ( $i \approx 3$ ). Different scaling ( $F^\alpha$ ) for 6P at (small) large  $F$  is attributed to (DLA) ALA dynamics, i.e.  $i = (5)7 \pm 2$ .<sup>2</sup> Our recent theoretical work considered monomers propagating ballistically before thermalizing or attaching to islands, leading to scaling, non-monotonic crossover, and activation energies that account for the data and reconciling the values of  $i$ .<sup>3</sup> We present applications to other experimental systems: 6P on SiO<sub>2</sub> and pentacene (5A) on amorphous mica. We describe useful simplifying approximations, and preliminary kinetic Monte Carlo simulations including transient effects on growth.

<sup>1</sup>Work at UMD supported by NSF CHE 13-05892

<sup>2</sup>L. Tumbek & A. Winkler, Surf. Sci. 606, L55 (2012)

<sup>3</sup>J. R. Morales-Cifuentes, T. L. Einstein, and A. Pimpinelli. Phys. Rev. Lett. 113, 246101 (2014)

**4:42PM C47.00012 Unravelling the “Silicene” Growth Mechanism Based on a Seeding Layer Approach<sup>1</sup>**, WEI JIANG, Univ of Utah, MIAO ZHOU, Chongqing University, FENG LIU, Univ of Utah, FENG LIU TEAM — Unlike *sp*<sup>2</sup> graphene, silicon atoms prefer to form *sp*<sup>3</sup> hybridized state that gives silicene a buckled geometry. To study how to grow flat silicene, we have investigated the structure and stability of multi-layer “silicene” using *ab initio* methods by introducing a “seeding layer” of silicene on which additional “silicene” layers are grown. The buckling height and the isotropic strain of the seeding layer is shown to play a key in affecting the structure, in particular the flatness of the growing layers. A phase diagram in the parameter space of buckling height and in-plane strain of the seeding layer is constructed to guide the growth of additional “silicene” layer. Furthermore, in contrast to monolayer silicene growth on Ag substrate which exhibits various patterns, only the  $\sqrt{3}\times\sqrt{3}$  pattern is found stable using large supercell calculations. Our calculations suggest that thermodynamically no silicene structures can survive beyond three layers. These results will shed useful lights on experimental growth of flat and low-buckled silicene and help explain existing experimental results.

<sup>1</sup>This work was supported by NSF-MRSEC (grant DMR-1121252) and DOE-BES (grant DE-FG02-04ER46148)

**4:54PM C47.00013 Current-Driven Nanowire Formation on Crystalline Conducting Substrate Surfaces**, DWAIPAYAN DASGUPTA, ASHISH KUMAR, DIMITRIOS MAROUDAS, Univ of Mass - Amherst — Using a simulation study, we demonstrate a new, driven-assembly-based approach to single-layer nanowire formation on fcc crystalline substrate surfaces. In this approach, we manipulate individual epitaxial islands using an external electric field to drive the formation of single nanowires or arrays of them. We have developed and validated a fully nonlinear model of current-driven island evolution mediated by diffusional mass transport along the island edge and accounting for edge diffusional anisotropy and island coalescence and breakup. Using a linear stability theory, we analyze the morphological stability of islands with equilibrium shapes and predict the occurrence of morphological instability for islands larger than a critical size under the action of an electric field along the slowest edge diffusion direction on {110}, {100}, and {111} substrate surfaces. Consistent with the theoretical prediction, dynamical simulations show that large-size islands undergo a fingering instability which, following finger growth and, depending on the substrate orientation, necking instability, leads to formation of single or multiple nanowires. We find that the nanowires have constant widths, on the order of tens of nanometers, and explain analytically the nanowire dimensions.

**5:06PM C47.00014 Nonlinear Analysis of the Surface Morphological Stability of Stressed Crystalline Materials and Coherently Strained Epitaxial Thin Films**, LIN DU, DWAIPAYAN DASGUPTA, DIMITRIOS MAROUDAS, University of Massachusetts Amherst — The competition between surface energy and elastic strain energy in surfaces of stressed solids may cause the Asaro-Tiller/Grinfeld (ATG) instability leading to surface cracking, which can be predicted by linear stability theory (LST). Self-consistent dynamical simulations based on a fully nonlinear surface evolution model reveal that, in addition to the ATG instability, long-wavelength perturbations from the planar surface morphology can also trigger a tip-splitting instability, causing the formation of a pattern of secondary ripples that cannot be predicted by LST. We have developed a weakly nonlinear stability theory that can explain the occurrence of such nonlinear rippling instabilities and predict the critical wavelength for secondary ripple formation as well as the number of secondary ripples that form on the surface as a function of perturbation wavelength. We also have applied the weakly nonlinear theory to study the surface morphological stability of a coherently strained epitaxial thin film on a crystalline elastic substrate. We find that, in addition to the Stranski-Krastanow instability, secondary rippling instabilities may also occur on the film surface, leading to formation of smaller-sized quantum dots (QDs) through tip splitting of larger QDs.

**5:18PM C47.00015 Triple line kinetics in solid-state dewetting<sup>1</sup>**, ASHWANI TRIPATHI, OLIVIER PIERRE-LOUIS, Univ Lyon I UA 442 CNRS — Solid-state dewetting has been studied in a large number of experimental systems, such as SOI (Si on amorphous SiO<sub>2</sub>)<sup>2</sup>, or metal films on various substrates<sup>3</sup>. Several theoretical approaches have been proposed in the past 10 years to understand this phenomena, ranging from Kinetic Monte Carlo to phase field, and continuum Mullins-like models. We present a continuum model<sup>4</sup> which addresses the question of the limit of validity of the usual approximation of a constant contact angle at the triple line between the solid, the film, and the vacuum (or vapor). Our results suggest that the Young relation is subject to systematic deviations, which could be measured in experiments. In addition, the so-called mass shedding effect, which leads to the breakup of the film at a finite distance from the triple-line, can be accelerated by orders of magnitude due to wetting effects.

<sup>1</sup>Supported by LOTUS Grant 11-13AP20

<sup>2</sup>E Bussmann, F Cheynis, F Leroy, P Müller and O. Pierre-Louis, New J. Phys. 13 043017 (2011).

<sup>3</sup>C.V. Thompson, Annu. Rev. Mater. Res. 42, 399 (2012).

<sup>4</sup>A. Tripathi, O. Pierre-Louis, preprint.

## Monday, March 14, 2016 2:30PM - 5:42PM –

**Session C48 GQI: Multimode Circuit QED and Strong Coupling** 349 - Benjamin Palmer, Laboratory of Physical Sciences, College Park

**2:30PM C48.00001 Multimode cavity QED 1: State preparation and readout**, RAVI NAIK, NELSON LEUNG, SRIVATSAN CHAKRAM, YAO LU, NATHAN EARNEST, Physics Department and James Franck Institute, University of Chicago, PETER GROSZKOWSKI, JENS KOCH, Department of Physics and Astronomy, Northwestern University, DAVID SCHUSTER, Physics Department and James Franck Institute, University of Chicago — Quantum information processing requires the creation of scalable architectures with long lived, highly coherent, readily addressable quantum states. A promising architecture consists of Fock states of photons in coupled superconducting microwave cavity arrays, with state preparation and readout achieved by coupling to superconducting qubits via circuit QED. We describe experiments on such multimode circuit QED devices consisting of 1D chains of 10-20 tunnel coupled 2D high-Q microwave resonators coupled to a single, flux-tunable transmon qubit. We use parametric sideband transitions [1], implemented via flux modulation of the transmon, to realize arbitrary states of the photonic qubits. We also discuss ongoing efforts to engineer multimode architectures comprised of coupled 3D microwave cavities in which photon lifetimes can exceed 10 ms [2]. [1] J. D. Strand et al, Physical Review B 87.22 (2013) [2] M. Reagor et al, Applied Physics Letters 102, 192604 (2013)

Multimode cavity QED 1: State preparation and readout

(Ravi Naik, Nelson Leung, Srivatsan Chakram, Yao Lu, Nate Earnest, Peter Groszkowski Jens Koch, David Shuster), but before a talk named:

Multimode cavity QED 3: Universal quantum gates

(Nelson Leung, Ravi Naik, Srivatsan Chakram, Yao Lu, Nate Earnest, Peter Groszkowski Jens Koch, David Shuster)

**2:42PM C48.00002 Multimode cavity QED 2: Parameter dependence of theoretical modeling**, PETER GROSZKOWSKI, Northwestern University, NELSON LEUNG, DAVID SCHUSTER, University of Chicago, JENS KOCH, Northwestern University — Superconducting circuits are a promising platform for future quantum information processing devices. While in recent years gate and readout fidelities have improved, they still benefit greatly from added intrinsic robustness and improved error resilience. In this talk, we present results from a new qubit array, where qubit manipulation and readout are achieved by interaction with a parametrically driven superconducting resonator. We provide insight into mode addressability as well as crosstalk, and their dependence on the system's size in various configurations.

Thank you!

**2:54PM C48.00003 Multimode cavity QED 3: Universal quantum gates**, NELSON LEUNG, RAVI NAIK, SRIVATSAN CHAKRAM, YAO LU, NATHAN EARNEST, Physics Department and James Franck Institute, University of Chicago, PETER GROSZKOWSKI, JENS KOCH, Department of Physics and Astronomy, Northwestern University, DAVID SCHUSTER, Physics Department and James Franck Institute, University of Chicago — A promising architecture for scalable quantum computation consists of photonic qubits in multimode superconducting cavities, coupled to superconducting qubits. In this talk, we describe schemes to implement pairwise universal gate operations between the photonic qubits. We use parametric sideband interactions [1] mediated by a superconducting qubit to realize arbitrary single photonic qubit gates, as well as the C-phase gate between arbitrary pairs of photonic qubits, thereby realizing universal gate operations. We also describe schemes to realize beam splitter and phase shifter elements in this multimode architecture, allowing for circuit QED realizations of linear optical quantum computation schemes. [1] J. D. Strand et al, Physical Review B 87.22 (2013)

**3:06PM C48.00004 Multimode cavity QED 4: Quantum state tomography**, SRIVATSAN CHAKRAM, NELSON LEUNG, RAVI NAIK, YAO LU, NATHAN EARNEST, Physics Department and James Franck Institute, University of Chicago, PETER GROSZKOWSKI, JENS KOCH, Northwestern University, DAVID SCHUSTER, Physics Department and James Franck Institute, University of Chicago — One of the challenges of large scale quantum information processing is the ability to perform quantum state tomography of massively entangled states. We implement multiplexed tomography of quantum states of multimode cavity arrays comprising several photonic qubits. Quantum state tomography is performed via sequential parametric transitions [1] with a single, flux-tunable transmon qubit, in conjunction with multimode photonic gates and transmon readout. We describe schemes to prepare and characterize W states of several modes of the multimode cavity, and our progress towards extending such schemes to multiphoton entangled states. The ability to create and measure arbitrary quantum states, in conjunction with the large coherence time of microwave cavities, makes multimode cavity QED a promising architecture for scalable quantum computation and bosonic quantum simulation. [1] J. D. Strand et al, Physical Review B 87.22 (2013)

**3:18PM C48.00005 Multimode Strong Coupling in Circuit QED**, NEEREJA SUNDARESAN, YANBING LIU, DARIUS SADRI, LASZLO SZOCS, DEVIN UNDERWOOD, MOEIN MALEKAKHLAGH, HAKAN TURECI, ANDREW HOUCK, Princeton University — We present experimental and theoretical studies in the multimode strong coupling (MMSC) regime of cavity quantum electrodynamics (QED). In MMSC, a single atom is simultaneously coupled to a large, but discrete, number of cavity harmonics, with atom-mode coupling strengths comparable to the free spectral range (FSR). This regime is readily accessible in circuit QED, by strongly coupling a transmon qubit to a low fundamental frequency microwave cavity. We present some key results from our original experiment (PRX 5, 021035, 2015), in which a transmon qubit, resonant with the 75th harmonic of a 90 MHz cavity, reached qubit-mode coupling strengths exceeding 30MHz. When this system is coherently driven, we observed complex multimode fluorescence, with the notable formation of ultra-narrow linewidths. To better understand these unique features of multimode resonance fluorescence we developed a quantum formalism, which attributes the spectral linewidth narrowing to the correlated spontaneous emission of doubly dressed states. Finally we will share preliminary experimental results from our continuing study of MMSC, this time from a system where qubit-mode coupling strengths approach and even exceed the FSR.

**3:30PM C48.00006 Multiphoton Quantum Rabi Oscillations in Ultrastrong Cavity QED**, ANTON FRISK KOCKUM, Center for Emergent Matter Science, RIKEN, Saitama 351-0198, Japan, LUIGI GARZIANO, ROBERTO STASSI, VINCENZO MACRI, SALVATORE SAVASTA, Dipartimento di Fisica e di Scienze della Terra, Università di Messina, I-98166 Messina, Italy, FRANCO NORI, Center for Emergent Matter Science, RIKEN, Saitama 351-0198, Japan — When an atom is strongly coupled to a cavity, the two systems can exchange a *single* photon through a coherent Rabi oscillation. This process enables precise quantum-state engineering and manipulation of atoms and photons in a cavity, which play a central role in quantum information and measurement. Recently, a new regime of cavity QED has been reached experimentally where the interaction between light and artificial atoms (qubits) becomes ultrastrong, *i.e.*, its strength is comparable to the atomic transition frequency or the resonance frequency of the cavity mode. Here we show that this regime can strongly modify the concept of vacuum Rabi oscillations, enabling multiphoton exchanges between the qubit and the resonator. We find that experimental state-of-the-art circuit-QED systems can undergo *two-* and *three-*photon vacuum Rabi oscillations. These anomalous Rabi oscillations can be exploited for the realization of efficient Fock-state sources of light and complex entangled states of qubits.

**3:42PM C48.00007 Ultrastrong coupling in a flux qubit-transmission line system**, POL FORN-DIAZ, JEAN-LUC ORGIAZZI, MARTIN OTTO, ALI YURTALAN, Institute for Quantum Computing, University of Waterloo, Waterloo, Canada, BORJA PEROPADRE, Department of Chemistry and Chemical Biology, Harvard University, Cambridge MA, USA, JUAN-JOSE GARCIA-RIPOLL, Instituto de Fisica Fundamental IFF-CSIC, Madrid, Spain, CHRISTOPHER WILSON, ADRIAN LUPASCU, Institute for Quantum Computing, University of Waterloo, Waterloo, Canada — Recent advances in circuit QED have enabled the study of light-matter interactions in new regimes of coupling strength. Experiments based on flux qubits coupled to resonators observed indications of the so-called ultrastrong coupling regime, where the coupling strength is comparable to the qubit energy splitting. We have realized an experiment where a flux qubit is coupled to an open transmission line with an adjustable coupling strength, which can be tuned into the ultrastrong coupling regime. When the coupling strength is low, the qubit behaves like an isolated dipole scatterer, reflecting over 97% of the incident coherent probe. At larger coupling strengths, the qubit linewidth exceeds its energy splitting, indicating that the system operates deeply in the ultrastrong coupling regime. We find that qualitative features of the qubit response evolve with the coupling strength in ways unexpected based on scattering calculations within the rotating-wave approximation. Some features of the evolution can be understood in the broader context of the spin-boson model.

**3:54PM C48.00008 Ultra-strong coupling in a transmon circuit architecture<sup>1</sup>**, SAL BOSMAN, MARIO GELY, VIBHOR SINGH, ALESSANDRO BRUNO, GARY STEELE, Delft Univ of Tech — New unexplored phenomena are predicted in cQED for the ultra-strong coupling (USC) regime and beyond. Here, we explore two strategies to increase the coupling between a transmon qubit and a microwave resonator. In the first approach, we increase the impedance of the resonator, enhancing its voltage zero-point fluctuations, and measure a vacuum Rabi splitting of 916 MHz. In a second approach, we create a transmon qubit by making a superconducting island suspended above the center conductor of the resonator and which is shorted to ground by two Josephson junctions. Doing so, we maximize the dipole moment of the qubit and observe a vacuum Rabi splitting of 1.2 GHz with a qubit linewidth of 1 MHz. This first transmon qubit in the USC regime improves the coherence time by a factor of 100 compared to other systems in the USC limit. Finally we predict that by combining both approaches, a coupling of  $\sim 3.6$  GHz is possible, reaching close to the deep strong coupling limit.

<sup>1</sup>The work was supported by the Dutch science foundation NWO/FOM.

**4:06PM C48.00009 Deep strong coupling in a circuit QED system (1) - Introduction**<sup>-1</sup>, KOUICHI SEMBA, TOMOKO FUSE, FUMIKI YOSHIHARA, National Institute of Information and Communications Technology, Koganei, Tokyo, Japan, SAHEL ASHHAB, Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, Qatar Foundation, Doha, Qatar — Recently, light-matter interaction at the single-photon level has been demonstrated in superconducting circuits (circuit-QED). The interaction energy between a superconducting artificial atom and an excitation quantum of a harmonic oscillator in the microwave region has been shown to be very large, at least a few thousand times that of the atom-photon interaction obtained using Rydberg atoms [1]. It is also intriguing that, depending on the circuit design, the relevant physical parameters of this system can be controlled at will. In particular, an interaction energy as large as the transition energy of a superconducting artificial atom or a harmonic oscillator is possible, where totally new states, such as a spontaneously generated Schrödinger-cat-like correlated ground state of light and matter, have been predicted [2,3]. In this talk, I will introduce the motivation and the significance of the research, methods to achieve such a strong interaction, and a brief overview of the obtained results. [1] J. Johansson, S. Saito, T. Meno, H. Nakano, M. Ueda, K. Semba, and H. Takayanagi, Phys. Rev. Lett. 96, 127006 (2006). [2] S. Ashhab and Franco Nori, Phys. Rev. A 81, 042311 (2010). [3] S. Ashhab Phys. Rev. A 87, 013826 (2013).

<sup>1</sup>This work was supported by JSPS KAKENHI Grant Number 25220601

**4:18PM C48.00010 Deep strong coupling in a circuit QED system (2) - experiment**<sup>-1</sup>, TOMOKO FUSE, FUMIKI YOSHIHARA, National Institute of Information and Communications Technology, Koganei, Tokyo, Japan, SAHEL ASHHAB, Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, Qatar Foundation, Doha, Qatar, KOUICHI SEMBA, National Institute of Information and Communications Technology, Koganei, Tokyo, Japan — Among a variety of cavity/circuit-QED systems, the superconducting flux qubit is a promising candidate for increasing the coupling strength further because of its huge magnetic moment. Using a flux qubit,  $g/\omega_r = 0.12$  ( $g$ : coupling strength,  $\omega_r$ : bare resonator frequency) has been reported [1]. However,  $g/\omega_r$  is still lower than 1. Here, instead of the widely used coplanar waveguide (CPW) resonators, we use a lumped-element resonator consisting of an inductor (L) and a capacitor (C). While CPW resonators are distributed-element circuits and are therefore restricted by impedance matching constraints, one can freely choose the ratio,  $L/C$ , of a lumped-element resonator. This allows us to design a much smaller inductance and to make the zero-point current fluctuation much larger. Using a flux qubit and a lumped-element resonator, we have achieved  $g/\omega_r$  comparable to or larger than 1, which is the deep strong coupling regime, where a variety of interesting physics is expected [2]. In this presentation, the sample design and spectroscopy data will be shown. [1] T. Niemczyk et al., nature physics 6, 772 (2010). [2] S. Ashhab and F. Nori, PRA 81, 042311 (2010).

<sup>1</sup>This work was supported by JSPS KAKENHI Grant Number 25220601

**4:30PM C48.00011 Deep strong coupling in a circuit QED system (3) - data and analysis**<sup>-1</sup>, FUMIKI YOSHIHARA, TOMOKO FUSE, KOUICHI SEMBA, National Institute of Information and Communications Technology, Koganei, Tokyo, Japan, SAHEL ASHHAB, Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, Qatar Foundation, Doha, Qatar — We have experimentally achieved deep-strong coupling between a superconducting flux qubit and a superconducting LC circuit, where the coupling energy,  $\hbar g$ , exceeds both the transition energy of the flux qubit,  $\hbar\omega_q$ , and the resonant energy of the LC circuit,  $\hbar\omega_r$ . At the optimal flux bias of the flux qubit, the qubit-resonator system is described by the Rabi model, which is one of the simplest quantum models of atom-cavity systems. The Hamiltonian of the Rabi model can be written as  $\mathcal{H}_{\text{Rabi}} = -\frac{\hbar}{2}\omega_q\sigma_z + \hbar\omega_r(a^\dagger a + \frac{1}{2}) + \hbar g\sigma_x(a + a^\dagger)$ , where  $\sigma_{x(z)}$  is a Pauli matrix and  $a(a^\dagger)$  is an annihilation (creation) operator. In this presentation, we will show the spectroscopy data of qubit-resonator systems in the deep-strong-coupling regime. Transition frequencies calculated from  $\mathcal{H}_{\text{Rabi}}$  fit the measured data well. We have also observed that  $\hbar\omega_q$  is largely suppressed due to the Lamb shift caused by the deep-strong coupling to the resonator. In this regime, the ground state is predicted to be an entangled state of the qubit's persistent-current states and the resonator's coherent states.

<sup>1</sup>This work was supported by JSPS KAKENHI Grant Number 25220601.

**4:42PM C48.00012 Quantum electrodynamics near a photonic band-gap**, YANBING LIU, ANDREW HOUCK, Princeton University — Quantum electrodynamics predicts the localization of light around an atom in photonic band-gap (PBG) medium or photonic crystal. Here we report the first experimental realization of the strong coupling between a single artificial atom and an one dimensional PBG medium using superconducting circuits. In the photonic transport measurement, we observe an anomalous Lamb shift and a large band-edge avoided crossing when the artificial atom frequency is tuned across the band-edge. The persistent peak within the band-gap indicates the single photon bound state. Furthermore, we study the resonance fluorescence of this bound state, again demonstrating the breakdown of the Born-Markov approximation near the band-edge. This novel architecture can be directly generalized to study many-body quantum electrodynamics and to construct more complicated spin chain models.

**4:54PM C48.00013 Experimental study of a 72-site Jaynes-Cummings lattice in the nonlinear dispersive regime**, MATTIAS FITZPATRICK, NEEREJA SUNDARESAN, Princeton University, ANDY C. Y. LI, JENS KOCH, Northwestern University, ANDREW HOUCK, Princeton University — The building blocks of circuit-QED provide useful tools for the study of nonequilibrium and highly nonlinear behavior. In particular, the inherent dissipation in circuit-QED systems naturally gives rise to crossovers between different steady-states and dynamical phase transitions in even as few as two-site lattices. We explore the steady-state behavior of a 72-site Jaynes-Cummings lattice in the dispersive regime, highlighting the sharp transition in fluorescence at critical drive powers as well as strong nonlinear wave-mixing phenomena.

**5:06PM C48.00014 The driven-dissipative Jaynes-Cummings lattice in the nonlinear dispersive regime**, ANDY C. Y. LI, Northwestern University, MATTIAS FITZPATRICK, NEEREJA SUNDARESAN, ANDREW HOUCK, Princeton University, JENS KOCH, Northwestern University — Experiments studying circuit-QED lattices have great potential for advancing our understanding of nonequilibrium many-body phenomena, including dissipative and dynamical phase transitions. One particular model realizable in this architecture is the driven-dissipative Jaynes-Cummings lattice. Motivated by the experimental measurements in the Houck lab, we theoretically investigate the dispersive regime including sub-leading nonlinear contributions from Kerr terms, employing a semi-classical approximation and numerics based on the quantum master equation. We explore the features of the experimentally detected crossover which is observed for an increase of the driving strength beyond a certain threshold.

**5:18PM C48.00015 Spin-boson model with an engineered reservoir in circuit QED**<sup>1</sup>, FRANK DEPPE, M. HAEBERLEIN, P. EDER, J. GOETZ, M. FISCHER, F. WULSCHNER, E. XIE, K. G. FEDOROV, A. MARX, R. GROSS, Walther-Meissner-Institut; Technische Universität München; Nanosystems Initiative Munich, Germany — A superconducting qubit coupled to an open transmission line represents an implementation of the spin-boson model with an engineered environment. Using a flux qubit with a large mutual inductance to the transmission line, we confirm in a resonance fluorescence experiment that the spectral function  $J(\omega)$  of this environment is Ohmic over a frequency range of several gigahertz. Furthermore, partial reflectors implemented into the transmission line modify the spectral function of the transmission line. For weak enough reflectors, we find that the resulting broad peak can be interpreted in terms of an enhanced spontaneous emission rate. Our work [M. Haeberlein et al., arXiv:1506.09114 (2015)] lays the ground for future quantum simulations of other, more involved, impurity models with superconducting circuits.

<sup>1</sup>We acknowledge support by the German Research Foundation through SFB 631 and FE 1564/1-1, the EU project PROMISCE, and Elite Network of Bavaria through the program ExQM.

**5:30PM C48.00016 Strongly Correlated Photons at Full Transmission<sup>1</sup>**, YAO-LUNG L. FANG, HAROLD U. BARANGER, Duke Univ — We show how to make strongly correlated photons in a fully transmitted pulse. The system consists of three-level qubits (3LS) coupled to a one-dimensional waveguide. Our two-photon scattering approach naturally connects photon correlations with inelastic scattering. We find that the total inelastically scattered flux is much larger than in the case of two-level systems, making 3LS better candidates for experimental study of non-classical light. Strikingly, there is a further substantial increase in inelastic flux upon adding either more 3LS or a mirror. Typically, resonant probe photons at electromagnetically induced transparency are not correlated — the correlations occur off resonance and so involve backscattering. Remarkably, we show that for three qubits, the qubit frequencies and the pump beam can be engineered such that correlated photons are fully transmitted, thereby greatly improving the efficiency of generating photon correlation.

<sup>1</sup>Work supported by U.S. NSF Grant No. PHY-14-04125.

**Monday, March 14, 2016 2:30PM - 5:30PM –**  
**Session C50 DAMOP: Many-Body Localization in Atomic Systems I** Hilton Baltimore Holiday Ballroom  
1 - Bela Bauer, Microsoft Station Q

**2:30PM C50.00001 Suppression and Revival of Weak Localization of Ultra-Cold Atoms by Manipulation of Time-Reversal Symmetry<sup>1</sup>**, ALAIN ASPECT, Institut d'Optique Palaiseau — In the early 1980's, observation of a magneto-resistance anomaly in metallic thin films was attributed to the phenomenon of weak localization of electrons and to time-reversal symmetry breaking due to a magnetic field acting upon charged particles. We have observed weak localization of ultra-cold atoms in a 2D configuration, placed in a disordered potential created by a laser speckle. In order to manipulate time-reversal symmetry with our neutral atoms, we take advantage of the slow evolution of our system, and we observe the suppression and revival of weak localization when time reversal symmetry is cancelled and reestablished. References: K. Muller, J. Richard, V. V. Volchkov, V. Denechaud, P. Bouyer, A. Aspect, and V. Josse, "Suppression and Revival of Weak Localization through Control of Time-Reversal Symmetry," Physical Review Letters 114 (20) (2015) and references in.

<sup>1</sup>Work supported by the ERC Advanced Grant Quantatop

**3:06PM C50.00002 Using subadditivity to reason about many-body localization on single disorder realizations.**, BRYAN CLARK, XIONGJIE YU, DAVID J. LUITZ, University of Illinois at Urbana Champaign — In the many-body localized (MBL) phase, the interplay of interactions and disorder prevents thermalization. Typically to reason about the many-body localized phase we average over many disorder realizations. It is interesting to ask in what ways we can we talk about MBL transitions for single disorder patterns. We show that subadditivity gives us a mechanism to make sense of MBL transitions on single disorder realizations and report what this implies for the average over disorder.

**3:18PM C50.00003 Many-Body Localization and Quantum Nonergodicity in a Model with a Single-Particle Mobility Edge<sup>1</sup>**, XIAOPENG LI, SRIRAM GANESHAN, J.H. PIXLEY, Univ of Maryland-College Park — We investigate many-body localization in the presence of a single-particle mobility edge. By considering an interacting deterministic model with an incommensurate potential in one dimension we find that the single-particle mobility edge in the noninteracting system leads to a many-body mobility edge in the corresponding interacting system for certain parameter regimes. Using exact diagonalization, we probe the mobility edge via energy resolved entanglement entropy (EE) and study the energy resolved applicability (or failure) of the eigenstate thermalization hypothesis (ETH). Our numerical results indicate that the transition separating area and volume law scaling of the EE does not coincide with the nonthermal to thermal transition. Consequently, there exists an extended nonergodic phase for an intermediate energy window where the many-body eigenstates violate the ETH while manifesting volume law EE scaling. We also establish that the model possesses an infinite temperature many-body localization transition despite the existence of a single-particle mobility edge. We propose a practical scheme to test our predictions in atomic optical lattice experiments which can directly probe the effects of the mobility edge.

<sup>1</sup>JQI-NSF-PFC, AROAtomtronics- MURI, and LPS-CMTC, UMD supercomputing resources

**3:30PM C50.00004 Early Breakdown of Area-Law Entanglement at the Many-Body Delocalization Transition**, TRITHEP DEVAKUL, Princeton University, RAJIV SINGH, University of California, Davis — We introduce the numerical linked cluster expansion as a controlled numerical tool for the study of the many-body localization transition in a disordered system with continuous nonperturbative disorder. Our approach works directly in the thermodynamic limit, in any spatial dimension, and does not rely on any finite size scaling procedure. We study the onset of many-body delocalization through the breakdown of area-law entanglement in a generic many-body eigenstate. By looking for initial signs of an instability of the localized phase, we obtain a value for the critical disorder, which we believe should be a lower bound for the true value, that is higher than current best estimates from finite size studies. This implies that most current methods tend to overestimate the extent of the localized phase due to finite size effects making the localized phase appear stable at small length scales. We also study the mobility edge in these systems as a function of energy density, and we find that our conclusion is the same at all examined energies. Work based on Phys. Rev. Lett. 115, 187201.

**3:42PM C50.00005 Exponential Orthogonality Catastrophe in Single-Particle and Many-Body Localized Systems<sup>1</sup>**, DONG-LING DENG, J. H. PIXLEY, XIAOPENG LI, Dept. of Physics, University of Maryland — We investigate the statistical orthogonality catastrophe (StOC) in single-particle and many-body localized systems by studying the response of the many-body ground state to a local quench. Using scaling arguments and exact numerical calculations, we establish that the StOC gives rise to a wave function overlap between the pre- and post-quench ground states that has an *exponential* decay with the system size, in sharp contrast to the well-known power law Anderson orthogonality catastrophe in metallic systems. This exponential decay arises from a statistical charge transfer process where a particle can be effectively "transported" to an arbitrary lattice site. We show that in a many-body localized phase, this non-local transport and the associated exponential StOC phenomenon persist in the presence of interactions. We study the possible experimental consequences of the exponential StOC on the Loschmidt echo and spectral function, establishing that this phenomenon might be observable in cold atomic experiments through Ramsey interference and radio-frequency spectroscopy.

<sup>1</sup>We thank S.-T. Wang, Z.-X. Gong, Y.-L. Wu, J. D. Sau, and Z. Ovadyahu for discussions. This work is supported by LPS-MPO-CMTC, JQI-NSF-PFC, and ARO-Atomtronics-MURI. The authors acknowledge the University of Maryland supercomputing resources.

**3:54PM C50.00006 Many-body localization effects in a disordered system coupled to a delocalized chain**, KATHARINE HYATT, University of California - Santa Barbara, JAMES R. GARRISON, Univ of California - Santa Barbara, BELA BAUER, Station Q, Microsoft Research — The possibility of closed quantum systems that robustly violate quantum statistical mechanics has received a tremendous amount of interest in recent years. Using both numerical and analytical techniques, it has been established that weakly interacting disordered systems can be brought into a many-body localized regime, where the system does not conduct and does not equilibrate even for arbitrarily long times. The starting point for such a phase is usually taken to be an Anderson insulator where in the limit of vanishing interactions, all degrees of freedom of the system are localized. Here, we revisit this problem in a model where in the non-interacting limit, some degrees of freedom are localized while others remain delocalized. Such a system can be viewed as a model for a many-body localized system brought into contact with a small bath of a comparable number of degrees of freedom. We numerically study the effect of interactions on this system and find that generically, the entire system delocalizes. However, we find certain parameter regimes where results are consistent with localization of the entire system, an effect recently termed many-body proximity effect.

**4:06PM C50.00007 Fractional transport and photonic sub-diffusion in aperiodic dielectric metamaterials**, LUCA DAL NEGRO, YU WANG, SANDEEP INAMPUDI, Boston University, ECE Department — Using rigorous transfer matrix theory and full-vector Finite Difference Time Domain (FDTD) simulations in combination with Wavelet Transform Modulus Maxima analysis of multifractal spectra, we demonstrate all-dielectric aperiodic metamaterial structures that exhibit sub-diffusive photon transport properties that are widely tunable across the near-infrared spectral range. The proposed approach leverages the unprecedented spectral scalability offered by aperiodic photonic systems and demonstrates the possibility of achieving logarithmic Sinai sub-diffusion of photons for the first time. In particular we will show that the control of multifractal energy spectra and critical modes in aperiodic metamaterials with nanoscale dielectric components enables tuning of anomalous optical transport from sub- to super-diffusive dynamics, in close analogy with the electron dynamics in quasi-periodic potentials. Fractional diffusion equations models will be introduced for the efficient modeling of photon sub-diffusive processes in metamaterials and applications to diffraction-free propagation in aperiodic media will be provided. The ability to tailor photon transport phenomena in metamaterials with properties originating from aperiodic geometrical correlations can lead to novel functionalities and active devices that rely on anomalous photon sub-diffusion to control beam collimation and non-resonantly enhance light-matter interaction across multiple spectral bands.

**4:18PM C50.00008 Many-body localization protected quantum state transfer**, CHRIS R LAUMANN, University of Washington, NORMAN Y YAO, ASHVIN VISHWANATH, University of California, Berkeley — In thermal phases, the quantum coherence of individual degrees of freedom is rapidly lost to the environment. Many-body localized (MBL) phases limit the spread of this coherence and appear promising for quantum information applications. However, such applications require not just long coherence times but also a means to transport and manipulate information. We demonstrate that this can be done in a one dimensional model of interacting spins at infinite temperature. Our protocol utilizes protected qubits which emerge at the boundary between topological and trivial phases. State transfer occurs via dynamic shifts of this boundary and is shown to preserve quantum information. As an example, we discuss the implementation of a universal, two-qubit gate based upon MBL-protected quantum state transfer.

**4:30PM C50.00009 Transport of Light in disordered random media**, REGINE FRANK, Serin Physics Laboratory, E273 Department of Physics and Astronomy Rutgers University 136 Frelinghuysen Road Piscataway, NJ 08854-8019, USA, ANDREAS LUBATSCH, Georg-Simon-Ohm University of Applied Sciences, Nuremberg, Germany — The Anderson transition was originally proposed for electrons, however it has been soon searched for all kinds of waves in disordered media. This physics became extremely interesting with the application of high amplitude excitations, where the medium is supposed to respond with non-linear effects. In theory it is ever since a challenge to treat large random ensembles numerically, even if the medium is completely non-resonant or passive. We discuss in this talk transport of light with respect to a quantum field theoretical approach and we explain through comparison to other existing theories, what the advantages of state of the art theory in that field is, and why it is exciting.

**4:42PM C50.00010 Many body localization in the presence of a single particle mobility edge**, SUBROTO MUKERJEE, RANJAN MODAK, Indian Institute of Science — In one dimension, noninteracting particles can undergo a localization-delocalization transition in a quasiperiodic potential. Recent studies have suggested that this transition transforms into a many body localization transition upon the introduction of interactions. It has also been shown that mobility edges can appear in the single particle spectrum for certain types of quasiperiodic potentials. Here we investigate the effect of interactions in models with such mobility edges. Employing the technique of exact diagonalization for finite-sized systems, we calculate the level spacing distribution, time evolution of entanglement entropy, optical conductivity and return probability to characterize the nature of localization. The localization that develops in the presence of interactions in these systems appears to be different from regular Many-Body Localization (MBL) in that the growth of entanglement entropy with time is linear (like in a thermal phase) but saturates to a value much smaller than the thermal value (like for MBL). All other diagnostics seem consistent with regular MBL.

**4:54PM C50.00011 Energy Dependence and Scaling Property of Localization Length near a Gapped Flat Band<sup>1</sup>**, LI GE, College of Staten Island, CUNY, HAKAN TURECI, Princeton University — Using a tight-binding model for a one-dimensional Lieb lattice, we show that the localization length near a gapped flat band behaves differently from the typical Urbach tail in a band gap: instead of reducing monotonically as the energy  $E$  moves away from the flat band energy  $E_f$ , the presence of the flat band causes a nonmonotonic energy dependence of the localization length. This energy dependence follows a scaling property when the energy is within the spread ( $W$ ) of uniformly distributed diagonal disorder, i.e. the localization length is only a function of  $(E-E_f)/W$ . Several other lattices are compared to distinguish the effect of the flat band on the localization length, where we eliminate, shift, or duplicate the flat band, without changing the dispersion relations of other bands. Using the top right element of the Green's matrix, we derive an analytical relation between the density of states and the localization length, which shines light on these properties of the latter, including a summation rule for its inverse.

<sup>1</sup>This work is partially supported by NSF under Grant No. DMR-1506987.

**5:06PM C50.00012 Spatial and temporal localization of light in two dimensions**, ROMAIN BACHELARD, Instituto de Física de São Carlos/Universidade de São Paulo — Despite decades of active research, punctuated by several contradictory experimental and theoretical claims, the mere existence of Anderson localization of light, a regime where light cannot propagate due to interference effects between randomly distributed scatterers, has not been demonstrated yet. Recent theoretical works suggest that the vectorial nature of light might actually prohibit localization. We here present a study on the scattering of light in two dimensions, a regime where both scalar or as a vectorial electromagnetic waves coexist. The scaling analysis reveals that although both kinds of wave present long-lived subradiant modes, only scalar ones do localize, supporting the theoretical claim in 3D. Yet we also observe a lack of correlation between lifetimes and localization length, calling for a differentiation between temporal (subradiant) and spatial (Anderson) localization. Finally, we discuss the implication of localization, following the original idea that the localization of the modes induces a metal to insulator transition, bringing transport to a halt. Indeed, in the case of light, the scattering is characterized by the presence of a few long-range (superradiant) modes, which appear to alter dramatically the transport properties.

**5:18PM C50.00013 Anderson Localization in Degenerate Spin-Orbit Coupled Fermi Gas with Disorder**<sup>1</sup>, SHENG LIU, XIANGFA ZHOU, GUANGCAN GUO, YONGSHENG ZHANG, Univ. of Sci. & Tech. of China — Competition between superconductivity and disorder plays an essential role in understanding the metal-insulator transition. Based on the Bogoliubov-de Gennes equation, we studied an *s*-wave superconductor with both spin-orbit coupling and disorder are presented. With increasing the strength of disorder, the mean superconducting order parameter will vanish while the energy gap will persist which indicates that the system undergoes a transition from a superconducting state to an insulating state which can be confirmed by calculating the inverse participation ratio. We also find that, if the strength of disorder is small, the superconducting order parameter and energy gap will decrease if we increase the strength of spin-orbit coupling and Zeeman field. In the large disorder limits, increasing the strength of spin-orbit coupling will increase the mean superconducting order parameter. This phenomena shows that the system is more insensitive to disorder if the spin-orbit coupling is presented. Numerical computing also shows that the whole system breaks up into several *superconducting islands* instead of being superconductive.

<sup>1</sup>This work was carried out with the support of National Natural Science Foundation of China (No. 61275122).

**Monday, March 14, 2016 2:30PM - 5:30PM –**  
**Session C51 FIAP: Applications Semiconductors & Dielectrics** Hilton Baltimore Holiday Ballroom 2 - Ichiro Takeuchi, University of Maryland

**2:30PM C51.00001 Fe<sub>2</sub>O<sub>3</sub> nanoparticles for airborne organophosphate detection**<sup>1</sup>, JOSHUA PHILLIPS, University of Alabama, JENNIFER SOLIZ, US Army Edgewood Chemical Biological Center, ADAM HAUSER, University of Alabama — Dire need for early detection of organophosphates (OP) exists in both civilian (pesticide/herbicide buildup) and military (G/V nerve agents) spheres. Nanoparticle materials are excellent candidates for the detection and/or decontamination of hazardous materials, owing to their large surface to volume ratios and tailored surface functionality. Within this category, metal oxides include structures that are stable with the range of normal environmental conditions (temperature, humidity), but have strong, specific reaction mechanisms (hydrolysis, oxidation, catalysis, stoichiometric reaction) with toxic compounds. In this talk, we will present on the suitability of Fe<sub>2</sub>O<sub>3</sub> nanoparticles as airborne organophosphate detectors. 23 nm particles were exposed to a series of organophosphate compounds (dimethyl methylphosphonate, dimethyl chlorophosphonate, diisopropyl methylphosphonate), and studied by x-ray magnetic circular dichroism and x-ray absorption spectroscopy to confirm the stoichiometric Fe<sub>2</sub>O<sub>3</sub> to FeO mechanism and determine magnetic sensor feasibility. AC Impedance Spectroscopy shows both high sensitivity and selectivity via frequency dependence in both impedance and resistivity, suggesting some feasibility for impedimetric devices.

<sup>1</sup>We acknowledge funding under Army Research Office STIR award W911F-15-1-0104. J.R.S. acknowledges funding from the Defense Threat Reduction Agency under Projects BA13PHM210 and BA07PRO104. J.R.S. also acknowledges funding under a NRC fellowship.

**2:42PM C51.00002 Towards a drift-free multi-level Phase Change Memory**, IBRAHIM CINAR, Bogazici University, SERVET OZDEMIR, University of Warwick, EGE CAN COGULU, New York University, AISHA GOKCE, Bogazici University, BARRY STIPE, JORDAN KATINE, HGST, A Western Digital Company, GULEN AKTAS, OZHAN OZATAY, Bogazici University — For ultra-high density data storage applications, Phase Change Memory (PCM) is considered a potentially disruptive technology. Yet, the long-term reliability of the logic levels corresponding to the resistance states of a PCM device is an important issue for a stable device operation since the resistance levels drift uncontrollably in time. The underlying mechanism for the resistance drift is considered as the structural relaxation and spontaneous crystallization at elevated temperatures. We fabricated a nanoscale single active layer-phase change memory cell with three resistance levels corresponding to crystalline, amorphous and intermediate states by controlling the current injection site geometry. For the intermediate state and the reset state, the activation energies and the trap distances have been found to be 0.021 eV and 0.235 eV, 1.31 nm and 7.56 nm, respectively. We attribute the ultra-low and weakly temperature dependent drift coefficient of the intermediate state ( $\nu=0.0016$ ) as opposed to that of the reset state ( $\nu=0.077$ ) as being due to the dominant contribution of the interfacial defects in electrical transport in the case of the mixed phase. Our results indicate that the engineering of interfacial defects will enable a drift-free multi-level PCM device design.

**2:54PM C51.00003 Sensing of NO<sub>2</sub> with Zirconium Hydroxide via Electrical Impedance Spectroscopy**<sup>1</sup>, COLEMAN HARRIS, The University of Alabama, JENNIFER SOLIZ, US Army Edgewood Chemical Biological Center, ANDREW KLEVITCH, The University of Alabama, JOSEPH ROSSIN, Guild Associates, Inc., AUGUSTUS FOUNTAIN III, GREGORY PETERSON, US Army Edgewood Chemical Biological Center, ADAM HAUSER, The University of Alabama — Nitrogen Dioxide (NO<sub>2</sub>) is a brown gas mainly produced as a byproduct of burning fossil fuels, such as automobiles and power plants. Nitrogen oxides can form acid rain and smog by reacting with air, can form toxic organic nitrates by reacting with soil, and can react with oxygen in water, destroying marine life due to a lack of breathable oxygen. Any concentration beyond 53 ppb (air quality standard) can cause irritation to the lungs and respiratory infections, and higher dosages can be fatal. As such, research in NO<sub>2</sub> detection is incredibly important to human welfare. Zirconium hydroxide (Zr(OH)<sub>4</sub>) has been investigated as a candidate NO<sub>2</sub> dielectric sensor using impedance spectroscopy analysis. Impedance changes of several orders of magnitude are seen down to our dosage minimum of 50 ppm•hr. Changes in impedance correlate with nitrogen and oxygen atomic ratio increases observed via X-ray photoelectron spectroscopy (XPS). The results indicate that Zr(OH)<sub>4</sub> may be a strong candidate for use in impedance-based NO<sub>2</sub> detection devices.

<sup>1</sup>A.J.H., J.R.S., A.W.F. and G.W. P. acknowledge funding under Army Research Office STIR award W911F-15-1-0104. J.R.S. acknowledges funding under a NRC fellowship and is advised by Dr. Christopher Karwacki, ECBC.

**3:06PM C51.00004 Laser Processing of Metal Oxides for Plasmonic Applications**<sup>1</sup>, HEUNGSOO KIM, Naval Research Laboratory, ERIC BRECKENFELD, National Research Council Fellow at Naval Research Laboratory, NICHOLAS CHARIPAR, ALBERTO PIQUE, Naval Research Laboratory — Noble metals such as Au and Ag have been used traditionally for plasmonic devices. However, conventional metals are not suitable for near infrared (IR) plasmonic applications due to their relatively large optical losses at these wavelengths. Metal oxides, on the other hand, have been considered for low loss metallic components in the near IR because they can provide a tunable carrier density by doping. The zero-cross-over permittivity values of these metal oxides, for example, can easily be tuned from 1.0 m to 3 m by adjusting doping levels. Optical losses in devices made from these metal oxide materials are generally found to be much lower than those obtained with conventional metals. We have investigated various laser processing techniques for synthesizing several types of metal oxides. First, pulsed laser deposition was used to grow metal oxide thin films such as, Al-doped ZnO, Sn-doped In<sub>2</sub>O<sub>3</sub> and VO<sub>2</sub>. Second, a laser sintering technique was used to improve the properties of solution-processed VO<sub>2</sub> coatings. Third, a laser printing technique was used to produce metal oxide films. We will present details on the use of laser processing techniques for synthesizing these metal oxides along with their electrical, optical, and structural properties.

<sup>1</sup>This work was funded by the Office of Naval Research (ONR) through the Naval Research Laboratory Basic Research Program.

**3:18PM C51.00005 Controlled Growth of Copper Oxide Nano-Wires through Direct Oxidation<sup>1</sup>**, JOANN HILMAN, RAVI NEUPANE, ANDREW J. YOST, TEYU CHIEN, Univ of Wyoming — Copper oxides, both Cu<sub>2</sub>O and CuO, have many applications in solar cells, sensors, and nano-electronics. The properties of the copper oxides are further influenced by the dimension of the materials, especially when made in nanoscale. In particular, the properties of the copper oxide nanowires could be tuned by their structures, lengths, and widths. While several methods have been reported to grow nanowires, direct oxidation is arguably the most economical one. This research examines the effects of oxidization duration and temperature in dry air environment on the development of copper oxide nanowires in order to achieve cost effective controllable growth. Using the direct oxidation method in dry air we have demonstrated growth of CuO nano-wires at temperatures as low as 300 C and as short as 1hr. Furthermore we have observed that the lengths and diameters of the CuO NWs can be controlled by the duration and temperature of the oxidation process.

<sup>1</sup>WY NASA Space Grant Consortium

**3:30PM C51.00006 Distinguishing the Photothermal and Photoinjection Effects in Vanadium Dioxide Nanowires<sup>1</sup>**, XI WANG, HANWEI GAO, Department of Physics, Florida State University — Vanadium dioxide (VO<sub>2</sub>) has drawn significant attention for its unique metal-to-insulator transition. The high electrical resistivity below the transition temperature is a result of the strong electron correlation with the assistance of lattice distortion. Theoretical calculations indicated that the strong inter-electron interactions might induce intriguing optoelectronic phenomena, such as the multiple exciton generation. However, the resistivity of VO<sub>2</sub> is temperature sensitive. Therefore, the light-induced conductivity in VO<sub>2</sub> has often been attributed to the photothermal effects. In this work, we distinguished the photothermal and photoinjection effects in VO<sub>2</sub> nanowires by varying the chopping frequency of the optical illumination. In our VO<sub>2</sub> nanowires, the relatively slow photothermal processes can be well suppressed when the chopping frequency >2 kHz, whereas the fast photoinjection component (direct photo-excitation of charge carriers) remains constant at all chopping frequencies. By separating the photothermal and photoinjection processes, our work set the basis for further studies of carrier dynamics under optical excitations in strongly correlated materials.

<sup>1</sup>This work is supported by the Start-Up Funds and the First-Year Assistant Professor Award from the Florida State University

**3:42PM C51.00007 Electronic properties of epitaxial Ge/AlAs heterostructures on Si and GaAs<sup>1</sup>**, J. J. HEREMANS, YUANTAO XIE, Virginia Tech, Department of Physics, M. K. HUDAIT, M. CLAVEL, P. S. GOLEY, Virginia Tech, Department of Electrical and Computer Engineering — Ge, with high electron and hole mobilities, has advantages over Si for low-power high-speed nanoscale logic. We report on the MBE growth of Ge/AlAs/GaAs and Ge/AlAs/GaAs/Si structures, where the Ge/AlAs band offsets provide carrier confinement inside the Ge layer. We studied the confinement of carriers in the Ge layer, the effect of the AlAs buffer layer, and the effects of a growth pause and growth temperature, correlated to structural and morphological properties. Magnetotransport and quantum transport measurements were obtained down to 390 mK and in magnetic fields up to 9 T. A weak-localization signal, in contrast to antilocalization, indicates absence of spin-orbit interaction and hence electron confinement in the Ge rather than in the III-V layers. For the Ge/AlAs/GaAs/Si structure a low-temperature sheet carrier density  $1.4 \times 10^{14} \text{ cm}^{-2}$  and mobility  $390 \text{ cm}^2/\text{Vs}$  were obtained, with similar values at 290 K, while at 200 K a maximum in mobility is reached of  $470 \text{ cm}^2/\text{Vs}$ . For the Ge/AlAs/GaAs structures a mobility up to  $260 \text{ cm}^2/\text{Vs}$  was obtained at  $2 \times 10^{13} \text{ cm}^{-2}$  at 290 K. The Ge/AlAs/GaAs structures have also shown phonon-limited scattering vs temperature, attesting to the quality of interfaces.

<sup>1</sup>Supported by DOE DE-FG02-08ER46532, NSF ECCS-1348653, Intel Corp.

**3:54PM C51.00008 Spectroscopic and structural studies of energetically efficient transport in nanocontacts to NiSi nanowires<sup>1</sup>**, A. STEIN, BNL-CFN, Upton, NY, 11973, USA, I. A. H. FARHAT, Khalifa University, AMS Dept. and KSRC, 127788, Abu Dhabi, UAE, N. LACEVIC, Univ. of Melbourne, Australia, S. K. BAZUHAIR, S. S. AZHAR, KSRC, 127788, Abu Dhabi, UAE, A. F. ISAKOVIC, Khalifa University, AMS Dept. and KSRC, 127788, Abu Dhabi, UAE — Understanding correlations between mechanical, thermal, structural and electronic transport properties of different nanocontact geometries to nanowires, such as Au/Cu-NiSi-Si, remain one of the major goals of nanodevices reliability and scalability research. Aiming to clarify the failure modes and processes that affect the energy efficiency of transport and switching in constrained nanocontact geometries, such as end contacts, we conducted the structural, spectroscopic, and noise correlation studies. We show how the spatial (in)homogeneity at and in the near vicinity of the interface affects the transport performance of the nanojunctions. Mobile Ni clusters are identified at the nanojunction interface via Raman spectromicroscopy and their influence on charge transport is analyzed. We also show that the noise correlation spectra and micro-X-ray stress-strain studies in the nanojunctions are effective tools in predicting the energy efficiency of the nanojunctions. A computational study of the interfacial properties of metal/Ni-Si via DFT and MD simulations is implemented.

<sup>1</sup>Work supported by Mubadala-SRC 2011-KJ-2190. A part of the work done at BNL-CFN, supported by DOE. A part of the work done at Cornell Univ.CFN and CCMR, supported by the NSF.

**4:06PM C51.00009 Memristive switching of ZnO nanorod mesh<sup>1</sup>**, PUZYREV YEVGENIY, Vanderbilt University, XIAO SHEN, University of Memphis, KAI NI, XUAN ZHANG, JORDAN HACHTEL, Vanderbilt University, BO CHOI, Vanderbilt Institute of Nanoscience, MATTHEW CHISHOLM, Oak Ridge National Laboratory, DANIEL FLEETWOOD, RONALD SCHRIMPF, SOKRATES PANTELIDES, Vanderbilt University — We present a combined experimental and theoretical study of memristive switching in a self-assembled mesh of ZnO nanorods. A ZnO nanorod mesh spans the area between Ag contacts in a device that exhibits hysteresis with large ON/OFF ratio, reaching ION/IOFF values of 104. We show that switching behavior depends critically on the geometry of the nanorod mesh. We employ density functional theory (DFT) calculations to deduce the mechanism for resistive switching for the nanorod mesh. Redistribution of Ag atoms, driven by an electrical field, leads to the formation and evolution of a conducting path through nanorods. Field-induced migration of Ag atoms changes the doping level of nanorods and modulates their conductivity. Using static DFT and nudged-elastic-band calculations, we investigate the energy of interaction between Ag clusters and a ZnO surface, including migration barriers of Ag atoms. Current-voltage (I-V) characteristics are modeled using percolation theory in a nanorod mesh. To describe the dynamics of SET/RESET phenomena, model parameters include the experimentally observed nanorod geometry and the energetics of Ag on ZnO surfaces, obtained from DFT calculations.

<sup>1</sup>This work was supported by NSF grant DMR-1207241, DOE grant DE-FG02-09ER46554, and the McMinn Endowment at Vanderbilt University. Computational support was provided by the NSF XSEDE under Grant DMR TG-DMR130121.

**4:18PM C51.00010 Field effect in perovskite heterostructures based on BaSnO<sub>3</sub> and BaHfO<sub>3</sub>**, YOUNG MO KIM, CHULKWON PARK, USEONG KIM, JUYEON SHIN, YOUJUNG KIM, KOOKRIN CHAR, Seoul National University — Perovskite La-doped BaSnO<sub>3</sub> (BLSO) was reported to possess high electron mobility and excellent oxygen stability [1]. We fabricated a field effect transistor on SrTiO<sub>3</sub> substrate using BLSO as a channel layer and BaHfO<sub>3</sub> (BHO) as a gate insulator. To reduce the threading dislocations and enhance the electrical properties of the channel, undoped BaSnO<sub>3</sub> (BSO) buffer layer was grown on SrTiO<sub>3</sub> substrates before the channel layer deposition. X-ray diffraction measurement confirms the epitaxial growth of BHO on BSO. We investigated optical and dielectric properties of the BHO gate insulator; the optical bandgap and the dielectric constant were measured to be 6.1 eV and 37.8, respectively. Using BHO as the gate insulator, we obtained the conductivity modulation in the channel by field effect. We will report on the electrical properties of the field effect transistor such as the output characteristics, the transfer characteristics, the  $I_{on}/I_{off}$  ratio, the subthreshold swing and the field effect mobility. [1] H. J. Kim, U. Kim *et al.*, Appl. Phys. Express **5**, 061102 (2012).

**4:30PM C51.00011 Characterization of Quasi-Metallic Tunnel-Field-Effect-Transistors**, ABDULRAHMAN ALHUSSAIN, FADHEL ALSAFFAR, King Abdulaziz City for Science and Technology, STEPHEN CRONIN, University of Southern California, MOH AMER, King Abdulaziz City for Science and Technology, KING ABDULAZIZ CITY FOR SCIENCE AND TECHNOLOGY TEAM, UNIVERSITY OF SOUTHERN CALIFORNIA COLLABORATION — Band-to-band tunneling mechanism has proven to be a promising alternative to thermionic diffusion for ultra-fast switching applications. Tunneling Field-Effect-Transistors (TFETs), which primarily operate based on tunneling current, can offer low turn-on voltage with low sub-threshold swing[1]. Here, we demonstrate TFETs based on suspended, ultra-clean, quasi-metallic carbon nanotube pn devices. These devices exhibit a subthreshold swing as low as 2mV/decade, with a current  $I_{on}/I_{off}$  ratio in the order of 105 at cryogenic temperatures. At room temperature, however, the current is dominated by the diffusion of carriers, which degrades the  $I_{on}/I_{off}$  ratio and the subthreshold swing. We also explore the effect of the schottky contacts on the tunneling current by adding two back-to-back diodes to the tunneling current model. Our results provide evidence that the effect of the schottky contacts can be significant when quasi-metallic nanotubes exhibit band-to-band tunneling. Our results show that quasi-metallic carbon nanotubes can be potential candidates for future nanoelectronics. References: [1] A. M. Ionescu and H. Riel, "Tunnel field-effect transistors as energy-efficient electronic switches," Nature, vol. 479, pp. 329-337, 2011.

**4:42PM C51.00012 Structural and electronic properties of BAlN alloy<sup>1</sup>**, JIMMY-XUAN SHEN, Dept. of Physics Univ of California - Santa Barbara, DARSHANA WICKRAMARATNE, CHRIS G VAN DE WALLE, Materials Dept., UC Santa Barbara — Designs of far-UV emitters using BAlN as the barrier layer and AlN as the active layer are being considered. Realization of BAlN alloys is complicated by the fact that BN is most stable in a hexagonal structure, which is different from the ground-state wurtzite structure of AlN. Enabling such designs requires a fundamental understanding of the composition dependent electronic structure of BAlN. Using first-principles simulations based on a hybrid functional, we investigate the band gaps, band-gap bowing, and miscibility of BAlN using explicit alloy calculations. The results from these calculations are used to determine the band offsets between AlN and BAlN that are essential to assess the performance of UV-emitting devices.

<sup>1</sup>This work is supported by NSF.

**4:54PM C51.00013 Sources of Shockley-Read-Hall recombination in III-nitride light emitters<sup>1</sup>**, CYRUS E. DREYER, Department of Physics and Astronomy, Rutgers University, AUDRIUS ALKAUSKAS, Center for Physical Sciences and Technology, Vilnius, Lithuania and Kaunas University of Technology, Kaunas, Lithuania, JOHN L. LYONS, Center for Functional Nanomaterials, Brookhaven National Laboratory, JAMES S. SPECK, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara — Group-III nitrides are the key materials for high efficiency light-emitting diodes in the blue part of the visible spectrum, and a large research effort is aimed at extending this success to the green and the yellow range, where nitride LEDs are significantly less efficient. Though it has been noted that the efficiency of III-nitride devices may be limited by Shockley-Read-Hall recombination at point defects, the microscopic mechanism and defects responsible are unknown. Based on first-principles calculations of defect formation energies, charge-state transition levels, and nonradiative capture coefficients, we describe a mechanism by which complexes between gallium vacancies and oxygen and/or hydrogen can act as efficient channels for nonradiative recombination in InGaN alloys. The dependence of these quantities on alloy composition is analyzed. We find that modest concentrations of the proposed defect complexes, around  $10^{16}\text{cm}^{-3}$ , can give rise to Shockley-Read-Hall coefficients  $A = (10^7 - 10^9)\text{s}^{-1}$ . The resulting nonradiative recombination can significantly reduce the internal quantum efficiency of optoelectronic devices.

<sup>1</sup>This work was supported by DOE and by EU Marie Skłodowska-Curie Action.

**5:06PM C51.00014 A first-principles study of pyroelectricity in GaN and ZnO**, JIAN LIU, MARIA V. FERNÁNDEZ-SERRA, PHILIP B. ALLEN, State Univ of NY- Stony Brook — We present first-principles calculations on the primary pyroelectric coefficients for wurtzite GaN and ZnO. The primary pyroelectricity is attributed to the anharmonic atomic displacements of the Born effective charges on the cations and anions. We show that the primary pyroelectricity is the major part of the total pyroelectricity at low temperatures, while the secondary pyroelectricity becomes comparable with the primary pyroelectricity at high temperatures. Our calculations show that contributions from the acoustic and the optical phonon modes to the primary pyroelectric coefficient can be well described by the corresponding Debye and Einstein functions respectively.

**5:18PM C51.00015 Resistive switching in nanodevices**, H. RAEBIGER, Yokohama Nat'l Univ., Yokohama, Japan and Univ. Federal do ABC, Santo André, SP, Brazil, A. C. M. PADILHA, Univ. Federal do ABC, Santo André, SP, Brazil, A. R. ROCHA, Univ. Estadual Paulista, São Paulo, SP, Brazil, G. M. DALPIAN, Univ. Federal do ABC, Santo André, SP, Brazil — A nanoscale metal/insulator/metal sandwich structure device may exhibit multiple resistive states, and switching between these states can be controlled by bias voltage. However, the underlying physical mechanism is poorly understood. We present an electronic mechanism that explains multiple resistive states in such devices due to multiple solutions of Poisson's equation. These solutions describe spontaneously charged states characterized by different (convex and concave) 'band bendings'. For an insulator with mainly donor type defects, the low-resistivity state is characterized by a negatively charged insulator due to convex band bending, and the high-resistivity state by a positively charged insulator due to concave band bending; vice versa for insulators with mainly acceptor type defects. We show that the coexistence of such states, and switching between them is determined by defect/impurity abundance, device size, and basic material properties.

**Monday, March 14, 2016 2:30PM - 5:30PM —**

**Session C52 DAMOP: Vortices, Rotation and Nonlinear Effects in BECs** Hilton Baltimore Holiday Ballroom 3 - Stephen Eckel, Joint Quantum Institute, University of Maryland

**2:30PM C52.00001 Melting of Vortex Lattice in Bose-Einstein Condensate in Presence of Disorder**<sup>1</sup>, BISHWAJYOTI DEY, Department of Physics, SP Pune University, Pune 411007, India. — We study the vortex lattice dynamics in Bose-Einstein condensate (BEC) in presence of single impurity as well as random impurities or disorder. The single impurity is modeled by a Gaussian function while disorder is introduced in the system by a uniform random potential. Such potentials can be created experimentally by lasers. We solve the time-dependent Gross-Pitaevskii equation in two-dimensions using split-step Crank-Nicolson method. We first show that a single vortex can be pinned by an impurity. We then show that even a single impurity can distort the vortex lattice. For sufficiently strong impurity potential, the vortex lattice gets pinned to the impurity. We also show that a new type of giant hole with hidden vortices inside it can be created in the vortex lattice by a cluster of impurities. In presence of random impurity potential or disorder, the vortices get pinned at random positions leading to melting of the vortex lattice. We further show that the vortex lattice melting can also be induced by the pseudorandom potential generated by the superposition of two optical lattices. The absence of long-range order in the melted vortex lattice is demonstrated from the structure factor profile and the histogram of the distance between each pair of vortices.

<sup>1</sup>I would like to thank DST, India and BCUD SPPU, for financial assistance through research grants.

**2:42PM C52.00002 From Vortex Rings to Hopfions in 3d Bose-Einstein Condensates**, PANAYOTIS KEVREKIDIS, UMass, Amherst — In this talk we report a number of recent results on three-dimensional topological states. Motivated by our earlier work on vortices, we develop a two-fold approach for studying vortex rings. We analytically and numerically explore their emergence through an instability from planar or ring dark soliton states in the small amplitude/weak nonlinearity limit. We also analytically and numerically explore the opposite, particle based limit of large density/large nonlinearity in the Thomas-Fermi regime. We connect these two analytically tractable limits through detailed numerical computations revealing the spectral and nonlinear stability of such states. We also explore a series of other states, including so-called Hopfions, and dark-soliton-shells examining both their regimes of stability in 3d atomic BECs, as well as their mechanisms and manifestations of dynamical instabilities.

**2:54PM C52.00003 Equation of Motion of a Quantum Vortex.**, TIMOTHY COX, University of British Columbia, PHILIP STAMP, University of British Columbia and the Pacific Institute of Theoretical Physics — Understanding the motion of vortices in quantum fluids is key to understanding the dynamics of such fluids. The motion of quantum vortices has long been understood in terms of the Hall-Vinen-Iordanski (HVI) equations. A fully quantum mechanical treatment of vortex motion in a two-dimensional Bose superfluid<sup>[1]</sup> leads to a modified version of the HVI equations which include significant history dependent forces and a fluctuating noise force. The dynamics deviates from that described by the HVI equations when the frequency of motion is higher than the temperature. We describe the consequences of the memory and noise for the motion of a single superfluid vortex as well as the circumstances under which their effects should be experimentally observable. <sup>[1]</sup> Thompson and Stamp, Phys Rev Lett. 108, 184501 (2012)

**3:06PM C52.00004 Helicity in superfluids**, HRIDESH KEDIA, DUSTIN KLECKNER, University of Chicago, DAVIDE PROMENT, University of East Anglia, WILLIAM T.M. IRVINE, University of Chicago — Ideal fluid flow conserves a special quantity known as helicity, in addition to energy, momentum and angular momentum. Helicity can be understood as a measure of the knottedness of vortex lines of the flow, providing an important geometric tool to study diverse physical systems such as turbulent fluids and plasmas. Since superfluids flow without resistance just like ideal (Euler) fluids, a natural question arises: Is there an extra conserved quantity akin to helicity in superfluids? We address the question of a "superfluid helicity" theoretically and examine its consequences in numerical simulations.

**3:18PM C52.00005 Finite temperature and density depletion effects on persistent current state transitions and critical velocity of a toroidal Bose-Einstein condensate**, AVINASH KUMAR, STEPHEN ECKEL, FRED JENDRZEJEWSKI<sup>1</sup>, Joint Quantum Institute, University of Maryland, GRETCHEN CAMPBELL, Joint Quantum Institute, University of Maryland, NIST — We study the decay of a persistent, quantized current state in a toroidal geometry. Our experiment involves trapping neutral <sup>23</sup>Na atoms in an all optical "target trap" shaped potential. This potential consists of a disc surrounded by an annular potential. A current in a superfluid can be sustained only below a critical current. This critical current can be tuned by introducing a density perturbation which depletes the local density. The decay time of a persistent current state can also be controlled by enhancing fluctuations of the system thermally. We study the decay at four different temperatures between 30 nK and 190 nK. For each temperature we record the decay at four different perturbation strengths. We find that increasing the magnitude of the density depletion or the temperature leads to a faster decay, and have seen the decay constant change by over two orders of magnitude. We also studied the size of hysteresis loop between different current states as a function of temperature, allowing us to extract a critical velocity. We find that the discrepancies between the experimentally extracted critical velocity and theoretically calculated critical velocity (using local-density approximation) decreases as the temperature is decreased.

<sup>1</sup>Now at University of Heidelberg

**3:30PM C52.00006 Finite-temperature energy landscapes in rotating ring BECs**<sup>1</sup>, BRENNAN COHELEACH, CLAYTON HELLER, MARK EDWARDS, Georgia Southern Univ, STEVE ECKEL, AVINASH KUMAR, CHARLES CLARK, GRETCHEN CAMPBELL, Joint Quantum Institute — In a recent experiment conducted at NIST a ring Bose-Einstein condensate (BEC) was prepared in a unit angular momentum circulation state. A barrier was then slowly raised and left on for a variable hold time and then turned off. The final circulation of the BEC was studied as a function of hold time and barrier energy height. This procedure was carried out for several well-characterized non-zero temperatures. We have studied the energetics of this process under the assumption that a vortex is initially present in the center of the ring BEC and then travels out of the ring through the density notch created by the barrier. We have computed the energy per particle of the condensate system for a variable location of the vortex by solving the time-dependent Generalized Gross-Pitaevskii (GGP) equation in imaginary time. To account for finite-temperature we solved self-consistently for the condensate fraction as a function of temperature in thermal equilibrium for fixed total particle number. This yielded the non-condensate density which appears in the GGP affecting the energy of the vortex. We also modeled the dynamics of the vortex using the ZNG formalism.

<sup>1</sup>Supported by NSF grants PHY-1413768 and ARO Atomtronics MURI

**3:42PM C52.00007 Cold atoms in one-dimensional rings: a Luttinger liquid approach to precision measurement.**<sup>1</sup>, STEPHEN RAGOLE, JQI, QuICS, and University of Maryland, JACOB TAYLOR, JQI, QuICS, University of Maryland, and National Institute of Standards and Technology — Recent experiments have realized ring shaped traps for ultracold atoms. We consider the one-dimensional limit of these ring systems with a moving weak barrier, such as a blue-detuned laser beam. In this limit, we employ Luttinger liquid theory and find an analogy with the superconducting charge qubit. In particular, we find that strongly-interacting atoms in such a system could be used for precision rotation sensing. We compare the performance of this new sensor to the state of the art non-interacting atom interferometry.

<sup>1</sup>Funding provided by the Physics Frontier Center at the JQI and by DARPA QUASAR

**3:54PM C52.00008 Resonant wavepackets and shock waves in an atomtronic SQUID<sup>1</sup>**, YI-HSIEH WANG, A. KUMAR, Joint Quantum Institute, F. JENDRZEJEWSKI, Ruprecht-Karls-Universität, RYAN M. WILSON, The United States Naval Academy, MARK EDWARDS, Georgia Southern University, S. ECKEL, G. K. CAMPBELL, CHARLES W. CLARK, Joint Quantum Institute — The fundamental dynamics of ultracold atomtronic devices are reflected in their phonon modes of excitation. We probe such a spectrum by applying a harmonically driven potential barrier to a <sup>23</sup>Na Bose-Einstein condensate in a ring-shaped trap<sup>2</sup>. This perturbation excites phonon wavepackets. When excited resonantly, these wavepackets display a regular periodic structure. The resonant frequencies depend upon the particular configuration of the barrier, but are commensurate with the orbital frequency of a Bogoliubov sound wave traveling around the ring. Energy transfer to the condensate over many cycles of the periodic wavepacket motion causes enhanced atom loss from the trap at resonant frequencies. Solutions of the time-dependent Gross-Pitaevskii equation exhibit quantitative agreement with the experimental data. We also observe the generation of supersonic shock waves under conditions of strong excitation, and collisions of two shock wavepackets.

<sup>1</sup>Work supported by the U. S. Army Research Office Atomtronics MURI program.

<sup>2</sup>Yi-Hsieh Wang, A. Kumar, F. Jendrzejewski, Ryan M. Wilson, Mark Edwards, S. Eckel, G. K. Campbell, and Charles W. Clark, arXiv: 1510.02968 (2015)

**4:06PM C52.00009 Anomalous hysteresis in a spinor atom-SQUID**, RANCHU MATHEW, Joint Quantum Institute, University of Maryland, EITE TIESINGA, Joint Quantum Institute, National Institute of Standards and Technology and University of Maryland — Over the past few years, there has been a concerted effort at NIST studying the atomic analogue of a Superconducting Quantum Interference Device (SQUID) [Eckel S. et al., Nature (London) 506, 200 (2014)]. The atom-SQUID consists of a Bose-Einstein condensate (BEC) in a ring trap with a rotating external potential or weak link. The system displays persistent currents and hysteresis as a function of rotation rate. We investigate the effect of the spin degree of freedom of an atom and a rotating vector potential, which mixes spin sublevels, on the hysteresis pattern by performing a numerical analysis of the Gross-Pitaevskii equation. For a spinless BEC the winding number of the BEC changes by one unit as the rotation of the potential is slowly changed beyond a critical value. In contrast, in a certain parameter regime for a spinor BEC with a vector potential the winding number changes by two units instead of one. To explain this anomalous phenomenon, we calculate the energies of the two saddle-points of the mean-field energy functional, which mediate the transitions to states which differs by one and two units of winding number.

**4:18PM C52.00010 Transport in a capacitive ultracold atomtronic circuit<sup>1</sup>**, MARK EDWARDS, BENJAMIN ELLER, Georgia Southern Univ, STEVE ECKEL, CHARLES CLARK, Joint Quantum Institute — A recent NIST experiment<sup>2</sup> studied the transport of a gaseous Bose-Einstein condensate (BEC) confined in an atomtronic “dumbbell” circuit. The optically created condensate potential consisted of a tight harmonic potential in the vertical direction confining the BEC to a horizontal plane. The horizontal potential consisted of two cylindrical wells separated by a channel produced by a harmonic oscillator potential transverse to the line joining the wells. The BEC, formed in the “source” well, was released to flow toward the “drain” well. The evolution of this system was shown to be reproduced by a model electronic circuit consisting of a charged capacitor,  $C$ , in series with an inductor,  $L$ , and a parallel combination of a resistor,  $R$ , and a Josephson junction. We modeled this system with the Gross-Pitaevskii (GP) equation and found good agreement with the data provided that the confining potential is carefully reproduced. The GP simulations show behavior, not detectable in the experiment, that atoms can jump out of the dumbbell area after filling up the drain well. We also present the dependence of  $R$  and  $L$  on the channel shape.

<sup>1</sup>Supported by NSF grants PHY-1413768 and ARO Atomtronics MURI

<sup>2</sup>J.G. Lee, et al., arXiv:1506.08413 (2015)

**4:30PM C52.00011 Collective modes of trapped Bose-Einstein condensates undergoing adiabatic deformation from filled-sphere to thin-shell geometries<sup>1</sup>**, COURTNEY LANNERT, Smith College, KUEI SUN, The University of Texas at Dallas, KARMELA PADAVI'C, SMITHA VISHVESHVARA, University of Illinois at Urbana-Champaign — Collective modes of a trapped Bose-Einstein condensate (BEC) are closely related to the ground-state density profile and are experimentally measurable. They are particularly useful for characterizing a BECs three-dimensional structure that cannot be well resolved by the two-dimensional absorption imaging. In this context, it is essential to understand the signatures of collective modes of a BEC in various typical geometries and how they change with the geometry. Here, we study a BEC confined in a spherical trap that is tunable to shape the BEC to be a filled sphere, a thin shell, or any crossover stage between them. We employ hydrodynamic treatments and real-time simulations of the Gross-Pitaevskii equation to obtain the collective modes. We find a set of radial modes that can distinguish a sphere from a shell, and an oscillation frequency dip in a crossover region where the central density becomes low. We also explore the angular modes and find a crucial role of the shell BECs inner boundary, which the sphere BEC lacks. Our findings ought to help future experimental investigations on recently realized BECs in bubble-trap potentials.

<sup>1</sup>Work supported by the National Science Foundation under award DMR-1243574

**4:42PM C52.00012 Gravitational Effects on Collective Modes of Superfluid Shells**, KARMELA PADAVI'C, University of Illinois at Urbana-Champaign, KUEI SUN, The University of Texas at Dallas, COURTNEY LANNERT, Smith College, SMITHA VISHVESHVARA, University of Illinois at Urbana-Champaign — We study the effects of gravity on collective excitations of shell-shaped Bose-Einstein condensates (BECs). Superfluid shells are of general interest as examples of hollow geometries that can be produced in ultracold atoms in bubble-trap potentials or optical lattices. Our approach to analyzing superfluid shells is based on a Gross-Pitaevskii mean field theory and hydrodynamic equations derived from it. Considering a spherically symmetric BEC in general, there are distinct collective excitation spectra for the cases of a fully filled sphere and a very thin shell. Furthermore, an adiabatic change in the potential producing a slow transition from one geometry to the other shows a characteristic evolution. Given that in most realistic experimental conditions gravity cannot be neglected we investigate its effects on the equilibrium profile and the collective modes in the very thin shell limit. We analytically obtain the full excitation spectrum for the thin shell geometry and account for gravity perturbatively at length and energy scales that describe a stable matter-wave bubble. We find that gravity breaks spherical symmetry of the equilibrium density profile and affects the collective excitations by coupling adjacent modes in the angular direction.

**4:54PM C52.00013 Classical and quantum dissipation of bright solitons in a bosonic superfluid**, DMITRY K. EFIMKIN, Condensed Matter Theory Center, University of Maryland, United States, JOHANNES B. HOFMANN, Condensed Matter Theory Center, University of Maryland, United States and TCM Group, Cavendish Laboratory, University of Cambridge, United Kingdom, VICTOR GALITSKI, Joint Quantum Institute and Condensed Matter Theory Center, University of Maryland, United States — We consider the quantum dissipation of a bright soliton in a quasi-one-dimensional bosonic superfluid. The dissipation appears due to interaction of the soliton with Bogoliubov excitations, which act as a bath for the soliton. Using a collective coordinate approach and the Keldysh formalism, we derive a Langevin equation for the soliton motion which contains both a friction and a stochastic force. We argue that due to the integrability of the original problem, Ohmic friction is absent, rendering the dynamics non-Markovian. We furthermore show that the resulting friction can be interpreted as the backreaction of Bogoliubov quasiparticles emitted by an accelerating soliton, which represents an analogue of the Abraham-Lorentz force known in electrodynamics.

**5:06PM C52.00014 Interacting multiple zero mode formulation for a dark soliton in a Bose-Einstein condensate** , JUNICHI TAKAHASHI, YUSUKE NAKAMURA, YOSHIYA YAMANAKA, Waseda Univ. — The system of Bose-Einstein condensate (BEC) has a zero-mode (ZM) associated with the spontaneous breakdown of the global phase symmetry. However, to formulate the ZMs in quantum field theory for a finite-size system with spontaneous breakdown of symmetries is not trivial, for in the naive Bogoliubov theory one encounters difficulties such as phase diffusion, the absence of a definite criterion for determining the ground state, and infrared divergences. In order to remove this difficulty, we have recently proposed the new treatment of the ZM, which enable us to introduce a unique ground state in the ZM sector<sup>1</sup>. Using this ground state, we have evaluated the quantum fluctuation for the phase of condensate. In this presentation, we consider an atomic BEC system with a dark soliton that contains two ZMs corresponding to spontaneous breakdown of the global phase and translational symmetries. In our treatment, the original non-linear interaction of the field operator brings us the interaction between the two ZMs. We evaluate the standard deviations of the ZM operators and see how the mutual interaction between the two ZMs affects them.

<sup>1</sup> J. Takahashi, Y. Nakamura, and Y. Yamanaka, Phys. Rev. A **92**, 023627 (2015).

**5:18PM C52.00015 Anomalous energetics and dynamics of moving vortices**<sup>1</sup> , LEO RADZIHOVSKY, Department of Physics, University of Colorado — Motivated by the general problem of moving topological defects in an otherwise ordered state and specifically, by the anomalous dynamics observed in vortex-antivortex annihilation and coarsening experiments in freely-suspended smectic-C films, I study the deformation, energetics and dynamics of moving vortices in an overdamped xy-model and show that their properties are significantly and qualitatively modified by the motion.

<sup>1</sup>supported by NSF through DMR-1001240, MRSEC DMR-0820579, and by Simons Investigator award from Simons Foundation

**Monday, March 14, 2016 2:30PM - 5:30PM —**  
**Session C53 DCOMP: Massively Parallel Simulations of Chemical, Materials and Biological Systems** Hilton Baltimore Holiday Ballroom 4 - Priya Vashisthta, University of Southern California

**2:30PM C53.00001 First-principles temperature-dependent phonons and elastic constants** , LIN YANG, Lawrence Livermore National Laboratory, CA — Calculations of thermodynamic properties of materials from first-principles are critical for equation of state and materials strength modeling. Here we present the thermodynamic properties of a select set of metals based on density functional theory. In particular, we present elastic constants and lattice dynamics for body-centered cubic metals obtained from first-principles molecular dynamics and a self-consistent phonon approach. In order to calculate the thermodynamic properties, we make use of fluctuation formulas associated with the canonical ensemble form of *ab initio* molecular dynamics (AIMD). This procedure is efficient and takes into account the anharmonic contributions to the equilibrium thermodynamic properties. In the self-consistent lattice dynamics approach, the phonon dispersions at finite temperature are determined from small displacements along normal modes associated with the chosen temperature. This method provides an efficient and accurate technique for phonon spectrum and finite-temperature acoustic sound speeds and elastic constants. We found that both methods provide consistent results for the temperature- and pressure-dependent elastic moduli. The AIMD include full anharmonicity but suffers from statistical errors of the order of 5%. The self-consistent phonon method, on the other hand, has less statistical uncertainty but does not explicitly account for electron-phonon coupling. At ambient pressure, our calculations (both methods) agree quite well with experimental data. This work performed under the auspices of the U.S. DOE by LLNL under Contract DE-AC52-07NA27344.

**3:06PM C53.00002 The ReaxFF method - new applications and developments** , ADRI VAN DUIN, Penn State — The ReaxFF method provides a highly transferable simulation method for atomistic scale simulations on chemical reactions at the nanosecond and nanometer scale. It combines concepts of bond-order based potentials with a polarizable charge distribution. Since its initial development for hydrocarbons in 2001, we have found that this concept is transferable to applications to elements all across the periodic table, including all first row elements, metals, ceramics and ionic materials. For all these elements and associated materials we have demonstrated that ReaxFF can reproduce quantum mechanics-based structures, reaction energies and reaction barriers with reasonable accuracy, enabling the method to predict reaction kinetics in complicated, multi-material environments at a relatively modest computational expense. This presentation will describe the current concepts of the ReaxFF method, the current status of the various ReaxFF codes, including parallel implementations and recently developed hybrid Grand Canonical Monte Carlo options - which significantly increase its application areas. Also, we will present an overview of recent applications to a range of materials of increasing complexity, with a focus on applications to combustion, biomaterials, batteries, tribology and catalysis.

**3:42PM C53.00003 Discovering chemistry with an ab initio nanoreactor** , TODD MARTINEZ, Stanford University and SLAC National Accelerator Laboratory — Traditional approaches for modeling chemical reaction networks such as those involved in combustion have focused on identifying individual reactions and using theoretical approaches to explore the underlying mechanisms. Recent advances involving graphical processing units (GPUs), commodity products developed for the videogaming industry, have made it possible to consider a distinct approach wherein one attempts to discover chemical reactions and mechanisms. We provide a brief summary of these developments and then discuss the concept behind the “ab initio nanoreactor” which explores the space of possible chemical reactions and molecular species for a given stoichiometry. The nanoreactor concept is exemplified with an example to the Urey-Miller reaction network which has been previously advanced as a potential model for prebiotic chemistry. We briefly discuss some of the future directions envisioned for the development of this nanoreactor concept.

**4:18PM C53.00004 Multi-petaflop/s quantum and reactive molecular dynamics simulations** , AIICHIRO NAKANO, University of Southern California — We have developed a divide-conquer-recombine algorithmic framework for large quantum molecular dynamics (QMD) and reactive molecular dynamics (RMD) simulations. The algorithms have achieved parallel efficiency over 0.98 on 786,432 IBM Blue Gene/Q processors for 39.8 trillion electronic degrees-of-freedom QMD in the framework of density functional theory and 67.6 billion-atom RMD. We will discuss several applications including (1) 16,616-atom QMD simulation of rapid hydrogen production from water using metallic alloy nanoparticles, (2) 6,400-atom nonadiabatic QMD simulation of exciton dynamics for efficient solar cells, and (3) 112 million-atom RMD simulation of nanocarbon synthesis by high temperature oxidation of SiC nanoparticles.

**4:54PM C53.00005 Massively parallel models of human hemodynamics** , AMANDA RANGLES, Duke University — No abstract available.

**Monday, March 14, 2016 2:30PM - 5:18PM —**  
**Session C54 FIAP: Ballistic Transport in Semiconductor Devices** Hilton Baltimore Holiday Ballroom 5 - Ernesto Marinero, Purdue University

**2:30PM C54.00001 Ballistic Hot Electron Transport in Heteroepitaxial SrRuO<sub>3</sub> Metal-Base Transistors**, BRIAN KIM, Stanford University, YASUYUKI HIKITA, SLAC National Accelerator Laboratory, TAKEAKI YAJIMA, The University of Tokyo, CHRISTOPHER BELL, University of Bristol, HAROLD HWANG, Stanford University — Perovskite oxide heterostructures is a rapidly emerging field significant for interface-induced electronic and magnetic reconstructions, resulting in novel phases distinct from those found in the bulk counterparts. Notably, utilizing device structures is an effective way to probe these interface-induced phases. One of the most prevalent device structures that has been adopted so far is a three-terminal field-effect geometry, used to probe in-plane electronic transport properties. However, the out-of-plane three-terminal device geometry, though less studied due to its complexity, is also useful in many aspects. In the metal-base transistor (MBT), for instance, ballistic transport of hot electrons injected across a Schottky diode emitter can be used to probe hot electron properties of the metal-base, providing information on inelastic scattering mechanisms, electron confinement effects, and intervalley transfer. One promising model system for the metal-base is SrRuO<sub>3</sub> (SRO), characterized by intermediate electron correlations with unusual transport properties. Here we present an all-perovskite oxide heteroepitaxial MBT using SRO as a metal-base layer. Successful MBT operation for various metal-base layer thicknesses was achieved, from which the hot electron attenuation length of SRO was deduced. These results form a foundation on which to examine the properties of hot electrons in strongly correlated systems using the out-of-plane three-terminal device geometry.

**2:42PM C54.00002 Nondiffusive thermal transport increases temperature rise in RRAM filaments**, KEITH REGNER, JONATHAN MALEN, Carnegie Mellon University — Resistive-switching memory (RRAM) offers benefits to nonvolatile memory systems due to scalability, fast switching, and easy fabrication. In RRAM, electrical stimulation switches the resistance of a metal-insulator-metal memory cell. A low-resistance state is achieved during the set process, when a conductive filament (CF) is formed by dielectric breakdown. During the reset process, disruption of the CF restores the device to a high-resistance state. Studies suggest that dissolution of the CF during the reset process occurs when the CF reaches a critical temperature due to Joule heating. Typically, the heat diffusion equation with bulk thermal properties is used to model the thermal processes both within the CF and the surrounding oxide. It is well known, however, that heat transport is nondiffusive when experimental length scales are comparable to energy carrier mean free paths (MFPs). We suggest that heat transport in RRAM is nondiffusive by determining the phonon MFP spectrum in TiO<sub>2</sub> (i.e., a promising material for RRAM) and showing that MFPs that contribute significantly to heat transport are comparable to the diameter of the CF. Thus, we approximate the CF as an infinitely long cylinder embedded in crystalline rutile TiO<sub>2</sub> and develop an approximate analytical solution to the BTE in the TiO<sub>2</sub>. We find that the surface temperature of the CF predicted by the BTE is larger than that predicted by the heat diffusion equation. If the heat diffusion equation is used to model thermal transport in RRAM, a reduced effective TiO<sub>2</sub> thermal conductivity should be used.

**2:54PM C54.00003 AC Josephson effect without superconductivity, and other effects of radio frequency quantum nanoelectronics**, XAVIER WAINANT, BENOIT GAURY, JOSEPH WESTON, INAC, CEA Grenoble, France — With single coherent electron sources and electronic interferometers now available in the lab, the time resolved dynamics of electrons can now be probed directly. I will discuss how a fast raise of voltage propagates inside an electronic interferometer and leads to an oscillating current of well controlled frequency. This phenomena is the normal counterpart to the AC Josephson effect. I will also briefly advertize our software for computing quantum transport properties, Kwant (<http://kwant-project.org>) and its time-dependent extension T-Kwant.

**3:06PM C54.00004 Orbital magnetoresistance of two-dimensional electron systems in the hydrodynamic regime<sup>1</sup>**, ANTON ANDREEV, University of Washington, ALEX LEVCHENKO, University of Wisconsin-Madison — We develop a theory of magnetoresistance of two-dimensional electron systems in the hydrodynamic regime. It applies to two-dimensional semiconductor structures with strongly correlated carriers when the electron-electron scattering length is sufficiently short. We find that the magnetoresistance is positive quadratic at weak fields. Although the resistivity is governed by both viscosity and thermal conductivity of the electron fluid, the temperature dependence of magnetoresistance depends on the viscosity only. This enables extraction of viscosity of the electron liquid from magnetotransport measurements.

<sup>1</sup>DE-FG02-07ER46452, NSF-DMR-1401908

**3:18PM C54.00005 The effect of split gate dimensions on the electrostatic potential and 0.7 anomaly within one-dimensional quantum wires on a modulation doped GaAs/AlGaAs heterostructure**, L. W. SMITH\*, H. AL-TAIE, A. A. J. LESAGE, K. J. THOMAS, F. SFIGAKIS, P. SEE, J. P. GRIFFITHS, I. FARRER, G. A. C. JONES, D. A. RITCHIE, M. J. KELLY, C. G. SMITH, University of Cambridge, Cavendish Laboratory — We use a multiplexing scheme to measure the conductance properties of 95 split gates of 7 different gate dimensions fabricated on a GaAs/AlGaAs chip, in a single cool down [1]. The number of devices for which conductance is accurately quantized reduces as the gate length increases. However, even the devices for which conductance is accurately quantized in units of  $2e^2/h$  show no correlation between the length of electrostatic potential barrier in the channel and the gate length, using a saddle point model to estimate the barrier length. Further, the strength of coupling between the gates and the 1D channel does not increase with gate length beyond 0.7  $\mu\text{m}$ . The background electrostatic profile appears as significant as the gate dimension in determining device behavior. We find a clear correlation between the curvature of the electrostatic barrier along the channel and the strength of the “0.7 anomaly” which identifies the electrostatic length of the channel as the principal factor governing the conductance of the 0.7 anomaly.

\* Present address: Wisconsin Institute for Quantum Information, University of Wisconsin-Madison, Madison, WI.

[1] L. W. Smith *et al.*, arXiv:1508.03085

**3:30PM C54.00006 Electron Energy Levels in the 1D-2D Transition<sup>1</sup>**, MICHAEL PEPPER, KUMAR SANJEEV, KALARIKAD THOMAS, GRAHAM CREETH, DAVID ENGLISH, London Centre for Nanotechnology, University College London, DAVID RITCHIE, University College London, JONATHAN GRIFFITHS, IAN FARRER, GERAINT JONES, Cavendish Laboratory, University of Cambridge — Using GaAs-AlGaAs heterostructures we have investigated the behaviour of electron energy levels with relaxation of the potential confining a 2D electron gas into a 1D configuration. In the ballistic regime of transport, when the conductance shows quantized plateaux, different types of behaviour are found according to the spins of interacting levels, whether a magnetic field is applied and lifting of the momentum degeneracy with a source-drain voltage. We have observed both crossing and anti-crossing of levels and have investigated the manner in which they can be mutually converted. In the presence of a magnetic field levels can cross and lock together as the confinement is altered in a way which is characteristic of parallel channels. The overall behaviour is discussed in terms of electron interactions and the wavefunction flexibility allowed by the increasing two dimensionality of the electron distribution as the confinement is weakened.

<sup>1</sup>Work supported by UK EPSRC

**3:42PM C54.00007 Single-electron devices fabricated using double-angle deposition and plasma oxidation**, Y. HONG, Z. S. BARCIKOWSKI, A. N. RAMANAYAKA, M. D. STEWART JR., N. M. ZIMMERMAN, J. M. POMEROY, National Institute of Standards and Technology, QUANTUM PROCESSES AND METROLOGY GROUP TEAM — We report on development of plasma oxidized, single-electron transistors (SETs) where we seek low-capacitance and small-area Al/AIOx/Al tunnel junctions with small charge offset drift. Performance of metal-based SET quantum devices and superconducting devices has suffered from long-term charge offset drift, high defect densities and charge noise. We use plasma oxidation to lower defect densities of the oxide layer, and adjustable deposition angles to control the overlapping areas for Al/AIOx/Al tunnel junctions. Current-voltage and charge offset drift measurements are planned for cryogenic temperatures. Other electrical properties will be measured at room temperature. We hope to see Coulomb blockade oscillations on these devices and better charge offset stability than typical Al/AIOx/Al SETs.

**3:54PM C54.00008 Quantum point contacts on two-dimensional electron gases with a strong spin-orbit coupling<sup>1</sup>**, JOON SUE LEE, California NanoSystems Institute, Univ of California, Santa Barbara, MIHIR PENDAHARKAR, Department of Electrical and Computer Engineering, Univ of California, Santa Barbara, BORZOYEH SHOJAEI, Materials Department, Univ of California, Santa Barbara, ANTHONY P. MCFADDEN, Department of Electrical and Computer Engineering, Univ of California, Santa Barbara, CHRIS PALMSTRM, Materials Department and Department of Electrical and Computer Engineering, Univ of California, Santa Barbara — Studies of electrical transport in one-dimensional semiconductors in a presence of a strong spin-orbit interaction are crucial not only for exploring the emergent phenomena, such as topological superconductivity, but also for potential spintronic applications by controlling of the electron spins. We investigate the electrical transport properties of one-dimensional confinement defined by electrostatic potentials on large area two-dimensional electron gases of InAs and InSb, which have a strong spin-orbit coupling. The high-quality InAs and InSb quantum wells are grown on antimonide buffers by molecular beam epitaxy, and the gate-tunable regions are created using Al<sub>2</sub>O<sub>3</sub> or HfO<sub>2</sub> gate dielectrics by atomic layer deposition. We will discuss the modulation of spin-orbit coupling in the two-dimensional electron gases and the spin-orbit-induced spin splitting by the split-gate quantum point contacts.

<sup>1</sup>This work was supported by Microsoft Research.

**4:06PM C54.00009 Quenching Plasma Waves in Two Dimensional Electron Gas by a Femtosecond Laser Pulse**, MICHAEL SHUR, Rensselaer Polytech Inst, SERGEY RUDIN AND GREG RUPPER COLLABORATION<sup>1</sup>, ANDREY MURAVIEV COLLABORATION<sup>2</sup> — Plasmonic detectors of terahertz (THz) radiation using the plasma wave excitation in 2D electron gas are capable of detecting ultra short THz pulses. To study the plasma wave propagation and decay, we used femtosecond laser pulses to quench the plasma waves excited by a short THz pulse. The femtosecond laser pulse generates a large concentration of the electron-hole pairs effectively shorting the 2D electron gas channel and dramatically increasing the channel conductance. Immediately after the application of the femtosecond laser pulse, the equivalent circuit of the device reduces to the source and drain contact resistances connected by a short. The total response charge is equal to the integral of the current induced by the THz pulse from the moment of the THz pulse application to the moment of the femtosecond laser pulse application. This current is determined by the plasma wave rectification. Registering the charge as a function of the time delay between the THz and laser pulses allowed us to follow the plasmonic wave decay. We observed the decaying oscillations in a sample with a partially gated channel. The decay depends on the gate bias and reflects the interplay between the gated and ungated plasmons in the device channel.

<sup>1</sup>Army Research Office

<sup>2</sup>Rensselaer Polytechnic Institute

**4:18PM C54.00010 Evidence for a New Intermediate Phase in a Strongly Correlated 2D System near Wigner Crystallization<sup>1</sup>**, XUAN GAO, RICHARD QIU, NICHOLAS GOBLE, Case Western Reserve University, ALEX SERAFIN, LIANG YIN, JIAN-SHENG XIA, NEIL SULLIVAN, National High Magnetic Field Laboratory and University of Florida, LOREN PFEIFFER, KEN WEST, Princeton University — How the two dimensional (2D) quantum Wigner crystal (WC) transforms into the metallic liquid phase remains an outstanding problem in physics. In theories considering the 2D WC to liquid transition in the clean limit, it was suggested that a number of intermediate phases might exist. We have studied the transformation between the metallic fluid phase and the low magnetic field reentrant insulating phase (RIP) which was interpreted as due to the WC [Qiu et al, PRL 108, 106404 (2012)], in a strongly correlated 2D hole system in GaAs quantum well with large interaction parameter  $r_s$  ( $\sim 20-30$ ) and high mobility. Instead of a sharp transition, we found that increasing density (or lowering  $r_s$ ) drives the RIP into a state where the incipient RIP coexists with Fermi liquid. This apparent mixture phase intermediate between Fermi liquid and WC also exhibits a non-trivial temperature dependent resistivity behavior which can be qualitatively understood by the reversed melting of WC in the mixture, in analogy to the Pomeranchuk effect in the solid-liquid mixture of Helium-3. Reference: R. Qiu et al, arXiv:1509.07463.

<sup>1</sup>X.G. thanks NSF (DMR-0906415) for supporting work at CWRU. Experiments at the NHMFL High B/T Facility were supported by NSF grant 0654118 and the State of Florida. L.P. thanks the Gordon and Betty Moore Foundation and NSF MRSEC (DMR-0819860) for support.

**4:30PM C54.00011 Electron bilayers in an undoped Si/SiGe double-quantum-well heterostructure**, TZU-MING LU, DOMINIQUE LAROCHE, Sandia National laboratories, SHIH-HSIEN HUANG, National Taiwan University, ERIK NIELSEN, Sandia National laboratories, YEN CHUANG, JIUN-YUN LI, CHEEWEE LIU, National Taiwan University — We report the design, fabrication, and the magneto-transport study of an undoped Si/SiGe double quantum well heterostructure. We show that employing asymmetric quantum wells for our single-side-gated devices allows us to observe a cross-over from single-layer-like to bi-layer-like behavior in the mobility-density dependence. We also observe an integer quantum Hall state at filling factor  $\nu = 2$ , which is expected to arise from inter-layer effects for Si electrons. This state could be due to either inter-layer coherence, or the symmetric-antisymmetric tunneling gap. This work has been supported by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy (DOE). Sandia National Laboratories is a multi program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. DOE's National Nuclear Security Administration under contract DE-AC04-94AL85000.

**4:42PM C54.00012 What carries heat in novel 2D semiconductors?**, ANDREA CEPPELLOTTI, Ecole Polytechnique Federale de Lausanne, Switzerland, GIORGIA FUGALLO, Ecole Polytechnique, Paris, France, LORENZO PAULATTO, FRANCESCO MAURI, Sorbonne Universites, Paris, France, NICOLA MARZARI, Ecole Polytechnique Federale de Lausanne, Switzerland — When materials are scaled down to the microscopic scale, or when dimensionality is reduced, thermal transport exhibits new intriguing behaviors that are not present in conventional bulk crystals. While phonons are typically considered to be the excitations responsible for carrying heat through a crystal, as dimensionality is reduced, the motion of phonons driven by a temperature perturbation becomes correlated, and collective excitations of many phonons arise [1]. This leads to a wealth of complex phenomena, such as very high thermal conductivity (the highest known conductivities are indeed found in 2D materials), or wave-like heat diffusion, with second sound, hitherto found only in a few exotic materials at cryogenic temperatures, routinely present at room temperature [2]. In this contribution, we show that heat transport in crystals can be described exactly with the kinetic theory of a gas of collective phonon excitations, termed relaxons. In this way, it is possible to recover a microscopic interpretation based on mean free paths and relaxation times without any simplification of the linearised phonon Boltzmann equation. [1] G. Fugallo, A. Cepellotti, et al., Nano Lett. 14, 6109 (2014) [2] A. Cepellotti, et al., Nat. Commun. 6, 6400 (2015)

**4:54PM C54.00013 Coherent dynamics of Landau-Levels in modulation doped GaAs quantum wells at high magnetic fields<sup>1</sup>** , CUNMING LIU, JAGANNATH PAUL, University of South Florida, JOHN RENO, CINT, Sandia National Laboratories, STEPHEN MCGILL, National High Magnetic Field Laboratory, DAVID HILTON, University of Alabama at Birmingham, DENIS KARAIKAI, University of South Florida — By using two-dimensional Fourier transform spectroscopy, we investigate the dynamics of Landau-Levels formed in modulation doped GaAs/AlGaAs quantum wells of 18 nm thickness at high magnetic fields and low temperature. The measurements show interesting dephasing dynamics and linewidth dependency as a function of the magnetic field. The work at USF and UAB was supported by the National Science Foundation under grant number DMR-1409473. The work at NHMFL, FSU was supported by the National Science Foundation under grant numbers DMR-1157490 and DMR-1229217. This work was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. Department of Energy, Office of Basic Energy Sciences user facility. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

1

**5:06PM C54.00014 Probing Carrier Transport across Patterned Interfaces with Ballistic Electron Emission Microscopy** , WESTLY NOLTING, CHRISTOPHER DURCAN, ROBERT BALSANO, College of Nanoscale Science and Engineering, VINCENT LABELLA, SUNY Polytechnic Institute — Electron scattering from sidewalls within aggressively scaled metallic interconnects dramatically increases the resistance, since the mean free path (~40 nm) is larger than the dimensions of the structure. One method to study hot-electron scattering in nm-thick metallic films is Ballistic Electron Emission Microscopy (BEEM), which is an STM based technique. In this work, we perform BEEM imaging and scattering measurements on lithographically patterned nanoscale oxide “fin” structures with a Schottky diode interface to determine its ability to measure sidewall scattering. This is accomplished by acquiring data from BEEM images and spectra on a regularly spaced grid and fitting the results to determine both the Schottky barrier height and the amplitude of the spectra. The amplitude of the spectra is related to the scattering in the film and interface. The position of fin structures is then determined by mapping both the Schottky height and amplitude over a square micron to observe scattering at the interface caused by the patterned structures. The fabrication of the patterned 50-nm-pitched sidewall structures and the preliminary BEEM imaging measurements on these structures will be presented.

## **Monday, March 14, 2016 2:30PM - 4:54PM –**

**Session C55 FPS DBIO: The Physics of Epidemics** Hilton Baltimore Holiday Ballroom 6 - Walter Beyerler, Sandia National Labs

**2:30PM C55.00001 Mitigating Infectious Disease Outbreaks<sup>1</sup>** , VICTORIA DAVEY, Department of Veterans Affairs — The emergence of new, transmissible infections poses a significant threat to human populations. As the 2009 novel influenza A/H1N1 pandemic and the 2014-2015 Ebola epidemic demonstrate, we have observed the effects of rapid spread of illness in non-immune populations and experienced disturbing uncertainty about future potential for human suffering and societal disruption. Clinical and epidemiologic characteristics of a newly emerged infectious organism are usually gathered in retrospect as the outbreak evolves and affects populations. Knowledge of potential effects of outbreaks and epidemics and most importantly, mitigation at community, regional, national and global levels is needed to inform policy that will prepare and protect people. Study of possible outcomes of evolving epidemics and application of mitigation strategies is not possible in observational or experimental research designs, but computational modeling allows conduct of ‘virtual’ experiments. Results of well-designed computer simulations can aid in the selection and implementation of strategies that limit illness and death, and maintain systems of healthcare and other critical resources that are vital to public protection.

<sup>1</sup>Mitigating Infectious Disease Outbreaks

**3:06PM C55.00002 TBD** , CHARLES MACAL, Director Center for Complex Adaptive Agent Sysys, Sim. Decis and Info. Sys. Div. — No abstract available.

**3:42PM C55.00003 TBD** , TIMOTHY LANT, Assistant Secretary for Preparedness and Response, BARDA — No abstract available.

**4:18PM C55.00004 What do public health officials expect from modelers during a response to an epidemic or outbreak?** , MARTIN MELTZER, Centers for Disease Control and Prevention — Since 2009, the CDC has participated in emergency responses ranging from small domestic outbreaks involving a few hundred people, to international public health emergencies affecting millions of individuals from around the world. Each response required unique skills from the CDC'S Modeling Task Force to address public health officials' questions and to help them make informed decisions. This presentation will discuss the roll of the Modeling Task Forces in the CDC's Incident Management structure and some of the models used to assist officials in making decisions about the potential size of the public health crisis, how effective interventions could be, and what resources are required.

## **Monday, March 14, 2016 5:45PM - 6:45PM –**

**Session D1 APS: APS Prizes and Awards Ceremonial Session** Hilton Baltimore Key Ballroom 11/12 -

**5:45PM D1.00001 Prizes & Awards Ceremony –**

## **Monday, March 14, 2016 6:45PM - 8:00PM –**

**Session D2 APS: APS Welcome Reception** Exhibit Hall EF -

**6:45PM D2.00001 APS Welcome Reception –**

## **Monday, March 14, 2016 5:45PM - 7:00PM –**

**Session D10 FGSA FIAP: Undergraduate Professional Skills Workshop for Non-Academic Careers** 303 -

5:45PM D10.00001 Undergraduate Professional Skills Workshop for Non-Academic Careers —

**Monday, March 14, 2016 7:30PM - 9:30PM —**

Session D20 DCMP FOEP: Special Outreach Session: Science and Cooking 310 -

**7:30PM D20.00001 Science and Cooking** — Many chefs are developing new approaches to prepare and present their cuisine using materials common to many physics labs, such as liquid nitrogen, foams, emulsions and hydrogels. In fact, the ingredients and methods of modern cooking can provide a wonderful inspiration to the teaching of introductory science. This talk will explore the physics of cooking and will include demonstrations. The science of several innovative techniques in cooking, including foams and the use of gelation, as well as more common processes, will be explored. The talk is inspired by a course taught at Harvard University through a collaboration of professors and well-known chefs. Presented by David Weitz, Harvard University.

**Tuesday, March 15, 2016 8:00AM - 11:00AM —**

Session E1 DCMP: Recent Developments in Hybrid Semiconductor-Superconductor Junctions

Ballroom I - Yong Chen, Purdue University

**8:00AM E1.00001 Finite Momentum Pairing and Spatially Varying Order Parameter in Proximitized HgTe Quantum Wells**, AMIR YACOBY, Harvard University — Conventional s-wave superconductivity is understood to arise from singlet pairing of electrons with opposite Fermi momenta, forming Cooper pairs whose net momentum is zero. Several recent studies have focused on structures where such conventional s-wave superconductors are coupled to systems with an unusual configuration of electronic spin and momentum at the Fermi surface. Under these conditions, the nature of the paired state can be modified and the system may even undergo a topological phase transition. Here we present measurements and theoretical calculations of several HgTe quantum wells coupled to either aluminum or niobium superconductors and subject to a magnetic field in the plane of the quantum well. By studying the oscillatory response of Josephson interference to the magnitude of the in-plane magnetic field, we find that the induced pairing within the quantum well oscillates between singlet and triplet pairing and is spatially varying. Cooper pairs acquire a tunable momentum that grows with magnetic field strength, directly reflecting the response of the spin-dependent Fermi surfaces to the in-plane magnetic field. Our new understanding of the interplay between spin physics and superconductivity introduces a way to spatially engineer the order parameter, as well as a general framework within which to investigate electronic spin texture at the Fermi surface of materials.

**8:36AM E1.00002 S-TI-S Josephson junction networks: a platform for exploring and exploiting topological states and Majorana fermions**, DALE J VAN HARLINGEN, Univ of Illinois - Urbana — We are studying the transport properties of hybrid superconductor-topological insulator nanoscale devices fabricated by depositing superconductor electrodes onto the surface of topological insulators. In top-gated lateral Nb-Bi<sub>2</sub>Se<sub>3</sub>-Nb junctions, we have measured the Josephson supercurrent and conductance as a function of geometry, temperature, and gate voltage in order to determine the nature of the electronic transport. The supercurrent exhibits a sharp drop as a function of gate voltage that may be explained by the relocation of the topological surface state from above to below trivial conducting surface states formed by band-banding near the surface. We find that the magnetic field modulation of the supercurrent in Josephson junctions and dc SQUIDs exhibits anomalous features consistent with a  $4\pi$ -periodic  $\sin(\varphi/2)$ -component in the junction current-phase relation that may arise from the nucleation of Majorana bound states in the junction. We are exploring circuits for imaging, manipulating, and braiding these exotic excitations and schemes for reading out their parity. In collaboration with Aaron Finck, Erik Huemiller, Cihan Kurter, Vladimir Oryanchik, Martin Stehno, and Can Zhang.

**9:12AM E1.00003 Induced superconductivity in high mobility two dimensional electron gas in GaAs heterostructures**, LEONID P. ROKHINSON, Purdue University — Search for Majorana fermions renewed interest in semiconductor-superconductor interfaces, while a quest for higher order non-Abelian excitations demands formation of superconducting contacts to materials with fractionalized excitations, e.g. a two-dimensional electron gas in a fractional quantum Hall regime. Here we report induced superconductivity in high mobility two-dimensional electron gas in GaAs heterostructures and development of highly transparent semiconductor-superconductor ohmic contacts. Supercurrent with characteristic temperature dependence of a ballistic junction has been observed across  $0.6 \mu\text{m}$ , a regime previously achieved only in point contacts but essential to the formation of well separated non-Abelian states. High critical fields ( $> 16 \text{ Tesla}$ ) in NbN contacts enables investigation of an interplay between superconductivity and strongly correlated states in a two dimensional electron gas at high magnetic fields.

**9:48AM E1.00004 Proximity induced topological superconductivity and Majorana fermions**, CARLO BEENAKKER, Leiden University — Topological states of matter are a source of low-energy quasiparticles, bound to a defect or propagating along the surface. In a superconductor these are Majorana fermions, described by a real rather than a complex wave function. The absence of complex phase factors promises protection against decoherence in quantum computations based on topological superconductivity. The early theoretical models that produced Majorana fermions relied on an exotic superconducting order, with spin-triplet Cooper pairs in a chiral  $p$ -wave orbital state. A recent alternative is to start from a conventional spin-singlet superconductor and use the proximity effect to induce a topologically nontrivial superconducting state in a material with strong spin-orbit coupling. In this talk we give an overview of some of the manifestations of a real Majorana wave function that are waiting to be observed. In particular, we discuss how shot noise measurements can provide for a purely electrical method of detection of charge-neutral Majorana edge modes.

**10:24AM E1.00005 Milestones toward Majorana-based quantum computing<sup>1</sup>**, JASON ALICEA, Caltech — Experiments on nanowire-based Majorana platforms now appear poised to move beyond the preliminary problem of zero-mode detection and towards loftier goals of realizing non-Abelian statistics and quantum information applications. Using an approach that synthesizes recent materials growth breakthroughs with tools long successfully deployed in quantum-dot research, I will outline a number of relatively modest milestones that progressively bridge the gap between the current state of the art and these grand longer-term challenges. The intermediate Majorana experiments surveyed in this talk should be broadly adaptable to other approaches as well.

<sup>1</sup>Supported by the National Science Foundation (DMR-1341822), Institute for Quantum Information and Matter, and Walter Burke Institute at Caltech.

**Tuesday, March 15, 2016 8:00AM - 11:00AM —**

Session E2 DCOMP DCMP: Computational Methods for Improved Transparent Conducting Oxides Ballroom II - Giulia Galli, Univ of Chicago

## 8:00AM E2.00001 Structure and Properties of Amorphous Transparent Conducting Oxides<sup>1</sup>,

JULIA MEDVEDEVA, Missouri University of Science and Technology — Driven by technological appeal, the research area of amorphous oxide semiconductors has grown tremendously since the first demonstration of the unique properties of amorphous indium oxide more than a decade ago. Today, amorphous oxides, such as a-ITO, a-IZO, a-IGZO, or a-ZITO, exhibit the optical, electrical, thermal, and mechanical properties that are comparable or even superior to those possessed by their crystalline counterparts, pushing the latter out of the market. Large-area uniformity, low-cost low-temperature deposition, high carrier mobility, optical transparency, and mechanical flexibility make these materials appealing for next-generation thin-film electronics. Yet, the structural variations associated with crystalline-to-amorphous transition as well as their role in carrier generation and transport properties of these oxides are far from being understood. Although amorphous oxides lack grain boundaries, factors like (i) size and distribution of nanocrystalline inclusions; (ii) spatial distribution and clustering of incorporated cations in multicomponent oxides; (iii) formation of trap defects; and (iv) piezoelectric effects associated with internal strains, will contribute to electron scattering. In this work, ab-initio molecular dynamics (MD) and accurate density-functional approaches are employed to understand how the properties of amorphous ternary and quaternary oxides depend on quench rates, cation compositions, and oxygen stoichiometries. The MD results, combined with thorough experimental characterization, reveal that interplay between the local and long-range structural preferences of the constituent oxides gives rise to a complex composition-dependent structural behavior in the amorphous oxides. The proposed network models of metal-oxygen polyhedra help explain the observed intriguing electrical and optical properties in In-based oxides and suggest ways to broaden the phase space of amorphous oxide semiconductors with tunable properties.

<sup>1</sup>The work is supported by NSF-MRSEC program

## 8:36AM E2.00002 Quasiparticle energies, excitonic effects, and dielectric screening in transparent conducting oxides ,

ANDRÉ SCHLEIFE, University of Illinois at Urbana-Champaign — Using the power of high-performance super computers, computational materials scientists nowadays employ highly accurate quantum-mechanical approaches to reliably predict materials properties. In particular, many-body perturbation theory is an excellent framework for performing theoretical spectroscopy on novel materials including transparent conducting oxides, since this framework accurately describes quasiparticle and excitonic effects.

We recently used hybrid exchange-correlation functionals and an efficient implementation of the Bethe-Salpeter approach to investigate several important transparent conducting oxides. Despite their exceptional potential for applications in photovoltaics and optoelectronics their optical properties oftentimes remain poorly understood: Our calculations explain the optical spectrum of bixbyite indium oxide over a very large photon energy range, which allows us to discuss the importance of quasiparticle and excitonic effects at low photon energies around the absorption onset, but also for excitations up to 40 eV. We show that in this regime the energy dependence of the electronic self energy cannot be neglected. Furthermore, we investigated the influence of excitonic effects on optical absorption for lanthanum-aluminum oxide and hafnium oxide. Their complicated conduction band structures require an accurate description of quasiparticle energies and we find that for these strongly polar materials, a contribution of the lattice polarizability to dielectric screening needs to be taken into account. We discuss how this affects the electron-hole interaction and find a strong influence on excitonic effects.

The deep understanding of electronic excitations that can be obtained using these modern first-principles techniques, eventually will allow for computational materials design, e.g. of band gaps, densities of states, and optical properties of transparent conducting oxides and other materials with societally important applications.

## 9:12AM E2.00003 Limits of transparency of transparent conducting oxides<sup>1</sup> ,

HARTWIN PEELAERS, University of California, Santa Barbara — A fundamental understanding of the factors that limit transparency in transparent conducting oxides (TCOs) is essential for further progress in materials and applications. These materials have a sufficiently large band gap, so that direct optical transitions do not lead to absorption of light within the visible spectrum. Since the presence of free carriers is essential for conductivity and thus for device applications, this introduces the possibility of additional absorption processes. In particular, indirect processes are possible, and these will constitute a fundamental limit of the material. The Drude theory is widely used to describe free-carrier absorption, but it is phenomenological in nature and tends to work poorly at shorter wavelengths, where band-structure effects are important.

We will present calculations of phonon- and defect-assisted free-carrier absorption in a TCO completely from first principles [1]. We will focus in detail on SnO<sub>2</sub>, but the methodology is general and we will also compare the results obtained for other TCO materials such as In<sub>2</sub>O<sub>3</sub>. These calculations provide not just quantitative results but also deeper insights in the mechanisms that govern absorption processes, which is essential for engineering improved materials to be used in more efficient devices.

[1] H. Peelaers, E. Kioupakis, and C.G. Van de Walle, Appl. Phys. Lett. 100, 011914 (2012).

<sup>1</sup>This work was performed in collaboration with E. Kioupakis and C.G. Van de Walle and was supported by ARO and NSF.

## 9:48AM E2.00004 High-throughput search for improved transparent conducting oxides ,

ANNA MIGLIO, Universit  catholique de Louvain — High-throughput methodologies are a very useful computational tool to explore the space of binary and ternary oxides. We use these methods to search for new and improved transparent conducting oxides (TCOs). TCOs exhibit both visible transparency and good carrier mobility and underpin many energy and electronic applications (e.g. photovoltaics, transparent transistors). We find several potential new n-type and p-type TCOs with a low effective mass. Combining different ab initio approaches, we characterize candidate oxides by their effective mass (mobility), band gap (transparency) and dopability. We present several compounds, not considered previously as TCOs, and discuss the chemical rationale for their promising properties. This analysis is useful to formulate design strategies for future high mobility oxides and has led to follow-up studies including preliminary experimental characterization of a p-type TCO candidate with unexpected chemistry. G. Hautier, A. Miglio, D. Waroquiers, G.-M. Rignanese, and X. Gonze, How Does Chemistry Influence Electron Effective Mass in Oxides? A High-Throughput Computational Analysis, Chem. Mater. 26, 5447 (2014). G. Hautier, A. Miglio, G. Ceder, G.-M. Rignanese, and X. Gonze, Identification and design principles of low hole effective mass p-type transparent conducting oxides, Nature Commun. 4, 2292 (2013).

## 10:24AM E2.00005 Hybrid functional studies of defects and hole polarons in oxides. ,

JOEL VARLEY, Lawrence Livermore Natl Lab — Transparent conducting oxides (TCOs) are ubiquitous, appearing in windows, flat-panel displays, solar cells, solid-state lighting, and transistors that all exploit TCOs' combination of high electrical conductivity and optical transparency. Thanks to this large and growing list of applications, there has been a surge of interest in the science of these materials, focusing on the fundamental properties and doping opportunities in traditional TCOs as well as the exploration of promising new candidate materials. Hybrid density functional theory has proven instrumental in elucidating the physics of TCOs. One example is the study of dopants and defects that determine the conductivity. Accurate formation energies and charge-state transition levels can now be obtained thanks to the accurate electronic structure provided by a hybrid functional. This allows us to address the origins of unintentional conductivity: for SnO<sub>2</sub>, In<sub>2</sub>O<sub>3</sub>, and Ga<sub>2</sub>O<sub>3</sub>, we demonstrate that this is *not* due to native defects such as oxygen vacancies, but must be attributed to unintentional incorporation of impurities. We can also provide guidelines for achieving higher doping levels, suggesting several impurities as candidate donors with high solubility. Limitations on doping due to the formation or incorporation of compensating centers are addressed as well. Hybrid functional calculations also overcome the shortcomings associated with traditional local or semi-local functionals, which do not properly describe charge localization. Hybrid functionals accurately describe polaron formation, i.e., the self-trapping of holes when p-type doping of the oxide materials is attempted. Consequences of polaron formation for optical characterization of the material will be discussed. This work was performed in collaboration with Anderson Janotti and Chris G. Van de Walle, and was in part under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

**Tuesday, March 15, 2016 8:00AM - 11:00AM –**

**Session E3 GMAG DCMF: A New Approach to the Kitaev Quantum Spin Liquid** Ballroom III -

Young-June Kim, Univ of Toronto

**8:00AM E3.00001 Possible Observation of fractionalized excitations in a Relativistic Mott Insulator**, KENNETH BURCH, Boston College — The combination of electronic correlation and spin-orbit coupling is thought to precipitate a variety of highly unusual electronic phases in solids, including topological and quantum spin liquid states. I will discuss our recent optical measurements that provide evidence for the relativistic Mott Insulating ground state of  $\alpha$ -RuCl<sub>3</sub>. Furthermore I will discuss the broad-continuum of scattering we observe, whose energy and temperature dependence suggest the presence of fractionalized excitations emerging from a quantum spin-liquid.

**8:36AM E3.00002 Inelastic neutron scattering evidence for Kitaev quantum spin liquid physics in  $\alpha$ -RuCl<sub>3</sub>**<sup>1</sup>, STEPHEN NAGLER, Oak Ridge National Laboratory — The magnetic semiconductor  $\alpha$ -RuCl<sub>3</sub> is composed of very weakly coupled honeycomb layers of edge-sharing RuCl<sub>6</sub> octahedra. The Ru<sup>3+</sup> ion has 5 *d* electrons in the low spin state, and the system is expected to have an effective  $J = \frac{1}{2}$  single ion ground state with an interacting spin Hamiltonian containing Kitaev-like terms. Inelastic neutron scattering [1] on powders and single crystals has been used to determine the energy scale of the magnetic interactions and the overall form of the magnetic fluctuations. The results indicate that the Kitaev term is significant. Moreover, detailed measurements of the response show evidence for the fractionalized excitations that are characteristic of the Kitaev quantum spin liquid.  
[1] A. Banerjee *et al.*, arXiv:1504.08037.

<sup>1</sup>Research supported by the Scientific User Facilities Division, Basic Energy Sciences, US Department of Energy

**9:12AM E3.00003 Magnetic and Crystal Structure of  $\alpha$ -RuCl<sub>3</sub>**, JENNIFER SEARS, University of Toronto — The layered honeycomb material  $\alpha$ -RuCl<sub>3</sub> has been proposed as a candidate material to show significant bond-dependent Kitaev type interactions [1]. This has prompted several recent studies of magnetism in this material that have found evidence for multiple magnetic transitions in the temperature range of 8-14 K [2,3,4]. We will present elastic neutron scattering measurements collected using a co-aligned array of  $\alpha$ -RuCl<sub>3</sub> crystals, identifying zigzag magnetic order within the honeycomb planes with an ordering temperature of  $\sim 8$  K [2]. It has been reported that the ordering temperature depends on the *c* axis periodicity of the layered structure, with ordering temperatures of 8 and 14 K for three and two-layer periodicity respectively [3]. While the in-plane magnetic order has been identified, it is clear that a complete understanding of magnetic ordering and interactions will depend on the three dimensional structure of the crystal. Evidence of a structural transition at  $\sim 150$  K has been reported [4] and questions remain about the structural details, in particular the stacking of the honeycomb layers. We will present x-ray diffraction measurements investigating the low and high temperature structures and stacking disorder in  $\alpha$ -RuCl<sub>3</sub>. Finally, we will present inelastic neutron scattering measurements of magnetic excitations in this material.

Work done in collaboration with K. W. Plumb (Johns Hopkins University), J. P. Clancy, Young-June Kim (University of Toronto), J. Britten (McMaster University), Yu-Sheng Chen (Argonne National Laboratory), Y. Qiu, Y. Zhao, D. Parshall, and J. W. Lynn (NCNR).

[1] K. W. Plumb *et al.*, Phys. Rev. B 90, 041112(R) (2014).

[2] J. A. Sears *et al.*, Phys. Rev. B 91, 144420 (2015).

[3] A. Banerjee *et al.*, arXiv:1504.08037 (2015).

[4] Y. Kubota *et al.*, Phys. Rev. B 91, 094422 (2015).

**9:48AM E3.00004 XY-like frustrated magnetic phase transitions in  $\alpha$ -RuCl<sub>3</sub>**, HIDEKAZU TANAKA, Tokyo Institute of Technology — It is known that a honeycomb-lattice antiferromagnet with the nearest-neighbor exchange interaction undergoes a conventional magnetic ordering even for the spin-1/2 case. However, when a certain amount of second-neighbor exchange interaction or anisotropic exchange interaction exists, the honeycomb-lattice quantum magnet exhibits an unusual ground state. In the last decade, spin-1/2 quantum magnets on honeycomb lattices have been attracting considerable attention from the viewpoints of the frustrated  $J_1 - J_2$  model and the Kitaev-Heisenberg model, both of which can exhibit the spin liquid state in some parameter range.

$\alpha$ -RuCl<sub>3</sub> is a layered compound, in which magnetic Ru<sup>3+</sup> ions with the 4*d*<sup>5</sup> electronic state form a honeycomb lattice. We have investigated the magnetic properties of  $\alpha$ -RuCl<sub>3</sub> via magnetization and specific heat measurements using single crystals. It was observed that  $\alpha$ -RuCl<sub>3</sub> undergoes a structural phase transition at  $T_t \simeq 150$  K accompanied by fairly large hysteresis. The magnetizations and magnetic susceptibilities are strongly anisotropic, which mainly arise from the anisotropic *g*-factors. These *g*-factors and the obtained entropy indicate that the effective spin of Ru<sup>3+</sup> is one-half, which results from the low-spin state. Specific heat data show that magnetic ordering occurs in four steps at zero magnetic field. The magnetic phase diagram is obtained. The successive magnetic phase transitions can be ascribed to the competition among exchange interactions. We discuss the strongly anisotropic *g*-factors and deduce that the exchange interaction is strongly XY-like. Main results of this talk was published in Phys. Rev. B 91, 094422 (2015).

**10:24AM E3.00005 Manifestations of Kitaev physics in thermodynamic properties of hexagonal iridates and  $\alpha$ -RuCl<sub>3</sub>**<sup>1</sup>, ALEXANDER TSIRLIN, Experimental Physics VI, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Germany — Kitaev model is hard to achieve in real materials. Best candidates available so far are hexagonal iridates M<sub>2</sub>IrO<sub>3</sub> (M = Li and Na) and the recently discovered  $\alpha$ -RuCl<sub>3</sub> featuring hexagonal layers coupled by weak van der Waals bonding. I will review recent progress in crystal growth of these materials and compare their thermodynamic properties. Both hexagonal iridates and  $\alpha$ -RuCl<sub>3</sub> feature highly anisotropic Curie-Weiss temperatures that not only differ in magnitude but also change sign depending on the direction of the applied magnetic field. Néel temperatures are largely suppressed compared to the energy scale of the Curie-Weiss temperatures. These experimental observations will be linked to features of the electronic structure and to structural peculiarities associated with deviations from the ideal hexagonal symmetry. I will also discuss how the different nature of ligand atoms affects electronic structure and magnetic superexchange.

<sup>1</sup>This work has been done in collaboration with M. Majumder, M. Schmidt, M. Baenitz, F. Freund, and P. Gegenwart

**Tuesday, March 15, 2016 8:00AM - 11:00AM –**

**Session E4 DPOLY: Polymer Physics Prize** Ballroom IV - Stephen Cheng, University of Akron

**8:00AM E4.00001 Polymer Physics Prize: Designing "Materials that Compute": Exploiting the Properties of Self-oscillating Polymer Gels**, ANNA BALAZS, University of Pittsburgh — Lightweight, deformable materials that can sense and respond to human touch and motion can be the basis of future wearable computers, where the material itself will be capable of performing computations. To facilitate the creation of "materials that compute", we draw from two emerging modalities for computation: chemical computing, which relies on reaction-diffusion mechanisms to perform operations, and oscillatory computing, which performs pattern recognition through synchronization of coupled oscillators. Chemical computing systems, however, suffer from the fact that the reacting species are coupled only locally; the coupling is limited by diffusion as the chemical waves propagate throughout the system. Additionally, oscillatory computing systems have not utilized a potentially wearable material. To address both these limitations, we develop the first model for coupling self-oscillating polymer gels to a piezoelectric (PZ) micro-electro-mechanical system (MEMS). The resulting transduction between chemo-mechanical and electrical energy creates signals that can be propagated quickly over long distances and thus, permits remote, non-diffusively coupled oscillators to communicate and synchronize. The oscillators can be organized into arbitrary topologies because the electrical connections lift the limitations of diffusive coupling. Using our model, we predict the synchronization behavior that can be used for computational tasks, ultimately enabling "materials that compute".

**8:36AM E4.00002 Reaction-Diffusion Patterns in Structured Media**, IRVING EPSTEIN, Department of Chemistry, Brandeis University, Waltham, MA — I will look at pattern formation in the Belousov-Zhabotinsky (BZ) oscillating chemical reaction in media that are structured at length scales ranging from ten nanometers to a few centimeters. A reverse microemulsion consisting of nanometer diameter droplets of water containing the reactants dispersed in oil allows the physical structure (size, spacing) of the droplets and their chemical composition to be controlled independently, enabling one to generate a remarkable variety of stationary and moving patterns, including Turing structures, ordinary and antispirals, packet waves and spatiotemporal chaos. One- and two-dimensional arrays of aqueous droplets in oil generated by microfluidic techniques have diameters of the order of 100 micrometers and produce a different array of patterns that can be precisely controlled with light. In particular, circular arrays of droplets provide a testing ground for some of Turing's ideas about morphogenesis. By attaching the BZ catalyst to a polymer that shrinks and swells in response to changes in the redox state of the catalyst, one can construct gel materials that transduce chemical changes to mechanical motion, a phenomenon modeled with considerable success by the Balazs group. If time permits, I will also discuss the BZ reaction in coupled macroscopic flow reactors that mimic small neural networks.

**9:12AM E4.00003 Modeling Anisotropic Self-Assembly of Isotropic Objects: from Hairy Nanoparticles to Methylcellulose Fibrils<sup>1</sup>**, VALERIY GINZBURG, The Dow Chemical Company — Spontaneous symmetry breaking and formation of anisotropic structures from apparently isotropic building blocks is an exciting and not fully understood topic. I will discuss two examples of such self-assembly. The first example is related to the assembly of "hairy" nanoparticles in homopolymer matrices<sup>1</sup>. The particles can assemble into long strings (they can also form other morphologies, as well) even though the shape of each particle and the distribution of ligands on the particle surface is spherically symmetric. Using the approach developed by Thompson, Ginzburg, Matsen, and Balazs<sup>2</sup>, we show that presence of other particles can re-distribute the ligands and effectively "polarize" the particle-particle interaction, giving rise to the formation of 1d particle strings<sup>3</sup>. In the second example, we consider aqueous solutions of methylcellulose (MC) polymers. It has been shown recently<sup>4</sup> that at high temperature, the polymers form high-aspect ratio "fibrils" with diameter ~15 nm and length in the hundreds of nanometers. Using coarse-grained Molecular Dynamics (CG-MD), we propose that the "fibrils" are result of one-dimensional self-assembly of single molecule "rings". Each MC polymer chain is forced into a ring because of the balance between internal chain rigidity (favoring more expanded configuration) and unfavorable polymer-water interactions (favoring more collapsed conformation). We also develop a theory predicting rheology and phase behavior of aqueous MC, and validate it against experimental data<sup>5</sup>. Both examples show that anisotropic self-assembly can show up in unexpected places, and various theoretical tools are needed to successfully model it. 1. P. Akcora et al., Nature Mater. 8, 354 (2009). 2. R. Thompson, V. Ginzburg, M. Matsen, and A. Balazs, Science 292, 2469 (2001). 3. V. Ginzburg, Macromolecules 46, 9898 (2013). 4. S. Arvidson et al., Macromolecules 46, 300 (2013). 5. V. Ginzburg, R. Sammler, W. Huang, and R. Larson, submitted for publication.

<sup>1</sup>Funded by The Dow Chemical Company through grant 223278AF. Collaborators: R. L. Sammler (Dow), W. Huang and R. Larson (U. of Michigan).

**9:48AM E4.00004 Functional, Responsive Materials Assembled from Recombinant Oleosin.**, DANIEL HAMMER, University of Pennsylvania — Biological cells are surrounded by a plasma membrane made primarily of phospholipids that form a bilayer. This membrane is permselective and compartmentalizes the cell. A simple form of artificial cell is the vesicle, in which a phospholipid bilayer membrane surrounds an aqueous solution. However, there is no a priori reason why a membrane needs to be made of phospholipids. It could be made of any surfactant that forms a bilayer. We have assembled membranes and other structures from the recombinant plant protein oleosin. The ability to assemble from a recombinant protein means that every molecule is identical, we have complete control over the sequence, and hence can build in designer functionality with high fidelity, including adhesion and enzymatic activity. Such incorporation is trivial using the tools of molecular biology. We find that while many variants of oleosin make membranes, others make micelles and sheets. We show how the type of supramolecular structure can be altered by the conditions of solvent, such as ionic strength, and the architecture of the surfactant itself. We show that protease cleavable domains can be incorporated within oleosin, and be engineered to protect other functional domains such as adhesive motifs, to make responsive materials whose activity and shape depend on the action of proteases. We will also present the idea of making "Franken"-oleosins, where large domains of native oleosin are replaced with domains from other functional proteins, to make hybrids conferred by the donor protein. Thus, we can view oleosin as a template upon which a vast array of designer functionalities can be imparted..

**10:24AM E4.00005 Moving HAIRS: Towards adaptive, homeostatic materials**, JOANNA AIZENBERG, Harvard — Dynamic structures that respond reversibly to changes in their environment are central to self-regulating thermal and lighting systems, targeted drug delivery, sensors, and self-propelled locomotion. Since an adaptive change requires energy input, an ideal strategy would be to design materials that harvest energy directly from the environment and use it to drive an appropriate response. This lecture will present the design of a novel class of reconfigurable materials that use surfaces bearing arrays of nanostructures put in motion by environment-responsive gels. Their unique hybrid architecture, and chemical and mechanical properties can be optimized to confer a wide range of adaptive behaviors. Using both experimental and modeling approaches, we are developing these hydrogel-actuated integrated responsive systems (HAIRS) as new materials with reversible optical and wetting properties, as a multifunctional platform for controlling cell differentiation and function, and as a first homeostatic system with autonomous self-regulation.

**Tuesday, March 15, 2016 8:00AM - 11:00AM —**

**Session E5 GMAG DMP: Magnetic Thin Films and Multilayers** 301 - Madhukar Reddy, Lam Research Corporation

**8:00AM E5.00001 Spin-orbit coupling of 3d transition metal atoms on MgO/Ag**, SHRUBA GANGOPADHYAY, University of California, Davis, BARBARA JONES, IBM Research Almaden — Spin-orbit coupling is normally predominant for high Z metal atoms, but we observe Fe and Co showing significant orbital moments on a MgO/Ag surface. DFT results show that on MgO/Ag both Co and Fe prefer O top binding sites. Calculation of orbital moments using DFT is always challenging, and we compare two DFT based protocols to calculate orbital moments. Our calculations show the magnitude of orbital moments strongly dependent on a number of factors including the number of Ag layers in our unit cell and the approximation we are using. Our results exhibit significant agreement with scanning tunneling microscopy (STM) and XMCD experiments. We show that Co retains its full atomic orbital moment on the O top site of MgO whereas the orbital moment for Fe is somewhat less than its atomic orbital moment.

**8:12AM E5.00002 Enhancement of the Co magnetic moment in bcc  $\text{Co}_{1-x}\text{Mn}_x$  on  $\text{MgO}^1$** , RYAN SNOW, HARSH BHATKAR, Montana State University, ALPHA N'DIAYE, ELKE ARENHOLZ, Lawrence Berkeley National Laboratories, YVES IDZERDA, Montana State University, MONTANA STATE UNIVERSITY TEAM, LAWRENCE BERKELEY NATIONAL LABORATORIES TEAM — Using X-ray absorption spectroscopy (XAS) and X-ray magnetic circular dichroism (MCD), we show that the elemental Co moment for MBE grown thin films of bcc  $\text{Co}_{1-x}\text{Mn}_x$  grown on  $\text{MgO}(001)$  is enhanced by 40% to a maximum value of  $2.1 \mu_B$  at  $x=0.24$ . The net Mn moment is found to align parallel with Co for all concentrations and remains roughly constant until  $x=0.3$ , then drops steadily, up to  $x=0.7$ , where the total moment of the film abruptly collapses to zero. Using a low-concentration Mn moment of  $3.0 \mu_B$ , the average magnetization lies directly on the Slater-Pauling (SP) curve for concentrations up to about  $x=0.25$ , where it reaches a maximum moment of  $2.3 \mu_B/\text{atom}$ . This peak is slightly shifted and the slope is steeper on the high-Mn concentration side of the peak relative to the standard SP curve. This is in stark contrast to the fcc CoMn and hcp CoCr bulk behavior which shows only a rapid total moment reduction with Mn concentration.

<sup>1</sup>This material is based upon work supported by the National Science Foundation under Grant ECCS-1542210. The Advanced Light Source is supported by the Director, Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Con

**8:24AM E5.00003 Cap-Induced Magnetic Anisotropy in Ultra-thin Fe/ $\text{MgO}(001)$  Films<sup>1</sup>**, TOBIAS BROWN-HEFT, Materials Department, University of California Santa Barbara, MIHIR PENDHARKAR, Electrical and Computer Engineering Department, University of California Santa Barbara, ELIZABETH LEE, Engineering Department, Harvey Mudd College, Claremont, CA, CHRIS PALMSTROM, Electrical and Computer Engineering Department & Materials Department, University of California Santa Barbara — Magnetic anisotropy plays an important role in the design of spintronic devices. Perpendicular magnetic anisotropy (PMA) is preferred for magnetic tunnel junctions because the resulting energy barrier between magnetization states can be very high and this allows enhanced device scalability suitable for magnetic random access memory applications. Interface induced anisotropy is often used to control magnetic easy axes. For example, the Fe/ $\text{MgO}(001)$  system has been predicted to exhibit PMA in the ultrathin Fe limit. We have used *in-situ* magneto optic Kerr effect and *ex-situ* SQUID to study the changes in anisotropy constants between bare Fe/ $\text{MgO}(001)$  films and those capped with  $\text{MgO}$ , Pt, and Ta. In some cases in-plane anisotropy terms reverse sign after capping. We also observe transitions from superparamagnetic to ferromagnetic behavior induced by capping layers. Perpendicular anisotropy is observed for Pt/Fe/ $\text{MgO}(001)$  films after annealing to 300C. These effects are characterized and incorporated into a magnetic simulation that accurately reproduces the behavior of the films.

<sup>1</sup>This work was supported in part by the Semiconductor Research Corporation programs (1) MSR-Intel, and (2) C-SPIN.

**8:36AM E5.00004 Thickness quantization in a reorientation transition**, DAVID VENUS, GENGMIN HE, HARRISON WINCH, RANDY BELANGER, McMaster University — The reorientation transition of an ultrathin film from perpendicular to in-plane magnetization is driven by a competition between shape and surface anisotropy. It is accompanied by a "stripe" domain structure that evolves as the reorientation progresses. Often, an  $n$  layer film has stable perpendicular magnetization and an  $n+1$  layer film has stable in-plane magnetization. If the domain walls are not pinned, the long-range stripe domain pattern averages over this structure so that the transition occurs at a non-integer layer thickness. We report *in situ* experimental measurements of the magnetic susceptibility (via MOKE) of the reorientation transition in Fe/2 ML Ni/W(110) films as a function of thickness as they are deposited at room temperature. In addition to a peak at the reorientation transition, we observe a strong precursor due to thickness quantization in atomic layers. This peak is described quantitatively by the response of small islands of thickness 3 layers with in-plane anisotropy in a sea of 2 layers Fe with perpendicular anisotropy. The fitted parameters give an estimate of the island size at which the response disappears. This size corresponds to a domain wall thickness, so that the islands become locally in-plane, demonstrating the self-consistency of the model.

**8:48AM E5.00005 Spin and orbital magnetic moments of Fe and Co in Co/Fe and Fe/Co multilayers on Si from  $L_{2,3}$  edge X-ray Magnetic Circular Dichroism Spectroscopy<sup>1</sup>**, KRISHNAMURTHY VEMURU, George Mason University, Fairfax, Virginia, RICHARD ROSENBERG, Advanced Photon Source, Argonne National Laboratory, Lemont, Illinois, GARY MANKEY, The University of Alabama, Tuscaloosa, Alabama — Nanostructured FeCo thin films are interesting for magnetic recording applications due to their high saturation magnetization, high Curie temperature and low magnetocrystalline anisotropy. It is desirable to know how the magnetism is modified by the nanostructure. We report Fe  $L_{2,3}$  edge and Co  $L_{2,3}$  edge x-ray magnetic circular dichroism (XMCD) investigations of element specific spin and orbital magnetism of Fe and Co in two multilayer samples: (S1) Si/ $\text{SiO}_2$ /[Co 0.8 nm/Fe 1.6 nm] $\times 32/\text{W}$  (2nm) and (S2) Si/ $\text{SiO}_2$ /[Co 1.6 nm/Fe 0.8 nm] $\times 32/\text{W}$  (2nm) thin films at room temperature. Sum rule analysis of XMCD at Fe  $L_{2,3}$  edge in sample S1 shows that the orbital moment of Fe is strongly enhanced and the spin moment is strongly reduced as compared to the values found in bulk Fe. Details of sum rule analysis will be presented to compare and contrast spin magnetic moments and orbital magnetic moments of Fe and Co in the two multilayer samples.

<sup>1</sup>This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

**9:00AM E5.00006 Direct Mapping of Magnetic and Structural Profiles of Electric Field Moderated Oxygen Migration**, DUSTIN A. GILBERT, ALEXANDER J. GRUTTER, BRIAN J. KIRBY, JULIE A. BORCHERS, BRIAN B. MARANVILLE, National Institute of Standards and Technology, ELKE ARENHOLZ, Lawrence Berkeley National Laboratory, KAI LIU, University of California, Davis — Recent studies on metal/oxide heterostructures have demonstrated control of interfacial magnetic anisotropy and saturation magnetization in ultrathin (5 ML) Co films through electric-field controlled oxygen migration. This approach presents a promising route to realizing next-generation, ultralow power sensor and data-storage technologies. Here we demonstrate magnetoelectric coupling moderated by electrically-driven oxygen migration in much thicker  $\text{AlOx}(1 \text{ nm})/\text{GdOx}(2 \text{ nm})/\text{Co}(15 \text{ nm})$  heterostructures. Using polarized neutron reflectometry, we present direct, quantitative depth profiling of the magnetization and oxygen concentration in these systems. Electro-thermal conditioning moves oxygen from  $\text{AlOx}$  and  $\text{GdOx}$  base-layers throughout the entire thickness of the 15 nm Co layer, resulting in a suppressed magnetization. Switching the electric field polarity semi-reversibly ejects oxygen preferentially from the  $\text{GdOx}/\text{Co}$  interface, partially recovering the magnetization and establishing a practical limit to this approach. First order reversal curve diagrams show that the conditioned samples exhibit two distinct magnetic phases, while the as-grown samples are single phase, suggesting that the treatments alters the Co film microstructure. X-ray spectroscopy confirms the oxidation states of the Co and Gd, and suggest that the  $\text{GdOx}$  acts to transmit oxygen but does not source or sink it.

**9:12AM E5.00007 Magnetic localization limit in  $T_C$  graded ferromagnetic thin films**, BRIAN KIRBY, National Institute of Standards and Technology, LORENZO FALLARINO, PATRICIA RIEGO, MATTEO PANCALDI, ANDREAS BERGER, CIC nanoGUNE Consolider, CASEY MILLER, Rochester Institute of Technology — We have recently demonstrated that the effective Curie temperature ( $T_C$ ) of a ferromagnetic alloy thin film can be continuously varied as a function of depth via a corresponding compositional gradient.[1] This work showed that the effective  $T_C$  can be made to vary continuously over tens of nm. However, over a short enough distance, the system must become localized, with exchange coupling dominating the effects of the compositional gradient. Understanding this localization limit is important for potential applications, as it dictates the length-scale below which this technique stops being a viable engineering tool (at least for itinerant ferromagnets and their thermodynamic properties). To determine the localization limit in this class of system, we have fabricated a series of  $\text{Co}[1-x]\text{Cr}[x]$  alloy films, where  $x$  varies sinusoidally between 0.28 (nominal  $T_C \approx 250 \text{ K}$ ) and 0.22 ( $T_C > 300 \text{ K}$ ), and have used polarized neutron reflectometry to study samples of differing oscillation wavelength. These measurements confirm the desired sinusoidal pattern was achieved, and reveal the temperature-dependence of the magnetic depth profile. Results will be presented in the context of mean-field simulations. [1] arXiv:1510.07535 [cond-mat.mtrl-sci].

**9:24AM E5.00008 Magnetic Irreversibility in VO<sub>2</sub>/Ni Bilayers.** , JOSE DE LA VENTA, JOSH LAUZIER, LOGAN SUTTON, Colorado State Univ — The temperature dependence of the coercivity and magnetization of VO<sub>2</sub>/Ni bilayers was studied. VO<sub>2</sub> exhibits a well-known Structural Phase Transition (SPT) at 330-340 K, from a low temperature monoclinic (M) to a high temperature rutile (R) structure. The SPT of VO<sub>2</sub> induces an inverse magnetoelastic effect that strongly modifies the coercivity and magnetization of the Ni films. In addition, the growth conditions allow tuning of the magnetic properties. Ni films deposited on top of VO<sub>2</sub> (M) show an irreversible change in the coercivity after the first cycle through the high temperature phase, with a corresponding change in the surface morphology of VO<sub>2</sub>. On the other hand, the Ni films grown on top of VO<sub>2</sub> (R) do not show this irreversibility. These results indicate that properties of magnetic films are strongly affected by the strain induced by materials that undergo SPT and that it is possible to control the magnetic properties by tuning the growth conditions.

**9:36AM E5.00009 Layer Resolved Imaging of Magnetic Domain Motion in Epitaxial Heterostructures** , SIOAN ZOHAR, YONGSEONG CHOI, Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, USA, DAVID LOVE, RHODRI MANSELL, CRISPIN BARNES, Cavendish Laboratory, University of Cambridge, J J Thomson Avenue, CB3 0HE Cambridge, United Kingdom, DAVID KEAVNEY, RICHARD ROSENBERG, Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, USA — We use X-ray Excited Luminescence Microscopy (XELM) to image the elemental and layer resolved magnetic domain structure of an epitaxial Fe/Cr wedge/Co heterostructure in the presence of large magnetic fields. The observed magnetic domains exhibit several unique behaviors that depend on the Cr thickness (tCr) modulated interlayer exchange coupling (IEC) strength. For Cr thickness tCr < 0.34 nm and tCr > 1.5 nm, strongly coupled parallel Co-Fe reversal and weakly coupled layer independent reversal are observed, respectively. The transition between these two reversal mechanisms for 0.34 < tCr < 1.5 nm is described by a combination of IEC guided domain wall motion and stationary zig zag domain walls. We observe domain walls nucleated at switching field minima are guided by IEC spatial gradients and collapse at switching field maxima.

**9:48AM E5.00010 Magnetic profile of a graphene wrapped ferromagnetic surface** , TIMOTHY CHARLTON, Science & Technology Facilities Council, DAVID LOVE, RAZAN ABOLJADAYEL, R. WEATHERUP, P. MONTEIRO, ADRIAN IONESCU, C. H. W BARNES, Cavendish Laboratory, Dept. of Physics, University of Cambridge — Graphene has one of the highest electron mobilities at room temperature, making it ideal for next generation electronic devices. However, due to its small spin-orbit coupling it is not possible to manipulate spins directly in a pristine graphene monolayer. This may be overcome by proximity to a ferromagnet. Recent theoretical and experimental publications [1] indicate that on a Ni surface the graphene band structure is spin split. The authors used XMCD to measure the magnetic moment induced on the  $\pi$ -electrons in graphene due to the proximity effect with Ni, obtaining a value between 0.05-0.10  $\mu_B$  per C atom. We have produced a uniform graphene layer grown by a CVD process directly a Ni coated substrate (the catalyst). By varying key growth parameters (temperature & pressure) the interaction between graphene and the catalyst can be tuned to provide strong epitaxial alignment between graphene and Ni or a more weakly oriented rotated alignment. We will present results showing a magnetic enhancement at the ferromagnet - C interface extracted from recent polarized neutron reflectivity measurement on both epitaxial and rotated graphene wrapped ferromagnetic surfaces. [1] V. Karpan, et al., Phys. Rev. B 78, 195419 (2008), M. Weser, et al., Appl. Phys. Lett. 96, 012504 (2010)

**10:00AM E5.00011 Self Exchange Bias and Bi-stable Magneto-Resistance States in Amorphous TbFeCo and TbSmFeCo Thin Films.**<sup>1</sup> , CHUNG MA, XIAOPU LI, JIWEI LU, JOSEPH POON, Univ of Virginia, RYAN COMES, ARUN DEVARAJ, STEVEN SPURGEON, Pacific Northwest National Laboratory — Amorphous ferrimagnetic TbFeCo and TbSmFeCo thin films are found to exhibit strong perpendicular magnetic anisotropy. Self exchange bias effect and bi-stable magneto-resistance states are observed near compensation temperature by magnetic hysteresis loop, anomalous Hall effect and transverse magneto-resistance measurements. Atom probe tomography, scanning transmission electron microscopy, and energy dispersive spectroscopy mapping have revealed two nanoscale amorphous phases with different Tb concentration distributed within the amorphous films. The observed exchange anisotropy originates from the exchange interaction between the two nanoscale amorphous phases. Exchange bias effect is used for increasing stability in spin valves and magnetic tunneling junctions. This study opens up a new platform for using amorphous ferrimagnetic thin films that require no epitaxial growth in nanodevices..

<sup>1</sup>The work was supported by the Defense Threat Reduction Agency grant and the U.S. Department of Energy.

**10:12AM E5.00012 Angular dependence of exchange bias and magnetization reversal controlled by electric-field-induced competing anisotropies.** , YONGGANG ZHAO, AITIAN CHEN, PEISEN LI, Tsinghua University, XU ZHANG, Beijing National Laboratory for Condensed Matter Physics, Chinese Academy of Sciences, RENCI PENG, Tsinghua University, HAO-LIANG HUANG, University of Science and Technology of China, LVKUAN ZOU, XIAOLI ZHENG, Beijing National Laboratory for Condensed Matter Physics, Chinese Academy of Sciences, SEN ZHANG, College of National University of Defense Technology, PEIXIAN MIAO, Tsinghua University, YALIN LU, University of Science and Technology of China, JIAN CAI, Beijing National Laboratory for Condensed Matter Physics, Chinese Academy of Sciences, CE-WEN NAN, Tsinghua University — Combination of exchange-biased systems and FE materials gives a new avenue to study angular dependence of exchange bias and achieve reversible electric-field-controlled magnetization reversal. We study the angular dependence of electric-field-controlled exchange bias and magnetization reversal in CoFeB/IrMn/Pb(Mg<sub>1/3</sub>Nb<sub>2/3</sub>)<sub>0.7</sub>Ti<sub>0.3</sub>O<sub>3</sub>. It is demonstrated that the ratio of the exchange-coupled unidirectional anisotropy and the uniaxial anisotropy of the FM layer, as well as their relative orientation can be dramatically and continuously tuned via electric fields. Simulations confirm that the electric-field-controlled exchange bias originates from the competition between the uniaxial anisotropy induced by the piezostain and the exchange-coupled unidirectional anisotropy. Moreover, electric-field-controlled magnetization reversal was realized at zero magnetic field.

**10:24AM E5.00013 Rationale for contrasting phonon confinement and interface localization effect in FeAg and FeCr multilayers**<sup>1</sup> , SAMPYO HONG, TALAT RAHMAN, University of Central Florida — We have performed density functional theory based calculations to investigate the propensity for formation of FeAg and FeCr multilayers. A perfect lattice match between Fe and Ag layers at the FeAg interface was obtained by modeling 45 rotated Ag(100) layers epitaxially on bcc Fe(100). In comparison, the FeCr interface was modeled by epitaxial layers of bcc Fe(100) and Cr(100). In FeAg, we find the signature peak of Fe bulk phonons (35 meV) to be substantially diminished and the low energy peaks to be remarkably enhanced, in qualitative agreement with experiment [1]. In contrast, the phonon density of state in the FeCr multilayers do not show any outstanding feature except a slight decrease in the 35 meV peak for the Fe layer at the interface, as compared to that of the middle Fe layer in excellent agreement with experiment [2]. The magnetic moment of the interfacial Fe atoms is larger than those Fe atoms in other layers, as a result of charge transfer from Fe to Ag at the interface. As compared to the middle layers, more spin-up and less spin-down states are occupied at the interface in such a way that Fe donates a large number of spin-down electrons to Ag but receives only a few spin-up electrons from the latter because of the almost fully occupied Ag d-band. [1] B. Roldan Cuenya et al., to be published. [2] Roldan et al, Phys. Rev. B 77, 165410 (2008).

<sup>1</sup>Work supported in part by DOE Grant No. DOE-DE-FG02-07ER4635

**10:36AM E5.00014 Magneto-optical mapping of the domain wall pinning potential in ferro-magnetic films<sup>1</sup>**, ROBERT BADEA, JESSE BEREZOVSKY, Case Western Reserve Univ — The propagation of domain walls in ferromagnetic films is influenced by defects which suppress and pin the motion of the domain walls. We map the nanoscale effective pinning potential in a ferromagnetic film by raster scanning a single ferromagnetic vortex domain and measuring the hysteretic displacement vs. applied magnetic field.[1] We use a differential magneto-optical microscopy technique which yields spatial sensitivity of  $\sim 10$  nm to measure the motion of the vortex domain.[2] Using a simple algorithm, we extract the effective pinning potential from the measured vortex displacement vs. applied field. The resulting effective pinning potential maps reveal different types of nanoscale pinning features which we attribute to different structural defects of the film. By comparing the pinning map to atomic force microscopy maps, we identify correlations between pinning sites and topographic features. [1] R. Badea, and J. Berezovsky, cond-mat/1510.07059, (2015). [2] R. Badea, J. A. Frey, and J. Berezovsky, Journal of Magnetism and Magnetic Materials 381, 463 (2015).

<sup>1</sup>This work was supported by DOE, award No. DE-SC008148

**10:48AM E5.00015 Kinetic Monte Carlo simulations of thermally activated magnetization reversal in dual-layer Exchange Coupled Composite recording media.**, M. L. PLUMER, A. M. ALMUDALLAL, J. I. MERCER, J. P. WHITEHEAD, Memorial University of Newfoundland, T. J. FAL, University of Colorado at Colorado Springs — The kinetic Monte Carlo (KMC) method developed for thermally activated magnetic reversal processes in single-layer recording media [1] has been extended to study dual-layer Exchange Coupled Composition (ECC) media used in current and next generations of disc drives [2]. The attempt frequency is derived from the Langer formalism with the saddle point determined using a variant of Bellman Ford algorithm. Complication (such as stagnation) arising from coupled grains having metastable states are addressed. MH-hysteresis loops are calculated over a wide range of anisotropy ratios, sweep rates and inter-layer coupling parameter. Results are compared with standard micromagnetics at fast sweep rates and experimental results at slow sweep rates.

1. T.J. Fal, J.I. Mercer, M.D. Leblanc, J.P. Whitehead, M.L. Plumer, and J. van Ek, Phys. Rev. B. 87, 064405 (2013).
2. Ahmad M. Al mudallal, J. I. Mercer, J. P. Whitehead, M. L. Plumer, J. van Ek, and T. J. Fal, Phys. Rev. B 92, 134418 (2015).

**Tuesday, March 15, 2016 8:00AM - 11:00AM –**  
**Session E6 GMAG DMP FIAP: Spin Excitations in Ultrathin Films, Nanostructures and Domain Walls** 302 - Behrouz Khodadadi, University of Alabama

**8:00AM E6.00001 Nonlinear spin-wave excitations at low magnetic bias fields**, GEORG WOLTERSDORF, Martin Luther University Halle — We investigate experimentally and theoretically the nonlinear magnetization dynamics in magnetic films at low magnetic bias fields. Nonlinear magnetization dynamics is essential for the operation of numerous spintronic devices ranging from magnetic memory to spin torque microwave generators. Examples are microwave-assisted switching of magnetic structures and the generation of spin currents at low bias fields by high-amplitude ferromagnetic resonance. In the experiments we use X-ray magnetic circular dichroism to determine the number density of excited magnons in magnetically soft  $\text{Ni}_{80}\text{Fe}_{20}$  thin films. Our data show that the common Suhl instability model of nonlinear ferromagnetic resonance is not adequate for the description of the nonlinear behavior in the low magnetic field limit. Here we derive a model of parametric spin-wave excitation, which correctly predicts nonlinear threshold amplitudes and decay rates at high and at low magnetic bias fields. In fact, a series of critical spin-wave modes with fast oscillations of the amplitude and phase is found, generalizing the theory of parametric spin-wave excitation to large modulation amplitudes. For these modes, we also find pronounced frequency locking effects that may be used for synchronization purposes in magnonic devices. By using this effect, effective spin-wave sources based on parametric spin-wave excitation may be realized. Our results also show that it is not required to invoke a wave vector-dependent damping parameter in the interpretation of nonlinear magnetic resonance experiments performed at low bias fields.

**8:36AM E6.00002 Spin torque ferromagnetic resonance in Heusler based magnetic tunnel junctions**, JIE ZHANG, TIMOTHY PHUNG, AAKASH PUSHUP, JAEWOO JEONG, YARI FERRANTE, CHARLES RETTNER, BRIAN P. HUGHES, SEE-HUN YANG, STUART S.P. PARKIN, IBM Almaden Res Ctr — Heusler compounds are of interest as electrode materials for use in magnetic tunnel junctions (MTJs) due to their half metallic character, which leads to high spin polarization and high tunneling magnetoresistance. Whilst much work has focused on the influence of the half metallic character of the Heusler compounds on the magnetoresistance of MTJs, there is much less work investigating the influence of this electronic structure on the spin transfer torque. Here, we investigate the bias dependence of the anti-damping like and field-like spin transfer torque components as a function of the bias voltage in symmetric ( $\text{CoMnSi}/\text{MgO}/\text{CoMnSi}$ ) and asymmetric ( $\text{CoMnSi}/\text{MgO}/\text{CoFe}$ ) structure magnetic tunnel junctions using spin transfer torque ferromagnetic resonance. Lastly, we report on the effect of asymmetric bias dependence of the differential conductance on the spin transfer torque.

**8:48AM E6.00003 Parametric excitation of magnetization by electric field**, YU-JIN CHEN, HAN KYU LEE, Univ of California - Irvine, ROMAN VERBA, Institute of Magnetism, Kyiv, Ukraine, JORDAN KATINE, HGST, VASIL TIBERKEVICH, ANDREI SLAVIN, Oakland University, IGOR BARSUKOV, ILYA KRIVOROTOV, Univ of California - Irvine — Manipulation of magnetization by electric field is of primary importance for development of low-power spintronic devices. We present the first experimental demonstration of parametric generation of magnetic oscillations by electric field. We realize the parametric generation in  $\text{CoFeB}/\text{MgO}/\text{SAF}$  nanoscale magnetic tunnel junctions (MTJs). The magnetization of the free layer is perpendicular to the sample plane while the magnetizations of the synthetic antiferromagnet (SAF) lie in the plane. We apply microwave voltage to the MTJ at  $2f$ , where  $f$  is the ferromagnetic resonance frequency of the free layer. In this configuration, the oscillations can only be driven parametrically via voltage-controlled magnetic anisotropy (VCMA) whereby electric field across the MgO barrier modulates the free layer anisotropy. The parametrically driven oscillations are detected via microwave voltage from the MTJ near  $f$  and show resonant character, observed only in a narrow range of drive frequencies near  $2f$ . The excitation also exhibits a well-pronounced threshold drive voltage of approximately 0.1 Volts. Our work demonstrates a low threshold for parametric excitation of magnetization by VCMA that holds promise for the development of energy-efficient nanoscale spin wave devices.

**9:00AM E6.00004 Control of Spin Wave Band Structure in YIG using Electric Fields<sup>1</sup>**, GLADE SIETSEMA, MICHAEL E. FLATTÉ, University of Iowa — It has previously been shown that a uniform electric field can be used to modify the dispersion relations of spin waves in a YIG slab<sup>2</sup>. The application of the electric field results in a Dzyaloshinsky-Moriya interaction, which then produces a linear shift of the spin wave frequencies<sup>3</sup>. In this work we consider the effects of a periodically varying electric field on a slab of YIG. The spin wave frequencies and linewidths of the system are obtained from the Landau-Lifshitz-Gilbert equation using the plane-wave expansion method. We demonstrate that the periodic variation of the electric field opens band gaps in the spin wave dispersion relations. A band gap width of several hundred MHz is observed when the electric field strength is alternating between 0 and  $8 \cdot 10^7$  V/m over a length scale of 200 nm. The frequency and width of these band gaps can be tuned by adjusting the electric field strength and the lattice constant associated with the periodicity, and quality factors on the order of 100 can be achieved.

<sup>1</sup>This work is supported in part by DARPA.

<sup>2</sup>X. Zhang et al., Phys. Rev. Lett. **113**, 037202 (2014)

<sup>3</sup>T. Liu et al., Phys. Rev. Lett. **106**, 247203 (2011)

**9:12AM E6.00005 Measuring magnon propagation in magnonic crystals at millikelvin temperatures<sup>1</sup>** , ALEXY KARENOWSKA, ARJAN VAN LOO, RICHARD MORRIS, SANDOKO KOSEN, University of Oxford, Department of Physics, ANDRII CHUMAK, ALEXANDER SERGA, BURKARD HILLEBRANDS, Technische Universitaet Kaiserslautern — Magnon systems are increasingly widely recognized as a potential basis for solid-state quantum information processing. Propagating magnons are readily excited over the same range of microwave frequencies as are used in established quantum circuit technologies, and couple readily to electromagnetic fields. These facts, in combination with the relatively slow speeds and highly tunable dispersion of the excitations, make them a particularly interesting proposition in the context of quantum devices. Here, we present the first experimental study of microwave-frequency magnonic crystals (magnon systems with an artificially engineered bandgap) at millikelvin temperatures. Our magnonic crystals were prepared by etching grooves into a magnon waveguide made from a film of the magnetic insulator, yttrium iron garnet. The high signal-to-noise afforded by our low-temperature measurement environment makes it possible to make detailed observations of the dispersion of externally excited propagating magnon modes within the crystals. Our results lead us to suggest a range of device applications of dispersion-engineered magnonic systems in the context of microwave-circuit based quantum information processing.

<sup>1</sup>The authors acknowledge support from the EPSRC (EP/K032690/1).

**9:24AM E6.00006 Torque-mixing Magnetic Resonance Spectroscopy** , JOSEPH LOSBY, FATEMEH FANI SANI, Univ. of Alberta, Dept. of Physics and National Institute for Nanotechnology, DYLAN GRANDMONT, Univ. of Alberta, Department of Physics, ZHU DIAO, Univ. of Alberta, Dept. of Physics and National Institute for Nanotechnology, MIRO BELOV, National Institute for Nanotechnology, JACOB BURGESS, SHAWN COMPTON, WAYNE HIEBERT, Univ. of Alberta, Dept. of Physics and National Institute for Nanotechnology, DOUG VICK, National Institute for Nanotechnology, KAVEH MOHAMMAD, ELHAM SALIMI, GREGORY BRIDGES, DOUGLAS THOMSON, Electrical and Computer Engineering, University of Alberta, MARK FREEMAN, Univ. of Alberta, Dept. of Physics and National Institute for Nanotechnology — A universal, mechanical torque method for magnetic resonance spectroscopy is presented. In analogy to resonance detection by induction, a signal proportional to the transverse component of a precessing dipole moment can be measured as a pure mechanical torque in broadband, frequency-swept spectroscopy. Comprehensive electron spin resonance of a single-crystal, mesoscopic yttrium iron garnet disk at room temperature are presented to demonstrate the method. The rich detail allows analysis of even complex 3D spin textures.

**9:36AM E6.00007 Ferromagnetic resonance of a YIG film in the low frequency regime** , JOHN KETTERSON, Northwestern University, Evanston, IL., SCOTT GRUDICHAK, Lawrence University, Appleton, WI., JOSEPH SKLENAR, Northwestern University, Evanston, IL., C. C. TSAI, Chang Jung Christian University, Tainan 71101, Taiwan., MOONGYU JANG, Hallym University, Chuncheon, 200-702 South Korea., QINGHUI YANG, HUAIWU ZHANG, State Key Laboratory of Electronic Films and Integrated Devices, University of Electronic Science and Technology, Chengdu, Sichuan, 610054, China., SEONGJAE LEE, Research Institute for Natural Sciences, Hanyang University, Seoul, 133-791 South Korea. — An improved method for characterizing the magnetic anisotropy of films with cubic symmetry is described and is applied to an yttrium iron garnet (111) film. Analysis of the FMR spectra performed both in-plane and out-of-plane from 0.7 to 8 GHz yielded the magnetic anisotropy constants as well as the saturation magnetization. The field at which FMR occurs is sensitive to anisotropy constants in the low frequency ( $\sim 2$  GHz) regime and when the orientation of the magnetic field is nearly normal to the sample plane; the restoring force on the magnetization arising from the magnetocrystalline anisotropy fields is then comparable to that from the external field, thereby allowing the anisotropy constants to be determined with greater accuracy. Work at Northwestern was supported by the US DOE, Office of Basic Energy Sciences, Materials Science and Engineering Division under grant number DE-SC0014424. The film growth was supported by the National Natural Science Foundation of China (NSFC) under Grants 51272036 and 51002021 and 51472046.

**9:48AM E6.00008 Current driven asymmetric domain wall propagation** , CHIRAG GARG, Max Planck Institute for Microstructure Physics, Halle, AAKASH PUSHP, TIMOTHY PHUNG, SEE-HUN YANG, BRIAN P. HUGHES, CHARLES RETTNER, IBM Almaden Research Center, San Jose, California, STUART S.P. PARKIN, Max Planck Institute for Microstructure Physics, Halle — In ultrathin magnetic heterostructures, the presence of spin-orbit coupling gives rise to chiral Neel walls which are stabilized by the Dzyaloshinskii-Moriya Interaction (DMI), and also to a highly efficient chiral spin torque mechanism. In straight nanowires, the current-driven propagation of alternating Néel DWs without the presence of an in-plane field is equivalent, leading to the lock-step motion of several DWs in a nanowire. Here, we show that by engineering the structure in which the domain walls propagate, which in our case is in the shape of a Y-shaped junction, the DW propagation process becomes selective to the polarity of the DWs even in the absence of any externally applied magnetic fields. We remarkably find that after splitting at the Y-shaped junction, the DW velocity in one branch remains largely unaffected compared to its initial velocity whereas simultaneously the DW velocity in the other branch decreases by as much as 10-90%. We show that this large change in the DW velocity in a particular branch depends on the relative angle between the local magnetization of the DW and the spin current emanating from the underlying heavy-metal layer in these nanowires.

**10:00AM E6.00009 Notch-Boosted Domain Wall Propagation in Magnetic Nanowires<sup>1</sup>** , XIANG RONG WANG, Hong Kong University of Science and Technology, HUIYANG YUAN, Hong Kong Univ of Sci & Tech — Magnetic domain wall (DW) motion along a nanowire underpins many proposals of spintronic devices. High DW propagation velocity is obviously important because it determines the device speed. Thus it is interesting to search for effective control knobs of DW dynamics. We report a counter-intuitive finding that notches in an otherwise homogeneous magnetic nanowire can boost current-induced domain wall (DW) propagation. DW motion in notch-modulated wires can be classified into three phases: 1) A DW is pinned around a notch when the current density is below the depinning current density. 2) DW propagation velocity above the depinning current density is boosted by notches when non-adiabatic spin-transfer torque strength is smaller than the Gilbert damping constant. The boost can be many-fold. 3) DW propagation velocity is hindered when non-adiabatic spin-transfer torque strength is larger than the Gilbert damping constant.

<sup>1</sup>This work was supported by Hong Kong GRF Grants (Nos. 163011151 and 605413) and the grant from NNSF of China (No. 11374249).

**10:12AM E6.00010 Magnetic domain walls as reconfigurable spin-wave nano-channels<sup>1</sup>**, KAI WAGNER, 1. Helmholtz-Zentrum Dresden - Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany. ;2. TU Dresden, Dresden, Germany — Research efforts to utilize spin waves as information carriers for wave based logic in micro- and nano-structured ferromagnetic materials have increased tremendously over the recent years [1,2]. However, finding efficient means of tailoring and downscaling guided spin-wave propagation in two dimensions, while maintaining energy efficiency and reconfigurability, still remains a delicate challenge.

Here we target these challenges by spin-wave transport inside nanometer-scaled potential wells formed along magnetic domain walls. For this, we investigate the magnetization dynamics of a rectangular-like element in a Landau state exhibiting a so called 180° wall along its center. By microwave antennae the rf-excitation is constricted to one end of the domain wall and the spin-wave intensities are recorded by means of Brillouin-Light Scattering microscopy revealing channelled transport. Additional micromagnetic simulations [3] with pulsed as well as cw-excitation are performed to yield further insight into this class of modes.

We find several spin-wave modes quantized along the width of the domain wall yet with well defined wave vectors along the wall, exhibiting positive dispersion. In a final step, we demonstrate the flexibility of these spin-wave nano-channels based on domain walls. In contrast to wave guides realised by fixed geometries, domain walls can be easily manipulated. Here we utilize small external fields to control its position with nanometer precision over a micrometer range, while still enabling transport. Domain walls thus, open the perspective for reprogrammable and yet non-volatile spin-wave waveguides of nanometer width.

[1]: A. V. Chumak, V. I. Vasyuchka, and B. Hillebrands, Nat. Phys. 11, 453-461 (2015).

[2]: D. Grundler, Nat. Phys. 11, 438-441 (2015).

[3]: A. Vansteenkiste, J. Leliaert, M. Dvornik, M. Helsen, F. Garcia-Sanchez and B. van Waeyenberge, AIP Advances 4, 107133 (2014).

[4]: K. Vogt, F. Y. Fradin, J. E. Pearson, T. Sebastian, S. D. Bader, B. Hillebrands, A. Hoffmann and H. Schultheiss H. , Nat. Comm. 5, 3727 (2014).

<sup>1</sup>Financial support by the Deutsche Forschungsgemeinschaft within project SCHU2922/1- 1 is gratefully acknowledged.

**10:48AM E6.00011 Studying Kittel-like modes in a 3D YIG disk using Torque-mixing Magnetic Resonance Spectroscopy**, FATEMEH FANI SANI, JOSEPH LOSBY, Univ. of Alberta, Department of Physics and National Institute for Nanotechnology, DYLAN GRANDMONT, Univ. of Alberta, Department of Physics, ZHU DIAO, Univ. of Alberta, Department of Physics and National Institute for Nanotechnology, MIRO BELOV, National Institute for Nanotechnology, JACOB BURGESS, SHAWN COMPTON, Univ. of Alberta, Department of Physics and National Institute for Nanotechnology, WAYNE HIEBERT, DOUG VICK, National Institute for Nanotechnology, KAVEH MOHAMMAD, ELHAM SALIMI, GREGORY BRIDGES, DOUGLAS THOMSON, Electrical and Computer Engineering, University of Manitoba, MARK FREEMAN, Univ. of Alberta, Department of Physics and National Institute for Nanotechnology — We report a study of ferrimagnetic resonance in a mesoscopic, single-crystalline YIG disk using torque-mixing magnetic resonance spectroscopy (TMRS). The Kittel model for magnetic resonance is a touchstone in measuring fundamental magnetic properties for magnetic films, which does not significantly depend on the film size. In 3D structures, ladders of confined resonance modes are observed, and these can exhibit the non-monotonic evolution of frequency with field familiar from Kittel modes. TMRS is a tool uniquely suited for observing this physics in individual 3D structures, on account of its combination of high sensitivity and broadband capability coupled with fine frequency resolution.

**Tuesday, March 15, 2016 8:00AM - 11:00AM —**

**Session E7 APS SPS: Undergraduate Research/SPS IV** 303 - Courtney Bougher, American Physical Society

**8:00AM E7.00001 Capacitance of thin film solar cells: violating the depletion approximation**, THADDEUS COX, ALEXANDER OGLE, JENNIFER HEATH, Linfield College — Capacitance measurements of solar cells are able to detect minute changes in charge in the material. For that reason, capacitance is used in many methods to electrically characterize the solar cell. Standard interpretations of capacitance relies on many assumptions, which, if wrong can skew the results. In some solar cells where a back contact barrier is suspected, measurements at high forward bias can be used. We have seen that apparent signatures of a back contact barrier in Cu(In,Ga)Se<sub>2</sub> may actually be the first signs of a negative contribution to capacitance. We will discuss the implications of negative capacitance, and its relationship to other electronic characteristics of the device.

**8:12AM E7.00002 Time-dependent efficiency measurements of donor-acceptor, dye-sensitized polymer solar cells.**, KYLE BANDACCARI, GRACE CHESMORE, PARISA TAJALLI-TEHRANI VALVERDE, MITCHEL BUGAJ, BRIAN MCNELIS, RICHARD BARBER, JR., Santa Clara University — The fullerene/polymer active layer pairing of PCBM/P3HT has become the model system within the field of polymer solar cell research. A large body of work concerned with reporting improved efficiencies for this system exists, but truly quantitative studies of device lifetime and long-term degradation tendencies are much rarer. Here, we report the effects of two donor-acceptor diazo dye sensitizers on efficiency and lifetime upon addition into the PCBM/P3HT active layer at varied concentrations. The electrical and efficiency measurements were supplemented by time-dependent UV-visible spectroscopy studies and morphology investigations via atomic-force microscopy (AFM). This pairing with spectroscopy offers an internal check on the data as the rate of change in absorbance of the active layer correlates almost exactly to the rate of power conversion efficiency decrease. Additionally, AFM imaging reveals different morphology patterns when dye concentrations and functionalities change. Such observations suggest that such small-molecule sensitizers exert yet undetermined effects on the organization of components within the active layer at the molecular level.

**8:24AM E7.00003 Quantitative study of stress levels in AT and BT cut quartz crystal microbalances associated with surface laser irradiation.<sup>1</sup>**, L.H. GOODMAN, E.S. BILILIGN, B.J. MCCANN, B.W. KELLER, K. STEVENS, S.G. KENNY, J. KRIM, North Carolina State University — The frequency response of an AT cut Quartz Crystal Microbalance (QCM) to laser irradiation has been increasingly studied in recent years, as the combination of photons with materials on a QCM's electrodes enables fundamental studies of topics that span biophysics to photovoltaics. In order for such studies to advance, however, the impact of heating effects associated with laser irradiation of the QCM must be accounted for. Prior studies reached qualitative conclusions that laser irradiation induces stress QCM's arising from non-uniform thermal expansion, but did not quantitatively measure the degree of stress. Secondary effects such as surface film desorption and/or changes in temperature were also reported to be present. We report here a study of the frequency response of AT and BT cut QCM's to laser irradiation. AT and BT cut QCM's have similar response to mass adsorption, but opposite frequency response to stress levels, allowing the stress levels induced by the laser light to be quantitatively measured when the results are compared. Studies were performed in both vacuum and air, to control for the presence of adsorbed films. As expected, system designs that minimize temperature gradients result in less of an effect.

<sup>1</sup>Work supported by NSF DMR-1310456

**8:36AM E7.00004 Photovoltaic performance parameters at the nanoscale from in situ I-V curve measurements**, SADIA NASEEM, ELIZABETH TENNYSON, MARINA LEITE, University of Maryland College Park — Monocrystalline photovoltaic (PV) devices exhibit higher efficiencies than polycrystalline devices, but the high manufacturing costs associated with single crystal solar cells pose a hindrance to their wide implementation. Polycrystalline  $\text{CuIn}_x\text{Ga}_{(1-x)}\text{Se}_2$  (CIGS) material with high optical absorbance and low cost/Watt, is a promising alternative. Yet, the efficiency of this low-cost technology is still substantially lower than the theoretical values estimated by the Shockley-Queisser limit. This is likely due to microstructural non-uniformities, which cannot be accessed by macroscopic light I-V measurements. Therefore, we spatially resolve the electrical response of these devices by 'local' I-Vs. For that, we utilize a 100x objective as a local excitation source and LabVIEW to map the PV performance with sub-microns scale resolution through extrapolation of key parameters from pixel by pixel I-V curves. Extraction of performance parameters such as short-circuit current, open-circuit voltage fill factor, and maximum power point can provide useful information regarding optimal microstructural characteristics. This information is not only valuable for CIGS-based devices, but also will be an essential tool for maximizing performance across all PV technologies.

**8:48AM E7.00005 Optimizing Hydrogen Storage by Doping the  $\text{LiBH}_4 + \text{MgH}_2$  Reaction with Various Niobium Based Oxides**, PAUL HORNUNG, ROBERT WALKO, ANDREW WENZEL, RICHARD WRIGHT, TABBETHA DOBBINS, Rowan University, Dept. of Physics & Astronomy — In this study, the effects of doping the dehydrogenation reaction of  $\text{MgH}_2 + 2\text{LiBH}_4$  was combined with 5 mole% of three different Niobium based oxides ( $\text{Nb}_2\text{O}_5$ ,  $\text{NbO}_2$ , and  $\text{LiNbO}_3$ ). The compounds were mixed using high energy ball milling, and then heated using an air tight heating stage. We looked for changes in the Raman spectra as temperature increased (up to 350C) as an indication of hydrogen desorption reaction. We found that milled  $\text{LiBH}_4$  undergoes significant changes in Raman spectra during heating to 130C.  $\text{MgH}_2$  undergoes significant changes when comparing before and after milling—but in each case, the spectral peaks remain unchanged during heating to 350C. The sample with  $\text{LiNbO}_3$  exhibited a concrete change in Raman spectrum at 300 C while the sample doped with  $\text{Nb}_2\text{O}_5$  underwent a change in spectra at 170C. The sample doped with  $\text{NbO}_2$  showed little change in spectra when the samples were heated up to 350C. Further studies are underway to examine the nature of the changes in the Raman spectra using X-ray diffraction and residual gas analysis.

**9:00AM E7.00006 Electromotive force and current in a superconducting solenoid with limited length induced by a bar magnet and a monopole<sup>1</sup>**, LIANXI MA, Blinn College - Bryan — The magnetic flux  $\Phi_B$ , electromotive force, EMF, and current  $I_{in}$ , induced by a moving magnetic bar and an imaginary magnetic monopole in a superconducting solenoid of multiple turns and length  $L$ , are numerically calculated. The magnetic field of the bar magnet is approximated with the magnetic field along  $z$  axis of a solenoid with length  $l$  and radius  $a$  and current  $I$ , while the magnetic field of the monopole is supposed to be inversely proportional to  $r^2$ . Calculations show that, for a bar magnet,  $\Phi_B$  and  $I_{in}$  essentially saturate when the bar moves inside superconducting solenoid, so EMF is zero while  $I_{in}$  is constant. EMF is only induced when the bar enters and exits the solenoid and  $I_{in}$  is zero after the bar leaves the solenoid. For a magnetic monopole,  $\Phi_B$  is discontinuous (from positive maximum to negative maximum) when it moves through each turn of the superconducting solenoid, but EMF caused by  $d\Phi_B/dt$  is continuous while the EMF induced by the a moving monopole is a delta function (moving monopole produces a ring-shaped  $E$  field). The total  $\text{EMF}_{Tot}$  in solenoid is the superposition of EMF of each turn of coil and the plateau appears. The current  $I_{in}$  continues to grow while the monopole leaves the solenoid.

<sup>1</sup>Thanks to Dr. Liancun Zheng and Mr. Lin Liu for verifying my calculation

**9:12AM E7.00007 Optimizing Production of Superconducting Bulk YBCO Crystals: Effects of Initial Temperature and Growth Time<sup>1</sup>**, ERIN JOLLEY, CONNOR SHEA, JANET HUNTING, M.C. SULLIVAN, Ithaca College — We present our work on increasing both pinning force and critical temperature of bulk YBCO superconducting crystals. We optimized temperature profiles for growing bulk  $\text{YBaCuO}$  superconductors by varying (a) temperature and (b) growth time. We synthesize the precursor materials, superconducting  $\text{Y}_1\text{Ba}_2\text{Cu}_3\text{O}_7$  (Y-123) and non-superconducting  $\text{Y}_2\text{Ba}_1\text{Cu}_1\text{O}_5$  (Y-211), and mix the two in a 1:0.4 molar ratio before beginning melt textured growth. We heat the mixture to a temperature above the melting point of Y-123 but below the melting point of Y-211, where it is held until the Y-123 melts and the Y-211 impurities disperse in the mixture. The mixture is then quickly cooled to an initial temperature (a) near the peritectic point, and is then slowly cooled for 30-100 hours (b) to allow steady growth of large domain Y-123 crystals. We will discuss the effects of different initial temperatures near the peritectic point and growth times on the pinning force and critical temperature of these samples.

<sup>1</sup>This work was supported by NSF grant DMR-1305637, and made use of the Cornell Center for Materials Research Shared Facilities which are supported through the NSF MRSEC program (grant DMR-1120296).

**9:24AM E7.00008 The Effect of Impurities on the Superconductivity of BSCCO-2212**, JOHN VASTOLA, RICHARD KLEMM, University of Central Florida — BSCCO-2212 is a high-temperature cuprate superconductor whose electronic structure is currently poorly understood. In particular, it is unclear whether its order parameter is consistent with s-wave or d-wave behavior. Leggett has suggested that its order parameter might take a certain form that is consistent with d-wave behavior. While some experiments on the surface of BSCCO seem to support this conclusion, other experiments have suggested that its order parameter is instead s-wave in the bulk. We present some quantum field theoretic calculations in the spirit of Abrikosov and Gorkov's approach to the theory of superconductivity that suggest that such an order parameter cannot be correct. We will demonstrate that having such an order parameter would mean that BSCCO's critical temperature would go to zero if it is sufficiently impure, contradicting experimental evidence otherwise. Because this would not happen with a d-wave order parameter, these calculations lend support to the hypothesis that BSCCO is s-wave.

**9:36AM E7.00009 Superconductivity and anti-ferromagnetism through Bose-Fermi mixture on optical lattices.**, JEREMY BRACKETT, THEJA DE SILVA, Augusta University — Motivated by the recent experimental progress with ultra-cold atoms, we investigate the physics of a Bose-Fermi mixture on a two dimensional optical lattice. We treat the system parameters such that 2-component fermions are in a deep external trap and weakly interacting bosons are in a shallow external trap, however both of these atoms are subjected to the same optical lattice. In this parameter regime, the bosons form a Bose-Einstein condensate and mediate an attractive interaction between fermions through low energy Bose excitations. As a result, the dynamics of the fermions can be described by the single band Hubbard model that involves on-site repulsive interaction and elementary excitation mediated attractive interactions. Using a mean field theory, we derive an effective action up to the quartic order in both d-wave superconducting and anti-ferromagnetic order parameters. Using this Landau energy functional, we then discuss the phase transition and study the competition and/or cooperation of anti-ferromagnetism and d-wave superconductivity in the system.

**9:48AM E7.00010 Coexistence of anti-ferromagnetism and anisotropic superconductivity in iron pnictides.**, JOSEPH NEWMAN, THEJA DE SILVA, Augusta University — By treating both anti-ferromagnetism (AFM) and superconductivity (SC) on an equal footing, we investigate the possible coexistence of AFM and SC of recently found high-temperature superconducting compounds. Assuming that the electron pairing is mediated by the spin fluctuations and using a mean-field theory, we derive a set of gap equations for both AFM and SC order parameters. In the spirit of the second order phase transition, we then linearize the gap equations using various base functions for superconducting order to include the different pairing symmetries. By analyzing the solution of our linearized equations, we then discuss the possible coexistence of AFM and anisotropic SC in these compounds.

**10:00AM E7.00011 Optimization of the high frequency magneto-impedance effect in Co-based amorphous ribbons<sup>1</sup>**, V. ORTIZ, Univ. of Puerto Rico at Mayaguez, T. EGGERS, M.H. PHAN, Univ. of South Florida — The magnetic field dependence of the impedance, known as magneto-impedance (MI), was measured as a function of excitation frequency in Co-based amorphous ribbons. An optimization of the MI profile on the high frequency regime (100 MHz – 1000 MHz) was attempted through annealing techniques. Current annealing was performed with different annealing amplitudes ranging from 200 mA up to 1 A. Field annealing was also performed by raising the temperature of the sample through Joule heating and applying an external magnetic field of 55 Oe transversal to the ribbon. It was found that annealing at low current improved the MI response at lower frequencies, between 100 MHz and 300 MHz. On the other hand annealing at higher amplitude, past the Curie temperature ( $T_c$ ) favored higher frequencies. These findings provide good guidance toward the optimization of the MI response of Co-based amorphous ribbons for high-frequency sensor applications.

<sup>1</sup>This project is supported by the NSF REU grant DMR 1263066: REU Site in Applied Physics at USF

**10:12AM E7.00012 Charge density wave phase transitions in Tantalum Disulfide<sup>1</sup>**, MARC REYNAUD, MICHAEL ALTVATER, ADITYA SRIPAL, ALICE HUANG, GUOHONG LI, EVA Y. ANDREI, Rutgers University, Physics and Astronomy, RUI ZHAO, JOSHUA ROBINSON, The Pennsylvania State University, Materials Science and Engineering, Center for Two- Dimensional and Layered Materials — The discovery of transition metal dichalcogenides has reopened the interest in charge density wave physics. By looking at the phase transition properties, it is possible to create switches with properties exceeding the traditional FETs. In this work, we fabricated 2D nanoscale switches made of 1T-TaS<sub>2</sub> and graphene. We tested the transport properties between the Mott insulating state and the conductive state of the switch. Our work will provide insight on possibilities for the production of ideal switches and transistor logic.

<sup>1</sup>The work is supported by DOE-FG02-99ER45742, NSF DMR 1207108, NSF EFRI2-DARE 13-583

**10:24AM E7.00013 Dielectric and electro-optic measurements of nematic liquid crystals doped with carbon nanotubes<sup>1</sup>**, MATTHEW PETERSON, Tufts University, GEORGI GEORGIEV, Assumption College, TIMOTHY ATHERTON, PEGGY CEBE, Tufts University — We studied the effects of carbon nanotubes (CNTs) on the dielectric and electro-optic properties of nematic 5CB liquid crystals (LCs). Samples containing 0.01%, 0.10% and 1.00% CNTs by weight were prepared. Anti- parallel rubbed cells with a nominal thickness of 10  $\mu$ m were prepared using indium tin oxide coated glass cells and a polyimide alignment layer. The capacitance and dissipation factor were measured using an Agilent 4284A precision LCR meter. From these measurements, the complex dielectric permittivity was determined as a function of frequency. Analysis of the low frequency regime ( $f < 1000$  Hz) indicates that 5CB samples containing CNTs have a higher conductance than neat samples. The Fréedericksz transition critical voltage was noted by a sharp increase in capacitance after an initial plateau. Numerical simulations of CNT-facilitated switching show that polarization induced on the nanotubes from capacitive effects can significantly reduce the critical voltage in DC electric fields, in agreement with experimental results. Measurements of the critical voltage over a range of frequencies will also be presented.

<sup>1</sup>Research was supported by the National Science Foundation, DMR1206010.

**10:36AM E7.00014 NaAlH<sub>4</sub> Mixed with Carbon Nanotubes, Fullerene, and Titanium to Yield the Lowest Temperature for Hydrogen Desorption.**, JENNIFER HILDEBRAND, PATRICK MCFADDEN, SANGA KIM, TABBETHA DOBBINS, Rowan University, Dept. of Physics & Astronomy — Recent research in hydrogen storage has improved dehydrogenation methods with solid-state compounds. NaAlH<sub>4</sub> is a complex hydrides which release hydrogen at a lower temperature making the compound a great candidate for hydrogen storage. However, a catalyst should be combined with NaAlH<sub>4</sub> to release the lowest desorption temperature. Prior research showed that interaction of NaAlH<sub>4</sub> with nanotube or fullerene effectively weakens the Al-H bonds causing hydrogen desorption at lower temperatures. In the present study, NaAlH<sub>4</sub> is ball milled with three of these catalysts: titanium, carbon nanotubes and fullerene and the milling time is varied from 10 to 30 minutes to compare the dehydrogenation rates in each setup. The phase structures were identified using the X-ray diffraction. Of these catalysts, the fullerene yielded the most interesting result showing nanostructuring of the hydride during ball milling. The possibility of “shot peening” of the NaAlH<sub>4</sub> by the fullerenes is explored.

**10:48AM E7.00015 Simulation of the Effects of Cooling Techniques on Turbine Blade Heat Transfer<sup>1</sup>**, VINCE SHAW, None, MARCO FATUZZO, Xavier University, Cincinnati, OH — Increases in the performance demands of turbo machinery has stimulated the development many new technologies over the last half century. With applications that spread beyond marine, aviation, and power generation, improvements in gas turbine technologies provide a vast impact. High temperatures within the combustion chamber of the gas turbine engine are known to cause an increase in thermal efficiency and power produced by the engine. However, since operating temperatures of these engines reach above 1000 K within the turbine section, the need for advances in material science and cooling techniques to produce functioning engines under these high thermal and dynamic stresses is crucial. As with all research and development, costs related to the production of prototypes can be reduced through the use of computational simulations. By making use of Ansys Simulation Software, the effects of turbine cooling techniques were analyzed.

<sup>1</sup>Simulation of the Effects of Cooling Techniques on Turbine Blade Heat Transfer

**Tuesday, March 15, 2016 8:00AM - 10:24AM –**

**Session E8 DCMP: Superconductivity: Transport Properties** 304 - Philip Adams, Louisiana State University

**8:00AM E8.00001 Charge transport in the electron-doped cuprate superconductors**, YANGMU LI, WOJCIECH TABIS, School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, USA, EUGENE MOTOYAMA, Department of Physics, Stanford University, Stanford, California 94305, USA, GUICHUAN YU, School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, USA, NEVEN BARIIC, Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria, MARTIN GREVEN, School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, USA — Recent studies of the normal-state charge transport of the hole-doped cuprates have revealed that, in the pseudogap phase at moderate doping, the behavior of the charge carriers is that of a Fermi-liquid: The scattering rate exhibits quadratic temperature and frequency dependencies [1,2], and the magnetoresistance obeys Kohlers rule [3]. The cotangent of the Hall angle, which in a parabolic single-band model corresponds to the scattering rate, is also quadratic in temperature, and moreover doping and compound independent, and hence universal [4]. Importantly, this observable is insensitive to the opening of the pseudogap. In light of these findings, we will revisit the charge-transport in the electron-doped cuprates [5]. [1] N. Bariic et al., Proc. Natl. Acad. Sci. USA 110, 12235 (2013); [2] S. I. Mirzaei et al., Proc. Natl. Acad. Sci. USA 110, 5774 (2013); [3] M. K. Chan et al., Phys. Rev. Lett. 113, 177005 (2014); [4] N. Bariic et al., arXiv:1507.07885 (2015); [5] N. P. Armitage et al., Rev. Mod. Phys. 82, 2421 (2010).

**8:12AM E8.00002 Multiple sign reversal of the Hall effect in electron-doped superconductor  $\text{Pr}_{0.9}\text{LaCe}_{0.1}\text{CuO}_{4\pm\delta}$  thin films**, BEIYI ZHU, Institute of Physics, Chinese Academy of Sciences — We have investigated the temperature and field dependence of the Hall resistivity of the electron-doped  $\text{Pr}_{0.9}\text{LaCe}_{0.1}\text{CuO}_{4\pm\delta}$  (PLCCO) superconducting thin films ( $T_{c0} = 22$  K). In the low magnetic field region ( $0.03 \sim 0.1$  T), a concrete triple sign reversal of the Hall resistivity  $\rho_{xy}$  has been observed in the  $\rho_{xy}(T)$  curve. With the increase of the magnetic field, the Hall resistivity  $\rho_{xy}(T)$  suffers triple, double, single sign reversal transitions and it will be completely disappear around 4.5 T. We contribute the triple sign reversal to the competition between the hole and the electron carriers in our electron-doped samples and a fourth sign reversal may be expected in the regime of the two-band system.

**8:24AM E8.00003 HIGH FIELD MAGNETORESISTANCE NEAR OPTIMAL DOPING IN  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$** , JOSE A. GALVIS, PAULA GIRALDO-GALLO, SCOTT RIGGS, ZACHARY STEGEN, National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL, USA, BRAD RAMSHAW, KIMBERLY MODIC, ROSS MCDONALD, National High Magnetic Field Laboratory, Los Alamos National Laboratory, Los Alamos, NM, USA., IVAN BOZOVIC, Brookhaven National Laboratory, Upton, NY 11973, USA., ARKADY SHEKHTER, GREG BOEBINGER, National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL, USA — An outstanding experimental feature of the metallic behavior of all high-temperature superconductors near optimal doping is the linear-in-temperature resistivity observed over a wide temperature range. Although metallic quantum criticality in these systems has been proposed to be the origin of this anomalous temperature dependence, its manifestation in the magnetotransport, yet to be determined, can become a source of important insight into the physics of these compounds. The experimental challenge is to measure normal state magnetoresistance in a broad range of magnetic fields, always limited by the  $H_{c2}$  on the lower side and the available magnetic fields on the higher. Here we report magnetoresistance measurements in thin films of  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ , for magnetic fields beyond 65 T — well above the highest fields used in previous studies of this system. We discuss the signature for quantum criticality based upon the high-field magnetoresistance measurements over a broad temperature range.

**8:36AM E8.00004 Fermi surface anisotropy in the cuprates**, BRAD RAMSHAW, Los Alamos Natl Lab — Broken rotational ( $C_4$ ) symmetry is a distinguishing feature for a number of experiments in the underdoped high- $T_c$  cuprates, including electrical resistivity, neutron scattering, Nernst coefficient, and scanning tunneling microscopy. This broken symmetry has not been observed on the Fermi surface, however, with or without the presence of an applied magnetic field. We measure the angle-dependent magnetoresistance—a quantity known to be extremely sensitive to the geometry and symmetry of the Fermi surface—of  $\text{YBa}_2\text{Cu}_3\text{O}_{6.58}$ , and find that the Fermi surface has a clear two-fold symmetry, breaking the  $C_4$  symmetry of the copper-oxide plane. We discuss the implications of this finding, including how it fits with recent X-ray measurements in high magnetic fields.

**8:48AM E8.00005 Onset field for Fermi-surface reconstruction in the cuprate superconductor  $\text{YBa}_2\text{Cu}_3\text{O}_y$** , GAEL GRISSONNANCHE, FRANCIS LALIBERTE, SOPHIE DUFOUR-BEAUSEJOUR, ALEXIS RIOPEL, SVEN BADOUX, MICHAEL CAQUETTE-MANSOUR, MARCIN MATUSIAK, ALEXANDRE JUNEAU-FECTEAU, PATRICK BOURGEOIS-HOPE, OLIVIER CYR-CHOINIRE, University of Sherbrooke, JAMES BAGLO, BRAD RAMSHAW, RUIXING LIANG, DOUG BONN, WALTER HARDY, University of British Columbia, STEFFEN KRAEMER, DAVID LEBOEUF, Laboratoire National des Champs Magnétiques Intenses (Grenoble), DAVID GRAF, National High Magnetic Field Laboratory (Tallahassee), NICOLAS DOIRON-LEYRAUD, LOUIS TAILLEFER, University of Sherbrooke — Discovery of quantum oscillations in underdoped cuprates [1] at low temperature and high magnetic field revealed the Fermi surface to contain a small closed electron pocket. It is thought to result from a reconstruction by charge order, but whether it is the order seen by NMR [2], and ultrasound [3] above a threshold field or the short-range modulations seen by X-ray diffraction in zero field is unclear [4]. Here we report measurements of the thermal Hall conductivity in  $\text{YBa}_2\text{Cu}_3\text{O}_y$  to show that Fermi-surface reconstruction occurs only above a sharply defined onset field, equal to the transition field seen in ultrasound. This reveals that electrons do not experience long-range broken translational symmetry in the zero-field ground state. [1] Doiron-Leyraud et al., Nature 447,565 (2007) [2] Wu et al., Nature 477,191 (2011) [3] LeBoeuf et al., Nat. Phys. 9,79 (2013) [4] Ghiringhelli et al. Science 337, 821-825 (2012)

**9:00AM E8.00006 Vortex creep and thermal depinning within strong pinning theory**, ROLAND WILLA, MARTIN BUCHACEK, VADIM B. GESHKENBEIN, GIANNI BLATTER, Institute for Theoretical Physics, ETH Zurich, 8093 Zurich, Switzerland — Vortex pinning in type-II superconductors can occur through the collective action of many pins (weak collective pinning scenario) or through plastic deformations induced by a low density of defects (strong pinning scenario). For the latter case, a new formalism has recently been developed [1-4] to provide a quantitative link between the microscopic pinning landscape and experimentally accessible quantities describing pinning on a macroscopic level. Examples are the critical current density  $j_c$ , the  $I$ - $V$  characteristics, or the  $ac$  Campbell length  $\lambda_C$ . Inspired by the original work of Larkin and Brazovskii [5,6] on density wave pinning, we have extended the strong pinning formalism to account for thermal depinning of flux lines and vortex creep. [1] G. Blatter, V. B. Geshkenbein, and J. A. G. Koopmann, Phys. Rev. Lett. **92**, 067009 (2004). [2] A. U. Thomann, V. B. Geshkenbein, and G. Blatter, Phys. Rev. Lett. **108**, 217001 (2012). [3] R. Willa, V. B. Geshkenbein, and G. Blatter, Phys. Rev. B **92**, 134501 (2015). [4] R. Willa, V. B. Geshkenbein, R. Prozorov and G. Blatter, Phys. Rev. Lett. (in press). [5] A. Larkin and S. Brazovskii, Solid State Communications **93**, 275 (1995). [6] S. Brazovskii and A. Larkin, Synthetic Metals **86**, 2223 (1997).

**9:12AM E8.00007 Anomalous high-field-induced phase in underdoped  $\text{La}_{1.7}\text{Eu}_{0.2}\text{Sr}_{0.1}\text{CuO}_4$** <sup>1</sup>, ZHENZHONG SHI, P. BAITY, DRAGANA POPOVIĆ, Dept. of Phys. & Natl. High Magnetic Field Lab., Florida State Univ., T. SASAGAWA, Tokyo Inst. of Tech. — We have investigated transport properties of the underdoped, stripe-ordered  $\text{La}_{1.7}\text{Eu}_{0.2}\text{Sr}_{0.1}\text{CuO}_4$  single crystals near their magnetic-field-driven superconducting transition for  $0.016 \leq T$  (K)  $\leq 40$  and magnetic fields  $H$  up to 18 T. At very low  $T$  ( $< 0.06$  K), an anomalous high-field-induced phase (HFIP) emerges in both the in-plane and out-of-plane resistivity measurements. Two temperature-independent crossing points in the magnetoresistance are identified near the boundaries of the HFIP. In addition, the HFIP exhibits signatures of glassiness, such as hysteretic behavior and memory of magnetic history. Differential resistance studies reveal nontrivial, non-Ohmic behavior, suggesting the possible presence of a vortex glass in the HFIP. A possible  $H$ - $T$  phase diagram for the underdoped  $\text{La}_{1.7}\text{Eu}_{0.2}\text{Sr}_{0.1}\text{CuO}_4$  and the nature of the HFIP will be discussed.

<sup>1</sup>Supported by NSF DMR-1307075 and NHMFL via NSF DMR-1157490 and the State of Florida.

**9:24AM E8.00008 Resistance Fluctuation Spectroscopy of Charge Stripes and Intertwined Orders in the Phase Diagram of  $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$** <sup>1</sup>, ADAM WEIS, MOUNIR FIZARI, DAVID HAMILTON, AZTON WELLS, JUSTIN LANE, University of Illinois at Urbana-Champaign, SO RA CHUNG, Belmont University, PATHIKUMAR SELLAPPAN, WALTRAUD KRIVEN, DALE VAN HARLINGEN, University of Illinois at Urbana-Champaign — The unusual phase diagram of  $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$  (LBCO) near  $x=1/8$  doping suggests a complex intertwined relationship between high-temperature superconductivity, charge stripes, spin order, and phase coherence. The charge stripe state's short-range conductance anisotropy may be observable as fluctuations in resistance. In thin film LBCO devices grown by pulsed laser deposition, our time-resolved resistance measurements have revealed an onset of resistance noise at dopings and critical temperatures consistent with charge stripes. The phase diagram of LBCO is explored by comparing the noise onset signature of charge order to measurements of superconductivity, the Hall effect, and other phenomena. I will briefly discuss the relevance of our results in LBCO thin films and crystals to a proposed "pair-density-wave" state near  $x=1/8$ .

<sup>1</sup>This research was supported by the DOE-BES under grant DE-SC0012368, through the Frederick Seitz Materials Research Laboratory at the University of Illinois at Urbana-Champaign. SRC was sponsored by NSF-REU 13-59126.

**9:36AM E8.00009 Avalanches and hysteresis at the structural transition in stripe-ordered  $\text{La}_{1.48}\text{Nd}_{0.4}\text{Sr}_{0.12}\text{CuO}_4$** <sup>1</sup>, P. G. BAITY, GARIMA SARASWAT, DRAGANA POPOVIĆ, Dept. of Phys. & Natl. High Magnetic Field Lab., Florida State Univ., T. SASAGAWA, Tokyo Inst. of Tech. — The coupling or intertwining of lattice, spin and charge orders and their effects on superconductivity are of great current interest in the physics of cuprates. The rare-earth-doped cuprate  $\text{La}_{1.48}\text{Nd}_{0.4}\text{Sr}_{0.12}\text{CuO}_4$  (LNSCO), for example, exhibits a first-order structural phase transition (SPT) from the low-temperature orthorhombic (LTO) to the low-temperature tetragonal (LTT) phase, with the onset of the static charge stripe order roughly coinciding with the SPT. We present out-of-plane magnetoresistance measurements around the LTO-LTT transition in LNSCO single crystals with  $H \parallel c$  up to 12 T and  $H \parallel ab$  up to 9 T. Hysteresis is observed for both field orientations, but for  $H \parallel c$  we also find evidence for the existence of metastable states and collective dynamics in the form of avalanches and return point memory. Such behavior indicates that, in LNSCO, the LTO-LTT structural transition can be driven with  $H$ . A detailed analysis of the avalanche statistics is used to determine their size and field dependence, and to extract information about the domain structure and dynamics of domain walls. Our results shed light on the interplay of lattice, spin and charge degrees of freedom in stripe-ordered La-based cuprates.

<sup>1</sup>Supported by NSF DMR-1307075 and NHMFL via NSF DMR-1157490 and the State of Florida.

**9:48AM E8.00010 Shot noise measurement in a strongly correlated material**, PANPAN ZHOU, WILL HARDY, Department of Physics and Astronomy, Rice University, ETHAN CHO, SHANE CYBART, ROBERT DYNES, Department of Physics, University of California, San Diego, DOUGLAS NATELSON, Department of Physics and Astronomy, Rice University — In strongly correlated materials, the motion of an electron is strongly affected by interactions with other electrons, leading to many interesting phenomena including metal-insulator transitions, colossal magnetoresistance, and high temperature superconductivity. Shot noise is one experimental probe for electronic correlations beyond simple electronic transport. Shot noise, which originates from the discrete nature of the charge-carrying particles, can be strongly affected by electronic correlations. Here we report initial shot noise measurements in tunnel junctions prepared from a  $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$  film sample, with nanoscale junctions written by focused helium ion beam. We will discuss a comparison of the shot noise between the YBCO film sample and standard tunnel junctions, as a function of temperature and bias, and the implications of these results.

**10:00AM E8.00011 Power-law Optical Conductivity from Unparticles: Application to the Cuprates**<sup>1</sup>, KRIDSANAPHONG LIMTRAGOOL, PHILIP PHILLIPS, Univ of Illinois - Urbana — We calculate the optical conductivity using several models for unparticle or scale-invariant matter. Within a Gaussian action for unparticles that is gauged with Wilson lines, we find that the conductivity computed from the Kubo formalism with vertex corrections yields no non-trivial deviation from the free-theory result. This result obtains because at the Gaussian level, unparticles are just a superposition of particle fields and hence any transport property must be consistent with free theory. Beyond the Gaussian approach, we adopt the continuous mass formulation of unparticles and calculate the Drude conductivity directly. We show that unparticles in this context can be tailored to yield an algebraic conductivity that scales as  $\omega^{-2/3}$  with the associated phase angle between the imaginary and real parts of  $\arctan \frac{\sigma_2}{\sigma_1} = 60^\circ$  as is seen in the cuprates. Our results indicate that at each frequency in the scaling regime, excitations on all energy scales contribute. Hence, incoherence is at the heart of the power-law in the optical conductivity in strongly correlated systems such as the cuprates.

<sup>1</sup>We thank NSF DMR-1461952 for partial funding of this project. KL is supported by a scholarship from the Ministry of Science and Technology, Royal Thai Government. PP thanks the Guggenheim Foundation for a 2015-2016 Fellowship.

**10:12AM E8.00012 Optical Measurements of Thermal Diffusivity in Strange Metals**, JIECHENG ZHANG, E. M. LEVENSON-FALK, AHARON KAPITULNIK, Stanford Univ — Thermal transport measurements of strongly correlated electronic systems provide key insight into their emerging collective behavior. For example, high- $T_c$  superconductors exhibit different regimes of unusual transport with bad metallicity at high temperatures, a pseudogap-dominated transport at intermediate temperatures, and the interplay with superconductivity at low temperatures. We present optical non-contact measurements of local thermal diffusivity in such materials. In our apparatus we focus a laser spot onto the surface of the investigated sample; the laser power is then modulated to create a periodic, point-like heat source. Another laser is focused nearby on the surface where the local reflectivity is measured. Since the reflectivity is temperature-dependent, it serves as a contactless probe of temperature oscillations due to the heat source. By measuring the temperature profile on the surface of the sample as a function of modulation frequency, we extract the thermal diffusivity of the material. We will present measurements of the temperature dependence and anisotropy of diffusivity in various strange metals, and discuss further applications of the apparatus.

**Tuesday, March 15, 2016 8:00AM - 11:00AM –**  
**Session E11 DMP GMAG: Electronic Structure and Magnetism in Fe-based Superconductors I**  
 307 - Qimiao Si, Rice University

**8:00AM E11.00001 The role of Hund's coupling in the correlations and the nematicity of iron superconductors**<sup>1</sup>, ELENA BASCONES, Instituto de Ciencia de Materiales de Madrid — Since their discovery in 2008 the strength and the nature of correlations in iron superconductors have been widely discussed [1]. Understanding the correlations is key to unveil the nature of the superconducting, nematic and magnetic instabilities which appear in the phase diagram. Due to their multi-orbital character, correlations in iron superconductors are strongly affected by Hund's coupling and these materials have been classified by some authors as Hund metals. For a long time there has been a strong controversy on the nature of correlations induced by Hund's coupling and its relation to Mott physics. While some authors describe Hund metals as strongly correlated systems which are not in proximity to a Mott insulating state, others, have described iron superconductors as doped Mott insulators. In the talk, after some introduction, I will first show our recent results which show that while the spin polarization of the atoms, promoted by Hund's coupling induces strong correlations, this does not necessarily mean that the total charge is more localized [2]. On the contrary, in some cases this polarization promotes itinerancy [2]. I will then present a generic framework to address the correlations in iron superconductors and discuss the role of Hund's coupling in the nematicity of iron superconductors, with special emphasis on FeSe. [1] Magnetic interactions in iron superconductors: a review, E. Bascones, B. Valenzuela and M.J. Calderon, (in press) arXiv:1503.04223 [2] Electronic correlations in Hund metals. L. Fanfarillo and E. Bascones, Phys. Rev. B 92, 075136 (2015)

<sup>1</sup>Funding from Ministerio de Ciencia y Tecnología FIS2011-29689, FIS2014-53219-P and Fundacion Ramon Areces

**8:36AM E11.00002 Itinerancy-Enhanced Quantum Fluctuation of Magnetic Moments in Iron-Based Superconductors<sup>1</sup>**, YU-TING TAM, DAO-XIN YAO, Sun Yat-sen university, WEI KU, Brookhaven National Laboratory — We investigate the influence of itinerant carriers on dynamics and fluctuation of local moments in Fe-based superconductors, via linear spin-wave analysis of a spin-fermion model containing both itinerant and local degrees of freedom. Surprisingly against the common lore, instead of enhancing the  $(\pi,0)$  order, itinerant carriers with well nested Fermi surfaces are found to induce a significant amount of *spatial* and temporal quantum fluctuation that leads to the observed small ordered moment. Interestingly, the underlying mechanism is shown to be intra-pocket nesting-associated long-range coupling rather than the previously believed ferromagnetic double-exchange effect. This challenges the validity of ferromagnetically compensated first-neighbor coupling reported from short-range fitting to the experimental dispersion, which turns out to result instead from the ferro-orbital order that is also found instrumental in stabilizing the magnetic order.  
\*Y.-T. Tam, D.-X. Yao and W. Ku, Phys. Rev. Lett. 115, 117001(2015)

<sup>1</sup>Work supported by US DOE No.DE-AC02-98CH10886 and CHN No. NBRPC-2012CB821400, No. NSFC-11275279

**8:48AM E11.00003 Competing magnetic fluctuations in iron pnictide superconductors: role of ferromagnetic spin correlations revealed by NMR<sup>1</sup>**, YUJI FURUKAWA, PAUL WIECKI, BEAS ROY, DAVID C. JOHNSTON, SERGEY L. BUD'KO, PAUL C. CANFIELD, Ames Laboratory, Dept. of Phys. and Astro, Iowa State Univ., COLLABORATION — The role of magnetic fluctuations in iron pnictide superconductors has been extensively studied since their discovery. As the parent materials have antiferromagnetic (AFM) ground states, attention has been focused on stripe-type AFM fluctuations, which are widely believed to give rise to the Cooper pairing in the systems. On the other hand, according to density functional theory calculations, the static magnetic susceptibility is enhanced at not only the stripe-type AFM but also ferromagnetic (FM) wavevectors. Nevertheless, FM fluctuations have not been investigated microscopically. In this talk, based on <sup>75</sup>As NMR data [1,2], we report clear evidence for the existence of strong FM correlations in the hole-doped  $(\text{Ba}_{1-x}\text{K}_x)\text{Fe}_2\text{As}_2$  and electron-doped  $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ . We will discuss the role of FM spin correlations in the occurrence of superconductivity in these systems. [1] P. Wiecki, et al., Phys. Rev. B **91**, 220406 (2015). [2] P. Wiecki, et al., Phys. Rev. Lett. **115**, 137001 (2015).

<sup>1</sup>Supported by USDOE under Contract No. DE-AC02-07CH11358.

**9:00AM E11.00004 Spin-liquid polymorphism in an underdoped iron-chalcogenide superconductor<sup>1</sup>**, IGOR ZALIZNYAK, Brookhaven National Laboratory, ANDREI SAVICI, MARK LUMSDEN, Oak Ridge National Laboratory, ALEXEI TSVELIK, Brookhaven Natl Lab, RONGWEI HU, Rutgers University, CEDOMIR PETROVIC, Brookhaven National Laboratory — We report neutron scattering measurements which reveal spin-liquid polymorphism in an 11 iron chalcogenide superconductor. It occurs when a poorly metallic magnetic state of FeTe is driven toward superconductivity by substitution of a small amount of tellurium with isoelectronic sulfur. We observe a liquid-like magnetic response, which is described by the coexistence of two disordered magnetic phases with different local structures whose relative abundance depends on temperature. One is the ferromagnetic (FM) plaquette phase observed in undoped, nonsuperconducting FeTe, which preserves the  $C_4$  symmetry of the underlying square lattice and is favored at high temperatures, whereas the other is the antiferromagnetic plaquette phase with broken  $C_4$  symmetry, which emerges with doping and is predominant at low temperatures. These findings suggest the coexistence of and competition between two distinct liquid states, and a liquid-liquid phase transformation between these states, in the electronic spin system of  $\text{FeTe}_{1-x}(\text{S,Se})_x$ . Our results shed light on many recent experimental data in unconventional superconductors. The phase with lower,  $C_2$  local symmetry, whose emergence precedes superconductivity, naturally accounts for a propensity to electronic nematic states.

<sup>1</sup>Work at BNL is supported by the Office of Basic Energy Sciences, US DOE, under Contract DE-SC00112704.

**9:12AM E11.00005 Studying the morphology of the magnetic  $C_4$  phase in the 122 superconductors.**, KEITH TADDEI, Northern Illinois University, JARED ALLRED, University of Alabama, DANIEL BUGARIS, Argonne National Laboratory, MATTHEW KROGSTAD, Northern Illinois University, SAUL LAPIDUS, Advanced Photon Source ANL, RYAN STADEL, Northern Illinois University, DUCK CHUNG, HELMUT CLAUS, Argonne National Laboratory, MERCOURI KANATZIDIS, Northwestern Illinois University, DENNIS BROWN, Northern Illinois University, STEPHAN ROSENKRANZ, RAYMOND OSBORN, Argonne National Laboratory, OMAR CHMAISSEM, Northern Illinois University — The iron based superconductors continue to prove an exciting system for the study of superconductivity: the recent discovery of a reentrant tetragonal phase with SDW magnetic ordering has opened new avenues to study the competition between microscopically coexistent superconductivity and magnetism. This intriguing new phase is not only an exceedingly rare example of a magnetic structure with two ordering vectors, and consequently a confirmation of itinerant magnetism, but has also allowed for the determination of spin fluctuations as the driving mechanism behind the phase evolution in these materials. Evidence has been mounting of the universality of  $C_4$  in the hole doped iron pnictides providing a useful playground for the comparison of how this phase behaves as it is stabilized out of different parent compounds and through different dopant atoms. Here all members of the hole doped family which show the  $C_4$  phase will be compared and the parameters which appear to tune the phase's extent in temperature and phase space will be discussed.

**9:24AM E11.00006 Itinerant Double-Q Spin-Density Wave in Iron Arsenide Superconductors<sup>1</sup>**, RAYMOND OSBORN, Argonne Natl Lab, JARED ALLRED, University of Alabama, OMAR CHMAISSEM, STEPHAN ROSENKRANZ, Argonne Natl Lab, DENNIS BROWN, Northern Illinois University, KEITH TADDEI, MATTHEW KROGSTAD, DANIEL BUGARIS, DUCK-YOUNG CHUNG, HELMUT CLAUS, SAUL LAPIDUS, MERCOURI KANATZIDIS, Argonne Natl Lab, JIAN KANG, RAFAEL FERNANDES, University of Minnesota, ILYA EREMIN, Ruhr-Universität Bochum — The recent observation of a tetragonal magnetic ( $C_4$ ) phase in hole-doped iron arsenide superconductors has provided evidence of a magnetic origin for the electronic nematicity in the  $C_2$  phase of these compounds. Now, Mössbauer data shows that the new phase also establishes the itinerant character of the antiferromagnetism of these materials and the primary role played by magnetic over orbital degrees of freedom. Neutron diffraction had shown that the magnetic order in the  $C_4$  phase was compatible with a double-Q structure arising from a collinear spin-density wave along both the X and Y directions simultaneously. The coherent superposition of the two modulations produces a non-uniform magnetic structure, in which the spin amplitudes vanish on half of the sites and double on the others, a uniquely itinerant effect that is incompatible with local moment magnetism. Mössbauer spectra in the  $C_4$  phase confirm this double-Q structure, with 50% of the spectral weight in a zero-moment peak and 50% with double the magnetic splitting seen in the  $C_2$  phase.

<sup>1</sup>Supported by the US DOE Office of Science, Materials and Engineering Division

**9:36AM E11.00007 ABSTRACT WITHDRAWN —**

**9:48AM E11.00008 Emergent Ising degrees of freedom in the  $J_1$ - $J_2$ - $J_3$  model for the iron tellurides**, GUANGHUA ZHANG, Ames Laboratory, Dept of Physics and Astronomy, Iowa State University, RAFAEL FERNANDES, School of Physics and Astronomy, University of Minnesota, REBECCA FLINT, Ames Laboratory, Dept of Physics and Astronomy, Iowa State University — The iron-telluride family of superconductors form a double-stripe [ $\mathbf{Q} = (\pi/2, \pi/2)$ ] magnetic order, which can be captured within a  $J_1 - J_2 - J_3$  Heisenberg model in the regime  $J_3 \gg J_2 \gg J_1$ . Intriguingly, besides breaking spin-rotational symmetry, the ground state manifold has three additional Ising degrees of freedom. Via their coupling to the lattice, they give rise to a monoclinic distortion and to two non-uniform lattice distortions with wave-vector  $(\pi, \pi)$ . Because the ground state is four-fold degenerate (mod rotations in spin space), only two of these Ising order parameters are independent. Here we introduce an effective field theory to treat all Ising order parameters, as well as magnetic order. All three transitions (corresponding to the condensations of two Ising and one magnetic order parameter) are simultaneous and first order in three dimensions, but lower dimensionality (or equivalently weaker interlayer coupling) and weaker magnetoelastic coupling can split the three transitions, and in some cases allows for two separate Ising phase transitions.

**10:00AM E11.00009 Non-Fermi liquid behavior in quantum critical iron-pnictide metal  $\text{Ba}(\text{Fe,Ni,Co})_2\text{As}_2$** , YASUYUKI NAKAJIMA, KEVIN KIRSHENBAUM, ALEX HUGHES, CHRISTOPHER ECKBERG, RENXIONG WANG, TRISTIN METZ, SHANTA SAHA, JOHNPIERRE PAGLIONE, Univ of Maryland-College Park — The breakdown of Landau's Fermi liquid theory has been believed to be induced by quantum fluctuations in the vicinity of a quantum critical point (QCP), occasionally accompanied by exotic superconductivity in the strongly correlated electron systems, such as cuprate and iron pnictide superconductors [1]. However, the superconducting dome of such materials with high  $T_c$  precludes us from investigating the interplay between quantum fluctuations and the exotic superconductivity. We report non-Fermi liquid behavior associated with quantum fluctuations in the transport and thermodynamic properties of the non-superconducting iron pnictide  $\text{Ba}(\text{Fe,Co,Ni})_2\text{As}_2$ , which allows us to elucidate the behavior on cooling down to near absolute zero without distractions from the superconductivity. We will discuss the evolution of non-Fermi liquid behavior with magnetic field, highlighting the presence of field tuned QCP. [1] T. Shibauchi et al., Annu. Rev. Condens. Matter Phys. 5, 113 (2014).

**10:12AM E11.00010 Spin-fluctuation induced non-Fermi-liquid behaviour with suppressed superconductivity in  $\text{LiFe}_{1-x}\text{Co}_x\text{As}$** , HU MIAO, YAOMIN DAI, Brookhaven National Laboratory, LINGYI XING, XIANCHENG WANG, Institute of physics, Chinese Academy of Sciences, PENGSHUAI WANG, Renmin University, HONG XIAO, TIAN QIAN, PIERRE RICHARD, XIANGGANG QIU, Institute of physics, Chinese Academy of Sciences, WEIQIANG YU, Renmin University, CHANGQING JIN, ZIQIANG WANG, Institute of physics, Chinese Academy of Sciences, P. D. JOHNSON, C. C HOMES, Brookhaven National Laboratory, HONG DING, Institute of physics, Chinese Academy of Sciences — We study a series of  $\text{LiFe}_{1-x}\text{Co}_x\text{As}$  compounds with different Co concentrations by transport, optical spectroscopy, angle-resolved photoemission spectroscopy, and nuclear magnetic resonance. We observe a Fermi-liquid to non-Fermi-liquid to Fermi-liquid (FL-NFL-FL) crossover alongside a monotonic suppression of the superconductivity with increasing Co content. In parallel to the FL-NFL-FL crossover, we find that both the low-energy spin fluctuations and Fermi surface nesting are enhanced and then diminished, strongly suggesting that the NFL behaviour in  $\text{LiFe}_{1-x}\text{Co}_x\text{As}$  is induced by low-energy spin fluctuations that are very likely tuned by Fermi surface nesting. Our study reveals a unique phase diagram of  $\text{LiFe}_{1-x}\text{Co}_x\text{As}$  where the region of NFL is moved to the boundary of the superconducting phase, implying that they are probably governed by different mechanisms.

**10:24AM E11.00011 Study of non-Fermi Liquid behavior from partial nesting in multi-orbital superconductors.**, CHANDAN SETTY, PHILIP PHILLIPS, University of Illinois at Urbana-Champaign — Partial nesting between two connected or disconnected regions of the Fermi surface leads to fractional powers of the Coulomb scattering lifetime as a function of temperature and frequency. This result is first demonstrated for a toy band structure where partial nesting occurs within a single band and between different regions of the Brillouin zone. A comparison is then made to a multiband scenario by studying the scattering rate of an effective two orbital model that was proposed in the context of multi-orbital superconductors. In the process, various model independent factors affecting the temperature exponent,  $n$ , are identified. The logarithmically divergent contributions of the lowest order vertex correction to the multi-orbital susceptibility, and the role played by nesting in suppressing these divergences is analyzed. The relevance of these results is discussed keeping the recently observed anomalous resistivity in the Co doped Iron superconductor  $\text{LiFeAs}$  as a backdrop.

**10:36AM E11.00012 Sensitivity of quantum critical pairing to Fermi surface topology: a Quantum Monte Carlo study**, XIAOYU WANG, University of Minnesota, YONI SCHATTNER, EREZ BERG, Weizmann Institute of Science, RAFAEL FERNANDES, University of Minnesota — In many iron-based and copper-based materials, unconventional superconductivity appears in close proximity to an antiferromagnetic instability. This fact has motivated intense theoretical investigations of the impact of magnetic fluctuations, particularly those associated with the putative quantum critical point (QCP), on the formation of the Cooper pairs. Although significant advance has been achieved using analytical methods to solve the so-called spin-fermion model, in which low-energy electronic states couple to quantum critical bosonic fluctuations, there remain significant challenges in establishing a perturbative scheme that accounts for both non-Fermi liquid behavior and superconductivity near the QCP. Here we present a sign-problem-free Quantum Monte Carlo (QMC) study of the spin-fermion model for a generic two-band Hamiltonian. We show that properties of the Fermi surface topology beyond the existence of hot spots play a fundamental role in determining the superconducting properties. In particular, we find that proximity to perfect nesting strongly suppresses the enhancement of the pairing susceptibility promoted by the QCP. We also compare our QMC results with an Eliashberg analysis of the quantum critical problem.

**10:48AM E11.00013 Density Functional Theory insights into the mechanism of noncollinear incommensurate spin density waves in Iron Arsenide.**, ROBERT SCHOONMAKER, STEWART CLARK, TOM LANCASTER, THOMAS FRAWLEY, PETER HATTON, Durham University — Iron arsenide intersects interesting physics between novel superconductors and other helical magnetic ordering in Pnma metal arsenide materials. Recent diffraction data has found a more complex ordering than a simple helical incommensurate spin density wave. Instead iron arsenide exhibits a definite chirality to the helimagnetism, an ellipticity in the spiral not aligned with the crystal axis, and resonant diffraction peaks forbidden by the Pnma symmetry. From non-magnetic and collinear density functional theory calculations we present insight into the mechanisms for the formation of this helimagnetic state. We find that ferromagnetic superexchange is a likely mechanism for the spin ordering and that the noncollinear ordering under this regime is caused by the spins on neighbouring irons arranging to minimise direct exchange between iron atoms, and also minimize disruption of the ferromagnetic superexchange between privileged iron-arsenic pairs. To explain the forbidden peaks in the diffraction we have performed second-order spin-orbit perturbation calculations on the nonmagnetic calculation, which finds that the orbital ordering on the iron atoms coupled to the helimagnetism will lead to the otherwise symmetry-forbidden peaks.

**Tuesday, March 15, 2016 8:00AM - 11:00AM —**  
Session E12 FIAP DMP: Mechanisms for Long Carrier Lifetimes and High Detectivities from Novel Ga-free Narrow Gap III-V Semiconductor Superlattices 308 - Michael Flatte, Univ of Iowa

**8:00AM E12.00001 Ga-free InAs/InAsSb type-II superlattice and its applications to IR lasers and photodetectors**, YONG-HANG ZHANG, Arizona State University — This talk will review the research on Ga-free InAs/InAsSb type-II superlattices (T2SL), especially their growth, structural and electronic properties, and applications to IR lasers and photodetectors with the following highlights: 1) Review of the previous study of InAs/InAsSb T2SL and its application to IR lasers and photodetectors in the 90's. 2) Long minority carrier lifetime up to 12.8  $\mu$ s in mid-wavelength infrared (MWIR) InAs/InAsSb T2SL was observed at 15 K, and 412 ns for long-wavelength infrared (LWIR) InAs/InAsSb T2SL were measured using time-resolved photoluminescence. The record long carrier lifetime in the MWIR range is due to carrier localization, which is confirmed by a 3 meV blue shift of the photoluminescence peak energy with increasing temperature from 15 K to 50 K, along with a photoluminescence linewidth broadening up to 40 K. In contrast, no carrier localization is observed in the LWIR T2SL. Modeling results show that carrier localization is stronger in shorter period (9.9 nm) MWIR T2SL as compared to longer period (24.2 nm) LWIR T2SL, indicating that the carrier localization originates mainly from InAs/InAsSb interface disorder. Although carrier localization enhances carrier lifetimes, it also adversely affects carrier transport. 3) Pressure-dependent photoluminescence (PL) experiments under hydrostatic pressures up to 2.16 GPa were conducted on a MWIR InAs/InAsSb T2SL structure at different pump laser excitation powers and sample temperatures. The results show a pressure coefficient of the T2SL transition was found to be  $93.2 \text{ meV/GPa}^{-1}$ ; a clear change in the dominant photo-generated carrier recombination mechanism from radiative to defect related, providing evidence for a defect level situated at 0.18 0.01 eV above the conduction band edge of InAs at ambient pressure. 4) LWIR InAs/InAsSb T2SL nBn photodetectors on GaSb substrates were demonstrated. The typical device consisted of a 2.2 micron thick absorber layer and has a 50% cutoff wavelength of 13.2  $\mu$ m, a measured dark current density of  $5 \times 10^{-4} \text{ A/cm}^2$  at 77 K under a bias of -0.3 V, a peak responsivity of 0.24 A/W at 12  $\mu$ m and a maximum RA product of 300 ohm-cm<sup>2</sup> at 77 K. The calculated generation-recombination noise limited specific detectivity ( $D^*$ ) and experimentally measured  $D^*$  at 12  $\mu$ m and 77 K are  $1 \times 10^{10} \text{ (cm-Hz}^{1/2})/\text{W}$  and  $1 \times 10^8 \text{ (cm-Hz}^{1/2})/\text{W}$ , respectively.

**8:36AM E12.00002 MWIR GaSb-based infrared detectors utilizing InAsPSb absorbers**, JIN KIM, Sandia National Lab — No abstract available.

**9:12AM E12.00003 Identification of dominant recombination mechanisms in narrow-bandgap InAs/InAsSb type-II superlattices and InAsSb alloys**, THOMAS BOGGESE, The University of Iowa — InAs/Ga(In)Sb type-II superlattices (T2SL) have been extensively studied for both advanced emitter and detector technologies associated with mid-wave (MWIR), long-wave (LWIR), and very-long-wave (VLWIR) infrared applications. The type-II band alignment, together with control of both the layer thicknesses and the alloy composition, provide a rich environment for band structure engineering, including band gap tuning and suppression of Auger recombination. Unfortunately, the InAs/Ga(In)Sb MWIR T2SLs have been found to have minority carrier lifetimes persistently below 100 ns, even at cryogenic temperatures. Such short lifetimes are problematic for detector applications and suggest that this material system will not compete with HgCdTe for IR detector applications. On the other hand, the report by Steenberg, et al., [1] of much longer minority carrier recombination lifetimes ( $>412 \text{ ns}$  at 77K) in a longwave (8.2  $\mu$ m) InAs/InAsSb T2SL suggests that the “Ga-free” superlattices could be competitive for IR detector applications. We will discuss all-optical measurements of carrier lifetimes as a function of temperature and injected carrier density in InAs/InAsSb T2SLs with a broad range of sample designs based on variations in alloy composition and/or layer thickness. Minority carrier lifetimes ranging from 4.5 s for a 9.2 m-band-gap T2SL to 18 s for a 4.2 m-band-gap T2SL have been measured at 77 K. This research was performed in collaboration with Y. Aytac, B.V. Olson, J.K. Kim, E.A. Shaner, J.F. Klem, S.D. Hawkins, and M.E. Flatté. [1] Steenberg, et al., Appl. Phys. Lett. Vol. 99, 251110 (2011).

**9:48AM E12.00004 Design of MWIR Type-II Superlattices for Infrared Photon Detectors<sup>1</sup>**, CHRISTOPH GREIN, University of Illinois at Chicago — The Type II InAs/GaInSb and InAs/InAsSb superlattices are material systems for implementation as photodetector absorbers in infrared imaging applications. In addition to cutoff wavelengths spanning the infrared spectrum, they offer degrees of freedom in their materials design (e.g. layer thicknesses, alloy compositions, number of layers in one superlattice period) that permit the optimization of an infrared photon detector's figures of merit such as detectivity through the tuning of material properties like generation/recombination lifetimes and optical absorption. We describe efforts to obtain accurate electronic band structures of superlattice semiconductors with infrared energy gaps, and employing them to evaluate nonradiative minority carrier lifetimes. Simple device models are utilized to suggest potential performance enhancements that arise from employing superlattices as infrared absorber. We also discuss current efforts to simulate the molecular beam epitaxial growth of InAs/InAsSb superlattices to predict dominant native point defects and other growth nonidealities.

<sup>1</sup>Design of MWIR Type-II Superlattices for Infrared Photon Detectors

**10:24AM E12.00005 Identification of Defect Candidates and their Effects on Carrier Lifetimes and Dark Currents in InAs/InAsSb Strained-Layer Superlattices for Infrared Detectors**, NICHOLAS KIOUSSIS, Physics Department, Cal State Univ - Northridge — The InAs/GaSb and InAs/InAsSb type-II strain-layer superlattices (T2SLS) are of great importance and show great promise for mid-wave and long-wave infrared (IR) detectors for a variety of civil and military applications. The T2SLS offer several advantages over present day detection technologies including suppressed Auger recombination relative to the bulk MCT material, high quantum efficiencies, and commercial availability of low defect density substrates. While the T2SLS detectors are approaching the empirical Rule-07 benchmark of MCT's performance level, the dark-current density is still significantly higher than that of bulk MCT detectors. One of the major origins of dark current is associated with the Shockley-Read- Hall (SRH) process in the depletion region of the detector. I will present results of ab initio electronic structure calculations of the stability of a wide range of point defects [As and In vacancies, In, As and Sb antisites, In interstitials, As interstitials, and Sb interstitials] in various charged states in bulk InAs, InSb, and InAsSb systems and T2SLS. I will also present results of the transition energy levels. The calculations reveal that compared to defects in bulk materials, the formation and defect properties in InAs/InAsSb T2SLS can be affected by various structural features, such as strain, interface, and local chemical environment. I will present examples where the effect of strain or local chemical environment shifts the transition energy levels of certain point defects either above or below the conduction band minimum, thus suppressing their contribution to the SRH recombination.

**Tuesday, March 15, 2016 8:00AM - 11:00AM —**  
**Session E13 DAMOP: Exploring Topological Physics with Cold Atoms** 309 -

**8:00AM E13.00001 From Berry's Phase to Wilson Lines in a Honeycomb Optical Lattice** , MONIKA SCHLEIER-SMITH, Department of Physics, Stanford University — I will report on methods for fully characterizing the topology and geometry of Bloch bands in optical lattices. Using a Bose-Einstein condensate as a momentum-resolved probe, we study a paradigmatic model system, the honeycomb lattice. Its salient features are two Dirac points, each producing a half-quantum of Berry flux similar to the magnetic flux of an infinitesimally narrow solenoid. We have detected this singular Berry flux by forming an Aharonov-Bohm-type interferometer in momentum space.<sup>1</sup> Our technique is broadly applicable to mapping out the Berry curvature or directly measuring the Chern number of a single band. I will furthermore show how interband dynamics can reveal the matrix-valued Wilson line, the generalization of Berry's phase to the multi-band setting.<sup>2</sup> In the simple case where the Wilson line is path-independent and Abelian, it serves as a powerful tool for tomographic reconstruction of the band eigenstates.

<sup>1</sup>L. Duca, T. Li, M. Reitter, I. Bloch, M. Schleier-Smith, and U. Schneider. *Science* **347**, 288 (2015).

<sup>2</sup>T. Li, L. Duca, M. Reitter, F. Grusdt, E. Demler, M. Endres, M. Schleier-Smith, I. Bloch, and U. Schneider. *arXiv:1509.02185[cond-mat/quant-gas]* (2015).

**8:36AM E13.00002 Geometric "charge" pumping with a Bose-Einstein condensate** , IAN SPIELMAN, JQI, NIST and the University of Maryland — We realized a quantum "charge" pump for a Bose-Einstein condensate (BEC) in a novel bipartite magnetic lattice, whose bands are characterized by non-trivial topological invariants: the Zak phases. For each band, the Zak phase is determined by that band's integrated Berry curvature, a geometric quantity defined at each crystal momentum. We probed this Berry curvature in a charge pump experiment, by periodically and adiabatically driving the system. Unlike topological charge pumps in filled bands that yield quantized pumping, our BEC occupied just a single crystal momentum state allowing us to access its band's local geometry. Like topological charge pumps, for each pump cycle we observed an overall displacement (here, not quantized) and a temporal modulation of the atomic wavepacket's position in each unit cell, i.e., the polarization. Our magnetic lattice enabled us to observe this modulation by measuring the BEC's magnetization. While our periodic drive shifted the lattice potential by one unit cell per cycle, the displacement of the BEC, solely determined by the underlying Berry curvature, was always less than the lattice's displacement.

**9:12AM E13.00003 Measuring Chern numbers in Atomic Gases: 2D and 4D Quantum Hall Physics in the Lab** , NATHAN GOLDMAN, Université Libre de Bruxelles (ULB) — Optical-lattice experiments have recently succeeded in probing the geometry of 2D Bloch bands with cold neutral atoms. Beyond these local geometrical effects, which are captured by the Berry curvature, 2D Bloch bands may also display non-trivial topology, a global property captured by a topological invariant (e.g. the first Chern number). Such topological properties have dramatic consequences on the transport of non-interacting atoms, such as quantized responses whenever the bands are uniformly populated. In this talk, I will start with the first experimental demonstration of topological transport in a gas of neutral particles, which revealed the Chern number through a cold-atom analogue of quantum-Hall measurements<sup>1</sup>. I will then describe how this Chern-number measurement could be extended in order to probe the topology of higher-dimensional systems. In particular, I will show how the *second Chern number* – an emblematic topological invariant associated with 4D Bloch bands – could be extracted from an atomic gas, using a 3D optical lattice extended by a synthetic dimension<sup>2</sup>. Finally, I will describe a general scheme by which optical lattices of subwavelength spacing could be realized<sup>3</sup>. This method leads to topological band structures with significantly enhanced energy scales, offering an interesting route towards the experimental realization of strongly-correlated topological states with cold atoms.

<sup>1</sup>*Measuring the Chern Number of Hofstadter Bands with Ultracold Bosonic Atoms*,

M. Aidelsburger, M. Lohse, C. Schweizer, M. Atala, J. T. Barreiro, S. Nascimbene, N. R. Cooper, I. Bloch and N. Goldman, *Nature Physics* **11**, 162 (2015).

<sup>2</sup>*Four-Dimensional Quantum Hall Effect with Ultracold Atoms*,

H. M. Price, O. Zilberberg, T. Ozawa, I. Carusotto and N. Goldman, *Phys. Rev. Lett.* **115**, 195303 (2015).

<sup>3</sup>*Dynamic Optical Lattices of Subwavelength Spacing for Ultracold Atoms*,

S. Nascimbene, N. Goldman, N. R. Cooper and J. Dalibard, *Phys. Rev. Lett.* **115**, 140401 (2015).

**9:48AM E13.00004 Experimental Realization of the Harper-Hofstadter Model** , COLIN KENNEDY, MIT — Extensions of Berry's phase and the quantum Hall effect have led to the discovery of new states of matter with topological properties. Traditionally, this has been achieved using magnetic fields or spin-orbit interactions, which couple only to charged particles. For neutral ultracold atoms, synthetic magnetic fields have been created that are strong enough to realize the Harper-Hofstadter model. In this talk, I report on work studying Bose-Einstein condensation in the Harper-Hofstadter Hamiltonian with one-half flux quantum per lattice unit cell. The diffraction pattern of the superfluid state directly shows the momentum distribution of the wavefunction, which is gauge-dependent, and it reveals both the reduced symmetry of the vector potential and the degeneracy of the ground state. I present an adiabatic, many-body state preparation protocol via the Mott insulating phase and show the superfluid ground state in a three-dimensional lattice with moderate interactions. I will discuss progress towards a triple-superlattice implementation as well as prospects for exploring exotic states close to the Mott transition.

**10:24AM E13.00005 Topological Charge Pumping with Cold Atoms** , YOSHIRO TAKAHASHI, Kyoto University — More than 30 years ago, Thouless considered an interesting phenomenon of quantum transport of an electron gas in an infinite one-dimensional periodic potential, driven in a periodic cycle. The charge pumped by this Thouless pump is a topological quantum number and does not depend on a smooth change of parameters. Importantly, this charge pumping shares the same topological origin as the integer quantum Hall effect. In spite of the importance in a topological quantum physics, this Thouless pump has never been realized in any system. In this study, we successfully realize the Thouless topological pump by exploiting the controllability of ultracold atoms in an optical superlattice. The charge pumping is detected as a shift of the center of mass of an atomic cloud measured with in situ absorption imaging. We extract the Chern number of the system from the average shift of the center of mass per pumping cycle. The topological nature of the pump is revealed by the clear dependence on the topology of the pumping trajectories in parameter space of our superlattice. We will describe the detail of our experiments using fermionic ytterbium atoms and also discuss the prospects of our research.

**Tuesday, March 15, 2016 8:00AM - 11:00AM –**

Session E14 CSWP: Understand and Improve the Status of Women in Physics 310 - Cha-Mei Tang, Creatv MicroTech. Inc.

**8:00AM E14.00001 Reversing into Meritocracy: Shifting the Culture of Physics** , EDMUND BERTSCHINGER, Massachusetts Institute of Technology — Culture is the dark energy of our lives: it is an invisible force that shapes our environment for work and life. Physics culture often includes the assumption that people have equal access to resources and opportunities regardless of gender, race, or any other demographic characteristic. Numerous studies show this is false, yet the invisible force of meritocracy shapes many departments, and its passive acceptance can foster inequitable working environments. Department chairs and other leaders play a key role in shifting institutional culture to leverage the power of diversity, improve student and employee success, and enhance the quality of life for everyone. I will describe steps taken at MIT to shift our cultural direction so that we are not driving in reverse on the highway of meritocracy.

**8:36AM E14.00002 New research on women's low participation in science and technology**<sup>1</sup> , JANE STOUT, Computing Research Association — It is well known that women have historically been and continue to be grossly underrepresented in technical fields (i.e., the physical sciences, engineering, and computing). This presentation will address the following research questions: What dissuades women from entering into a technical career track, and what are women's experiences like within technical fields? At the same time, this presentation will acknowledge a shortcoming of decades of social science research and interventions designed to improve women's interest and persistence in technical fields: a narrow definition of "women". Given that the majority of women in colleges and universities (i.e., the typical sites of social science research) tend to be affluent and/or White, STEM education research that relies on convenience samples at colleges and universities paints a skewed picture of gender issues in technical fields. This presentation will showcase research findings that call into question conventional conceptions of gender disparities in technical fields. Specifically, the presentation will emphasize the importance of recognizing that women constitute more than their gender; women come from a diverse array of backgrounds, which no doubt play a role in the experience of being a woman in technical fields. By understanding the experiences of women from a broad array of demographics groups, the STEM education community can develop a corresponding set of strategies to recruit and retain women with diverse interests, experiences, and values (e.g., first generation versus second college students; women of different racial/ethnic backgrounds). The aim of this presentation is to promote social science research and interventions that acknowledge the nuanced experiences of diverse women in technical fields, in order to address the seemingly intractable problem of women's underrepresentation in technical fields.

<sup>1</sup>NSF DUE-1431112, NSF CNS-1246649

**9:12AM E14.00003 Interactive Leadership Training: "Be the Leader You Already Are"** , JOHN RIORDAN, Cindy Zook Associates — No abstract available.

**10:20AM E14.00004 Panel Discussion** —

**Tuesday, March 15, 2016 8:00AM - 11:00AM** —

**Session E15 DMP: 2D Devices: Mobility and Energy Relaxation** 314 - Wenjuan Zhu, University of Illinois at Urbana-Champaign

**8:00AM E15.00001 Graphene based GHz detectors.**<sup>1</sup> , ANTHONY K BOYD, ASEE Postdoctoral Fellow in-residence at U.S. Naval Research Lab, Washington DC, ABDEL EL FATIMY, PAOLA BARBARA, Georgetown University, ANINDYA NATH, George Mason University Postdoctoral fellow in-residence at U.S. Naval Research Lab, Washington DC, PAUL M CAMPBELL, RACHAEL MYERS-WARD, U.S. Naval Research Laboratory, KEVIN DANIELS, NRC Postdoctoral fellow in-residence at U.S. Naval Research Lab, Washington DC, D. KURT GASKILL, U.S. Naval Research Laboratory — Graphene demonstrates great promise as a detector over a wide spectral range especially in the GHz range. This is because absorption is enhanced due to the Drude contribution. In the GHz range there are viable detection mechanisms for graphene devices. With this in mind, two types of GHz detectors are fabricated on epitaxial graphene using a lift off resist-based clean lithography process to produce low contact resistance.[1] Both device types use asymmetry for detection, consistent with recent thoughts of the photothermoelectric effect (PTE) mechanism. The first is an antenna coupled device. It utilizes two dissimilar contact metals and the work function difference produces the asymmetry. The other device is a field effect transistor constructed with an asymmetric top gate that creates a PN junction and facilitates tuning the photovoltaic response. The response of both device types, tested from 100GHz to 170GHz, are reported. 1. Nath Anindya et al Applied Physics Letters 104, 224102 (2014)

<sup>1</sup>This work was sponsored by the U.S. Office of Naval Research (award number N000141310865)

**8:12AM E15.00002 Optimization of thermoelectric power factor in ion-gated ultrathin WSe2 single crystals** , YIJIN ZHANG, MASARO YOSHIDA, TAKAHIKO IIZUKA, RYUJI SUZUKI, YOSHIHIRO IWASA, Department of Applied Physics, The University of Tokyo, SUNAO SHIMIZU, RIKEN Center for Emergent Matter Science — We report an electric field tuning of the thermopower in ultrathin WSe2 single crystals over a wide range of carrier concentration by using electric double-layer (EDL) technique. We fabricated a micro-sized EDL transistor with on-chip heaters and thermometers for an ultrathin flake of WSe2. We succeeded in the optimization of power factor not only in the hole but also in the electron side, which has never been chemically accessed. The maximized values of power factor are one-order larger than that obtained by changing chemical composition, reflecting the clean nature of electrostatic carrier doping.

**8:24AM E15.00003 Quantum lifetime in BN-encapsulated graphene devices** , JESSE BALGLEY, SCOTT DIETRICH, Columbia University, LEI WANG, Cornell University, VITTO HAN, BO WEN, YUANDA GAO, JAMES HONE, CORY DEAN, Columbia University — Encapsulating monolayer graphene in BN has lead to vastly enhanced device quality, leading to significantly increased mobility and quantum lifetimes on the order of picoseconds. However, magnetoresistance measurements in the quantum Hall regime reveal remnant disorder that continues to inhibit transport measurement. Here we report a study of the Shubnikov-de Haas oscillations in very high mobility devices. Comparison of the mean scattering and quantum lifetimes suggest that remote impurities remain the dominant scattering mechanism. The source of this remnant disorder, and the consequence for mobility enhancement in BN-supported 2D materials beyond graphene is discussed.

**8:36AM E15.00004 Velocity Saturation of Hot Carriers in Two-Dimensional Transistors<sup>1</sup>**, JONATHAN BIRD, University at Buffalo — Two-dimensional (2D) materials, including graphene and transition-metal dichalcogenides, have emerged in recent years as possible “channel-replacement” materials for use in future generations of post-CMOS devices. Realizing the full potential of these materials requires strategies to maximize their current-carrying capacity, while minimizing Joule losses to its environment. A major source of dissipation for hot carriers in any semiconductor is spontaneous optical-phonon emission, resulting in saturation of the drift velocity. In this presentation, I discuss the results of studies of velocity saturation in both graphene and molybdenum-disulphide transistors, emphasizing how this phenomenon impacts resulting transistor operation. While in graphene the large intrinsic optical-phonon energies promise high saturation velocities, experiments to date have revealed a significant degradation of the drift velocity that arises from the loss of energy from hot carriers to the underlying substrate. I discuss here how this problem can be overcome by implementing a strategy of nanosecond electrical pulsing [H. Ramamoorthy et al., Nano Lett., under review], as a means to drive graphene’s hot carriers much faster than substrate heating can occur. In this way we achieve saturation velocities that approach the Fermi velocity near the Dirac point, and which exceed those reported for suspended graphene and for devices fabricated on boron nitride substrates. Corresponding current densities reach those found in carbon nanotubes, and in graphene-on-diamond transistors. In this sense we are able to “free” graphene from the influence of its substrate, revealing a pathway to achieve the superior electrical performance promised by this material. Velocity saturation is also found to be important for the operation of monolayer molybdenum-disulphide transistors, where it limits the drain current observed in saturation [G. He et al., Nano Lett. **15**, 5052 (2015)]. The implications of these results for 2D transistor performance will be explored in my presentation.

<sup>1</sup>This research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02-04ER46180

**9:12AM E15.00005 Electrical Transport in Ultra-Short Atomically Thin Devices**, MATHIAS BOLAND, M. JAVAD FARROKHI, MOHSEN NASSERI, DOUGLAS STRACHAN, University of Kentucky — Ultra-short nanoscale devices that incorporate atomically-thin materials have the potential to be the smallest electronics. These materials represent the ultimate size-scaling in the vertical dimension and could be ideal as channel, electrode, and dielectric materials for a variety of applications – especially for ultrafast electronics. Such extremely-scaled devices can show unique transport characteristics that depended sensitively on their atomic-scale configurations. Here we report several atomically-thin ultra-short device schemes we have been developing which includes those consisting of single and bilayer graphene channels. Electrical transport measurements show very unique characteristics between these ultra-short devices that are highly sensitive to the atomic layer number. This sensitivity suggests that these ultra-short devices are strongly dependent on the unique chiral nature of the charge carriers in these atomically-thin channel materials.

**9:24AM E15.00006 Chemical assembly of atomically thin transistors and circuits in a large scale**, MERVIN ZHAO, YU YE, Univ of California - Berkeley, YIMO HAN, Cornell University, YANG XIA, HANYU ZHU, YUAN WANG, Univ of California - Berkeley, DAVID MULLER, Cornell University, XIANG ZHANG, Univ of California - Berkeley — Next-generation electronics calls for new materials beyond silicon for increased functionality, performance, and scaling in integrated circuits. 2D gapless graphene and semiconducting TMDCs have emerged as promising electronic materials due to their atomic thickness, chemical stability and scalability. However, difficulties in the assembly of 2D electronic structures arise in the precise spatial control over the conducting and semiconducting crystals, typically relying on physically transferring them. Ultimately, this renders them unsuitable for an industrial scale and impedes the maturity of integrating atomic elements in modern electronics. Here, we report the large-scale spatially controlled synthesis of the single-layer MoS<sub>2</sub> laterally in electrical contact with graphene using a seeded growth method. TEM studies reveal that the single-layer MoS<sub>2</sub> nucleates at the edge of the graphene, creating a lateral van der Waals heterostructure. The graphene allows for electrical injection into MoS<sub>2</sub>, creating 2D atomic transistors with high transconductance, on-off ratios, and mobility. In addition, we assemble 2D logic circuits, such as a heterostructure NMOS inverter with a high voltage gain, up to 70.

**9:36AM E15.00007 Nonlinear Ballistic Transport in Graphene Devices**, M. JAVAD FARROKHI, MATHIAS BOLAND, MOHSEN NASSERI, DOUGLAS STRACHAN, University of Kentucky — Through the extreme size scaling of electronic devices, there is great potential to achieve highly efficient and ultrafast electronics. By scaling down the channel length in graphene transistors to the point where the mean free path exceeds the relevant channel length, the electron transport can transition from a diffusive regime to an intrinsic ballistic regime. In such a regime, both quantum tunneling at the electrode-channel interface and the screening length, as determined by electrode-channel barrier width, can have a strong effect on current nonlinearity and asymmetric gate response. Here we discuss our experimental results on nanogap electrodes to graphene channels that show quantitative agreement with an intrinsic ballistic model. Moreover, this behavior persists to room temperature and on standard oxide substrates, providing strong evidence for a new regime of nonlinearity in graphene devices that could be of potential use for electronic applications.

**9:48AM E15.00008 Resonant high harmonic generation in a ballistic graphene transistor with an AC driven gate**, TOMAS LOFWANDER, YEVGENIY KORNIYENKO, OLEKSII SHEVTSOV, Chalmers University of Technology — We report a theoretical study of time-dependent transport in a ballistic graphene field effect transistor. We develop a model based on Floquet theory describing Dirac electron transmission through a harmonically driven potential barrier. Photon-assisted tunneling results in excitation of quasibound states at the barrier. Under resonance condition, the excitation of the quasibound states leads to promotion of higher-order sidebands and enhanced higher harmonics of the source-drain conductance. The resonances in the main transmission channel are of the Fano form, while they are of the Breit-Wigner form for sidebands. We discuss the possibility of utilizing the resonances in prospective ballistic high-frequency devices, in particular frequency multipliers.

**10:00AM E15.00009 Substrate dependence of Hall and Field-effect mobilities in few-layer MoS<sub>2</sub> field-effect transistors<sup>1</sup>**, BHIM CHAMLAGAIN, MEEGHAGE PERERA, HSUEN-JEN CHUANG, ARTHUR BOWMAN, UPENDRA RIJAL, KRAIG ANDREWS, JOSEPH KLESKO, CHARLES WINTER, ZHIXIAN ZHOU, Wayne State University — In this work, we systematically study the Hall and field-effect mobilities of few-layer MoS<sub>2</sub> FETs fabricated on different substrates. Hall bar devices were fabricated on SiO<sub>2</sub> and hBN to directly measure carrier density. Standard four-probe transport measurement and Hall effect measurement were carried out for a wide temperature range to determine the carrier mobility and understand the scattering mechanisms. By comparing field-effect and Hall mobilities, we demonstrate that the intrinsic drift mobility of multi-layer MoS<sub>2</sub> in the high carrier density metallic region is independent of substrate and sample thickness. While the optical-phonon scattering remains the dominant scattering mechanism in MoS<sub>2</sub> devices on h-BN down to ~100 K, extrinsic scattering mechanisms start to degrade the carrier mobility of MoS<sub>2</sub> on all other substrates below ~200 K.

<sup>1</sup>NSF grant number DMR-1308436

**10:12AM E15.00010 ABSTRACT WITHDRAWN —**

**10:24AM E15.00011 What Makes Effective Gating Possible in Two-Dimensional Heterostructures?**<sup>1</sup>, IGOR ZUTIC, University at Buffalo, PREDRAG LAZIC, Rudjer Boskovic Institute, KIRILL D. BELASHCHENKO, University of Nebraska-Lincoln — Electrostatic gating provides a way to obtain key functionalities in modern electronic devices and to qualitatively alter materials properties. While electrostatic description of such gating gives guidance for related doping effects, inherent quantum properties of gating provide opportunities for intriguing modification of materials and unexplored devices. Using first-principles calculations for Co/bilayer graphene, Co/BN, and Co/benzene, as well as a simple physical model, we show that magnetic heterostructures with two-dimensional layered materials can manifest tunable magnetic proximity effects [1]. van der Waals bonding is identified as a requirement for large electronic structure changes by gating. In particular, the magnitude and sign of spin polarization in physisorbed graphene can be controlled by gating, which is important for spintronic devices [2,3]. [1] P. Lazić, K. D. Belashchenko, and I. Žutić, arXiv:1510.05404. [2] P. Lazić, G. M. Sipahi, R. K. Kawakami, and I. Žutić, Phys. Rev. B **90**, 085429 (2014). [3] H. Dery et al., IEEE Trans. Electron. Dev. **59**, 259 (2012).

<sup>1</sup>Supported by U.S. ONR Grant N000141310754, U.S. DOE-BES Award DE-SC0004890, NSF DMR-1124601, the Center for NanoFerroic Devices, the Nanoelectronics Research Initiative, and NSF DMR-1308751.

**10:36AM E15.00012 Highly sensitive hBN/graphene hot electron bolometers with a Johnson noise readout**, DMITRI EFETOV, Massachusetts Institute of Technology, YUANDA GAO, Columbia University, EVAN WALSH, REN-JYE SHIUE, GABRIELE GROSSO, CHENG PENG, Massachusetts Institute of Technology, JAMES HONE, Columbia University, KIN CHUN FONG, BBN Raytheon, DIRK ENGLUND, Massachusetts Institute of Technology — Graphene has remarkable opto-electronic and thermo-electric properties that make it an exciting functional material for various photo-detection applications. In particular, owed to graphenes unique combination of an exceedingly low electronic heat capacity and a strongly suppressed electron-phonon thermal conductivity  $G_{th}$ , the electronic and phononic temperatures are highly decoupled allowing an operation principle as a hot electron bolometer (HEB). Here we demonstrate highly sensitive HEBs made of high quality hBN/graphene/hBN stacks and employ a direct electronic temperature read out scheme via Johnson noise thermometry (JNT). We perform combined pump-probe and JNT measurements to demonstrate strongly damped  $C_e$  and  $G_{th}$  in the ultra-low impurity  $\sigma_i = 10^9 \text{ cm}^{-2}$  hBN/G/hBN stacks, which result in unprecedented photo-detection sensitivity and noise equivalent power for graphene HEBs.

**10:48AM E15.00013 Design and fabrication of an antenna-coupled graphene terahertz mixer**<sup>1</sup>, EDWARD LEONG, Univ of Maryland-College Park, JAKE CONNERS, CHEUK-YU E. TONG, PAUL K. GRIMES, LINGZHEN ZENG, Harvard-Smithsonian Center for Astrophysics, MARTIN MITTENDORFF, THOMAS E. MURPHY, Univ of Maryland-College Park — Graphene has shown promise for tunable terahertz (THz) technology, including detectors, modulators, filters, and emitters. Graphene exhibits a significant change in conductivity when the Fermi energy is altered by applying a gate voltage. Near the Dirac point, graphene field effect transistors (FETs) show a strongly nonlinear response (i.e. a strong change in resistivity with applied voltage) that can be exploited to provide efficient rectification and mixing of THz signals. Although rectification in graphene field-effect transistors has been demonstrated, heterodyne mixing in the THz band has not been explored. We examine a THz graphene mixer using an antenna-coupled graphene FET configuration. We will discuss the antenna and graphene device design optimized for heterodyne mixing 0.35 THz. In addition, fabrication and preliminary measurements of a lower frequency prototype will be presented to demonstrate the principle of the operation.

<sup>1</sup>Supported by the UMD/SI Seed Grant Research Program

**Tuesday, March 15, 2016 8:00AM - 10:48AM –**  
**Session E16 DMP: Graphene and Graphene Nanoribbons** 315 - Jing Kong, MIT

**8:00AM E16.00001 Observation of dopant-induced impurity states in bottom-up graphene nanoribbons**, ZAHRA PEDRAMRAZI, CHEN CHEN, TOMAS MARANGONI, RYAN CLOKE, TING CAO, STEVEN LOUIE, FELIX FISCHER, MICHAEL CROMMIE, Univ of California - Berkeley — Graphene nanoribbons (GNRs) provide a means for inducing energy gaps in graphene and are a promising candidate for many nanotechnological applications. New bottom-up fabrication techniques allow the structure of GNRs to be tuned with atomic precision, thus providing new opportunities for modifying their electronic structure. Here we report the synthesis of bottom-up armchair GNRs (AGNRs) with isolated substitutional boron-dopant centers; thus creating localized impurity states in the GNR. These impurities are realized via dilute doping of pristine  $n=7$  AGNRs with sparse boron-containing monomer units, resulting in uniform-width  $n=7$  AGNR segments where only two carbon atoms have been substitutionally replaced by boron atoms. Scanning tunneling microscopy (STM) and spectroscopy (STS) were performed to study the electronic structure of these AGNR impurity systems, enabling us to observe localized mid-gap impurity states.

**8:12AM E16.00002 Bottom-up Synthesis of N=13 Sulfur-doped Graphene Nanoribbons.**, TRINITY JOSHI, GIANG NGUYEN, FRANCESCA TOMA, TING CAO, ZAHRA PEDRAMRAZI, CHEN CHEN, DANIEL RIZZO, CHRISTOPHER BRONNER, YEN-CHIA CHEN, STEVEN LOUIE, FELIX FISCHER, MICHAEL CROMMIE, University of California, Berkeley — Substitutional doping of graphene nanoribbons (GNRs) with heteroatoms is a principal strategy to fine-tune the electronic structure of GNRs for future device applications. Up to now, however, edge-doping in bottom-up fabricated GNRs has exclusively relied on the introduction of nitrogen heteroatoms in the form of pyridine and pyrimidine rings along the edges of chevron GNRs. Here we report the bottom-up synthesis and characterization of atomically-precise  $N=13$  armchair graphene nanoribbons (S-13-AGNRs) wherein alternating  $(CH)_2$  groups lining the edges of the GNRs have been replaced by sulfur atoms. We study the resultant GNR with scanning tunneling microscopy (STM) and spectroscopy (STS). Our experimental results are consistent with first-principles simulations of the S-13-AGNR electronic structure.

**8:24AM E16.00003 Bottom-up fabrication and characterization of boron doped N=7 armchair graphene nanoribbons**, GIANG D. NGUYEN, ARASH A. OMRANI, HSIN-ZON TSAI, DANIEL J. RIZZO, TRINITY JOSHI, CHRISTOPHER BRONNER, RYAN R. CLOKE, TOMAS MARANGONI, TING CAO, GRIFFIN F. RODGERS, WON-WOO CHOI, Univ of California - Berkeley, STEVEN G. LOUIE, Univ of California - Berkeley and Lawrence Berkeley National Laboratory, FELIX R. FISCHER, MICHAEL F. CROMMIE, Univ of California - Berkeley and Kavli Energy NanoSciences Institute, and Lawrence Berkeley National Laboratory — Graphene nanoribbons (GNRs) have recently attracted great interest because of their novel electronic and magnetic properties, as well as the significant potential they have for device applications. Although several top-down techniques exist for fabricating GNRs, only bottom-up synthesis of GNRs from molecular precursors yields nanoribbons with atomic-scale structural control. Here we report the successful bottom-up fabrication boron doped  $N=7$  armchair graphene nanoribbons. Substitutional boron atoms were incorporated into the GNRs' central backbone, thus placing boron's empty p-orbital in conjugation with the extended  $\pi$  system of the GNR. Topographic and local electronic structure characterization was performed via STM and CO-tip-functionalized nc-AFM, and compared to DFT simulations.

**8:36AM E16.00004 Structure and Electronic Properties of Polymer Chains and Graphene Nanoribbon Formed by Molecular Self-Assembly on Au(111).** , CHUANXU MA, MIGUEL A. FUENTES-CABRERA, BOBBY G. SUMPTER, KUNLUN HONG, AN-PING LI, Oak Ridge National Laboratory, ZHONGCAN XIAO, WENCHANG LU, J. BERNHOLC, North Carolina State University — Graphene nanoribbons (GNRs) with bandgaps are promising building blocks for ultra-fast electronics. Bottom-up synthesis of GNRs from aromatic hydrocarbon molecules has been proven to be an effective way to control GNR's width with atomically precise edge structures. Using scanning tunneling microscopy (STM), we study the formation of both linear polymer chains and narrow GNRs in the bottom-up self-assembly process with the DBBA molecules as the precursor on Au(111). The linear polymer chains are formed after the deposition of DBBA and 200 C annealing for 30 min. The polymers can be converted to 7-AGNRs (seven-carbon wide armchair GNRs) after 400 C annealing. Interestingly, second-layer polymer is seen to survive on the GNRs during the annealing process. This result indicates that the Au(111) substrate plays an important role in the dehydrogenation process and the formation of GNRs, which is confirmed by our DFT calculations. Electronically, the polymers show a bandgap of 3.4 eV, much larger than that of GNRs. After annealing at 500 C for 30 min, wider GNRs can form: 14-AGNR, 21-AGNR. The 7-AGNR shows a typical edge state at -1.1 eV, while for 14-AGNR it is at -1.35 eV. Moreover, junctions of GNRs with different widths can be formed with pronounced boundary states.

**8:48AM E16.00005 Graphene Nanoribbons Anchored to a SiC Substrate.** , LILIA WOODS, NAM LE, University of South Florida, Department of Physics — Due to their exceptional fundamental characteristics graphene nanoribbons play a major role in the development of future nano-technological applications. The high chemical reactivity of the graphene nanoribbon edges can be utilized to create modified materials. Using first principles simulations we explore this possibility to construct patterned systems composed of anchored ribbons of zigzag edges covalently bonded to a SiC substrate. The hybrid edge states are found to possess interesting electronic and magnetic properties, which alter the overall behavior of the entire system as compared to the behavior of the individual components. It is found that the van der Waals interactions are important for the overall stability and structure of the anchored ribbons. Also, spin-polarization effects play a profound role in the electronic structure and associated density of states. The hybrid graphene/SiC zigzag edges are analyzed in terms of their transport characteristics as well.

**9:00AM E16.00006 Pseudospin dephasing in relaxed shape armchair graphene nanoribbons** , SANJAY PRABHAKAR, RODERICK MELNIK, Wilfrid Laurier University, LUIS BONILLA, Universidad Carlos III de Madrid — In this presentation, we argue that the Zeeman pseudospin splitting energy might not be neglected for smaller widths of the graphene nanoribbons (GNRs). Mathematically valid study shows that the pseudospin splitting energy breaks the symmetry of degeneracy due to ripple induced Zeeman effect in GNRs originating from electromechanical effects. We estimate the spin relaxation time caused by in-plane phonon modes for possible application in straintronics and quantum information processing. We acknowledge Natural Sciences and Engineering Research Council of Canada and Canada Research Chair programs for their financial support.

**9:12AM E16.00007 Decay patterns of edge states at reconstructed armchair graphene edges<sup>1</sup>** , CHANGWON PARK, ORNL, USA, JISOON IHM, Seoul National Univ., Korea, GUNN KIM, Sejong Univ., Korea — Density functional theory calculations are used to investigate the electronic structures of localized states at reconstructed armchair graphene edges. We consider graphene nanoribbons with two different edge types and obtain the energy band structures and charge densities of the edge states. By examining the imaginary part of the wave vector in the forbidden energy region, we reveal the decay behavior of the wave functions in graphene. The complex band structures of graphene in the armchair and zigzag directions are presented in the first-principles framework.

<sup>1</sup>G.K. acknowledges the support of the Basic Science Research Program through the National Research Foundation of Korea funded by the Ministry of Education (Grant No. 2013R1A1A2009131) and the Priority Research Center Program (Grant No. 2010-0020207).

**9:24AM E16.00008 Orientationally Misaligned Zipping of Lateral Graphene and Boron Nitride Nanoribbons with Minimized Strain Energy and Enhanced Half-Metallicity<sup>1</sup>** , JIANG ZENG, University of Science and Technology of China, WEI CHEN, Harvard University, PING CUI, University of Science and Technology of China, DONG-BO ZHANG, Beijing Computational Science Research Center, ZHENYU ZHANG, University of Science and Technology of China — Lateral heterostructures of two-dimensional materials may exhibit various intriguing emergent properties. Yet when specified to the orientationally aligned heterojunctions of zigzag graphene and hexagonal boron nitride (hBN) nanoribbons, realizations of the high expectations on their properties encounter two standing hurdles. First, the rapid accumulation of strain energy prevents large-scale fabrication. Secondly, the pronounced half-metallicity predicted for freestanding graphene nanoribbons is severely suppressed. By properly tailoring orientational misalignment between zigzag graphene and chiral hBN nanoribbons, here we present a facile approach to overcome both obstacles. Our first-principles calculations show that the strain energy accumulation in such heterojunctions is significantly diminished for a range of misalignments. More strikingly, the half-metallicity is substantially enhanced from the orientationally aligned case, back to be comparable in magnitude with the freestanding case. The restored half-metallicity is largely attributed to the recovered superexchange interaction between the opposite heterojunction interfaces. The present findings may have important implications in eventual realization of graphene-based spintronics.

<sup>1</sup>This work was supported by the National Natural Science Foundation of China and the National Key Basic Research Program of China.

**9:36AM E16.00009 First principles-based moiré model for incommensurate graphene on BN<sup>1</sup>** , CATALIN SPATARU, KONRAD THURMER, Sandia National Labs — Various properties of supported graphene films depend strongly on the exact positions of carbon atoms with respect to the underlying substrate. While density functional theory (DFT) can predict atom position in many systems, it cannot be applied straightforwardly to systems that are incommensurate or have large unit cells, such as graphene on a BN surface. We address these limitations by developing a simple moiré model with parameters derived from DFT calculations for systems strained into commensurate structures with manageable unit cell sizes. Our moiré model, which takes into account the flexural rigidity of graphene and includes the influence of the substrate, is able to reproduce the DFT-relaxed carbon positions with an accuracy of <0.01 Å. We then apply this model to the unstrained C/BN system and predict how structure and energy vary with azimuthal orientation of the graphene sheet with respect to the BN substrate.

<sup>1</sup>Work supported by the Laboratory Directed Research and Development program at Sandia National Laboratories, a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Co., for the U.S. DOE under contract DE-AC04-94AL85000.

Structure and Electronic Properties of Polymer Chains and Graphene Nanoribbon Formed by Molecular Self-Assembly on Au(111)

submitted by Dr. Chuanxu Ma, with ID 61213787, and this talk following Dr. Ma's?

**10:00AM E16.00011 A first-principles study on Magnetic and Electronic properties of Graphane vacancies Dots.**

, BI-RU WU, Department of Natural science, Center for General Education, Chang Gung University, Kueishan 333, CHIH-KAI YANG, Graduate Institute of Applied Physics, National Chengchi University, Taipei 11605 — Graphane is the end product of the complete hydrogenation of graphene. The incomplete hydrogenation of graphene produces hydrogen vacancies in graphane. Hydrogen vacancies can alter the electronic structure of graphane and therefore tune the electronic, magnetic, and optical properties of the composite. In this paper, we use a first-principles density functional calculation to investigate a variety of well-separated clusters of hydrogen vacancies in graphane with magnetism, including the geometrical shapes of triangles, parallelograms, and rectangles. The results indicate that energy levels caused by the missing H are generated in the broad band gap of pure graphane. All triangular clusters of H vacancies are magnetic, the larger the triangle the higher the magnetic moment. The defect levels introduced by the missing H in triangular and parallelogram clusters are spin-polarized and can find application in optical transition. Parallelograms and open-ended rectangles are antiferromagnetic and can be used for nanoscale registration of digital information.

**10:12AM E16.00012 Influence of Spatial Inhomogeneity on Electronic and Magneto Transport in Graphene.**<sup>1</sup>

, BERNARD MATIS, BRIAN HOUSTON, JEFFREY BALDWIN, Naval Research Laboratory — We discuss room temperature electronic and magnetotransport measurements of polycrystalline graphene, grown by chemical vapor deposition, on a SiO<sub>2</sub> dielectric. The measured graphene devices are intentionally spatially inhomogeneous such that the length of the sample is much greater (>1000 times) than the average grain size. At magnetic field  $B = 0$  T the electronic transport is well described by a diffusive transport model with contributions from grain boundary scattering significantly larger in the high charge carrier density limit. We find the largest percent change in the magnetoresistivity occurs at the film's Dirac point where the magnetotransport is largely dependent upon charge disorder. Away from the Dirac point we find a modified expression for the charge carrier density dependence of the magnetoresistivity with respect to the case of single-crystal graphene.

<sup>1</sup>This work was supported by the Office of Naval Research.

**10:24AM E16.00013 Spontaneous and Thermally Enhanced Charge Transfer at Graphene-Silica Interface**

, KWANGHEE PARK, Department of Chemistry, Pohang University of Science and Technology, SUNMIN RYU<sup>1</sup>, Department of Chemistry, Division of Advanced Materials Science, Pohang University of Science and Technology — Low dimensional carbon materials undergo spontaneous hole doping in the ambient conditions. Thermal annealing enhances the degree of the charge transfer in silica-supported graphene exposed to oxygen and water vapor. In this work, we investigated the mechanisms responsible for the charge transfer using Raman spectroscopy and water contact angle measurements. Mechanically exfoliated graphene samples were annealed at various temperatures in a range of 100 to 1000 °C to induce the hole doping. While the annealing-induced charge density of graphene increased with increasing annealing temperature up to 700 °C, it decreased as increasing the temperature further higher. Graphene samples prepared in a low humidity condition lead to significantly decreased hole doping suggesting that water contained in the samples plays a key role. We will propose and discuss a charge transfer mechanism that involves thermal hydroxylation and rehydroxylation of silica surfaces.

<sup>1</sup>corresponding author

**10:36AM E16.00014 Scrolling of Suspended CVD Graphene Sheets**

, OLEG MARTYNOV, SINCHUL YEOM, MARC BOCKRATH, Univ of California - Riverside, UC: RIVERSIDE TEAM — Carbon Nanoscrolls, one dimensional spiral forms of graphitic carbon, have attracted recent interest due to their novel proposed properties [1]. Although various production methods and studies of carbon nanoscrolls have been performed, low yield and poor controllability of their synthesis have slowed progress in this field. Suspended graphene membranes and carbon nanotubes have been predicted as promising systems for the formation of graphene scrolls [2]. We have suspended chemical vapor deposition (CVD)-grown graphene over large holes in a Si/SiO<sub>2</sub> substrate to make suspended membranes upon which nanotubes are placed. Initial experiments have been performed showing that tears or cuts of the suspended sheet can initiate scrolling. Our latest progress towards carbon nanotube initiated formation of graphene scrolls and suspended CVD graphene scrolling, along with measurements of these novel structures will be presented. [1] E. Perim et al., Front. Mater., 1:31 (2014); [2] E. Perim et al., J. Appl. Phys. 113, 054306 (2013)

**Tuesday, March 15, 2016 8:00AM - 10:48AM –**

**Session E17 DCMP DMP: Strained Graphene** 316 - Masahiro Ishigami, University of Central Florida

**8:00AM E17.00001 Quasi-bound states in strained graphene**

, DARIO BAHAMON, Mackenzie Presbyterian University, ZENAN QI, HAROLD PARK, Boston University, VITOR PAREIRA, National University of Singapore, DAVID CAMPBELL, Boston University — In this work, we explore the possibility of manipulating electronic states in graphene nanostructures by mechanical means. Specifically, we use molecular dynamics and tight-binding models to access the electronic and transport properties of strained graphene nanobubbles and graphene kirigami. We establish that low energy electrons can be confined in the arms of the kirigami and within the nanobubbles; under different load conditions the coupling between confined states and continuous states is modified creating different conductance line-shapes.

**8:12AM E17.00002 Probing Graphene on Micropatterned Strain Arrays**

, JOHN HENRY HINNEFELD, NADYA MASON, Univ of Illinois - Urbana — The generation of enormous pseudo-magnetic fields in graphene by the application of carefully designed strain profiles opens a promising window onto an otherwise unattainable high-field regime. A central challenge in exploiting graphene's access to this regime is the difficulty of controllably generating the required strain profiles. Here, we report the tunable fabrication of nano-scale strain feature arrays, as well as optical, mechanical, and other measurements of graphene deposited on substrates prepared by this method. We describe the signatures of strain present in our measurements, and discuss the potential for further experimental exploration of this system.

**8:24AM E17.00003 Current and Noise Saturation in Graphene Superlattice.**<sup>1</sup>, WEI YANG, Laboratoire Pierre Aigrain, ENS-CNRS, XIAOBO LU, Institute of Physics, Chinese Academy of Sciences, SIMON BERTHOU, QUENTIN WILMART, MOHAMED BOUKHICHA, CHRISTOPHE VOISIN, Laboratoire Pierre Aigrain, ENS-CNRS, GUANGYU ZHANG, Institute of Physics, Chinese Academy of Sciences, BERNARD PLACAIS, Laboratoire Pierre Aigrain, ENS-CNRS — One of the merits of graphene is that the Fermi level can be easily tuned by electrical gating, which render charge carriers n type or p type, or even insulating around the Dirac point (DP). By aligning graphene on top of Boron Nitride (BN), the presence of graphene superlattice makes transport properties even more versatile owing to the emergence of secondary Dirac points (SDPs). Here we present a study of high electric field performance of graphene superlattice obtained from epitaxial approach. By using microwave cavity, noise produced from graphene by joule heating is recorded up to 5GHz. Current and noise saturation are observed and investigated. Depending on Fermi energy, saturation can be attributed to intrinsic optical or remote surface polar phonon scattering at a doping far away from DP, while no saturation are found around DP. Moreover, noise saturation is identified around Fermi energy between DP and SDP, which can be attributed to the influence of van Hove singularity arising from the superlattice. Lastly, saturation due to the bias induced shift of DP, or so called Dirac fermion pinch-off, is well observed by local top gate technique.

<sup>1</sup> EU Graphene flagship project (contract no. 604391)

**8:36AM E17.00004 Valley polarization in graphene with out-of-plane deformations**<sup>1</sup>, DAWEI ZHAI, NANCY SANDLER, Department of Physics and Astronomy, Ohio University — At low energy, the energy dispersion of graphene shows a conical valley structure with the conduction and valence bands touching at the Dirac points. The existence of two inequivalent Dirac points in the Brillouin zone, thus two valleys, suggests they may be used as new degrees of freedom to carry information. Several schemes based on different mechanisms have been advanced to achieve valley separation in this material, however the proposed setups remain challenging for experimental observation. In this work we investigate graphene with out-of-plane deformations- one of the most naturally occurring and practically realizable settings, as a candidate system to produce valley polarization. Local strains produced by the deformations serve as scattering potentials for electronic states. A second-order Born approximation calculation based on the continuum model reveals the existence of valley polarization and its dependence on the geometrical parameters of the deformations. We characterize the efficiency of valley filtering for different geometries and energies and discuss their implementation in currently available experimental setups.

<sup>1</sup>Work supported by NSF-DMR 1508325.

**8:48AM E17.00005 Tuning transport properties on graphene multiterminal structures by mechanical deformations**, ANDREA LATGE, VANESSA TORRES, Univ. Federal Fluminense, RJ-Brazil, DAIARA FARIA, Univ. do Estado do Rio de Janeiro, RJ-Brazil — The realization of mechanical strain on graphene structures is viewed as a promise route to tune electronic and transport properties such as changing energy band-gaps and promoting localization of states. Using continuum models, mechanical deformations are described by effective gauge fields, mirrored as pseudomagnetic fields that may reach quite high values. Interesting symmetry features are developed due to out of plane deformations on graphene; lift sublattice symmetry was predicted and observed in centrosymmetric bumps and strained nanobubbles [1]. Here we discuss the effects of Gaussian-like strain on a hexagonal graphene flake connected to three leads, modeled as perfect graphene nanoribbons. The Green function formalism is used within a tight-binding approximation. For this particular deformation sharp resonant states are achieved depending on the strained structure details. We also study a fold-strained structure [2] in which the three leads are deformed extending up to the very center of the hexagonal flake. We show that conductance suppressions can be controlled by the strain intensity and important transport features are modeled by the electronic band structure of the leads. [1]RC-Bastos et al., Phys. Rev. B 91, 125408 (2015).[2]HLim et al., Nat. Commun. 6, 8601(2015).

**9:00AM E17.00006 Fold assisted transport in graphene systems**<sup>1</sup>, RAMON CARRILLO-BASTOS, Univ. Autonoma de Baja California, BC, Mexico, DAIARA FARIA, Univ. do Estado de Rio de Janeiro, RJ, Brazil, YUHANG JIANG, JINHAI MAO, GUOHONG LI, EVA Y. ANDREI, Rutgers Univ., NJ, USA, ANDREA LATGE, Univ. Federal Fluminense, RJ, Brazil, NANCY SANDLER, Ohio University, OH, USA — Sasaki pointed out that a constant uniaxial strain applied along the zigzag direction in graphene causes localized states, akin to edge states in nanoribbons[1]. These states are dispersionless and can carry ballistic transport. Recent experiments reported the presence of ballistic channels in graphene grown on SiC characterized with STM spectroscopy[2, 3]. In this work, we show that out-of plane deformations in the form of folds produce states as those predicted by Sasaki. Using tight-binding calculations and recursive Greens function methods, we obtain conductance, density of states (DOS), local density of states, and band structure (BS) for graphene nanoribbons with zigzag termination. Regions with enhanced DOS are identified in the deformed area corresponding to states in new flattened bands in the BS and new ballistic channels in the conductance. Adjusting the fold parameters, desired properties of these states can be tailored. Our results show that folds could serve as pathways for electronic transport and open the possibility of circuitry design within a simple graphene membrane. [1]Sasaki et al., J. Phys. Soc. Jpn. 75 (2006). [2]Baringhaus et al., Nature 506 (2014). [3]Palacio et al., Nano Lett. 15 (2015).

<sup>1</sup>Support: DOE-FG02-99ER45742, NSF-DMR 1207108 and 1508325.

**9:12AM E17.00007 Helium adsorption potential near mechanically deformed graphene**, NATHAN NICHOLS, VALERI KOTOV, ADRIAN DEL MAESTRO, University of Vermont — Mechanical strain modifies the van der Waals interactions of neutral adatoms near two-dimensional materials like graphene and commonly used parameters for helium interacting with carbon do not capture these effects. Using the polarization function of strained graphene, we have compared the long-distance Lifshitz dispersion force with an effective potential computed from the sum of two-body interactions. The resulting optimized many-body adsorption potential exhibits an anisotropic minimum that is displaced higher above the graphene sheet as uniaxial strain is increased. The competing energy scales introduced by strain open up the possibility of mechanically tuning novel anisotropic adsorbed superfluid phases of helium on graphene.

**9:24AM E17.00008 Elastic Solitons and Vortices in Bilayer Graphene**, JOSEPHINE YU, Montgomery Blair High School, HARSH MATHUR, Case Western Reserve University — Using electron microscopy Alden et al [PNAS 110, 11256 (2013)] find that in strained bilayer graphene regions of stable AB and BA stacking are separated by domain walls. Vortex-like defects are also observed at the intersections of three domain walls; scanning transmission electron microscopy reveals that the vortex cores have an unstable AA stacking. We develop a continuum elasticity model that describes the relative displacement of the two layers of graphene. In addition to the usual gradient energy cost we posit a nonlinear potential for the displacement field that favors AB and BA stackings and disfavors the AA stacking. In our model the domain walls appear as soliton solutions to a double sine-Gordon equation. We find that the ratio of the width of domain walls with tensile strain to those with shear strain is  $\sim 1.63$ , in excellent agreement with observations. We study the stability and oscillatory modes of the domain walls motivated by experimental observations that show the domain walls undergoing damped oscillations. Estimates of the vortex core size based on our model are in agreement with the experiment. A homotopy analysis of bilayer graphene vortices shows that they carry non-abelian topological charge.

**9:36AM E17.00009 Graphene on a curved substrate with a controllable curvature: Device fabrication and transport measurements**, YIXUAN CHEN, SHAUN MILLS, YING LIU, Pennsylvania State University — In monolayer graphene, the local deviation of carbon positions from the perfect lattice has been predicted to lead to a pseudo magnetic field with measurable effects. A striking confirmation of this effect is the observation of Landau levels that are attributed to a pseudo magnetic field in excess of 300 T in graphene nanobubbles. However, typical experimental methods of generating such local deviations in graphene rely on strain accompanied by a surface curvature. Whether a surface curvature alone can produce measurable effects in graphene has not been explored experimentally. It is therefore of interest to study graphene in a system that decouples strain from surface curvature. Of particular interest is its response to an external magnetic field. We developed a grayscale electron beam lithography technique for preparing PMMA substructures with a continuously variable radius of curvature from  $\sim 100$  nm to  $\sim 1$   $\mu$ m. Magnetoelectrical transport measurements on exfoliated graphene supported by these substructures are being carried out. The flexibility of this process may be further exploited in the study of the bilayer and trilayer graphene systems. We will also study hybrid structures of 2D superconductors and graphene.

**9:48AM E17.00010 Graphene with out-of-plane deformations and external magnetic fields<sup>1</sup>**, DAIARA FARIA, UERJ, RJ Brazil, RAMON CARRILLO BASTOS, Univ. Autonoma de Baja California, BC Mexico, FRANCISCO MIRELES, Univ. Nacional de Mexico, BC Mexico, ANDREA LATGE, Univ. Federal Fluminense, RJ Brazil, NANCY SANDLER, Ohio University, OH USA — Microscopic measurements in corrugated graphene have helped to elucidate how its electronic properties are affected in deformed regions, confirming the pseudomagnetic description for strained graphene. As the pseudofields reverse sign at each valley, an enhancement of the local density of states (LDOS) was found with broken sublattice symmetry in strained regions[1,2]. As a consequence, these systems have been proposed as a viable way to obtain valley filters. In graphene ribbons with a centrosymmetric deformation, the LDOS modification was predicted to be accompanied with a decrease in conductance, pointing to the presence of confined states [3]. To further characterize these states, we investigate the effect of strain in the presence of an external magnetic field, using a tight-binding model and recursive Greens function techniques. Anomalous conductance and DOS features are consistent with interpretation in terms of Fano resonances appearing for bound states in the continuum. We discuss the robustness of the sublattice asymmetry against the magnetic field and the possibility of exploring the valley separation in chosen spatial regions. [1]Mashoff et al. NanoLetters 10 (2010). [2]Schneider et al. 91 (2015). [3]Carrillo-Bastos et al. PRB 90 (2014).

<sup>1</sup>Work supported by NSF grant DMR 1508325.

**10:00AM E17.00011 Towards Quantum Strain Engineering in Ultra-short Ballistic Graphene Devices**, ANDREW MCRAE, VAHID TAYARI, SIMEON HANKS, ALEXANDRE CHAMPAGNE, Concordia University — We report our progress towards combining ultra-short and clean suspended graphene transistors [1] with mechanical breakjunction (MCBJ) instrumentation to create a widely tunable quantum strain engineering platform for graphene electronics. We first present data from our electromigrated ultra-short ( $\sim 10$  to 50 nm) suspended graphene transistors, which show ballistic transport [1], and demonstrate that we can tailor the length and shape of the suspended graphene by adjusting the electromigration parameters. We observe Fabry-Pérot interferences, which correspond to coherent transport not only in the suspended graphene channel, but also in the suspended graphene contacts connecting to the channel. We then describe the MCBJ assembly we use to bend the substrate in-situ at low temperature. Using long suspended cantilever contacts, this instrumentation allows strains up to  $\sim 10\%$  for device lengths  $\sim 10$  nm. The assembly is hosted in a cryostat operating down to 0.3 K and in magnetic fields up to 9 T. We finally report on our progress towards the application of large uniaxial strain for graphene strain transistors, and graphene NEMS with tunable frequencies approaching the THz range. [1] V. Tayari *et al.*, Nano. Lett. 15, 1 (2015)

**10:12AM E17.00012 Local Probes of Strain Texture and Individual Atomic Dopant Sites in Monolayer MoS<sub>2</sub>**, ALEX H. FRAGAPANE, ALEX W. CONTRYMAN, HONG LI, Stanford University, XIAOFENG QIAN, SINA MOEINI ARDAKANI, MIT, YONGJI GONG, XINGLI WANG, Rice University, JEFFREY M. WEISSE, CHI HWAN LEE, JIHENG ZHAO, Stanford University, PULICKEL M. AJAYAN, Rice University, JU LI, MIT, XIAOLIN ZHENG, HARI C. MANOHARAN, Stanford University — The 2D semiconductor MoS<sub>2</sub> is an optically active material uniquely responsive to local perturbations. As an atomically thin membrane with exceptional strength, it can embed wide band gap variations overlapping the visible light spectrum when subjected to biaxial strain, where the modified electronic potential emanating from point-induced tensile strain perturbations mimics the Coulomb potential in a mesoscopic atom. We have realized this “artificial atom” concept via monolayer nanoindentation, and demonstrate that a synthetic superlattice of these building blocks forms an optoelectronic crystal capable of broadband light absorption and efficient funneling of photogenerated excitons to points of maximum strain at the artificial-atom nuclei. We also investigate the effects of individual atomic dopant sites through STM/STS, and visualize the atomic-scale local band structure changes. The modification of 2D semiconductors through methods such as strain texturing and doping connects to applications in next generation optoelectronics and photovoltaics.

**10:24AM E17.00013 Effects of Strain on CVD-Grown Few-Layered Terrace Structures of MoS<sub>2</sub><sup>1</sup>**, AMBER MCCREARY, Penn State University, R. GHOSH, Univ. Texas at Austin, M. AMANI, U.S. Army Research Lab, J. WANG, Univ. of Connecticut, K.-A. DUERLOO, Stanford Univ., A. SHARMA, K. JARVIS, Univ. of Texas at Austin, E. REED, Stanford Univ., A. DONGARE, Univ. of Connecticut, S.K. BANERJEE, Univ. of Texas at Austin, M. TERRONES, Penn State Univ., R. NAMBURU, M. DUBEY, U.S. Army Research Lab — In this report, we used CVD-grown terrace MoS<sub>2</sub> layers to study how the number and size of the layers affected the physical properties under uniaxial and biaxial tensile strain. Interestingly, we observed significant shifts in both the Raman in-plane mode (as high as  $-5.2$   $\text{cm}^{-1}$ ) and photoluminescence (PL) energy (as high as  $-88$  meV) for the few-layered MoS<sub>2</sub> under approximately 1.5% applied uniaxial tensile strain. The observed results were compared to monolayers and few-layers of MoS<sub>2</sub> previously reported. We also observed slippage between the layers which resulted in a hysteresis of the Raman and PL spectra during further applications of strain. Through DFT calculations, we contended that this random layer slippage was due to defects present in CVD-grown materials. This work demonstrates that the properties of CVD-grown few-layered MoS<sub>2</sub> studied here can be tuned under strain as well as, if not better than, it's exfoliated monolayered counterpart.

<sup>1</sup>Funded by ARL DSI on stacked 2D atomic layered materials, ARO MURI Grant W911NF-11-1-0362, ARO STTR Award W911NF-14-P-0030, and ARL Cooperative Agreement Number W911NF-14-2-0059

**10:36AM E17.00014 First-Principles Computation of Graphene's Phonon Anharmonicity**, MORDECHAI KORNBLUTH, CHRIS A. MARIANETTI, Columbia University, Department of Applied Physics and Applied Mathematics — Here we use density-functional theory to compute an interatomic potential for graphene, including anharmonicities up to at least fourth order. We generate all group-theoretically allowed terms within a hexagon via the recently-developed slave mode expansion. This expands the potential in terms of the normal modes of overlapping hexagons, while obeying the space group symmetry and homogeneity of free space. We further introduce the notion of cooperative modes, which combine strain and  $q = 0$  phonons to yield the same pure mode amplitude on each hexagon. Within the cooperative subspace, cooperative modes allow for arbitrarily-precise meshing to directly compute energies, or calculation of the anharmonic coefficients via finite-difference. We demonstrate the power of our approach in the context of strained graphene, which is known to have a novel strain-driven soft mode at the  $K$ -point. We identify the dominant anharmonic terms which drive the soft  $K$  mode, and study the role of finite temperatures using molecular dynamics and Monte-Carlo simulations.

**Tuesday, March 15, 2016 8:00AM - 11:00AM —**

**Session E18 GMAG DMP FIAP: Spin-Hall II** 317 - Se Kwon Kim, UC Los Angeles

**8:00AM E18.00001 Role of transparency of platinum-ferromagnet interface in determining intrinsic magnitude of spin Hall effect** , WEI HAN, International Center for Quantum Materials, Peking University — The spin Hall effect (SHE) converts charge current to pure spin currents in orthogonal directions in materials that have significant spin-orbit coupling. The efficiency of the conversion is described by the spin Hall Angle (SHA). The SHA can most readily be inferred by using the generated spin currents to excite or rotate the magnetization of ferromagnetic films or nano-elements via spin-transfer torques. Some of the largest spin torque derived spin Hall angles (ST-SHA) have been reported in platinum. In this talk, I will discuss that the transparency of the Pt-ferromagnet interface to the spin current plays a central role in determining the magnitude of the ST-SHA [1]. Using spin torque ferromagnetic resonance (ST-FMR) measurements, we measure a much larger ST-SHA in Pt/cobalt (0.11) compared to Pt/permalloy (0.05) bilayers when the interfaces are assumed to be completely transparent. Taking into account the transparency of these interfaces, as derived from spin-mixing conductances, we find that the intrinsic SHA in platinum has a much higher value of 0.19 0.04 as compared to the ST-SHA. The importance of the interface transparency is further exemplified by the insertion of atomically thin magnetic layers at the Pt/permalloy interface that we show strongly modulates the magnitude of the ST-SHA. Improving the interface transparency can make the SHE more effective for spintronic applications and is critical to understanding the fundamental origin of the SHE. [1] W. Zhang\*, Wei Han\*, Xin Jiang, See-Hun Yang and Stuart S. P. Parkin, Nature Physics, 11, 496–502 (2015).

**8:36AM E18.00002 Multi-directional Spin Transport at Interfaces with Spin-Orbit Coupling** , VIVEK AMIN, Center for Nanoscale Science and Technology, NIST / Maryland NanoCenter, Univ. of Maryland, MARK STILES, Center for Nanoscale Science and Technology, NIST — Spin transport remains poorly understood in multilayer systems with interfacial spin-orbit coupling. Currently, drift-diffusion models cannot accurately treat this phenomenon, since the important consequences of interfacial spin-orbit scattering remain uncharacterized in a systematic way. Here we present boundary conditions suitable for drift-diffusion models that capture the phenomenology of interfacial spin-orbit coupling. To access their viability we compare solutions of the drift-diffusion and Boltzmann equations in a Co/Pt bilayer, since the latter approach yields a momentum-dependent distribution function equipped to describe spin-orbit scattering. A key result is that in-plane electric fields create spin accumulations and spin currents polarized in all directions, which describes a generalization of the Rashba-Edelstein and spin Hall effects. In heavy metal/ferromagnet bilayers, this phenomenon provides a mechanism for the creation of damping-like and field-like torques; it also leads to possible reinterpretations of experiments in which interfacial torques are thought to be suppressed. We discuss the interpretation of experiments involving spin orbit torque, spin pumping/memory loss, the Rashba-Edelstein effect, and the spin Hall magnetoresistance.

**8:48AM E18.00003 Spin-Hall Non-Local Transport Mediated by a Magnetic Insulator<sup>1</sup>** , MASSOUD RAMEZANI MASIR, HUA CHEN, Department of physics, University of Texas at Austin, Texas 78712, USA, INTI SODEMANN, Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA, ALLAN. H. MACDONALD, Department of physics, University of Texas at Austin, Texas 78712, USA — Magnetic systems with easy-plane order support dissipationless spin supercurrents that can lead to non-local coupling between electrically separated conductors. Recently the electrical properties of a system containing two magnetic multilayer stacks with perpendicular magnetic anisotropy electrodes and a shared easy-plane magnetic layer have been discussed. In this research we discuss a closely related system in which the two conducting channels that are coupled by the easy-plane magnetic layer are co-planar thin film metals with large spin Hall effects. We theoretically explained the non-local relationship between the current-voltage relationships of two thin film metallic conductors. Coupling occurs because both conductors inject spins into the magnetic insulator and because this information is communicated between conductors via exchange interactions within the magnetic system. We investigate the non-local transport properties of the system in the macrospin and long thin nanomagnet limits, deriving conditions for the critical currents and using solutions to the Landau-Lifshitz-Gilbert equation to characterize the dynamic steady state case.

<sup>1</sup>This work was supported by as part of SHINES, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award SC0012670.

**9:00AM E18.00004 Nonlocal anomalous Hall effect<sup>1</sup>** , SHULEI ZHANG, GIOVANNI VIGNALE, Department of Physics and Astronomy, University of Missouri — Anomalous Hall effect (AHE) is a distinctive transport property of ferromagnetic metals arising from spin orbit coupling (SOC) in concert with spontaneous spin polarization. Nonetheless, recent experiments have shown that the effect also appears in a nonmagnetic metal in contact with a magnetic insulator. The main puzzle lies in the apparent absence of spin polarized electrons in the non-magnetic metal. Here, we theoretically demonstrate that the scattering of electrons from a rough metal-insulator interface is generally spin-dependent, which results in mutual conversion between spin and charge currents flowing in the plane of the layer. It is the current-carrying spin polarized electrons and the spin Hall effect in the bulk of the metal layer that conspire to generate the AH current. This novel AHE differs from the conventional one only in the spatial separation of the SOC and the magnetization, so we name it as nonlocal AHE. In contrast to other previously proposed mechanisms (e.g., spin Hall AHE and magnetic proximity effect (MPE)), the nonlocal AHE appears on the *first order* of spin Hall angle and does *not* rely on the induced moments in the metal layer, which make it experimentally detectable by contrasting the AH current directions of two layered structures such as Pt/Cu/YIG and  $\beta$ -Ta/Cu/YIG (with a thin inserted Cu layer to eliminate the MPE). We predict that the directions of the AH currents in these two trilayers would be *opposite* since the spin Hall angles of Pt and  $\beta$ -Ta are of opposite signs.

<sup>1</sup>Work supported by NSF Grants DMR-1406568.

**9:12AM E18.00005 Spin Hall effects from mesoscopic ferromagnetic NiFe thin films** , CHUAN QIN, SHUHAN CHEN, YUNJIAO CAI, YI JI, University of Delaware — The spin Hall effect (SHE) and inverse spin Hall effect (ISHE) have been explored primarily in nonmagnetic heavy metals such as Pt. In this work, we probe SHE/ISHE from mesoscopic ferromagnetic NiFe (Py) films in nonlocal lateral structures. The structure consists of a Py spin injector/detector (F1), a Cu channel, and a second Py stripe (F2) where SHE/ISHE occurs. Low-resistance AlOx layers are placed at all interfaces. For SHE, a charge current passes through F2, and a nonlocal voltage is detected between F1 and Cu. For ISHE, a charge current is injected from F1 into Cu, and the nonlocal voltage is measured between two ends of F2. The in-plane magnetic field is applied perpendicular to F1/F2 stripes. For both measurements, the nonlocal signal for large positive field is different from that of large negative field owing to the SHE/ISHE. Using a simple model, the apparent spin Hall angle (assuming long Py spin diffusion length) of Py is estimated to be 0.010 at 295K and 0.017 at 4.5K.

**9:24AM E18.00006 Demonstration of Kirchhoff's First Law for Pure Spin Currents** , JOSEPH BATLEY, M. C. ROSAMOND, M. ALI, E. H. LINFIELD, G. BURNELL, B. J. HICKEY, University of Leeds — In conventional electronics a fundamental component of circuit design is the principle of fan-out, which allows multiple operations to be performed in order to build up complex logical procedures. A fan-out device relies on the condition that electrical currents obey Kirchhoff's laws and in order for spin-logic to be viable, the same must be shown for pure spin currents. Both fan-out and fan-in experiments have been performed to observe how spin currents behave in a multi-terminal circuit. The development of a 3-dimensional nonlocal IV and matrix fitting method provides information about each spin current, along with the thermal current generated at the injection point, and how they interact with each other. The fan-out geometry demonstrates that a pure spin current will divide between the different branches in a circuit, with a magnitude determined through the spin resistances of each arm. The fan-in measurements demonstrate that two pure spin currents will add and subtract with each other in a conventional manner expected from Kirchhoff's first law. These experiments have demonstrated the symmetry of pure spin currents with respect to the injection current and shown that they obey Kirchhoff's current law.

**9:36AM E18.00007 ABSTRACT WITHDRAWN —**

**9:48AM E18.00008 Anomalous Hall effect driven by dipolar spin waves in uniform ferromagnets**, KOJI SATO, AIMR, Tohoku University, KEI YAMAMOTO, Kobe University, EIJI SAITOH, AIMR, Tohoku University, HIROSHI KOHNO, Nagoya University — An anomalous Hall effect is shown to arise from the exchange interaction of conduction electrons with dipolar spin waves in ferromagnets. This effect exists even in homogeneous ferromagnets without relativistic spin-orbit coupling. The leading contribution to the Hall conductivity is proportional to the chiral spin correlation of dynamical spin textures and is physically understood in terms of the skew scattering by dipolar magnons.

**10:00AM E18.00009 Strong Spin Hall effect in PtMn**, YONGXI OU, SHENGJIE SHI, DANIEL RALPH, ROBERT BUHRMAN, Cornell Univ — Recent reports indicate that certain metallic antiferromagnets (AFM) can exhibit a significant spin Hall effect. Here we report a large damping-like spin torque efficiency ( $\xi_{DL}$ ) in PtMn/ferromagnet(FM) bilayer structures, determined from both FM-thickness-dependent spin-torque ferromagnetic resonance (ST-FMR), and harmonic response (HR) measurements of layers with perpendicular magnetic anisotropy (PMA). We find that  $\xi_{DL}$  can vary from  $<0.1$  to  $>0.15$ , depending on the thickness of PtMn, the stacking order of the samples, and the choice of the FM material. The field-like spin torque efficiency ( $\xi_{FL}$ ) is also quite variable,  $0 < |\xi_{FL}| < 0.5$ . The large broadening of the ST-FMR linewidth suggests extra spin attenuation at the AFM/FM interface that is possibly due to intermixing. The PtMn/FeCoB/MgO structures that exhibit PMA have a comparatively low switching current density and an unusual asymmetric switching phase diagram. These results indicate that AFM PtMn has significant potential both for advancing the understanding the physics of the spin Hall effect in Pt alloys, and for enabling new spintronics functionality.

**10:12AM E18.00010 Large anomalous Hall effect in Pt interfaced with perpendicular anisotropy ferrimagnetic insulator<sup>1</sup>**, CHI TANG, PATHIKUMAR SELLAPPAN, YAWEN LIU, JAVIER GARAY, JING SHI, University of California-Riverside, SHINES TEAM — We demonstrate the strain induced perpendicular magnetic anisotropy (PMA) in a ferrimagnetic insulator (FMI),  $Tm_3Fe_5O_{12}$  (TIG) and the first observation of large anomalous Hall effect (AHE) in TIG/Pt bilayers. Atomically flat TIG films were deposited by a laser molecular beam epitaxy system on (111)-orientated substituted gadolinium gallium garnet substrates. The strength of PMA could be effectively tuned by controlling the oxygen pressure during deposition. Sharp squared anomalous Hall hysteresis loops were observed in bilayers of TIG/Pt over a range of thicknesses of Pt, with the maximum AHE conductivity reaching 1 S/cm at room temperature. The AHE vanishes when a 5 nm Cu layer was inserted between Pt and TIG, strongly indicating the proximity-induced ferromagnetism in Pt. The large AHE in the bilayer structures demonstrates a potential use of PMA-FMI related heterostructures in spintronics.

<sup>1</sup>This work was supported as part of the SHINES, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award SC0012670.

**10:24AM E18.00011 Direct measurement of spin accumulation in the Cu layer due to spin currents from Co**, ROOPALI KUKREJA, UC San Diego — Spin transport is the key for reading or writing bits in spintronic devices by utilizing the Giant Magnetoresistance effect or the spin transfer torque effect. Spin currents have also been shown to play important role in the ultrafast manipulation of magnetization via all optical switching. Hence, detailed understanding of spin currents from ferromagnet to non-magnets is a crucial step in development of spintronic devices. However, directly observing these spin currents is extremely challenging due to magnetic moment injected into non-magnet being very small, less than 1/10000 of a regular ferromagnet. In this talk, I will present our recent measurements on the spin currents from a thin film Co ferromagnet into non-magnetic Cu metal in a nanopillar device. We have developed an extremely sensitive spectro-microscopy detection method based on element specific x-ray magnetic circular dichroism where current pulses driving the spin currents into the Cu layer are synchronized with the synchrotron x-ray photons. The sensitivity of this 'lock-in' technique has allowed us to detect the extremely small transient Cu magnetization. We observe two spin currents induced effects in the Cu layer. The first effect is the transiently induced magnetization which occurs in bulk of the Cu layer due to spin accumulation and has a magnitude of 0.00003  $\mu B$  per atom. The second effect occurs at the Co/Cu interface where we observe a 10% increase or 0.004  $\mu B$  per atom for the hybridized Cu atoms due to spin torque-alignment.

**Tuesday, March 15, 2016 8:00AM - 10:48AM –**

**Session E19 GMAG DMP: Magnetic Oxide Thin Films and Heterostructures: Novel Interfacial Phenomena** 318 - Ho Nyung Lee, Oak Ridge National Laboratory

**8:00AM E19.00001 Controlled lateral anisotropy in correlated manganite heterostructures by interface-engineered oxygen octahedral coupling**, MARK HUIJIBEN<sup>1</sup>, MESA+ Institute for Nanotechnology, University of Twente — Ultimate miniaturization of magnetic random access memory (MRAM) devices is expected by the utilization of spin-transfer torques, because they present an efficient means to switch elements with a very high magnetic anisotropy. To overcome the low switching speed in current collinearly magnetized devices, new routes are being explored to realize magnetic tunnel junction stacks with non-collinear magnetization between two magnetic electrodes. Controlled in-plane rotation of the magnetic easy axis in manganite heterostructures by tailoring the interface oxygen network would provide a promising direction for non-collinear magnetization in correlated oxide magnetic tunneling junctions. Here, we demonstrate how to manipulate magnetic and electronic anisotropic properties in manganite heterostructures by engineering the oxygen network on the unit-cell level. The strong oxygen octahedral coupling is found to transfer the octahedral rotation, present in the NdGaO<sub>3</sub> (NGO) substrate, to the La<sub>2</sub>/3Sr<sub>1</sub>/3MnO<sub>3</sub> (LSMO) film in the interface region. This causes an unexpected realignment of the magnetic easy axis along the short axis of the LSMO unit cell as well as the presence of a giant anisotropic transport in these ultrathin LSMO films. As a result we possess control of the lateral magnetic and electronic anisotropies by atomic scale design of the oxygen octahedral rotation.

<sup>1</sup>Membership Pending

**8:36AM E19.00002 Interfacial Control of Magnetic Properties at LaMnO<sub>3</sub>/LaNiO<sub>3</sub> Interfaces**, MARTA GIBERT, University of Geneva, MICHEL VIRET, CEA Saclay, ALMUDENA TORRES-PARDO, University of Paris-Sud, Complutense University of Madrid, CINTHIA PIAMONTEZE, SLS-PSI, PAVLO ZUBKO, University of Geneva, University College London, NICOLAS JAOUEN, Synchrotron SOLEIL, JEAN-MARC TONNERRE, CNRS Institut Neel, ALEXANDRA MOUGIN, University of Paris-Sud, JENNIFER FOWLIE, SARA CATALANO, University of Geneva, ALEXANDRE GLOTER, ODILE STPHAN, University of Paris-Sud, JEAN-MARC TRISCONI, University of Geneva — The functional properties of oxide heterostructures ultimately rely on how the electronic and structural mismatches occurring at interfaces are accommodated by the chosen materials combination. We discuss here LaMnO<sub>3</sub>/LaNiO<sub>3</sub> heterostructures, which display an intrinsic interface structural asymmetry depending on the growth sequence with the LaMnO<sub>3</sub>-on-LaNiO<sub>3</sub> interface being sharper than the LaNiO<sub>3</sub>-on-LaMnO<sub>3</sub> one, which exhibits 2-3 unit cells intermixing [1]. Using a variety of synchrotron-based techniques, we show that the degree of intermixing at the monolayer scale allows interface-driven properties such as charge transfer and the induced magnetic moment in the nickelate layer to be controlled. Further, our results demonstrate that the magnetic state of strained LaMnO<sub>3</sub> thin films dramatically depends on interface reconstructions. [1] Gibert *et al.*, NanoLetters in press.

**8:48AM E19.00003 Understanding the Origin of Ferromagnetism in  $\text{LaNiO}_3/\text{CaMnO}_3$  Superlattices**, CHARLES FLINT, Stanford University, ALPHA N'DIAYE, PADRAIC SHAFER, ELKE ARENHOLZ, Advanced Light Source, YURI SUZUKI, Stanford University — Interfacial ferromagnetism (FM) in transition metal oxide heterostructures is a promising route for engineering new low-dimensional devices. In 2001, FM was discovered in  $\text{CaRuO}_3/\text{CaMnO}_3$  superlattices (SLs), which is attributed to an itinerant electron-mediated Mn-Mn double-exchange (DE). Since then we have discovered interfacial FM in  $(\text{LaNiO}_3)_N/(\text{CaMnO}_3)_8$  SLs that is consistent with this DE interaction<sup>1</sup>. Now we have explored even further reduced dimensionality by fabricating  $[(\text{LNO})_{n=2-7}/(\text{CMO})_4]_{10}$  SLs. Transport measurements confirmed a thickness dependent metal-insulator transition, with insulating films for  $N < 4$ . Bulk magnetometry measurements reveal interfacial FM in insulating and conducting SLs. Since there are no itinerant electrons in the insulating SLs, this FM must arise from a different source. Using x-ray absorption spectroscopy and magnetic circular dichroism, we have identified the coexistence of  $\text{Ni}^{2+}$  and  $\text{Ni}^{3+}$  and Ni magnetism. We therefore speculate that the FM in insulating SLs originates from a Mn-Ni superexchange interaction. We discuss the role of these interactions in interfacial FM and methods for controlling them.

<sup>1</sup>A.J. Grutter et al., *Phys. Rev. Lett.* **111**, 087202 (2013)

**9:00AM E19.00004 Exploring interfacial ferromagnetism in manganite-based superlattices**, DI YI, CHARLES FLINT, YURI SUZUKI, Department of Applied Physics, Stanford University — Heterointerface of complex oxides provides a rich playground to explore the emergent phenomena that are not found in bulk. In particular, emergent interfacial ferromagnetism has been successfully demonstrated in heterostructures composed of materials which are paramagnetic and antiferromagnetic in bulk. In our previous work, leakage of itinerant electrons from a paramagnetic metal to an antiferromagnetic insulator has been shown to give rise to interfacial ferromagnetism in  $\text{CaMnO}_3$ -based superlattices. However interfacial ferromagnetism in insulating superlattices suggests a more complicated scenario. Therefore a thorough investigation of coupling between charge, lattice and spin degrees of freedom is necessary. In this talk, we focus on the  $\text{NdNiO}_3/\text{CaMnO}_3$  system. By choosing a paramagnetic layer that undergoes a metal-insulator transition, we can explore the role of electron itinerancy in interfacial ferromagnetism in the same sample to eliminate the inconsistencies that may originate from the deposition of multiple samples. We demonstrate that  $\text{NdNiO}_3$  exhibits a metal-insulator transition as a function of temperature, which can be tuned as a function of film thickness. We have also grown  $\text{NdNiO}_3/\text{CaMnO}_3$  heterostructures with excellent crystallinity. Preliminary transport measurements indicate that the presence of an adjacent  $\text{CaMnO}_3$  layer also affects the transport in  $\text{NdNiO}_3$  so that charge transfer from the itinerant layer into the adjacent antiferromagnetic insulating  $\text{CaMnO}_3$  is likely not the only contribution to interfacial ferromagnetism.

**9:12AM E19.00005 Magnetotransport in  $\text{LaNiO}_3/\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$  superlattices with non-collinear magnetic ordering**, JASON HOFFMAN, University of British Columbia, STEPHEN WU, Argonne National Laboratory, BRIAN KIRBY, National Institute of Standards and Technology, ANAND BHATTACHARYA, Argonne National Laboratory — Non-collinear magnetic textures can give rise to exotic charge and spin transport behaviors, and may allow for the control of magnetism using small electric currents. While these textures have been observed in a number of bulk materials and in thin films, realizing non-collinear magnetism in heterostructures presents new avenues to tune their properties using tailored interfaces and gate electric fields. We have previously used polarized neutron reflectometry (PNR) to demonstrate that superlattices of paramagnetic  $\text{LaNiO}_3$  (LNO) and ferromagnetic  $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$  (LSMO) adopt a non-collinear magnetic structure. In this work, we characterize the non-collinearity as a function of temperature and magnetic field using anisotropic magnetoresistance (AMR) and Nernst effect measurements. We observe rotational hysteresis at low fields, while the magnitude of the AMR is found to vary non-monotonically with applied field. To understand this behavior, we develop a simple free-energy model that includes contributions from biaxial anisotropy, Zeeman energy, and exchange coupling between the LSMO and the LNO layers. From this analysis, we are able to extract the orientation of the magnetization of the individual LSMO layers, which agrees well with the values measured using PNR.

**9:24AM E19.00006 Influence of quantum confinement and strain on orbital polarization of strained four-layer  $\text{LaNiO}_3$  superlattices: a DFT+DMFT study**<sup>1</sup>, HYOWON PARK, University of Illinois at Chicago, ANDREW MILLIS, CHRIS MARIANETTI, Columbia University — Here we use the combination of density functional theory and dynamical mean field theory to study Ni d orbital polarization in strained  $\text{LaNiO}_3/\text{LaAlO}_3$  superlattices consisting of four layers of nominally metallic  $\text{NiO}_2$  and four layers of insulating  $\text{AlO}_2$  separated by  $\text{LaO}$  layers. The layer-resolved orbital polarization is calculated as a function of strain and analysed in terms of structural, quantum confinement, and correlation effects. The overall dependence of orbital polarization on strain in superlattices is qualitatively consistent with recent X-ray absorption spectroscopy and resonant reflectometry data. However, interesting differences of detail are found depending on the sign of strain. Under tensile strain, the two inequivalent Ni ions display orbital polarization similar to that calculated for strained bulk  $\text{LaNiO}_3$  and observed in experiment. Compressive strain produces a larger dependence of orbital polarization on Ni position and even the inner Ni layer exhibits orbital polarization different from that calculated for strained bulk  $\text{LaNiO}_3$ . The quantum confinement effect is as important as the strain effect and more stronger for tensile strain.

<sup>1</sup>This work is supported by DOE ER-046169 and FAME, one of six centers of STARnet, a Semiconductor Research Corporation program sponsored by MARCO and DARPA.

**9:36AM E19.00007 Interfacial Symmetry Control of Emergent Ferromagnetism**, ALEXANDER GRUTTER, JULIE BORCHERS, BRIAN KIRBY, Natl Inst of Stds and Tech, CHUNYONG HE, University of California, Berkeley, ELKE ARENHOLZ, Lawrence Berkeley National Lab, ARTURAS VAILIONIS, CHARLES FLINT, YURI SUZUKI, Stanford University — Atomically precise complex oxide heterostructures provide model systems for the discovery of new emergent phenomena since their magnetism, structure and electronic properties are strongly coupled. Octahedral tilts and rotations have been shown to alter the magnetic properties of complex oxide heterostructures, but typically induce small, gradual magnetic changes. Here, we demonstrate sharp switching between ferromagnetic and antiferromagnetic order at the emergent ferromagnetic interfaces of  $\text{CaRuO}_3/\text{CaMnO}_3$  superlattices. Through synchrotron X-ray diffraction and neutron reflectometry, we show that octahedral distortions in superlattices with an odd number of  $\text{CaMnO}_3$  unit cells in each layer are symmetry mismatched across the interface. In this case, the rotation symmetry switches across the interface, reducing orbital overlap, suppressing charge transfer from Ru to Mn, and disrupting the interfacial double exchange. This disruption switches half of the interfaces from ferromagnetic to antiferromagnetic and lowers the saturation magnetic of the superlattice from 1.0 to 0.5  $\mu_B$ /interfacial Mn. By targeting a purely interfacial emergent magnetic system, we achieve drastic alterations to the magnetic ground state with extremely small changes in layer thickness.

**9:48AM E19.00008 4d electron Ruthenate systems: their unique and new magnetic properties**, SEUNGRAN LEE, YEONGJAE SHIN, CCES-IBS, Seoul 151-747, Republic of Korea, M.S. ANWAR, YUSUKE SUGIMOTO, Dept. of Physics, Graduate School of Science, Kyoto Uni., Kyoto 606-8502, MINCHEOL LEE, SUNGJIN KANG, CCES-IBS, Seoul 151-747, Republic of Korea, SHINGO YONEZAWA, YOSHITERU MAENO, Dept. of Physics, Graduate School of Science, Kyoto Uni., Kyoto 606-8502, TAEWON NOH, CCES-IBS, Seoul 151-747, Republic of Korea — The Ruddlesden-Popper series (PR) of  $\text{Sr}_{n+1}\text{Ru}_n\text{O}_{3n+1}$  has attract much interest of their unique physical properties. Among them,  $\text{SrRuO}_3$  ( $n = \infty$ ) (SRO) is the only ferromagnetic metallic oxide especially in Ru 4d transition metal oxides. Bulk SRO has orthorhombic structure showing the Curie temperature ( $T_C$ )  $\sim 160$  K. It is well known that  $\text{RuO}_6$  octahedral distortion plays critical roles in its magnetic properties. In film systems, such  $\text{RuO}_6$  octahedra can be easily controlled by strain-engineering. In this talk, with high quality SRO films fully strained (-1.7%-1%) using various substrates, we systematically studied their structural changes and associated magnetic properties. Compared to theoretical predictions, the structural changes can be explained, while the magnetic property changes cannot be understood. Surprisingly, when SRO113 is grown on its PR series of  $\text{Sr}_2\text{RuO}_4$  ( $n=1$ ) (SRO214) single crystal, the exact substrate of SRO214 magnetization results in strongly enhanced magnetization ( $M \propto 3 \mu_B/\text{Ru}$ ,  $T_C \sim 160$  K), which has never found SRO113 (001) since the low-spin configuration of SRO113 prevent M never exceed  $2 \mu_B/\text{Ru}$ . The mystery of M in SRO113 (especially SRO113/SRO214) will be further discussed.

**10:00AM E19.00009 Chemical Ordering Modulated Electronic Phase Separation and Macroscopic Properties in Colossal Magnetoresistance Manganites**, YINYAN ZHU, KAI DU, LIFENG YIN, JIAN SHEN, Fudan University, LOW-DIMENSIONAL MATERIAL PHYSICS TEAM — Using unit cell by unit cell superlattice growth technique, we determine the role of chemical ordering of the Pr dopant in a colossal magnetoresistance  $(\text{La}_{1-y}\text{Pr}_y)_{1-x}\text{Ca}_x\text{MnO}_3$  (LPCMO) system, which has been well known for its large length scale electronic phase separation (EPS) phenomena. Our experimental results show that the chemical ordering of Pr leads to dramatic reduction of the length scale of EPS. Moreover, compared to the conventional Pr-disordered LPCMO system, the Pr-ordered LPCMO system has ~100 K higher metal-insulator transition temperature. We have further investigated the n-dependence of the physical properties of the  $(\text{LCMO})_{2n}/(\text{PCMO})_n$  superlattices. Magnetic and transport measurements indicate that the physical properties change nonmonotonically with increasing n, reaching a minimum for both the Curie temperature and the meta-insulator transition temperature. The crossover thickness thus reflects the characteristic correlation length scale along the vertical direction of the superlattice. For superlattices with n smaller than the correlation length, we combine MFM studies and model calculations to explain the weakened ferromagnetism and metallicity with increasing n.

**10:12AM E19.00010 Polarized Neutron Reflectometry Study of Tunable Metal-insulator Superlattices<sup>1</sup>**, QIANG WANG, YAOHUA LIU, SUZANNE TE VELTHUIS, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA, MICHAEL FITZSIMMONS, Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge TN 37831, USA, DAISUKE OKUYAMA, Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University, Sendai 980-8577, Japan, MASAO NAKAMURA, MASASHI KAWASAKI, YOSHINORI TOKURA, RIKEN Center for Emergent Matter Science (CEMS), Wako, 351-0198, Japan — Superlattices composed of equal thickness of ferromagnetic (FM) metal  $\text{La}_{0.5}\text{Sr}_{0.5}\text{MnO}_3$  (LSMO) and charge-orbital ordered (COO) insulator  $\text{Pr}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$  (PCMO) on (011)-oriented  $(\text{LaAlO}_3)_{0.3}(\text{Sr}_2\text{AlTaO}_6)_{0.7}$  substrate have been investigated using polarized neutron reflectometry. In a 200-Oe magnetic field, the magnetization depth profile shows strong temperature dependence. Between the FM transition temperature of LSMO and the COO transition temperature of PCMO, a uniform magnetization throughout the superlattices was obtained. Below the COO transition temperature of PCMO, the magnetization depth profile shows a strong contrast between the LSMO and PCMO regions. At 5000 Oe, both LSMO and PCMO show magnetizations close to their bulk saturation value at low temperature. Our result demonstrates the tunability of the PCMO/LSMO superlattices' magnetic structure with field and temperature and the behavior of this system could be explained as the result of coexistence of the FM and COO phases and their competition.

<sup>1</sup>Work at Argonne was supported by DOE, Office of Science, BES, MSE.

**10:24AM E19.00011 Superparamagnetism at oxide interfaces revealed by scanning SQUID-on-tip microscopy**, YONATHAN ANAHORY, L. EMBON, Weizmann Institute of Science, C.J. LI, National University of Singapore, S. BANERJEE, A. MELTZER, H. R. NAREN, A. YAKOVENKO, J. CUPPENS, Y. MYASOEDOV, M. L. RAPPAPORT, Weizmann Institute of Science, M. E. HUBER, University of Colorado Denver, K. MICHAELI, Weizmann Institute of Science, T. VENKATESAN, A. ARIANDO, National University of Singapore, E. ZELDOV, Weizmann Institute of Science — Our novel scanning SQUID-on-tip technique[1] is used to study nanoscale magnetism present in systems such as atomically sharp oxide heterostructures. Here we report a new emergent phenomenon at the  $\text{LaMnO}_3/\text{SrTiO}_3$  interface in which an antiferromagnetic insulator abruptly transforms into a magnetic state that exhibits unexpected nanoscale superparamagnetic dynamics. Upon increasing the thickness of  $\text{LaMnO}_3$  above five unit cells, our scanning nanoSQUID-on-tip microscopy shows spontaneous formation of isolated magnetic islands of 10 to 50 nm diameter, which display random moment reversals by thermal activation or in response to an in-plane magnetic field[2]. Our charge reconstruction model of the polar  $\text{LaMnO}_3/\text{SrTiO}_3$  heterostructure describes the sharp emergence of thermodynamic phase separation leading to nucleation of metallic ferromagnetic islands in an insulating antiferromagnetic matrix. The model further suggests that the nearby superparamagnetic-ferromagnetic transition can be gate tuned, holding potential for applications in magnetic storage and spintronics. [1] D. Vasyukov *et al*, Nature Nanotech. 8, 639 (2013) [2] Y. Anahory *et al*, arXiv:1509.01895

**10:36AM E19.00012 Giant structural modulation & abnormal ferromagnetism in ferroelectric & ultrathin ferromagnetic digital superlattices<sup>1</sup>**, HANGWEN GUO, ZHEN WANG, MOHAMMAD SAGHAYEZHIAN, LINA CHEN, RONGYING JIN, WARD PLUMMER, JIANDI ZHANG, Louisiana State University, SHUAI DONG, Southeast University, China — The nature of magnetoelectric coupling in oxide heterostructure remains interesting but illusive, largely because the complex nature of interface intermixing and diffusion. In this work, we present our ability to fabricate superlattices consist of ferroelectric BTO & ferromagnetic LSMO, with minimum interfacial intermixing confined within half a unit cell. Such high quality superlattices with sharp interfaces allow us to explore magnetoelectric coupling effect into ultrathin region (reduced dimensionality) and observe ferroelectric induced abnormal magnetic behavior. A detailed STEM study reveals that the traditional electron/hole carrier doping scenario does not play a major role. Instead, distinct modulation of lattice displacement and octahedron tilting is responsible for the coupling effect and abnormal magnetic behavior. Our study highlights the importance of structural-property relationship in oxide heterostructures.

<sup>1</sup>Supported by U.S. DOE under Grant No. DOE DE-SC0002136

**Tuesday, March 15, 2016 8:00AM - 10:36AM —**

**Session E20 GMAG DCMP FIAP: II-VI Magnetic Semiconductors** 319 - Denis Kochan, U. Regensburg

**8:00AM E20.00001 Dynamics of the matrix in DMS Type-II quantum dot systems<sup>1</sup>**, COLLIN R. BROWN, VINCE R. WHITESIDE, IAN R. SELLERS, Department of Physics & Astronomy, University of Oklahoma, Norman, Oklahoma 73019, USA, ATHOS PETROU, Department of Physics, University at Buffalo SUNY, Buffalo, New York 14260, USA, W-C. CHOU, Department of Electro-physics, National Chiao Tung University, Hsinchu 300, Taiwan — Magnetic field, temperature, and polarization dependent continuous wave photoluminescence spectroscopy (PL) is used to study two related Type-II quantum dots (QDs). These techniques were used to study how the location of magnetic impurities affects the formation of magnetic polarons in these two (related) systems. The  $\text{ZnMnTe}/\text{ZnSe}$  system has Mn impurities located within the QDs, with (ideally) no Mn in the surrounding ZnSe matrix. The  $\text{ZnTe}/\text{ZnMnSe}$  QDs have Mn impurities grown within the matrix, which ideally is excluded from the QDs. For both these systems, the holes are confined within the dots, while the electrons are located in the surrounding matrix. The location of the Mn and its coupling with the spin of the corresponding carrier leads to distinct characteristics for each system. Due to difficulties growing these systems, some diffusion of Mn during the growth of these samples is suspected, leading to a percentage of magnetic impurities unintentionally located in the non-magnetic region for both samples. The emission from the matrix in particular was studied to determine the effect/composition of Mn in this region and its contribution to the characteristics of the QDs.

<sup>1</sup>This work is supported by NSF DMR-1305770

**8:12AM E20.00002 Mn<sup>2+</sup>-Doped CdSe/CdS Core/Multishell Colloidal Quantum Wells Enabling Tunable Carrier-Dopant Exchange Interactions<sup>1</sup>**, SAVAS DELIKANLI, Bilkent University, THOMAS SCRACE, JOSEPH MURPHY, BIBLOP BARMAN, YUTSUNG TSAI, PEIYAO ZHANG, State University of New York, University at Buffalo, PEDRO LUDWIG HERNANDEZ-MARTINEZ, Nanyang Technological University, JOSEPH CHRISTODOULIDES, Naval Research Laboratory, ALEXANDER N. CARTWRIGHT, ATHOS PETROU, State University of New York, University at Buffalo, HILMI VOLKAN DEMIR, Nanyang Technological University — We report the manifestations of carrier-dopant exchange interactions in colloidal Mn<sup>2+</sup>-doped CdSe/CdS core/multishell quantum wells. In our solution-processed quantum well heterostructures, Mn<sup>2+</sup> was incorporated by growing a Cd<sub>0.985</sub>Mn<sub>0.015</sub>S monolayer shell on undoped CdSe nanoplatelets using the colloidal atomic layer deposition technique. The carrier-magnetic ion exchange interaction effects are tunable through wave function engineering. This is realized by controlling the spatial overlap between the carrier wave functions with the manganese ions through adjusting the location, composition, and number of the CdSe, Cd<sub>1-x</sub>Mn<sub>x</sub>S, and CdS layers. Our colloidal quantum wells, which exhibit magneto-optical properties analogous to those of epitaxially grown quantum wells, offer new opportunities for solution-processed spin-based semiconductor devices.

<sup>1</sup>H.V.D. acknowledges support from EU-FP7 Nanophotonics4Energy NoE, TUBITAK, NRF-CRP-6-2010-02 and A\*STAR of Singapore. Work at the University at Buffalo was supported by NSF DMR 1305770.

**8:24AM E20.00003 Time resolved photoluminescence study of CdSe/CdMnS/CdS core/shell/shell nanoplatelets heterostructures<sup>1</sup>**, THOMAS SCRACE, State Univ of NY - Buffalo, SAVAS DELIKANLI, MEHMET ZAFER AKGUL, Bilkent University, JOSEPH MURPHY, TIM THOMAY, PEIYAO ZHANG, TENZIN NORDEN, ALEXANDER CARTWRIGHT, ATHOS PETROU, State Univ of NY - Buffalo, HILMI VOLKAN DEMIR, Bilkent University — We have recorded the time evolution of the photoluminescence (PL) for CdSe/CdMnS/CdS core/shell/shell solution-processed nanoplatelets (NP) using ultrafast pulses at 400 nm and 514 nm. Our NPs consist of a core with 5 monolayers (1.5 nm) of CdSe and average lateral dimensions of 55 × 10 nm<sup>2</sup>. Using 400 nm pulses we excite electron-hole pairs above the CdS shell bandgap; with 514 nm pulses we excite only in the CdSe core. The holes are primarily localized in the CdSe core, while the electrons are delocalized. Our measurements show that at  $\Delta t = 0$ , the peak PL energy for both kind of excitations is the same. As a function of time, both types of excitations result in a red-shift. The red shift of with 400 nm excitation is 60 meV and is described by two time scales:  $\tau_1 = 270$  ps and  $\tau_2 = 2.5$  ns. The red shift with the 514 nm excitation is 30 meV and is described by a single time scale:  $\tau_2 = 2.5$  ns. These results are discussed in terms of dipole layer formation[1]. [1] Gu, Y et. al. Phys. Rev. B 71 045340 (2005).

<sup>1</sup>H.V.D. is supported by EU-FP7 Nanophotonics4Energy NoE, and TUBITAK EEEAG 109E002, 109E004, NRF-RF-2009-09, NRF-CRP-6-2010-02 and A\*STAR of Singapore. A.P. is supported by NSF DMR 1305770

**8:36AM E20.00004 Spin-orbit twisted spin-flip waves in CdMnTe quantum wells<sup>1</sup>**, SHAHRZAD KARIMI, University of Missouri, FLORENT PEREZ, Institut des Nanosciences de Paris, CNRS/Universite Paris VI, FLORENT BABOUX, Laboratoire de Photonique et de Nanostructures, LPN/CNRS, IRENE D'AMICO, University of York, GIOVANNI VIGNALE, CARSTEN ULLRICH, University of Missouri — We present a numerical study of spin-flip wave dispersions in a spin-polarized electron gas in a dilute magnetic semiconductor heterostructure, using time-dependent density-functional response theory. The system under study is an n-doped CdMnTe quantum well with an in-plane magnetic field. Rashba and Dresselhaus spin-orbit coupling induces a wavevector-dependent spin splitting in the conduction bands. The spin waves hence travel through a spin-orbit twisted medium. We calculate the spin-wave dispersion to second order in spin-orbit coupling, including impurity scattering effects. Our results are compared with recent inelastic light scattering experiments.

<sup>1</sup>Work supported by DOE Grant No. DE-FG02-05ER46213

**8:48AM E20.00005 Magnetic properties of nano-patterned GaMnAs films grown on ZnCdSe buffer layers<sup>1</sup>**, SINING DONG, XIANG LI, VASILY KANZYUBA, TAEHEE YOO, XINYU LIU, MALGORZATA DOBROWOLSKA, JACEK FURDYNA, Physics Department, University of Notre Dame — Magnetic semiconductor nanostructures are attracting intense attention, both because of their fundamental physical properties, and because of the promise which they hold for building smaller, faster and more energy-efficient devices. In this study we report successful MBE growth of GaMnAs films on the GaAs (100) substrates with ZnCdSe buffer layers, which results in perpendicular magnetic easy axis in the GaMnAs films. The GaMnAs/ZnCdSe films have been etched into nano-stripe shapes with various widths below 200nm by e-beam lithography, which resulted in a new geometry of interest for perpendicular magnetic recording. Magnetic anisotropy of as-grown GaMnAs films and nano-stripes was then studied by SQUID magnetometry. The results indicate that the GaMnAs films consist of magnetic domains with magnetization normal to the film plane, having rather high coercivity, which survives after nanofabrication. This is also confirmed by the dynamics of the domain motion as shown by AC susceptibility measurements. These findings are of interest for understanding the magnetic anisotropy mechanisms in GaMnAs and its domain structures, as well as for designing of nano-sized spintronic devices which require hard ferromagnetic behavior with perpendicular easy axes.

<sup>1</sup>This work was supported by the National Science Foundation Grant DMR1400432.

**9:00AM E20.00006 Gate tunable spin exchange interaction and inversion of magnetoresistance in ferromagnetic ZnO nanowire**, VIJAYAKUMAR MODEPALLI, MI-JIN JIN, JUNGMIN PARK, JUNHYEON JO, JI-HYUN KIM, JEONG MIN BAIK, Ulsan national institute of science and technology, JEONGYONG KIM, Sungkyunkwan University, JUNG-WOO YOO, Ulsan national institute of science and technology — Tuning magnetism in diluted magnetic semiconductor (DMS) is one of the central issue to the development of future spintronic device applications. Particularly, realizing such control in nanostructure has received growing attention. Here, we report the dramatic change of MR in ferromagnetic ZnO nanowire with varied gate voltages (+50 V to -40 V) at different temperatures (2 K to 50 K). The MR signal was greatly influenced by the gate voltage induced carrier concentrations which results the inversion of MR from positive to negative sign while pertaining the coexistence of both parts before inversion in the range of -2T to 2T. The origin of negative MR is mainly due to spin scattering while the positive one is due to a field induced change in relative populations of conduction bands with different conductivities. The extracted spin exchange related parameter was well tuned with the varied gate voltages at different temperatures. More importantly this type of gate tuning of spin exchange interactions in ferromagnetic single ZnO nanowire is well suitable for future spintronic device applications.

**9:12AM E20.00007 The State of the Art in (Cd,Mn)Te Heterostructures: Fundamentals and Applications**<sup>1</sup>, TOMASZ WOJCIOWICZ, Institute of Physics, Polish Academy of Sciences, Warsaw, Poland — In my talk I will review recent progress in the MBE technology of (Cd,Mn)Te nanostructures containing two dimensional electron gas (2DEG) that led to the first ever observation of fractional quantum Hall effect in magnetic system [1]. This opens new directions in spintronics. I will first discuss already demonstrated applications of such high mobility magnetic-2DEG system for: a) THz and microwave radiation induced zero-bias generation of pure spin currents and very efficient magnetic field induced conversion of them into spin polarized electric current [2]; b) clear demonstration of THz radiation from spin-waves excited via efficient Raman generation process [3]; c) experimental demonstration of working principles of a new type of spin transistor based on controlling the spin transmission via tunable Landau-Zener transitions in spatially modulated spin-split bands [4]. I will also explain the possibility to use magnetic-2DEG for developing of a new system where non-Abelian excitations can not only be created, but also manipulated in a two-dimensional plane. The system is based on high mobility CdTe quantum wells with engineered placement of Mn atoms, where sign of the Lande g-factor can be locally controlled by electrostatic gates at high magnetic fields. Such a system may allow for building a new platform for topologically protected quantum information processing. I will also present results demonstrating electrostatic control of 2D gas polarization in a quantum Hall regime [5].

[1] C. Betthausen, *et al.*, Phys. Rev. B **86**, 085310 (2014).

[2] P. Olbrich, *et al.*, Phys. Rev. B **86**, 085310 (2012).

[3] R. Rungsawang, *et al.*, Phys. Rev. Lett. **110**, 177203 (2013).

[4] C. Betthausen, *et al.*, Science **337**, 324 (2012).

[5] A. Kazakov, *et al.*, APS March Meeting 2015, <http://meetings.aps.org/link/BAPS.2015.MAR.A7.13>.

<sup>1</sup>The research was partially supported by National Science Centre (Poland) grant DEC-2012/06/A/ST3/00247 and by ONR grant N000141410339.

**9:48AM E20.00008 Structural and Optical properties of Er doped ZnO diluted magnetic semiconductor nano thin films produced by sol gel method.**<sup>1</sup>, A. TOLGA TASCI, OZGUR OZTURK, ELIF ASIKUZUN, KASTAMONU UNIVERSITY, LUTFI ARDA, Bahcesehir University, SUKRU CELIK, Sinop University, CABIR TERZIOGLU, Abant Izzet Baysal University — Undoped and Er doped ZnO ( $Zn_{1-x}Er_xO$ ) transparent semiconductor thin films were coated using sol-gel method on non-alkali glass. Erbium was doped 1%, 2%, 3%, 4% and 5% ratio. Methanol and monoethanolamine were used as solvent and stabilizer. In this study, the effect of Er doping was examined on the structural and optical properties of ZnO DMS thin films. XRD, SEM and UV-VIS-NIR spectrometer measurements were performed for the structural and optical characterization. XRD results showed that, all of Er doped ZnO thin films have a hexagonal structure. The optical transmittance of rare earth element (Er) doped ZnO thin films were increased. The Er doped ZnO thin films showed high transparency ( $>84$ ) in the visible region (400-700 nm).

<sup>1</sup>This research has been supported by the Kastamonu University Scientific Research Projects Coordination Department under the Grant No. KUBAP-03/2013-41 and the Scientific and Technological Research Council of Turkey (TUBITAK) Project No. 114F259.

**10:00AM E20.00009 Microstructural and Optical properties of transition metal (Cu) doped ZnO diluted magnetic semiconductor nano thin films fabricated by sol gel method.**<sup>1</sup>, OZGUR OZTURK, ELIF ASIKUZUN, A. TOLGA TASCI, Kastamonu University, LUTFI ARDA, Bahcesehir University, SEVIM DEMIROZU SENOL, Abant Izzet Baysal University, SUKRU CELIK, Sinop University, CABIR TERZIOGLU, Abant Izzet Baysal University — Undoped and Cu (Copper) doped ZnO ( $Zn_{1-x}Cu_xO$ ) semiconductor thin films were produced by using sol-gel method. Cu was doped 1%, 2%, 3%, 4% and 5% ratio. Methanol and monoethanolamine (MEA) were used as solvent and stabilizer. In this study, the effect of Cu doping was investigated on microstructural and optical properties of ZnO DMS thin films. XRD, SEM, AFM and UV-VIS spectrometer measurements were performed for the microstructural and optical characterization. XRD, SEM and AFM results were showed that all of Cu doped ZnO based thin films have a hexagonal structure. The grain size of Cu doped ZnO thin films and morphology of surface were changed with increasing Cu doping. The optical transmittance of transition metal (Cu) doped ZnO thin films were decreased with doping. **Keywords:** Diluted Magnetic Semiconductor (DMS), Thin Film, Cu-doping, Bandgap Energy, ZnO.

<sup>1</sup>This research has been supported by the Kastamonu University Scientific Research Projects Coordination Department under the Grant No. KU-BAP-05/2015-12 and the Scientific and Technological Research Council of Turkey (TUBITAK) Project No. 114F259.

**10:12AM E20.00010 Oxygen vacancies induced Spin polarized current in Co-doped ZnO by Andreev reflection technique**, KUNG-SHANG YANG, HSIUNG CHOU, WEN LING CHAN, BO-YU CHEN, Department of Physics, NSYSU, Kaohsiung 804, Taiwan, SHANG-FAN LEE COLLABORATION<sup>1</sup> — Dilute magnetic semiconductor (DMO) is a semiconducting system with spin-polarized carriers and magnetic properties. However, since most studies had been focused on existence of FM, the proportion of spin-polarized current (SPC) in DMO is far from being determined. We used Point-contact Andreev reflection measurements on various  $Zn_{0.95}Co_{0.05}O$  thin films, with controlled oxygen vacancies by sputtering in various  $H_2$  partial pressure with Ar atmosphere. We found that conductance versus voltage (G-V) spectra suppresses as oxygen vacancy concentration increases. It indicates oxygen vacancies play significant role in inducing the SPC. To understand the origin of spin polarized current at the interface of the superconducting tip/CZO system, we use modified Blonder-Tinkham-Klapwijk (MBTK) model in ballistic and diffusive regime to interpret GV curve. The extracted SPC value were up to 70% in ballistic regime and 65% in diffusive regime. The results suggest tiny routes have been formed by oxygen vacancies which are extended throughout the whole films. This result confirmed that MBTK model in ballistic regime is more suitable for our GV spectra and this explains the observation of such a high SPC

<sup>1</sup>Institute of Physics, Academia Sinica Taiwan

**10:24AM E20.00011 Study of the new diluted magnetic semiconductors based on the doping of iron-based superconductors**, LI ZHANG, SHAN FENG, LINXIAN LI, SHAOLEI WANG, YUKE LI, China Jiliang University — Diluted magnetic semiconductors(DMSs) have attracted increasing attention because of their potential applications in spintronics. Recently, a series of new bulk DMS materials [1,2] were synthesized by doping in the 122 and 1111 phases of iron-based superconductors(Fe-SC), which sheds light on the DMS research[3]. In this report, we have synthesized two systems of 1111 phases of DMSs based on Fe-SC materials ( $La_{1-x}Sr_x$ ) ( $Ag_{0.925}Mn_{0.075}SO$  ( $x=0, 0.025, 0.05, 0.075$  and  $0.1$ ) and ( $Y_{1-x}Sr_x$ ) ( $Cu_{0.925}Mn_{0.075}SO$  ( $x=0, 0.025, 0.05, 0.075$  and  $0.1$ ) by solid state method. The structure and electrical, magnetic and optical properties have been investigated by means of XRD, 4KCCS, MPMS, PL, UV-Vis and Raman technique, respectively. Some interesting phenomena are found (Such as the Curie temperature  $T_c$  and band-gap energy  $E_g$  change regularly with the dopants addition). The results are helpful to clarify the intrinsic mechanism of the DMSs, and will provide new insights on the fabrication and application of devices based on these materials. This work was supported by the National Science Foundation of China (Grant No 61376094). Li Zhang would like to acknowledge a scholarship granted by China Scholarship Council (CSC-201408330028) **References:** [1] K.Zhao,Z.Deng and X.C.Wang et al., Nature Communications 4, 1442 (2013). [2] X.J. Yang, Y.K. Li, C.Y. Shen et al., Appl. Phys. Lett. 103, 022410 (2013). [3]T. Ditel and H.Ohno, Rev.Mod.Phys., 86,187(R)(2014).

**Tuesday, March 15, 2016 8:00AM - 10:48AM –**

**Session E21 DCMP DCOMP: Experimental Techniques and Results: Static and Dynamic High-Pressure Physics** 320 - Audrey Grockowiak, National High Magnetic Field Laboratory

**8:00AM E21.00001 High-Pressure Electrical, Raman, and Structural Measurements on Lithium Sulfide<sup>1</sup>**, KATHRYN HAM, YOGESH VOHRA, GEORGIY TSOI, Univ of Alabama - Birmingham — High-Pressure studies have been conducted on Lithium Sulfide ( $\text{Li}_2\text{S}$ ) to 55 GPa, with electrical, structural, and Raman measurements. Due to the highly reactive nature of the sample in air, the loading was conducted in a glove bag under an inert Argon atmosphere. Four probe electrical measurements using designer diamond anvils showed characteristic semiconducting behavior in  $\text{Li}_2\text{S}$  up to 33 GPa from ambient temperature to 10 K.  $\text{Li}_2\text{S}$  was compressed to 55 GPa and angle dispersive X-Ray data was collected at the Advanced Photon Source, Argonne National Lab, which showed a phase transition from a face centered cubic phase to a primitive orthorhombic phase. Raman data was obtained for  $\text{Li}_2\text{S}$  at ambient conditions after decompression from 55 GPa. The Raman Spectrum showed the characteristic peak for  $\text{Li}_2\text{S}$  at 372.5 wavenumbers, but had an additional uncharacteristic peak at 327.4 wavenumbers. There is a possibility that the additional uncharacteristic Raman peak is due to the decomposition of  $\text{Li}_2\text{S}$  at high pressure.

<sup>1</sup>This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Lab, Contract No. DE-AC02-06CH11357.; DOE-NNSA Grant No. DE-NA0002014.

**8:12AM E21.00002 Pressure tuning the lattice and optical response of  $\text{Ag}_2\text{S}$** , ZHAO ZHAO, Department of Physics, Stanford University, HUA WEI, Department of Materials Science and Engineering, University of Tennessee, WENDY MAO, Photon Science, SLAC; Department of Geological Sciences, Stanford University — Silver chalcogenides  $\text{Ag}_2\text{E}$  ( $\text{E} = \text{S}, \text{Se}, \text{and Te}$ ) is a group of materials attracting intense scientific and industrial interest recently. The ability to tune their crystal structure and electronic structure away from their pristine states opens up new optics and opto-electronics applications. In this work, we systematically studied the high pressure structural and optical behavior of  $\text{Ag}_2\text{S}$  by in-situ angle dispersive X-ray Diffraction (XRD) and Infrared (IR) measurements in a diamond anvil cell. Though a series of structural transitions and lattice contractions, the structural symmetrization of  $\text{Ag}_2\text{S}$  is seen from the decrease of  $\beta$  from  $99^\circ$  to  $90^\circ$ . The IR transmission and reflection measurements showed that pressure continuously tuned semiconducting  $\text{Ag}_2\text{S}$  to metallic at around 22 GPa. By Drude model analysis of the IR reflectivity, the optical conductivity shows radical evolution. In particular, the highest DC conductivity reaches  $100 \Omega^{-1}\text{cm}^{-1}$  at 40 GPa. Our results highlight pressure's dramatic role in tuning the lattice and electronic state of silver chalcogenides.

**8:24AM E21.00003 Synthesis and Characterization of Bulk BC8 Si**, HAIDONG ZHANG, TIMOTHY STROBEL, Geophysical Laboratory, Carnegie Institution of Washington — Silicon, an essential element for modern industry, has several allotropes existing at ambient conditions. Among them, one of the most important phases is the metastable Si-III (BC8) structure. Although it has been known since 1960s, experimental characterization of its properties is still rare primarily due to lack of large bulk samples. Common methods produce BC8 Si samples with the size of micrometers in dimension, preventing definitive experimental measurements. In this work we report synthesis of phase pure bulk BC8 Si with the size of a few millimeters through the multi-anvil press method. The structure was confirmed by powder X-ray diffraction and further supported by the Raman spectrum. Its electrical resistance exhibits clear temperature dependence, increasing from 300 K to 2K. A crossover region occurs around 80 K to 100 K, showing a stronger dependence below 80 K. We also report its optical properties, thermal stability and phonon density of states.

**8:36AM E21.00004 Experimental Equation of State of Hafnium Metal to 210 GPa<sup>1</sup>**, YOGESH VOHRA, JEFFREY MONTGOMERY, SPENCER SMITH, GEORGIY TSOI, University of Alabama at Birmingham — The equation of state of hafnium metal has been measured using a platinum pressure marker to 210 GPa. Beveled diamonds with 35 micron central flats were used to compress a sample consisting of a mixture of platinum and hafnium that was packed with 6 nm diamond powder. It was hoped that this geometry would provide an alternative method of creating a second-stage pressure region to reach multi-megabar pressures. Powder diffraction patterns were collected across the high-pressure region using an x-ray beam collimated to  $1 \times 2$  microns in a grid with a spacing of 1 micron. At the highest loads, a pressure gradient of 90 GPa was observed across the sample. This gradient allows for the construction of an equation of state over this range from data collected in only 3 minutes of synchrotron x-ray time. A new analysis program suite employing a measurement of spectral overlap has been developed to identify the multiple structures present, fit lattice parameters, and analyze the newly available gradient information.

<sup>1</sup>This work was supported by the Department of Energy (DOE) National Nuclear Security Administration under grant number DE-NA0002014.

**8:48AM E21.00005 Molecular crystals as precursors for poly-nitrogen<sup>1</sup>**, GUSTAV BORSTAD, JENNIFER CIEZAK-JENKINS, US Army Research Laboratory — The application of pressure to matter results in dramatic modifications of its properties. The compression of molecular crystals first eliminates “empty” space between the molecules. It then alters the electron density distribution, favoring the increase of atomic coordination and the formation of polymers. The polymerization of low-Z compounds into covalently-bonded networks in three dimensions tend to generate materials characterized by superconductivity, super-hardness, and high-energy density.<sup>1</sup> Poly-nitrogen (analogous to diamond) has been synthesized under extreme conditions above 100 GPa and 2000 K in diamond anvil cells, but could not be recovered to ambient conditions.<sup>2</sup> A useful form of poly-nitrogen would have to be synthesized at low-pressure with enhanced stability at ambient conditions. The changes in the intermolecular and intramolecular interactions with pressure play a crucial role in the synthesizing and stabilizing of the structure as well as in tuning its properties. In this talk, we provide Raman and x-ray diffraction data on nitrogen-containing compound biuret and compare it to work on other possible poly-nitrogen precursors. References [1] W. Grochala *et al.*, *Angew. Chem. Int. Ed.* **46**, 3620 (2007). [2] M. I. Eremets *et al.*, *Nat. Mater.* **3**, 558 (2004).

<sup>1</sup>During this project, coauthor GB was supported in part by an appointment to the Postdoctoral Research Program at the US Army Research Laboratory administered by the Oak Ridge Associated Universities.

**9:00AM E21.00006 High-pressure thermal properties of liquid, crystalline, and amorphous  $\text{H}_2\text{O}$** , ZACHARY GEBALLE, VIKTOR STRUZHUKIN, Carnegie Inst of Washington — We have developed a new technique to measure thermal conductivity and heat capacity of any insulator compressed inside a diamond anvil cell. The method uses Joule heating of a platinum foil or thin-film that is pressed against the sample. Electrical current oscillates at frequencies up to 300 kHz and we infer the amplitude of temperature oscillation via a third-harmonic voltage measurement. The melting and freezing of water in a diamond cell, including 30 K hysteresis, is documented with this new technique when temperature is varied over hours. We will also present calorimetry results using cooling timescales from seconds to milliseconds, which may be short enough to pass through “no-man’s land” into the stability field of glassy water.

**9:12AM E21.00007 High Pressure XANES studies on Mn doped Bi<sub>2</sub>Te<sub>3</sub>**, BRIAN LIGHT, RAVHI KUMAR, JASON BAKER, Univ of Nevada - Las Vegas, PRABHAKARAN DHARMALINGAM, Clarendon Laboratory, University of Oxford, UK, CHANGYONG PARK, Univ of Nevada - Las Vegas, UNLV TEAM, HPCAT AND CARNEGIE INSTITUTE OF WASHINGTON COLLABORATION — Bi<sub>2</sub>Te<sub>3</sub>, Bi<sub>2</sub>Se<sub>3</sub>, and Sb<sub>2</sub>Te<sub>3</sub> are narrow band-gap semiconductors have been extensively studied along with their alloys due to their promising technological applications as thermoelectric materials. More recently pressure induced superconductivity and structural transition have been observed in these materials around 7 GPa [1,2]. Here we have performed high pressure x-ray near edge spectroscopy (XANES) measurements at Bi L-III edge on Mn (0.1) doped Bi<sub>2</sub>Te<sub>3</sub> samples to understand the variation of the Bi valence across the pressure induced superconductivity regime. We have inferred notable changes in the Bi valence at high pressure conditions. The results will be discussed in detail. Work at the University of Nevada Las Vegas (ALC) is funded by U.S. Department of Energy Award DE-SC0001928. Portions of this work were performed at HPCAT (Sector 16), Advanced Photon Source (APS), Argonne National Laboratory. HPCAT is supported by DOE-BES, DOE-NNSA, NSF, and the W.M. Keck Foundation. APS is supported by DOE-BES, under Contract No. DE-AC02-06CH1135.

**9:24AM E21.00008 Equation of state of palladium hydride and deuteride to 100 GPa<sup>1</sup>**, KEENAN BROWNSBERGER, Whitworth University, MUHTAR AHART, MADDURY SOMAYAZULU, STEPHEN GRAMSCH, RUSSELL HEMLEY, Carnegie Institution of Washington — To study the behavior of palladium hydrides under pressure, we loaded palladium foils in hydrogen or deuterium environments in two separate diamond anvil cells. We subsequently measured x-ray diffraction up to 100 GPa at room temperature. No structural phase transition was observed for either PdD<sub>x</sub> or PdH<sub>x</sub> between 0 GPa and 100 GPa. The pressure-volume data were fitted with the third-order Birch-Murnaghan equation of state, which gave an initial volume of 10.8 cm<sup>3</sup>/mol, a bulk modulus of 153 GPa, and its derivative of 4.3 for palladium hydride. An initial volume of 10.6 cm<sup>3</sup>/mol, a bulk modulus of 162 GPa, and its pressure derivative of 4.6 were determined for palladium deuteride. From initial volumes, we conclude that  $x=1$  for both PdD<sub>x</sub> and PdH<sub>x</sub>. This work is supported by the Carnegie-DOE Alliance Center.

<sup>1</sup> EOS of palladium hydride and deuteride to 100 GPa

**9:36AM E21.00009 Development of safety containment system for experiments on radioactive and other hazardous materials with large volume Paris-Edinburgh press at APS and first measurements on depleted-uranium**, MATTHEW JACOBSEN, NENAD VELISAVLJEVIC, Los Alamos National Laboratory — Recent technical developments using the large volume Paris-Edinburgh press platform have enabled x-ray synchrotron studies at high pressure and temperature conditions (Kono, Y. *et al. Rev. Sci. Instrum.* **83**, 033905 (2012)). However, application for hazardous materials requires special handling due to safety issues, reactivity, or other challenges. Facility safety requirements require adequate containment for operation in the variety of environments available. In this talk, we will present a containment setup developed to enable studies of such materials. In particular, studies of the phase diagram of uranium using ultrasonic interferometry to determine the elasticity, mechanical, and thermal properties will be discussed. These results present the first high pressure studies of combined elasticity and thermal properties of depleted uranium metal as well as demonstration of a containment system for making such measurements.

**9:48AM E21.00010 NMR in a Diamond Anvil Pressure Cell**, MATTHEW LAWSON, Univ of California - Davis, ADAM DIOGUARDI, Los Alamos National Lab, SAMUEL WEIR, LLNL, BLAINE BUSH, Univ of California - Davis, MIHINDRA DUNUWILLE, SHANTI DEEMYAD, University of Utah, NICHLAS CURRO, Univ of California - Davis — We present recent advances in the use of diamond anvil pressure cells in nuclear magnetic resonance measurements. This technique allows access to new regions of the phase diagrams of iron pnictide and heavy fermion materials, and promises to allow NMR experiments under pressures not previously accessible.

**10:00AM E21.00011 Reactive decomposition of low density PMDI foam subject to shock compression<sup>1</sup>**, SCOTT ALEXANDER, WILLIAM REINHART, AARON BRUNDAGE, DAVID PETERSON, Sandia National Laboratories — Low density polymethylene diisocyanate (PMDI) foam with a density of 5.4 pounds per cubic foot (0.087 g/cc) was tested to determine the equation of state properties under shock compression over the pressure range of 0.58 - 3.4 GPa. This pressure range encompasses a region approximately 1.0-1.2 GPa within which the foam undergoes reactive decomposition resulting in significant volume expansion of approximately three times the volume prior to reaction. This volume expansion has a significant effect on the high pressure equation of state. Previous work on similar foam was conducted only up to the region where volume expansion occurs and extrapolation of that data to higher pressure results in a significant error. It is now clear that new models are required to account for the reactive decomposition of this class of foam. The results of plate impact tests will be presented and discussed including details of the unique challenges associated with shock compression of low density foams.

<sup>1</sup>Sandia National Labs is a multi-program lab managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corp., for the U.S. Dept. of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

**10:12AM E21.00012 Modeling shock-driven reaction in low density PMDI foam<sup>1</sup>**, AARON BRUNDAGE, C. SCOTT ALEXANDER, WILLIAM REINHART, DAVID PETERSON, Sandia National Laboratories — Shock experiments on low density polyurethane foams reveal evidence of reaction at low impact pressures. However, these reaction thresholds are not evident over the low pressures reported for historical Hugoniot data of highly distended polyurethane at densities below 0.1 g/cc. To fill this gap, impact data given in a companion paper for polymethylene diisocyanate (PMDI) foam with a density of 0.087 g/cc were acquired for model validation. An equation of state (EOS) was developed to predict the shock response of these highly distended materials over the full range of impact conditions representing compaction of the inert material, low-pressure decomposition, and compression of the reaction products. A tabular SESAME EOS of the reaction products was generated using the JCZS database in the TIGER equilibrium code. In particular, the Arrhenius Burn EOS, a two-state model which transitions from an unreacted to a reacted state using single step Arrhenius kinetics, as implemented in the shock physics code CTH, was modified to include a statistical distribution of states. Hence, a single EOS is presented that predicts the onset to reaction due to shock loading in PMDI-based polyurethane foams.

<sup>1</sup>Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's NNSA under contract DE-AC04-94AL85000.

**10:24AM E21.00013 Static Pressure Above 300 GPa Using Chemical Vapor Deposited Two-stage Diamond Micro-anvils<sup>1</sup>**, JEFFREY MONTGOMERY, GOPI SAMUDRALA, GEORGIY TSOI, SPENCER SMITH, YOGESH VOHRA, University of Alabama at Birmingham — Two-stage diamond micro-anvils were grown via chemical vapor deposition (CVD) on beveled diamond anvils with 30 micron central flats. These anvils were used to compress a pre-indented rhenium foil to pressures in excess of 300 Gigapascals (GPa) at relatively small applied loads. Powder diffraction patterns were collected across the high-pressure region using an x-ray beam collimated to 1x2 microns in a grid with a spacing of 1 micron. While multi-megabar pressures were seen across the entire second stage, the highest pressure regions were confined to areas of a few microns in diameter. These were observed at points near the edge of the second stage with nearby pressure gradients as high as 100 GPa/micron. The transmitted x-rays show that the second stage plastically deformed while maintaining multi-megabar pressures. This may have created a second-stage gasket consisting of CVD diamond and rhenium that supported the pressure gradient without substantial external confining pressure. Further improvements in two-stage diamond micro-anvils would require controlling the geometry and microcrystalline/nanocrystalline diamond content during CVD growth process.

<sup>1</sup>This work was supported by the Department of Energy (DOE)/National Nuclear Security Administration under grant number DE-NA0002014.

**10:36AM E21.00014 High-pressure X-ray diffraction, Raman, and computational studies of MgCl<sub>2</sub> up to 1 Mbar: Extensive pressure stability of the  $\beta$ -MgCl<sub>2</sub> layered structure.<sup>1</sup>**, ELISSAIO STAVROU, JOSEPH ZAUG, SORIN BASTEA, I-FENG KUO, JONATHAN CROWHURST, Lawrence Livermore National Laboratory, BORA KALKAN, MARTIN KUNZ, Advanced Light Source, Lawrence Berkeley Laboratory, ZUZANA KONOPKOVA, Deutsches Elektronen-Synchrotron (HASYLAB) — Magnesium chloride with the rhombohedral layered CdCl<sub>2</sub>-type structure ( $\alpha$ -MgCl<sub>2</sub>) has been studied using x-ray diffraction and Raman spectroscopy up to 1 Mbar. The results reveal a second-order phase transition to a hexagonal layered CdI<sub>2</sub>-type structure at 0.7 GPa. This phase transition affects the stacking of the Cl anions, resulting to a shorter *c*-axis. An anisotropic compression along *c*-axis was observed during initial compression; altered above 10 GPa due to the repulsion between adjacent Cl-layers. According to previous theoretical studies, a series of phase transitions towards, initially, the 3D rutile (6-fold Mg cations) at 17 GPa and to fluorite structure (8-fold Mg cations) at 70 GPa are proposed. According to our experimental study MgCl<sub>2</sub> remains in a 2D layered structure up to 1Mbar keeping the 6-fold coordination of Mg cations. This observation contradicts with the general structural behavior of compressed AB<sub>2</sub> compounds; we conducted *ab-initio* calculations to elucidate the mechanisms that extend the remarkable structural stability of MgCl<sub>2</sub>.

<sup>1</sup>This work was performed under the auspices of the U. S. Department of Energy by Lawrence Livermore National Security, LLC under Contract DE-AC52-07NA27344.

**Tuesday, March 15, 2016 8:00AM - 11:00AM –**  
**Session E22 DCOMP: Predicting and Classifying Materials via High-Throughput Databases and Machine Learning I** 321 - Gus Hart, Brigham Young University

**8:00AM E22.00001 Novel energy materials through structural search**, MAXIMILIAN AMSLER, Northwestern University, STEFAN GOEDECKER, Basel University, CHRIS WOLVERTON, Northwestern University — Sophisticated structure prediction methods have been developed and become essential tools when designing new materials with desired properties. Their successful applications to many systems at various conditions and the increasing amount of available computational power have strongly contributed to their popularity. The Minima Hopping Method (MHM) is a powerful tool to find low energy structures given only the chemical composition of a system and allows the prediction of structures at any boundary condition. Recently, not only the thermodynamic ground states, but also metastable phases accessible through various synthesis methods have drawn considerable interest for energy applications. We present the discovery of novel energy materials, ranging from low-density silicon allotropes with improved absorption in the visible to thermoelectric materials, by optimizing the MHM to imitate synthesis pathways.

**8:12AM E22.00002 High-throughput Screening and Statistical Learning for the Design of Transparent Conducting Oxides**, CHRISTOPHER SUTTON, LUCA GHIRINGHELLI, MATTHIAS SCHEFFLER, Fritz Haber Institute of the Max Planck Society — Transparent conducting oxides (TCOs) represent a class of well-developed and commercialized wide-bandgap semiconductors that are crucial for many electronic devices. Al, Ga, and In-based sesquioxides are investigated as new TCOs motivated by very intriguing recent experimental work that has demonstrated bandgap engineering in ternary (Al<sub>x</sub>Ga<sub>1-x</sub>Y)2O<sub>3</sub> ranging from 3.8 eV to 7.5 eV by adjusting the ratio of In/Ga[1] and Ga/Al.[2] We employed DFT-based cluster expansion (CE) models combined with fast stochastic optimization techniques (e.g., Wang-Landau and diffusive nested sampling) in order to efficiently search for stable and metastable configurations of (Al<sub>x</sub>Ga<sub>1-x</sub>Y)2O<sub>3</sub> at various lattice structures. The approach also allows for a consideration of the effect of entropy on the relative stability of ternary TCOs. Statistical learning/compressed sensing is being used to efficiently identify a structure-property relationship between the targeted properties (e.g., mobilities and optical transparency) and the fundamental chemical and physical parameters that control these properties. [1] Zhang et al., Solid State Commun, 186, 28 (2014). [2] Ito et al., Jpn. J. Appl. Phys., 51, 100207 (2012); Zhang et al., Appl. Phys. Lett., 105, 162107 (2014).

**8:24AM E22.00003 Many-body physics via machine learning<sup>1</sup>**, LOUIS-FRANCOIS ARSENAULT, Columbia Univ, O. ANATOLE VON LILIENFELD, Basel Univ, ANDREW J. MILLIS, Columbia Univ — We demonstrate a method for the use of machine learning (ML) to solve the equations of many-body physics, which are functional equations linking a bare to an interacting Greens function (or self-energy) offering transferable power of prediction for physical quantities for both the forward and the reverse engineering problem of materials. Functions are represented by coefficients in an orthogonal polynomial expansion and kernel ridge regression is used. The method is demonstrated using as an example a database built from Dynamical Mean Field theory (DMFT) calculations on the three dimensional Hubbard model. We discuss the extension to a database for real materials. We also discuss some new area of investigation concerning high throughput predictions for real materials by offering a perspective of how our scheme is general enough for applications to other problems involving the inversion of integral equations from the integrated knowledge such as the analytical continuation of the Greens function and the reconstruction of lattice structures from X-ray spectra.

<sup>1</sup>Office of Science of the U.S. Department of Energy under Subcontract DOE No. 3F-3138 and FG-ER04169

### 8:36AM E22.00004 Deep Wavelet Scattering for Quantum Energy Regression<sup>1</sup>, MATTHEW HIRN,

Michigan State University — Physical functionals are usually computed as solutions of variational problems or from solutions of partial differential equations, which may require huge computations for complex systems. Quantum chemistry calculations of ground state molecular energies is such an example. Indeed, if  $x$  is a quantum molecular state, then the ground state energy  $E_0(x)$  is the minimum eigenvalue solution of the time independent Schrödinger Equation, which is computationally intensive for large systems. Machine learning algorithms do not simulate the physical system but estimate solutions by interpolating values provided by a training set of known examples  $\{(x_i, E_0(x_i))\}_{i \leq n}$ . However, precise interpolations may require a number of examples that is exponential in the system dimension, and are thus intractable. This curse of dimensionality may be circumvented by computing interpolations in smaller approximation spaces, which take advantage of physical invariants. Linear regressions of  $E_0$  over a dictionary  $\Phi = \{\phi_k\}_k$  compute an approximation  $\tilde{E}_0$  as:  $\tilde{E}_0(x) = \sum_k w_k \phi_k(x)$ , where the weights  $\{w_k\}_k$  are selected to minimize the error between  $E_0$  and  $\tilde{E}_0$  on the training set. The key to such a regression approach then lies in the design of the dictionary  $\Phi$ . It must be intricate enough to capture the essential variability of  $E_0(x)$  over the molecular states  $x$  of interest, while simple enough so that evaluation of  $\Phi(x)$  is significantly less intensive than a direct quantum mechanical computation (or approximation) of  $E_0(x)$ . In this talk we present a novel dictionary  $\Phi$  for the regression of quantum mechanical energies based on the *scattering transform* of an intermediate, approximate electron density representation  $\rho_x$  of the state  $x$ . The scattering transform has the architecture of a deep convolutional network, composed of an alternating sequence of linear filters and nonlinear maps. Whereas in many deep learning tasks the linear filters are learned from the training data, here the physical properties of  $E_0$  (invariance to isometric transformations of the state  $x$ , stable to deformations of  $x$ ) are leveraged to design a collection of linear filters  $\rho_x * \psi_\lambda$  for an appropriate wavelet  $\psi$ . These linear filters are composed with the nonlinear modulus operator, and the process is iterated upon so that at each layer stable, invariant features are extracted:  $\phi_k(x) = |||\rho_x * \psi_{\lambda_1} * \psi_{\lambda_2} * \dots * \psi_{\lambda_m}|||$ ,  $k = (\lambda_1, \dots, \lambda_m)$ ,  $m = 1, 2, \dots$ . The scattering transform thus encodes not only interactions at multiple scales (in the first layer,  $m = 1$ ), but also features that encode complex phenomena resulting from a cascade of interactions across scales (in subsequent layers,  $m \geq 2$ ). Numerical experiments give state of the art accuracy over data bases of organic molecules, while theoretical results guarantee performance for the component of the ground state energy resulting from Coulombic interactions.

<sup>1</sup>Supported by the ERC InvariantClass 320959 grant.

### 9:12AM E22.00005 Machine learning bandgaps of double perovskites<sup>1</sup>, GHANSHYAM PILANIA, Los Alamos

Natl Lab, ARUN MANNODI-KANAKKITHODI, University of Connecticut, BLAS UBERUAGA, Los Alamos Natl Lab, RAMPI RAMPRASAD, University of Connecticut, JAMES GUBERNATIS, TURAB LOOKMAN, Los Alamos Natl Lab — The ability to make rapid and accurate predictions of bandgaps for double perovskites is of much practical interest for a range of applications. While quantum mechanical computations for high-fidelity bandgaps are enormously computation-time intensive and thus impractical in high throughput studies, informatics-based statistical learning approaches can be a promising alternative. Here we demonstrate a systematic feature-engineering approach and a robust learning framework for efficient and accurate predictions of electronic bandgaps for double perovskites. After evaluating a set of nearly 1.2 million features, we identify several elemental features of the constituent atomic species as the most crucial and relevant predictors. The developed models are validated and tested using the best practices of data science (on a dataset of more than 1300 double perovskite bandgaps) and further analyzed to rationalize their prediction performance.

<sup>1</sup>Los Alamos National Laboratory LDRD program and the U.S. Department of Energy, Office of Science, Basic Energy Sciences

### 9:24AM E22.00006 A Multi-Objective Optimization Technique to Model the Pareto Front of Organic Dielectric Polymers<sup>1</sup>, J. E. GUBERNATIS, Theoretical Division, Los Alamos National Laboratory, A. MANNODI-KANAKKITHODI,

R. RAMPRASAD, Department of Materials Science and Engineering, University of Connecticut, G. PILANIA, Materials Science and Engineering Division, Los Alamos National Laboratory, T. LOOKMAN, Theoretical Division, Los Alamos National Laboratory — Multi-objective optimization is an area of decision making that is concerned with mathematical optimization problems involving more than one objective simultaneously. Here we describe two new Monte Carlo methods for this type of optimization in the context of their application to the problem of designing polymers with more desirable dielectric and optical properties. We present results of applying these Monte Carlo methods to a two-objective problem (maximizing the total static band dielectric constant and energy gap) and a three objective problem (maximizing the ionic and electronic contributions to the static band dielectric constant and energy gap) of a 6-block organic polymer. Our objective functions were constructed from high throughput DFT calculations of 4-block polymers, following the method of Sharma et al., Nature Communications 5, 4845 (2014) and Mannodi-Kanakkithodi et al., Scientific Reports, submitted. Our high throughput and Monte Carlo methods of analysis extend to general N-block organic polymers.

<sup>1</sup>This work was supported in part by the LDRD DR program of the Los Alamos National Laboratory and in part by a Multidisciplinary University Research Initiative (MURI) grant from the Office of Naval Research.

### 9:36AM E22.00007 A New Silicon Allotrope with a Direct Band Gap for Optoelectronic Ap-

plications, YAGUANG GUO, QIAN WANG, Peking University, YOSHIYUKI KAWAZOE, Tohoku University, PURU JENA, Virginia Commonwealth University, PEKING UNIVERSITY TEAM, KAWAZOE COLLABORATION, JENA COLLABORATION — Silicon structures with direct band gaps have been hotly pursued for solar cell applications. To effectively harvest the sunlight in the whole frequency region, it is a good strategy to use arrays consisting of Si structures with different direct band gaps. However, the structure with a direct band gap about 0.6 eV has been missing according to current progress made in the direction. Here we report our findings that the missing structure can be constructed by using Si triangles as the building blocks, which is stable dynamically and thermally, not only exhibiting the desirable band gap, but also showing high intrinsic mobility and low mass density. These advantages over the existing Si structures would motivate new experimental effort in this direction.

### 9:48AM E22.00008 A comprehensive polymer dataset for accelerated property prediction and design, HUAN TRAN, ARUN KUMAR MANNODI-KANAKKITHODI, CHIHO KIM, University of Connecticut, VINIT SHARMA, Oak Ridge National

Laboratory, GHANSHYAM PILANIA, Los Alamos National Laboratory, RAMPI RAMPRASAD, University of Connecticut — Emerging computation- and data-driven approaches are particularly useful for rationally designing materials with targeted properties. In principle, these approaches rely on identifying structure-property relationships by learning from a dataset of sufficiently large number of relevant materials. The learned information can then be used to rapidly predict the properties of materials not already in the dataset, thus accelerating the design of materials with preferable properties. Here, we report the development of a dataset of 1,065 polymers and related materials, which is available at <http://khazana.uconn.edu/>. This dataset is uniformly prepared using first-principles calculations with structures obtained either from other sources or by using structure search methods. Because the immediate target of this work is to assist the design of high dielectric constant polymers, it is initially designed to include the optimized structures, atomization energies, band gaps, and dielectric constants. The dataset will be progressively expanded by accumulating new materials and including additional properties calculated for the optimized structures provided. We discuss some information “learned” from the dataset and suggest that it may be used as the playground for further data-mining work.

**10:00AM E22.00009 Application of Machine Learning tools to recognition of molecular patterns in STM images<sup>1</sup>**, ARTEM MAKSOV, UT/ORNL Bredesen Center, MAXIM ZIATDINOV, ORNL, SHINTARO FUJII, MANABU KIGUCHI, Tokyo Institute of Technology, SHUHEI HIGASHIBAYASHI, Institute for Molecular Science, HIDEHIRO SAKURAI, Osaka University, SERGEI KALININ, BOBBY SUMPTER, ORNL — The ability to utilize individual molecules and molecular assemblies as data storage elements has motivated scientist for years, concurrent with the continuous effort to shrink a size of data storage devices in microelectronics industry. One of the critical issues in this effort lies in being able to identify individual molecular assembly units (patterns), on a large scale in an automated fashion of complete information extraction. Here we present a novel method of applying machine learning techniques for extraction of positional and rotational information from scanning tunneling microscopy (STM) images of  $\pi$ -bowl sumanene molecules on gold. We use Markov Random Field (MRF) model to decode the polar rotational states for each molecule in a large scale STM image of molecular film. We further develop an algorithm that uses a convolutional Neural Network combined with MRF and input from density functional theory to classify molecules into different azimuthal rotational classes. Our results demonstrate that a molecular film is partitioned into distinctive azimuthal rotational domains consisting typically of 20-30 molecules. In each domain, the “bowl-down” molecules are generally surrounded by six nearest neighbor molecules in “bowl-up” configuration, and the resultant overall structure form a periodic lattice of rotational and polar states within each domain.

<sup>1</sup>Research was supported by the US Department of Energy.

**10:12AM E22.00010 Accurate Models of Formation Enthalpy Created using Machine Learning and Voronoi Tessellations**, LOGAN WARD, ROSANNE LIU, AMAR KRISHNA, VINAY HEGDE, ANKIT AGRAWAL, ALOK CHOUDHARY, CHRIS WOLVERTON, Northwestern Univ — Several groups in the past decade have used high-throughput Density Functional Theory to predict the properties of hundreds of thousands of compounds. These databases provide the unique capability of being able to quickly query the properties of many compounds. Here, we explore how these datasets can also be used to create models that can predict the properties of compounds at rates several orders of magnitude faster than DFT. Our method relies on using Voronoi tessellations to derive attributes that quantitatively characterize the local environment around each atom, which then are used as input to a machine learning model. In this presentation, we will discuss the application of this technique to predicting the formation enthalpy of compounds using data from the Open Quantum Materials Database (OQMD). To date, we have found that this technique can be used to create models that are about twice as accurate as those created using the Coulomb Matrix and Partial Radial Distribution approaches and are equally as fast to evaluate.

**10:24AM E22.00011 Description of interatomic interactions with neural networks<sup>1</sup>**, SAMAD HAJINAZAR, JUNPING SHAO, ALEKSEY N. KOLMOGOROV, Physics Department, Binghamton University — Neural networks are a promising alternative to traditional classical potentials for describing interatomic interactions. Recent research in the field has demonstrated how arbitrary atomic environments can be represented with sets of general functions which serve as an input for the machine learning tool. We have implemented a neural network formalism in the MAISE package [1] and developed a protocol for automated generation of accurate models for multi-component systems. Our tests illustrate the performance of neural networks and known classical potentials for a range of chemical compositions and atomic configurations. [1] Module for Ab Initio Structure Evolution, <http://maise-guide.org>

<sup>1</sup>Supported by NSF Grant DMR-1410514

**10:36AM E22.00012 Learning targeted materials properties from data**, TURAB LOOKMAN, PRASANNA V BALACHANDRAN, XUE DEZHEN, JAMES THEILER, JOHN HOGDEN, Los Alamos Natl Lab — We compare several strategies using a data set of 223 M<sub>2</sub>AX family of compounds for which the elastic properties [bulk (B), shear (G), and Young's (E) modulus] have been computed using density functional theory. The strategy is decomposed into two steps: a *regressor* is trained to predict elastic properties in terms of elementary orbital radii of the individual components of the materials; and a *selector* uses these predictions to choose the next material to investigate. The ultimate goal is to obtain a material with desired elastic properties. We examine how the choice of data set size, regressor and selector impact the results.

**10:48AM E22.00013 Neural-network-biased genetic algorithms for materials design<sup>1</sup>**, TARAK PATRA, VENKATESH MEENAKSHISUNDARAM, DAVID SIMMONS, The University of Akron — Machine learning tools have been progressively adopted by the materials science community to accelerate design of materials with targeted properties. However, in the search for new materials exhibiting properties and performance beyond that previously achieved, machine learning approaches are frequently limited by two major shortcomings. First, they are intrinsically interpolative. They are therefore better suited to the optimization of properties within the known range of accessible behavior than to the discovery of new materials with extremal behavior. Second, they require the availability of large datasets, which in some fields are not available and would be prohibitively expensive to produce. Here we describe a new strategy for combining genetic algorithms, neural networks and other machine learning tools, and molecular simulation to discover materials with extremal properties in the absence of pre-existing data. Predictions from progressively constructed machine learning tools are employed to bias the evolution of a genetic algorithm, with fitness evaluations performed via direct molecular dynamics simulation. We survey several initial materials design problems we have addressed with this framework and compare its performance to that of standard genetic algorithm approaches.

<sup>1</sup>We acknowledge the W. M. Keck Foundation for support of this work.

**Tuesday, March 15, 2016 8:00AM - 11:00AM —**

**Session E23 DMP: Metamaterial Devices and Applications** 322 - Jeremy Munday, University of Maryland

**8:00AM E23.00001 Dielectric metasurfaces**, JASON VALENTINE, Vanderbilt University — While plasmonics metasurfaces have seen much development over the past several years, they still face throughput limitations due to ohmic losses. On the other hand, dielectric resonators and associated metasurfaces can eliminate the issue of ohmic loss while still providing the freedom to engineer the optical properties of the composite. In this talk, I will present our recent efforts to harness this freedom using metasurfaces formed from silicon and fabricated using CMOS-compatible techniques. Operating in the telecommunications band, I will discuss how we have used this platform to realize a number of novel functionalities including wavefront control, near-perfect reflection, and high quality factor resonances. In many cases the optical performance of these silicon-based metasurfaces can surpass their plasmonic counterparts. Furthermore, for some cases the surfaces are more amenable to large-area fabrication techniques.

**8:36AM E23.00002 Reconfigurable Infrared Phased-Array Semiconductor Metasurfaces**, JON SCHULLER, Univ of California - Santa Barbara — The ability to engineer the scattering *phase* of metamaterial constituents offers tremendous potential for constructing new classes of beam steering, shaping, and focusing technologies. Current methods for engineering phase rely on static geometry-based effects. In this talk we describe methods to *dynamically* tune the scattering phase of infrared semiconductor nanoantennas. We fabricate spherical silicon and germanium nanoparticles via femtosecond laser ablation and demonstrate size-dependent multipolar resonances throughout the infrared frequency range. We experimentally demonstrate that the resonance frequencies shift with doping, according to simple Drude models of free-carrier refraction. Using a combination of theoretical and analytical calculations we show that dynamically tuning free-carrier concentration can enable reconfigurable optical antennas and metasurfaces. Such dynamic tuning will enable reconfigurable photonic devices based on optical antenna and metamaterial concepts.

**8:48AM E23.00003 Electromechanical control of flat optical devices**, TAPASHREE ROY, Argonne National Lab, SHUYAN ZHANG, John A. Paulson School of Engineering and Applied Sciences, Harvard University, IL WOONG JUNG, Argonne National Lab, FEDERICO CAPASSO, John A. Paulson School of Engineering and Applied Sciences, Harvard University, DANIEL LOPEZ, Argonne National Lab — In the recent times flat optical elements, like lenses and beam deflectors, have come to the forefront of scientific research. These devices, also referred to as metasurfaces, use metal or dielectric resonators, arbitrarily spaced with subwavelength resolution on a two dimensional plane, to mimic the phase profile of any conventional bulk optical device and beyond. Such metasurface-based planar devices are compact and lightweight compared to their conventional bulky counterparts. However, most of these nanostructured devices have so far been passive. In this work we introduce an important concept of actively controlling these flat optical devices. A prototype: an electromechanically controlled plasmonic flat lens focusing mid infrared signal in reflection will be presented. The lens is fabricated on a 2.8 micron thin membrane following photolithography processes and integrated with a micro electromechanical system (MEMS) device. When electrostatically actuated, the MEMS platform controls the mechanical tilt angle of the lens along two orthogonal axes by about 16 degrees that in turn controls the scanning of the focal spot. Such actively controlled miniaturized optical devices promise to provide faster, more efficient and often enhanced functionalities.

**9:00AM E23.00004 Dynamic tuning of lattice plasmon lasers with long coherence characteristics**, THANG HOANG, Department of Physics, Duke University, ANKUN YANG, Department of Materials Science and Engineering, Northwestern University, GEORGE SCHATZ, Department of Chemistry, Northwestern University, TERI ODOM, Department of Materials Science and Engineering, Department of Chemistry, Northwestern University, MAIKEN MIKKELSEN, Department of Physics, Department of Electrical and Computer Engineering, Duke University — Here, we experimentally demonstrate dynamic tuning of an optically-pumped lattice plasmon laser based on arrays of gold nanoparticles and liquid gain materials [A. Yang, T. B. Hoang et al., Nature Communications 6, 6939 (2015)]. The structure consists of an array of 120 nm diameter gold disks with a height of 50 nm and 600 nm spacing. A liquid gain material composed of IR-140 dye molecules dissolved in a variety of organic solvents is placed on top of the disks and held in place by a thin glass coverslip. At a lasing wavelength of 860 nm, time-resolved measurements show a dramatic reduction of the decay time from 1 ns to less than 20 ps when the optical excitation power density increases from below to above the lasing threshold, indicating the transition from spontaneous to stimulated emission. By changing the dielectric environment surrounding the gold disks in real time, the lasing wavelength can be dynamically tuned over a 55 nm range. Finally, we will discuss recent experiments where we probe both the temporal and spatial coherence properties of the lattice plasmon laser. This advance of tunable plasmon lasers offer prospects to enhance and detect weak physical and chemical processes on the nanoscale in real time.

**9:12AM E23.00005 Nanophotonic interactions between organic excitons and plasmonic metasurfaces**, DEIRDRE OCARROLL, Rutgers University — Thin-film organic semiconductor materials are emerging as energy-efficient, versatile alternatives to inorganic semiconductors for display and solid-state lighting applications. Additionally, thin-film organic laser and photovoltaic technologies, while not yet competitive with inorganic semiconductor-based analogues, can exhibit small device embodied energies (due to comparatively low temperature and low energy-use fabrication processes) which is of interest for reducing overall device cost. To improve energy conversion efficiency in thin-film organic optoelectronics, light management using nanophotonic structures is necessary. Here, our recent work on improving light trapping and light extraction in organic semiconductor thin films using nanostructured silver plasmonic metasurfaces will be presented [1,2]. Numerous optical phenomena, such as absorption induced scattering, out-of-plane waveguiding and morphology-dependent surface plasmon outcoupling, are identified due to exciton-plasmon coupling between the organic semiconductor and the metasurface. Ways in which these phenomena can be controlled and optimized for particular optoelectronic applications will be presented. Work done in collaboration with C. Petoukhoff and Z. Shen. [1] C. E. Petoukhoff, D. M. O'Carroll, Absorption-Induced Scattering and Surface Plasmon Out-Coupling from Absorber-Coated Plasmonic Metasurfaces. Nat. Commun. 6, 7899-1-13 (2015). [2] Z. Shen, D. M. O'Carroll, Nanoporous Silver Thin Films: Multifunctional Platforms for Influencing Chain Morphology and Optical Properties of Conjugated Polymers. Adv. Funct. Mater. 25, 3302-3313 (2015).

**9:48AM E23.00006 High sensitivity plasmonic sensor based on sharp cavities**, MICHAEL J. NAUGHTON, JUAN M. MERLO, CHAOBIN YANG, YITZI M. CALM, MICHAEL J. BURNS, Boston College — Surface plasmon resonance sensors have been demonstrated as among the most useful applications of the surface plasmon phenomena. SPR sensors are sensitive enough to detect low refractive index shifts, a critical factor in many biological applications [1]. We present a SPR sensor based on sharp cavities. An antipillar template is fabricated in PDMS and the resulting cavities are coated with a thin film of Ag. Optimization of the Ag film thickness allows one to tune and enhance the optical transmittance and response sensitivity. We also report that the proposed sensor demonstrates sensitivity at one, and likely several, orders of magnitude higher than the maximum sensitivity reported in the literature for different, similar, devices [2]. Numerical calculations show that the sensitivity is due to the strong confinement of localized plasmons inside the cavities, particularly at the sharpest ends. [1] S. Zeng, D. Baillargeat, H. P. Hod, K. T. Yong, Chem. Soc. Rev. 43, 3426 (2014). [2] M. R. Gartia, A. Hsiao, A. Pokhriyal, S. Seo, G. Kulsharova, B. T. Cunningham, T. C. Bond, G. L. Liu. Adv. Opt. Mat., 1, 68 (2013).

**10:00AM E23.00007 An ultrathin invisibility skin cloak for visible light**, ZI JING WONG, XINGJIE NI, MICHAEL MREJEN, YUAN WANG, XIANG ZHANG, University of California, Berkeley — Metamaterial-based optical cloaks have thus far used volumetric distribution of the material properties to gradually bend light and thereby obscure the cloaked region. Hence, they are bulky and hard to scale up to macroscopic sizes. In addition, typical carpet cloaks introduce unnecessary phase shifts in the reflected light, making the cloaks detectable. Here, we demonstrate experimentally an ultrathin invisibility skin cloak wrapped over an object. This skin cloak conceals a three-dimensional arbitrarily shaped object by complete restoration of the phase of the reflected light at 730-nanometer wavelength. The skin cloak comprises a metasurface with distributed phase shifts rerouting light and rendering the object invisible. In contrast to bulky cloaks with volumetric index variation, our device is only 80 nanometer (about one-ninth of the wavelength) thick and potentially scalable to hide macroscopic objects.

**10:12AM E23.00008 Fabrication of tunable infrared metamaterials using atomic calligraphy**<sup>1</sup>, JEREMY REEVES, THOMAS STARK, LAWRENCE BARRETT, RICHARD LALLY, DAVID BISHOP, Boston University — Metamaterials with dynamically variable spectral response to incident radiation through the use of a deformable substrate have so far been limited to the IR and longer wavelength regimes. Such materials, with unit cells a few to tens of microns across, can readily be fabricated using existing lithography techniques. Extending these metamaterials to shorter wavelengths and into the visible spectrum requires a proportional shrinking of the unit cell to be patterned over a large area. The reduced structure size leads to a strong reduction in the throughput of the chosen fabrication technique [1]. Here, we investigate the prospects for the use of atomic calligraphy [2] to pattern arbitrary infrared metamaterials with high throughput. Atomic calligraphy provides a scalable technique for the manufacture of metamaterials with high precision while allowing for writing on a variety of substrates, including deformable materials. We consider the electromagnetic response of these tunable materials and possibilities to develop metamaterials with resonances in the visible spectrum.

[1] M. Imboden, and D. Bishop, Physics Today **67**, 45 (2014)

[2] M. Imboden, et. al., Nano Lett. **13**, 3379 (2013)

<sup>1</sup>This work is funded by the DARPA A2P program.

**10:24AM E23.00009 Wireless transmission by plasmonic antennas**, JUAN M MERLO, YITZI M. CALM, AARON H. ROSE, MICHAEL J. BURNS, MICHAEL J. NAUGHTON, Boston College — Radio frequency (RF) communication is fundamental to many modern technologies. The idea of a simple rescaling of RF theory to the visible frequency range is not a direct issue [1,2], due in part to the finite conductivity in the optical range of commonly-used metals (e.g. Ag, Au). In this context, wireless communication using plasmonic antennas is a very recent concept with potential importance in an on-chip technology application. Here, we propose a plasmonic antenna system capable of wireless transmission-at-a-distance equivalent to at least four free-space wavelengths from the emitter. We demonstrate that it is possible to transmit information with maximum signal strength of -6.9 dB at three free-space wavelengths with a signal-to-noise ratio of -13 dB, good enough to be considered as an efficient wireless system. Theoretical calculations agree with our experimental results and open the possibility to future optimizations of the proposed plasmonic wireless system. [1] Y. Wang, K. Kempa, B. Kimball, J. B. Carlson, G. Benham, W. Z. Li, T. Kempa, J. Rybczynski, A. Herczynski, Appl. Phys. Lett. 85, 2607 (2004). [2] L. Novotny, Phys. Rev. Lett. 98, 266802 (2007).

**10:36AM E23.00010 A Metamaterial-Inspired Approach to RF Energy Harvesting**, CLAYTON FOWLER, JIANGFENG ZHOU, University of South Florida — We demonstrate an RF energy harvesting rectenna design based on a metamaterial perfect absorber (MPA). With the embedded Schottky diodes, the rectenna converts captured RF energy to DC currents. The Fabry-Perot cavity resonance of the MPA greatly improves the amount of energy captured and hence improves the rectification efficiency. Furthermore, the FP resonance exhibits high Q-factor and significantly increases the voltage across the Schottky diodes. This leads to a factor of 16 improvement of RF-DC conversion efficiency at ambient intensity level.

**10:48AM E23.00011 Influences of the Mie resonance on reflectance spectra of Si nanopillar arrays with different wetting states**, SUJUNG KIM, MINJI GWON, Ewha Womans University, JIAQI LI, imec, KU Leuven, XIUMEI XU, imec, SUN-KYUNG KIM, Kyung Hee University, EUNSONGYI LEE, University of Manchester, DONG-WOOK KIM, Ewha Womans University, CHANG CHEN, imec, KU Leuven — The reflectance spectra of crystalline Si nanopillar (SiNP) arrays with various diameters were investigated by finite-difference time-domain (FDTD) simulations. The spectra exhibited distinct features depending on the wetting states. The FDTD-simulated reflectance dips of the 40-nm-diameter SiNP array were in good agreement with those estimated from destructive interference conditions at the top and bottom of the SiNPs: the SiNP arrays and the surrounding medium were treated as one optically homogeneous medium with an effective permittivity estimated from the effective medium approximation (EMA) model. However, the dip positions of the simulated spectra for 70-, 100-, and 130-nm-diameter SiNP arrays deviated from the results of interference calculations, particularly for short wavelengths. The optical reflectance spectra were significantly affected by the strong diameter-dependent Mie resonances in SiNPs, which were sensitive to the refractive index of the surrounding medium (i.e., the wetting state). Optical reflectance measurements provide an easy and efficient means of inspecting the wetting behavior of nano-patterned surfaces.

**Tuesday, March 15, 2016 8:00AM - 11:00AM –**  
**Session E24 DMP DCOMP: Many-Body Perturbation Theory for Electronic Excitations: Computational Advances** 323 - Volker Blum, Duke University

**8:00AM E24.00001 Plasmon Pole Approximations within a GW Sternheimer implementation**, VINCENT GOSSELIN, MICHEL COTE, Univ of Montreal — We use an implementation of the GW approximation that exploits a Sternheimer equation and a Lanczos procedure to circumvent the resource intensive sum over all bands and inversion of the dielectric matrix. I will present further improvement of the method that uses Plasmon Pole approximations to evaluate the integral over all frequencies analytically. A comparison study between the von Linden-Horsh and Engel-Farid approaches for energy levels of various molecules along with benchmarking of the computational resources needed by the method will be discussed.

**8:12AM E24.00002 Inclusion of the electron-phonon interaction in the BerkeleyGW computational package<sup>1</sup>**, DEREK VIGIL-FOWLER, STEPHAN LANY, Natl Renewable Energy Lab — The BerkeleyGW package is a highly optimized and efficient code for calculating, among others, the dielectric response, bandstructures, lifetimes, and optical absorption of materials from nanostructures and two-dimensional sheets to bulk materials. In the past the only interactions included in BerkeleyGW were electron-electron interactions, with other packages being used to include the effect of, say, electron-phonon interactions. One common approach is to use Wannier functions to interpolate all needed quantities to a very fine grids in energy and momentum, which leads to very accurate electron-phonon couplings and lifetimes. However, in materials with complex, even unknown, chemical environments the generation of Wannier functions can be quite time consuming and constitutes another step in an already difficult calculation. The BerkeleyGW package has a wavefunction-based interpolation scheme that is used in solving the Bethe-Salpeter equation and which is much more easily automated than Wannier interpolation. In this talk, we discuss results for the carrier lifetimes due to the electron-phonon interaction using this interpolation scheme. In particular, we discuss the computational efficiency and scalability, and the prospects for applying this method to a wide range of materials to get first principles lifetimes, and related quantities, such as mobilities and diffusion lengths.

<sup>1</sup>Derek Vigil-Fowler's work is supported by the National Renewable Energy Laboratory's Director's Postdoctoral Fellowship

**8:24AM E24.00003 Large-scale GW software development<sup>1</sup>**, MINJUNG KIM, SUBHASISH MANDAL, Department of Applied Physics, Yale University, ERIC MIKIDA, PRATEEK JINDAL, ERIC BOHM, NIKHIL JAIN, LAXMIKANT KALE, Department of Computer Science, University of Illinois at Urbana-Champaign, GLENN MARTYNA, IBM T. J. Watson Research Center, SOHRAB ISMAIL-BEIGI, Department of Applied Physics, Yale University — Electronic excitations are important in understanding and designing many functional materials. In terms of *ab initio* methods, the GW and Bethe-Salpeter Equation (GW-BSE) beyond DFT methods have proved successful in describing excited states in many materials. However, the heavy computational loads and large memory requirements have hindered their routine applicability by the materials physics community. We summarize some of our collaborative efforts to develop a new software framework designed for GW calculations on massively parallel supercomputers. Our GW code is interfaced with the plane-wave pseudopotential *ab initio* molecular dynamics software "OpenAtom" which is based on the Charm++ parallel library [1]. The computation of the electronic polarizability is one of the most expensive parts of any GW calculation. We describe our strategy that uses a real-space representation to avoid the large number of fast Fourier transforms (FFTs) common to most GW methods. We also describe an eigendecomposition of the plasmon modes from the resulting dielectric matrix that enhances efficiency. [1] Bohm *et al.*, IBM J. RES. & DEV. vol. 52 no. 1/2, 2008

<sup>1</sup>This work is supported by NSF through grant ACI-1339804.

**8:36AM E24.00004 Towards highly scalable GW calculations<sup>1</sup>**, SUBHASISH MANDAL, MINJUNG KIM, Department of Applied Physics, Yale University, ERIC MIKIDA, ERIC BOHM, PRATEEK JINDAL, NIKHIL JAIN, Department of Computer Science, University of Illinois at Urbana Champaign, LAXMIKANT V. KALE, Department of Computer Science, University of Illinois at UrbanaChampaign, GLENN J. MARTYNA, IBM T. J. Watson Research Center, SOHRAB ISMAIL-BEIGI, Department of Applied Physics, Yale University — The GW and Bethe-Salpeter Equation (GW-BSE) approach is an accurate and useful method beyond DFT to describe excited states of materials. However over the past few decades, most *ab initio* GW calculations used have been confined to small units of cells of bulk-like materials due to the extreme computational demands of the approach. We will present our collaborative efforts to develop new software that permits large scale GW calculations more efficiently: our GW software is interfaced with the *ab initio* plane wave pseudopotential OpenAtom software (<http://charm.cs.uiuc.edu/OpenAtom/>) that uses the Charm++ parallel framework. Here, we focus on describing our work on computing the static (so called “COHSEX”) GW self-energy. We describe the advantages of our real-space approach for quasi-particle calculations and provide information on scaling behavior of the resulting algorithms.

<sup>1</sup> NSF ACI-1339804

**8:48AM E24.00005 Accurate Ionization Potentials and Electron Affinities of Acceptor Molecules: A Benchmark of GW Methods**, NOA MAROM, JOSEPH KNIGHT, XIAOPENG WANG, Tulane University, LUKAS GALLANDI, University of Potsdam, Germany, OLGA DOLGOUNITCHEVA, Auburn University, XINGUO REN, USTC, VINCENT ORTIZ, Auburn University, PATRICK RINKE, Aalto University, Finland, THOMAS KORZDORFER, University of Potsdam, Germany — The performance of different GW methods is assessed for a set of 24 organic acceptors. Errors are evaluated with respect to coupled cluster singles, doubles, perturbative triples [CCSD(T)] reference data for the vertical ionization potentials (IPs) and electron affinities (EAs), extrapolated to the complete basis set limit. Additional comparisons are made to experimental data, where available. We consider fully self-consistent GW (scGW), partial self-consistency in the Green's function (scGW<sub>0</sub>), non-self-consistent G<sub>0</sub>W<sub>0</sub> based on several mean-field starting points, and a “beyond GW” second order screened exchange (SOSEX) correction to G<sub>0</sub>W<sub>0</sub>. The best performers overall are G<sub>0</sub>W<sub>0</sub>+SOSEX and G<sub>0</sub>W<sub>0</sub> based on an IP-tuned long range corrected hybrid functional with the former being more accurate for EAs and the latter for IPs. Both provide a balanced treatment of localized vs. delocalized states and valence spectra in good agreement with photoemission spectroscopy (PES) experiments.

**9:00AM E24.00006 Extrapolation of G<sub>0</sub>W<sub>0</sub> energy levels from small basis sets for elements from H to Cl**, TONG ZHU, VOLKER BLUM, MEMS Department, Duke University, Durham, NC 27708 — G<sub>0</sub>W<sub>0</sub> calculations based on orbitals from a density-functional theory reference are widely used to predict carrier levels in molecular and inorganic materials. Their computational feasibility, however, is limited by the need to evaluate slow-converging sums over unoccupied states, requiring large basis sets paired with unfavorable scaling exponents to evaluate the self-energy. In the quantum chemistry literature, complete basis set (CBS) extrapolation strategies have been used successfully to overcome this problem for total energies. We here apply the principle of basis set extrapolation to G<sub>0</sub>W<sub>0</sub> energy levels. For a set of 49 small molecules and clusters containing the elements H, Li through F, and Na through Cl, we test established extrapolation strategies based on Dunning's correlation-consistent (cc) basis sets (aug)-cc-pVNZ (N=2-5), as well as numeric atom-centered NAO-VCC-nZ (n=2-5) basis sets in the FHI-aims all-electron code. For the occupied and lowest unoccupied levels, different extrapolation strategies agree within ±50 meV based on large 4Z and 5Z basis sets. We show that extrapolation based on much smaller 2Z and 3Z basis sets with largest errors ± 100 meV based on a refinement of the NAO-VCC-nZ basis sets.

**9:12AM E24.00007 The Sternheimer-GW method and the spectral signatures of plasmonic polarons<sup>1</sup>**, FELICIANO GIUSTINO, University of Oxford — During the past three decades the GW method has emerged among the most promising electronic structure techniques for predictive calculations of quasiparticle band structures. In order to simplify the GW work-flow while at the same time improving the calculation accuracy, we developed the Sternheimer-GW method [1]. In Sternheimer-GW both the screened Coulomb interaction and the electron Green's function are evaluated by using exclusively occupied Kohn-Sham states, as in density-functional perturbation theory. In this talk I will review the basics of Sternheimer-GW, and I will discuss two recent applications to semiconductors and superconductors. In the case of semiconductors we calculated complete energy- and momentum-resolved spectral functions by combining Sternheimer-GW with the cumulant expansion approach. This study revealed the existence of band structure replicas which arise from electron-plasmon interactions [2]. In the case of superconductors we calculated the Coulomb pseudo-potential from first principles, and combined this approach with the Eliashberg theory of the superconducting critical temperature [3]. [1] H. Lambert, F. Giustino, Phys. Rev. B 88, 075117 (2013). [2] F. Caruso, H. Lambert, F. Giustino, Phys. Rev. Lett. 114, 146404 (2015). [3] E. R. Margine, F. Giustino, Phys. Rev. B 87, 024505 (2013).

<sup>1</sup>This work was supported by the Leverhulme Trust (RL-2012- 001), the European Research Council (EU FP7/ERC 239578), the UK Engineering and Physical Sciences Research Council (EP/J009857/1), and the Graphene Flagship (EU FP7/604391)

**9:48AM E24.00008 Combination of Hedin's GW and dynamical mean-field theory tested on H<sub>2</sub> molecule**, JUHO LEE, KRISTJAN HAULE, Rutgers University — We compare various flavors of “GW+DMFT” approach with LDA+DMFT for the simplest strongly correlated system, the H<sub>2</sub> molecule. The following GW+DMFT methodologies are compared: (i) the fully self-consistent GW+DMFT, (ii) the quasi-particle self-consistent QS-GW+DMFT with dynamic double-counting, (iii) QS-GW+DMFT with static double-counting schemes. We found that fully self-consistent GW+DMFT with exact double-counting yields very precise spectra around equilibrium H-H distance, as well as reasonable total energy (comparable to LDA+DMFT). However, this scheme breaks down in the correlated regime due to causality violation. The QS-GW+DMFT approaches, which are not derivable from a functional, yield similar spectra as full GW+DMFT near equilibrium distance, and in static double-counting schemes, can also be extended into correlated regime. However, the total energy of these approaches is much worse than the total energy of LDA+DMFT. In summary, this toy model of correlated physics suggests that QS-GW+DMFT with constant double-counting should give accurate predictions of spectra, but not total energy, while LDA+DMFT gives very precise total energy, but somewhat less precise spectra.

**10:00AM E24.00009 Electron-phonon coupling using many-body GW theory<sup>1</sup>**, BARTOMEU MONSER-RAT, DAVID VANDERBILT, Rutgers University — Electron-phonon coupling drives a plethora of phenomena, such as superconductivity in metals, or the temperature dependence of optical properties in semiconductors. There is increasing evidence that semi-local density functional theory (DFT) is not adequate for the description of electron-phonon coupling, and instead effects such as electronic correlation need to be included. Unfortunately, methods beyond semi-local DFT are computationally demanding, limiting the study of these phenomena. In this talk we will introduce the idea of “thermal lines”, which can be used to explore the vibrational phase space of solids and molecules at small computational cost. In particular, we will describe how thermal lines can be exploited to calculate the temperature dependence of band structures beyond semi-local DFT, by using many-body GW theory, or by including the effects of spin-orbit coupling. We will present first-principles results showing the effects of electron correlation on the strength of electron-phonon coupling, and the effects of electron-phonon coupling on topological states of matter.

<sup>1</sup>Supported by Robinson College, Cambridge, and the Cambridge Philosophical Society.

**10:12AM E24.00010 Plane wave based selfconsistent solution of the GW Dyson equation<sup>1</sup>**, LIN-WANG WANG, HUAWEI CAO, Lawrence Berkeley Natl Lab — We have developed a selfconsistent procedure to calculate the full Dyson equation based on plane wave basis set. The whole formalism is based on the Greens function matrix of the plane wave G-vector. There is no truncation of the conduction band when the dielectric function is calculated. The Dyson equation is the variational minimum solution of the total energy in terms of the Greens function. The calculation uses the "space-time" method, with special algorithm for imaginary time integration and Fourier transformation. We have tested isolated molecules and periodic systems. The effects of selfconsistency compared to the G0W0 results will be presented. We will also discuss some special techniques used in the k-point summation for the periodic system. Massive parallelization is used to carry out such calculations.

<sup>1</sup>This work is supported by the Director, SC/BES/MSED of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231, through the Material Theory program at Lawrence Berkeley National Laboratory.

**10:24AM E24.00011 Post-GW energies from an extended Bethe-Salpeter scheme**, EMANUELE MAGGIO, Univ of Vienna, GEORG KRESSE, University of Vienna — Hedin's breakthrough in many-body physics is a computationally manageable scheme to implicitly account for many-body effects thanks to the introduction of a self-energy, whose expression is known but in practice approximated by truncation at some order in the inter-particle interaction. Hedin's scheme allows the computation of quasi-particle addition and removal energies. The introduction of an added particle (or hole) to the system will trigger the formation of higher order neutral excitations (particle/hole pairs formation). The widespread GW approximation only partially accounts for these effects by replacing the bare interparticle interaction with a dressed one. Other effects are contained in the vertex function and are typically disregarded. In the present work, we move beyond the GW level by including vertex effects in the self-energy. This is implemented by expressing the self-energy in terms of the reducible two-particle scattering amplitude. The latter is related to the kernel of the Bethe-Salpeter equation and to the corresponding polarisation propagator. The proposed implementation allows us to evaluate the quality of quasi-particle spectra for a range of realistic solids and molecular systems.

**10:36AM E24.00012 GW Calculations of Materials on the Intel Xeon-Phi Architecture<sup>1</sup>**, JACK DESLIPPE, LBNL, FELIPE H. DA JORNADA, UC Berkeley and LBNL, DEREK VIGIL-FOWLER, NREL, ARIEL BILLER, Weizmann Institute of Science, JAMES R. CHELIKOWSKY, UT Austin, STEVEN G. LOUIE, UC Berkeley and LBNL — Intel Xeon-Phi processors are expected to power a large number of High-Performance Computing (HPC) systems around the United States and the world in the near future. We evaluate the ability of GW and pre-requisite Density Functional Theory (DFT) calculations for materials on utilizing the Xeon-Phi architecture. We describe the optimization process and performance improvements achieved. We find that the GW method, like other higher level Many-Body methods beyond standard local/semilocal approximations to Kohn-Sham DFT, is particularly well suited for many-core architectures due to the ability to exploit a large amount of parallelism over plane-waves, band-pairs and frequencies.

<sup>1</sup>Support provided by the SCIDAC program, Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Sciences. Grant Numbers DE-SC0008877 (Austin) and DE-AC02-05CH11231 (LBNL)

**10:48AM E24.00013 Recent Advances in Modeling Transition Metal Oxides for Photo-electrochemistry<sup>1</sup>**, MAYTAL CASPARY TOROKER, Department of Materials Science and Engineering, Technion - Israel Institute of Technology — Computational research offers a wide range of opportunities for materials science and engineering, especially in the energy arena where there is a need for understanding how material composition and structure control energy conversion, and for designing materials that could improve conversion efficiency. Potential inexpensive materials for energy conversion devices are metal oxides. However, their conversion efficiency is limited by at least one of several factors: a too large band gap for efficiently absorbing solar energy, similar conduction and valence band edge characters that may lead to unfavorably high electron-hole recombination rates, a valence band edge that is not positioned well for oxidizing water, low stability, low electronic conductivity, and low surface reactivity. I will show how we model metal oxides with ab-initio methods, primarily DFT+U. Our previous results show that doping with lithium, sodium, or hydrogen could improve iron (II) oxide's electronic properties, and alloying with zinc or nickel could improve iron (II) oxide's optical properties. Furthermore, doping nickel (II) oxide with lithium could improve several key properties including solar energy absorption. In this talk I will highlight new results on our understanding of the mechanism of iron (III) oxide's surface reactivity. Our theoretical insights bring us a step closer towards understanding how to design better materials for photo-electrochemistry. References: 1. O. Neufeld and M. Caspary Toroker, "Pt-doped Fe<sub>2</sub>O<sub>3</sub> for enhanced water splitting efficiency: a DFT+U study", J. Phys. Chem. C 119, 5836 (2015). 2. M. Caspary Toroker, "Theoretical Insights into the Mechanism of Water Oxidation on Non-stoichiometric and Ti - doped Fe<sub>2</sub>O<sub>3</sub>(0001)", J. Phys. Chem. C, 118, 23162 (2014).

<sup>1</sup>This research was supported by the Morantz Energy Research Fund, the Nancy and Stephen Grand Technion Energy Program, the I-CORE Program of the Planning and Budgeting Committee, and The Israel Science Foundation (Grant No. 152/11).

**Tuesday, March 15, 2016 8:00AM - 10:48AM —**

**Session E25 DCMP: Superconductivity: Vortex matter** 324 - Valentin Taufour, Ames Laboratory

**8:00AM E25.00001 A quantitative model for flux flow resistivity and Nernst effect of vortex fluid in high-temperature superconductors**, RONG LI, ZHEN-SU SHE, College of Engineering, Peking University, LAN YIN, School of Physics, Peking University, STATE KEY LABORATORY FOR TURBULENCE AND COMPLEX SYSTEMS TEAM — Transport properties of vortex fluid in high-temperature superconductors have been described in terms of viscous dynamics of magnetic and thermal vortices. We have constructed a quantitative model by extending the Bardeen-Stephen model of damping viscosity to include the contributions of flux pinning in low temperature and vortex-vortex interaction in high magnetic field. A uniformly accurate description of flux flow resistivity and Nernst signal is achieved for empirical data over a wide range of temperature and magnetic field strength. A discrepancy of three orders of magnitude between data and Anderson model of Nernst signal is pointed out, suggesting the existence of anomalous transport in high-temperature superconductor beyond mere quantum and thermal fluctuations. The model enables to derive a set of physical parameters characterizing the vortex dynamics from the Nernst signal, as we illustrate with an analysis of six samples of Bi<sub>2</sub>Sr<sub>2- $\gamma$</sub> La <sub>$\gamma$</sub> CuO<sub>6</sub> and Bi<sub>2</sub>Sr<sub>2</sub>CaCu<sub>2</sub>O<sub>8+ $\delta$</sub> .

**8:12AM E25.00002 In-plane electronic anisotropy from core states of tilted vortices.**, HERMANN SUDEROW, Univ Autonoma de Madrid, JOSE AUGUSTO GALVIS, National high magnetic field laboratory, EDWIN HERRERA, ISABEL GUILLAMON, SEBASTIAN VIEIRA, Univ Autonoma de Madrid — Magnetic field enters type II superconductors in form of quantized vortices. Each vortex has a core with the superconducting wavefunction vanishing at its center. Quasiparticles at the vortex core form bound states whose radial extension depends on the superconducting gap value and Fermi surface shape. In the layered superconductor 2H-NbSe<sub>2</sub> vortex cores have been studied using scanning tunneling microscopy (STM) mostly with magnetic fields applied perpendicular to the layers. It is found that vortices have a six-fold star shape due to the in-plane anisotropy of the superconducting gap and of the electronic density of states. Here we study vortex core states with the magnetic field applied parallel to the layers. We find that the vortex cores change their shape depending on the angle of the tilted magnetic field with respect to the in-plane crystalline directions, providing a lateral view of the electronic structure.

**8:24AM E25.00003 Characterization of vortex pinning through the Campbell length**, ROLAND WILLA, VADIM B. GESHKENBEIN, GIANNI BLATTER, Institute for Theoretical Physics, ETH Zurich, 8093 Zurich, Switzerland — Vortex pinning is decisive in establishing dissipation-free current flow in a type-II superconductor; knowledge and optimization of the pinning landscape (pinscape) is of major importance for applications. The *ac* magnetic response, characterized by the Campbell penetration depth  $\lambda_C$  [1], provides valuable information on the pinscape, besides the critical current density  $j_c$ . While microscopic derivations of  $j_c$  are available both in the weak and strong pinning limits, this is not the case for the Campbell length, whose understanding has remained on a phenomenological level so far. Based on the microscopic theory of strong pinning, we have established a proper link between the Campbell length and the pinscape parameters. This new quantitative formalism [2] captures all experimentally observed signatures [3], among which are the dependence of  $\lambda_C$  on the vortex state preparation and the hysteresis in  $\lambda_C$  upon thermal cycling the field-cooled state. [1] A.M. Campbell, J Phys C: Solid State Physics 2, 1492 (1969), *ibid.* 4, 3186 (1971) [2] R. Willa, V.B. Geshkenbein, and G. Blatter, PRB 92, 134501 (2015), R. Willa, V.B. Geshkenbein, R. Prozorov and G. Blatter, PRL in press [3] R. Prozorov et al., PRB 67, 184501 (2003), H. Kim et al., PRB 87, 094515 (2013)

**8:36AM E25.00004 Observation of RF-induced flux lattice annealing (RIFLA) in cuprate high temperature superconductors**, GUOQING WU, XIANGHUA ZENG, XIAO-SHAN YE, Yangzhou Uni., BING WU, Fayetteville State Uni., GERARD GAIDOS, W. G. CLARK, UCLA — We report the annealing of a strained flux lattice (FL) in cuprate high temperature superconductors, by the RF pulses used to obtain the NMR spin-echo signal and by a series of RF pulses that are input into the sample coil in a tuned NMR probe circuit. The strained FL is prepared by changing the alignment and/or magnitude of the applied magnetic field at temperatures well below the superconducting transition temperature, which leaves the FL pinned in a non-equilibrium configuration. We provide a very sensitive measure of the phenomenon. This new observation enriches the phenomenon of FL, and indicates that shaking the flux lattice by the applied RF pulses (including both the spin-echo pulses and the pulses input to the sample coil circuit) progressively causes the flux lattice to change to a lower free energy configuration. Supported by NSF China grant : 61474096

**8:48AM E25.00005 Dynamic and Structural Studies of Metastable Vortex Lattice Domains in  $\text{MgB}_2$** <sup>1</sup>, E.R. DE WAARD, S.J. KUHN, C. RASTOVSKI, M.R. ESKILDSEN, University of Notre Dame, A. LEISHMAN, Kent State University, C.D. DEWHURST, Institut Laue-Langevin, France, L. DEBEER-SCHMITT, K. LITTRELL, Oak Ridge National Laboratory, J. KARPINSKI, EPFL, Switzerland, N.D. ZHIGADLO, ETH, Switzerland — Small-angle neutron scattering (SANS) studies of the vortex lattice (VL) in the type-II superconductor  $\text{MgB}_2$  have revealed an unprecedented degree of metastability that is demonstrably not due to vortex pinning, [C. Rastovski *et al.*, Phys. Rev. Lett. 111, 107002 (2013)]. The VL can be driven to the GS through successive application of an AC magnetic field. Here we report on detailed studies of the transition kinetics and structure of the VL domains. Stroboscopic studies of the transition revealed a stretched exponential decrease of the metastable volume fraction as a function of the number of applied AC cycles, with subtle differences depending on whether the AC field is oriented parallel or perpendicular to the DC field used to create the VL. We speculate the slower transition kinetics for the transverse AC field may be due to vortex cutting. Spatial studies include scanning SANS measurements showing the VL domain distribution within the  $\text{MgB}_2$  single crystal as well as measurements of VL correlation lengths.

<sup>1</sup>This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences under Award DE-FG02-10ER46783.

**9:00AM E25.00006 Enhancement of long-range correlations in a 2D vortex lattice by an incommensurate 1D disorder potential**<sup>1</sup>, I. GUILLAMON, S. VIEIRA, H. SUDEROW, Universidad Autonoma de Madrid, Spain, R. CORDOBA, J. SESE, J.M. DE TERESA, R. IBARRA, Instituto de Nanociencia de Aragon, Spain — In two dimensional (2D) systems, theory has proposed that random disorder destroys long range correlations driving a transition to a glassy state. Here, I will discuss new insights into this issue obtained through the direct visualization of the critical behaviour of a 2D superconducting vortex lattice formed in a thin film with a smooth 1D thickness modulation [1]. Using scanning tunneling microscopy at 0.1K, we have tracked the modification in the 2D vortex arrangements induced by the 1D thickness modulation while increasing the vortex density by three orders of magnitude. Upon increasing the field, we observed a two-step order-disorder transition in the 2D vortex lattice mediated by the appearance of dislocations and disclinations and accompanied by an increase in the local vortex density fluctuations. Through a detailed analysis of correlation functions, we find that the transition is driven by the incommensurate 1D thickness modulation. We calculate the critical points and exponents and find that they are well above theoretical expectation for random disorder. Our results show that long range 1D correlations in random potentials enhance the stability range of the ordered phase in a 2D vortex lattice. [1] I. Guillamon et al., Nature Physics 10, 851856 (2014)

<sup>1</sup>Work supported by Spanish MINECO, CIG Marie Curie grant, Axa Research Fund and FBBVA.

**9:12AM E25.00007 Study of vortex states and dynamics in mesoscopic superconducting samples with MFM**, GREGORY POLSHYN, TYLER NAIBERT, VICTOR CHUA, RAFFI BUDAKIAN, University of Illinois at Urbana-Champaign — Vortex states in superconducting (SC) structures, their dynamics and ways to manipulate them are topics of great interest. We report a new method of magnetic force microscopy (MFM) that allows the study of vortex states in mesoscopic SC samples. For the case of a SC ring, which is biased to a half-integer flux quantum, the flux modulation through the ring caused by the motion of the magnetic tip drives the ring between two consecutive fluxoid states. The corresponding current switching in the ring produces strong position-dependent forces on the cantilever. In the regime where the frequency of the thermally activated jumps between fluxoid states is close to the frequency of the cantilever, large changes in the cantilever frequency and dissipation are observed. This effect may be understood as a stochastic resonance (SR) process. These changes in the cantilevers mechanical properties are used to image the barrier energies between fluxoid states. Additionally, SR imaging of the barrier energies are used to study the effect of the locally applied magnetic field from the MFM tip on the barrier heights. We report the results of measurements for Al rings. Further, the same imaging technique can be applied to more sophisticated SC structures such as arrays of Josephson junctions.

**9:24AM E25.00008 History Dependence of the Vortex Lattice Rotation in the B-phase of  $\text{UPt}_3$  with  $\mathbf{H} \parallel \mathbf{c}^1$** , K.E. AVERS, Northwestern Univ, M.R. ESKILDSEN, Notre Dame University, W.P. HALPERIN, W.J. GANNON, Northwestern Univ, J.L. GAVILANO, G. NAGY, U. GASSER, Paul Scherrer Institute — The unconventional superconductor  $\text{UPt}_3$  is widely believed to be a triplet superconductor, where the low temperature superconducting B-phase is a chiral state. We have performed small angle neutron scattering (SANS) from the vortex lattice (VL) in  $\text{UPt}_3$  at the Paul Scherrer Institute with the magnetic field parallel to the hexagonal *c*-axis in the 0.5 T to 0.9 T range. The diffraction pattern of the VL rotates away from a high symmetry direction producing two domains of different orientation. Our field dependent measurements show a subtle magnetic field history dependence of this orientation; VLs prepared with the magnetic field parallel or anti-parallel with respect to the angular momentum from the circulating screening currents show different field-history dependence. These results suggest a coupling of a chiral superconducting order parameter with the applied magnetic field.

<sup>1</sup>US DOE, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Awards DE-FG02-10ER46783 (University of Notre Dame; neutron scattering) and DE-FG02-05ER46248 (Northwestern University; crystal growth, characterization, neutron

**9:36AM E25.00009 Vortex matter in superconductors: solid or gas?** , VLADIMIR KOZHEVNIKOV, Tulsa Community College, ANNE-MARIE VALENTE-FELICIANO, Thomas Jefferson National Lab, PETER CURRAN, University of Bath, GUNTHER RICHTER, Max-Planck-Institut for Intelligent Systems, HAOLIANG LIU, ALEXANDER VOLODIN, Solid State Physics and Magnetism Section, KU Leuven, SIMON BENDING, University of Bath, CHRIS VAN HAESENDONCK, Solid State Physics and Magnetism Section, KU Leuven — We will report on results of our recent study of the equilibrium magnetic properties of the mixed state in type-II superconductors performed with high purity bulk and film niobium samples in parallel and perpendicular magnetic fields using dc magnetometry and scanning Hall-probe microscopy. Equilibrium magnetization data for the perpendicular geometry were obtained for the first time. It was found that none of the existing theories is consistent with these new data. To address this problem a theoretical model is developed and verified experimentally. The new model describes the magnetic properties of the mixed state in an averaged limit, i.e. without detailing the samples' magnetic structure and therefore ignoring interactions between the structural units (vortices). Nevertheless, it is quantitatively consistent with the data obtained in a perpendicular field. At low values of the Ginzburg-Landau parameter, the model converts to that of Peierls and London for the intermediate state in type-I superconductors, valid in the limit of non-interacting normal domains. We will show that description of the vortex matter in type-II superconductors in terms of a 2D gas is more appropriate than the frequently used crystal- and glass-like scenarios.

**9:48AM E25.00010 Orientational Ordering, Buckling, and Dynamic Transitions for Vortices Interacting with a Periodic Quasi-One Dimensional Substrate** , MINH QUAN LE THIEN, DANIELLE MCDERMOTT, Department of Physics, Wabash College, Crawfordsville, Indiana 47933 USA, CYNTHIA OLSON REICHHARDT, CHARLES REICHHARDT, Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545 USA — We examine the statics and dynamics of vortices in the presence of a periodic quasi-one dimensional substrate, focusing on the limit where the vortex lattice constant is smaller than the substrate lattice period. As a function of the substrate strength and filling factor, within the pinned state we observe a series of order-disorder transitions associated with buckling phenomena in which the number of vortex rows that fit between neighboring substrate maxima increases. These transitions coincide with steps in the depinning threshold, jumps in the density of topological defects, and changes in the structure factor. For weaker substrate strengths we find that the vortices retain triangular ordering but can show changes in the orientation of the triangular lattice with respect to the substrate. Under an applied drive the system exhibits a rich variety of distinct dynamical phases, including plastic flow, a density-modulated moving crystal, and moving floating solid phases. We also discuss how these results are related to recent experiments by I. Guilamon et al, Nature Physics 10, 751 (2014), for vortices interacting on quasi-one-dimensional periodic modulated substrates.

**10:00AM E25.00011 The dynamics and pinning of single vortices in type-II superconductors investigated using a scanning SQUID-on-tip microscope** , LIOR EMBON, YONATHAN ANAHORY, ALEX SUHOV, DORRI HALBERTAL, JO CUPPENS, ANTON YAKOVENKO, AVIRAM URI, YURI MYASOEDOV, MICHAEL RAPPAPORT, Weizmann Institute of Science, MARTIN HUBER, University of Colorado Denver, ALEX GUREVICH, Old Dominion University, ELI ZELDOV, Weizmann Institute of Science — The electromagnetic properties of superconductors, particularly their ability to carry non-dissipative currents, are governed by the dynamics of quantized magnetic vortices and their pinning due to material defects. Despite recent advances in the understanding of the complex physics of vortex matter, the behavior of vortices driven by current through a potential created in an actual material is still not well understood, mostly due to the scarcity of adequate experimental tools. Using a novel scanning SQUID-on-tip microscope we have investigated the controlled dynamics of vortices in Pb films with sub-Angstrom sensitivity to vortex displacement. Using the ability to trace vortex trajectories on nanometer scales, we measured, for the first time, the fundamental dependence of the elementary pinning force of multiple defects on the vortex displacement, revealing a far more complex behavior than has previously been recognized. Our results indicate the importance of thermal fluctuations even at 4.2 K, and of the vital role of small and seemingly unimportant ripples in the pinning potential. These give new insights into the mechanisms of magnetic relaxation and electromagnetic response of superconductors.

**10:12AM E25.00012 Dissipative vortex dynamics in overdamped superconducting arrays** , MALCOLM DURKIN, IAN MONDRAGON-SHEM, University of Illinois at Urbana-Champaign, SERENA ELEY, Los Alamos National Laboratory, TAYLOR HUGHES, NADYA MASON, University of Illinois at Urbana-Champaign — We study 2D superconductor-normal-superconductor (SNS) arrays consisting of regularly spaced Nb islands on Au films, measuring the current-driven voltage response. SNS arrays provide a highly tunable platform for studying classical vortex behavior and we are able to access a number of vortex regimes, including edge pinning and site pinning regimes at low fields and commensurate vortex lattice behavior at higher fillings. Focusing on the low vortex filling regime, we study the current driven transition from pinned vortices to flux flow, finding that the differential resistance peak predicted by current driven vortex models is absent in our arrays. While the absence of a differential resistance peak is typically associated with finite temperature effects, this explanation is not consistent with our data. Instead, we find that the dynamic behavior of our system is consistent with the presence of time delayed dissipative forces in an overdamped array.

**10:24AM E25.00013 ABSTRACT WITHDRAWN —**

**10:36AM E25.00014 <sup>93</sup>Nb NMR investigation of vortex- glass transition in layered NbSe<sub>2</sub><sup>1</sup>** , DOUGLAS WILSON, GARIMA SARASWAT, National High Magnetic Field Laboratory, PARASHARAM SHIRAGE, Indian Institute of Technology, PHILIP KUHNS, MICHAEL J. R. HOCH, ARNEIL REYES, National High Magnetic Field Laboratory — We report a detailed low temperature investigation of vortex glass transition in layered superconducting compound NbSe<sub>2</sub> using <sup>93</sup>Nb NMR at fields below H<sub>c2</sub>. Preliminary measurements show that spin-lattice relaxation rate 1/T<sub>1</sub> demonstrates a classic Korringa behavior 1/T<sub>1</sub> ~ T above the superconducting transition T<sub>c</sub>, consistent with previous measurements on this compound. However, for field H perpendicular to the layers, we observed that 1/T<sub>1</sub> exhibits an anomalous plateau between T<sub>c</sub> (H = 0) and T<sub>c</sub>(H) and a suppression of the superconducting enhancement expected below T<sub>c</sub>. Instead, a power law behavior, 1/T<sub>1</sub> ~ T<sup>1.2</sup> below T<sub>c</sub> down to 360mK was observed which suggests a strong anisotropy in the low energy excitations. However, the possibility of enhancement in 1/T<sub>1</sub> due to vortex fluctuations which competes with electronic mechanisms cannot be excluded. The implications of these results with regards to vortex-glass transition will be discussed.

<sup>1</sup>This work was performed at the National High Magnetic Field Laboratory, which is supported by NSF DMR-1157490 and the State of Florida.

**Tuesday, March 15, 2016 8:00AM - 11:00AM —**

**Session E27 DCMP: Heavy Fermion Superconductors** 326 - Paula Giraldo Gallow, Florida State University

**8:00AM E27.00001 Tuning the electronic state in  $\text{CeCu}_2\text{Si}_2$ :  $\text{Si} \rightarrow \text{P}$  substitution**, YOU LAI, SCOTT SAUNDERS, ANDREW GALLAGHER, KUAN WEN CHEN, SHENGZHI ZHANG, LUCAS NELSON, DAVID GRAF, FUMITAKE KAMETANI, ARKADY SHEKHTER, RYAN BAUMBACH, FSU-NHMFL — The chemical substitution series  $\text{CeCu}_2\text{Si}_{2-x}\text{Ge}_x$  hosts two distinct superconducting regions that are accessed under applied pressure. The first of these surrounds an antiferromagnetic quantum critical point, while the second does not appear to be associated with the zero-temperature collapse a line of phase transitions. It has been speculated that the second superconducting dome encompasses a quantum phase transition that is associated with a Ce  $4f$ -electron valence collapse, but this has yet to be established. We report a study of the chemical substitution series  $\text{CeCu}_2\text{Si}_{2-x}\text{P}_x$  for  $x \leq 0.2$ , which may expose a new dimension for investigation of quantum valence transitions. This ligand site tuning strategy has the advantage that it changes the number of  $s/p$  electrons without strongly modifying other important variables such as the strength of Coulomb, spin orbit, crystal electric field interactions, and the hybridization between  $f$ - and conduction electrons. We find that the superconductivity is rapidly suppressed and is replaced by strengthening antiferromagnetism with increasing  $x$ . An unexpected additional hysteretic phase transition (V) appears at temperatures below the antiferromagnetic ordering temperature for  $x \geq 0.13$ , which shows several characteristics of Ce valence physics. We will discuss this  $T-x$  phase diagram and consider implications for understanding the proposed valence instability region of  $\text{CeCu}_2\text{Si}_{2-x}\text{Ge}_x$  alloys at high pressure.

**8:12AM E27.00002 Evidence for fully-gapped superconductivity in heavy-fermion  $\text{CeCu}_2\text{Si}_2$** , Y. KASAHARA, D. TERAZAWA, T. YAMASHITA, T. ONISHI, Y. TOKIWA, T. TERASHIMA, Y. MATSUDA, Kyoto Univ., T. TAKENAKA, Y. MIZUKAMI, T. SHIBAUCHI, Univ. of Tokyo, J. WILCOX, C. PUTZKE, A. CARRINGTON, Univ. of Bristol, S. KITAKA, T. SAKAKIBARA, ISSP, Univ. of Tokyo, H. S. JEEVAN, S. SEIRO, C. GEIBEL, Max Planck Institute, Y. HAGA, JAEA — The discovery of superconductivity in heavy-fermion  $\text{CeCu}_2\text{Si}_2$  in 1979 has opened a new playground for unconventional superconductivity in strongly-correlated systems. However, even in this archetypal heavy-fermion superconductor, the symmetry and the structure of the superconducting gap, which are intimately related to the pairing mechanism, are still elusive. Here, to investigate the low-energy quasiparticle excitations in the superconducting state of  $\text{CeCu}_2\text{Si}_2$  ( $T_c = 0.6$  K), we performed specific heat, thermal conductivity, and penetration depth measurements down to 60 mK. We found that specific heat and penetration depth exhibit exponential  $T$ -dependence at low  $T$ . Moreover, thermal conductivity has no residual  $T$ -linear term and shows little  $H$ -dependence. These behavior are in marked contrast to nodal superconductors. From the data taken with different experimental configurations, the detailed superconducting gap structure will be discussed.

**8:24AM E27.00003 Thermal expansion and magnetostriction under extreme conditions of an archetypal heavy fermion system.**<sup>1</sup>, AUDREY GROCKOWIAK, DAVID GRAF, WILLIAM CONIGLIO, National High Magnetic Field Laboratory, TAKAO EBIHARA, Shizuoka University, TIMOTHY MURPHY, STANLEY TOZER, National High Magnetic Field Laboratory, TALLAHASSEE TEAM, PR EBIHARA COLLABORATION — Several dilatometry techniques [1] have been developed and used for low temperature and high magnetic field measurements, but do not permit the use of high pressures. Following the experimental development of R.Daou[2], we successfully coupled Fiber Bragg Gratings (FBG) with pressure cells enabling us to map the magnetic field-pressure-temperature phase space of various systems. FBG measurements permit us to achieve a resolution of  $\Delta L/L \approx 3.10^{-7}$  making it a very sensitive technique. Piston-cylinder cells developed at the NHMFL permit us to reach a pressure of 3 GPa, and their compact size allows them to be used in highly constrained sample volume, giving us the ability to do high pressure dilatometry studies in pulsed and dc high magnetic field facility at temperatures as low as 25 mK. Along with the setup we will present our results on the high pressure, high magnetic field dilatometry of  $\text{CeCu}_2\text{Ge}_2$ . [1] Schmiedeshoff, G., Review of Scientific Instruments, 77(12) (2006) [2] Daou, R., Review of Scientific Instruments, 81(3) (2010)

<sup>1</sup>Part of this work was funded by the US DoE NNSA SSAA DE-NA0001979, and performed at the National High Magnetic Field Laboratory, which is supported by National Science Foundation Cooperative Agreement No. DMR-1157490 and the State of Florida.

**8:36AM E27.00004 Optical Kerr Measurements of  $\text{PrOs}_4\text{Sb}_{12}$** , E. M. LEVENSON-FALK, Stanford University, M. BRIAN MAPLE, UC San Diego, YUJI AOKI, Tokyo Metropolitan University, AHARON KAPITULNIK, Stanford University — By probing the symmetries of a superconducting order parameter, it is possible to gain insight into the microscopic physics underlying superconductivity. This approach is especially important for unconventional superconductors, such as heavy fermion materials, where the pairing mechanisms are poorly understood. Time reversal symmetry breaking plays a large role in many heavy fermion systems, due to their strong magnetic interactions; however, TRS is an especially difficult symmetry to probe. Using a zero-loop-area Sagnac interferometer, we measure the polar Kerr effect in materials and thus extract information about TRSB via the optical conductivity. We present measurements of the polar Kerr effect in the multi-phase heavy fermion material  $\text{PrOs}_4\text{Sb}_{12}$ , and discuss applications to other materials.

**8:48AM E27.00005 Superconducting gap symmetry in  $\text{Pr}_{1-x}\text{Ce}_x\text{Pt}_4\text{Ge}_{12}$  studied through specific heat and resistivity measurements**<sup>1</sup>, R. B. ADHIKARI, Y. P. SINGH, S. ZHANG, Kent State University, K. HUANG, D. YAZICI, I. JEON, M. B. MAPLE, University of California, San Diego, M. DZERO, C. C. ALMASAN, Kent State University — We present results of a systematic study of polycrystalline samples of  $\text{Pr}_{1-x}\text{Ce}_x\text{Pt}_4\text{Ge}_{12}$  ( $0 \leq x \leq 0.2$ ) through low-temperature specific heat and electrical resistivity measurements, which allow us to explore the nature of the superconducting gap symmetry and its evolution with Ce concentration  $x$ . As reported earlier, Ce substitution on the Pr site suppresses monotonically the superconducting (SC) transition temperature  $T_c$ : a small Ce concentration of  $x = 0.14$  suppresses  $T_c$  from 7.8 K in the parent compound to 0.6 K. This study points toward a two-band SC gap scenario for the parent compound, in which the larger gap is nodeless, whereas the smaller gap is nodal. While the larger gap remains nodeless irrespective of the amount of Ce substitution, a rather dramatic effect of Ce substitution is seen in the evolution of the smaller gap: a small amount of Ce substitution ( $x < 0.04$ ) increases the value of this gap, while for  $x > 0.04$ , the data suggest that the nodal character of this gap disappears and both SC order parameters become nodeless. We will discuss our findings in the context of other recent results on this series of filled skutterudite compounds.

<sup>1</sup>This work has been supported by the US NSF (Grant Nos. DMR-1506547 and DMR-1505826) at KSU and by the US DOE (Grant No. DE-FG02-04-ER46105) and US NSF (Grant No. DMR-1206553) at UCSD.

**9:00AM E27.00006 Heavy fermion superconductivity under strong orbital fluctuations in  $\text{PrV}_2\text{Al}_{20}$** , YOSUKE MATSUMOTO, MASAKI TSUJIMOTO, TAKAHIRO TOMITA, AKITO SAKAI, SATORU NAKATSUJI, ISSP, Univ. of Tokyo — Novel quantum phases formed in the vicinity of a magnetic quantum critical point (QCP) have been studied extensively in  $4f$  based intermetallics. On the other hand, it is an interesting open question what types of ground state emerges in the vicinity of a QCP of orbital orderings if the  $f$  electrons' orbital degrees of freedom strongly hybridize with conduction electrons. In order to study this, it is important to choose a material with purely orbital degrees of freedom in the ground state. In addition, the material should be clean and the hybridization should be large. Recent our studies have revealed that  $\text{PrTi}_2\text{Al}_{20}$  ( $T = \text{Ti, V}$ ) are ideal systems. Both systems have the nonmagnetic cubic  $\Gamma_3$  crystal electric field doublet. In addition, the hybridization is strong as is evident in many physical properties. We found that both exhibit heavy fermion superconductivity inside the multipole ordering phases. Especially, in the case of  $\text{PrV}_2\text{Al}_{20}$ , the effective mass is highly enhanced ( $m^*/m_0 \sim 140$ ) even at ambient pressure, revealing even stronger hybridization. This observation indicates the first realization of the novel superconductivity arising from the orbital fluctuation of the  $f$  electrons at ambient pressure, suggesting a proximity to an orbital QCP.

### 9:12AM E27.00007 Superconducting Pairing Correlations near a Kondo-destruction Quantum Critical Point in Cluster Impurity Models

ANG CAI, Rice University, JEDEDIAH PIXLEY, University of Maryland, QIMIAO SI, Rice University — Heavy fermion metals represent a canonical system to study superconductivity driven by quantum criticality. We are particularly motivated by the properties of  $\text{CeRhIn}_5$ , which shows the characteristic features of a Kondo destruction quantum critical point (QCP) in its normal state, and has one of the highest  $T_c$ 's among the heavy fermion superconductors. As a first step to study this problem within a cluster-EDMFT approach [1], we analyze a four-site Anderson impurity model with the antiferromagnetic spin component of the cluster coupled to a sub-Ohmic bosonic bath. We find a QCP that belongs to the same universality class as the single-site Bose-Fermi Anderson model. Together with previous work on a two-site model [2], our result suggests that the Kondo destruction QCP is robust as cluster size increases. More importantly, we are able to calculate the  $d$ -wave pairing susceptibility, which we find to be enhanced near the QCP. Using this model as the effective cluster model of the periodic Anderson model, we are also able to study the superconducting pairing near the Kondo-destruction QCP of the lattice model; preliminary results will be presented. [1] J. H. Pixley, A. Cai, Q. Si, Phys. Rev. B 91, 125127 [2] J. H. Pixley, L. Deng, K. Ingersent, Q. Si, Phys. Rev. B 91, 201109

### 9:24AM E27.00008 Visualization of Ce atoms and surface-induced magnetism in $\text{CeCoIn}_5$

YASUO YOSHIDA, HOWON KIM, The institute for solid state physics, The University of Tokyo, CHI-CHENG LEE, HSIN LIN, Graphene Research Centre, National University of Singapore, YOSHINORI HAGA, NAOYUKI TATEIWA, Advanced Science Research Center, Japan Atomic Energy Agency, ZACHARY FISK, Department of Physics and Astronomy, University of California, Irvine, YUKIO HASEGAWA, The institute for solid state physics, The University of Tokyo —  $\text{CeCoIn}_5$  is known as a heavy fermion compound naturally born at the quantum critical point having an unconventional  $d$ -wave superconducting phase at low temperatures. Recently, several STM works on a cleaved surface of this compound reported visualization of emerging heavy fermion bands and consistency of the bulk superconducting properties reported previously. However, reported STM images in those works only visualized In atoms on the Ce-In plane even though the Ce-In plane contains Ce and In atoms. By performing precise low-temperature STM measurements on  $\text{CeCoIn}_5$ , we successfully visualize Ce atoms on the Ce-In plane and, in addition, surface-induced staggered dumbbell-shaped order on the Co plane. This ordered structure locally has  $C_{2v}$  symmetry but retaining  $C_4$  symmetry. This structure coexists with the superconductivity, and is robust against temperatures ( $>T_c$ ) and an external magnetic field ( $>H_{c2}$ ). In the talk, we will discuss the origin of the peculiar ordered structure based on our experimental observations together with first principles calculations.

### 9:36AM E27.00009 Mapping Dimensionality and Directionality of Electronic Behavior in $\text{CeCoIn}_5$ : the Normal State

ANDRAS GYENIS, BENJAMIN E. FELDMAN, MALLIKA T. RANDERIA, GABRIEL A. PETERSON, Princeton University, PEGOR AYNAJIAN, Binghamton University, ERIC D. BAUER, Los Alamos National Laboratory, ALI YAZDANI, Princeton University — Materials made from alternating layers of different constituents can exhibit dramatic variability in their electronic properties depending on which layer is probed. This is evident in the heavy fermion compound  $\text{CeCoIn}_5$ , where scanning tunneling microscopy (STM) has revealed preferential coupling to either light or heavy electron states depending on the surface termination. Here we report STM measurements of  $\text{CeCoIn}_5$  cleaved perpendicular to its basal plane that clearly shows the quasi-two-dimensional nature of the electronic behavior on a single (100) surface. We observe atomic scale modulation of tunneling into the light and heavy electron bands in the  $c$ -axis direction, with no variation visible along the basal planes in the  $b$ -axis direction. In addition, conductance maps reveal preferential scattering along the two-dimensional basal planes. Our measurements highlight the reduced effective dimensionality of electronic states in  $\text{CeCoIn}_5$ , and underscore the potential insight that can be gained by imaging layered materials perpendicular to their  $c$ -axis.

### 9:48AM E27.00010 Mapping Dimensionality and Directionality of Electronic Behavior in $\text{CeCoIn}_5$ : the Superconducting State

BENJAMIN E. FELDMAN, ANDRAS GYENIS, MALLIKA T. RANDERIA, GABRIEL A. PETERSON, Princeton University, PEGOR AYNAJIAN, Binghamton University, ERIC D. BAUER, Los Alamos National Laboratory, ALI YAZDANI, Princeton University — Unconventional superconductors often exhibit anisotropic physical properties that arise from the directional dependence of their order parameters. A prime example is  $\text{CeCoIn}_5$ , a heavy fermion  $d$ -wave superconductor with a rich low-temperature phase diagram consisting of competing and coexisting magnetic and superconducting orders. Here we present dilution refrigerator scanning tunneling microscopy of  $\text{CeCoIn}_5$  cleaved perpendicular to its basal plane. We study superconductivity on the (100) surface, whose normal vector points along the antinode of the superconducting energy gap. The gap magnitude is similar to that observed in the basal plane, with a key difference: it does not exhibit any suppression near step edges. Application of a magnetic field along the [100] direction leads to the formation of anisotropic vortices, and the vortex lattice undergoes a transition at high field before the superconducting state gives way to a pseudogap phase. Our measurements illustrate the directional dependence of the superconducting properties in  $\text{CeCoIn}_5$ , and more generally, demonstrate the utility of imaging  $d$ -wave superconductors along their nodal and antinodal directions.

### 10:00AM E27.00011 Zero-field magnetism in Nd-doped $\text{CeRhIn}_5$ under pressure<sup>1</sup>

PRISCILA ROSA, Los Alamos National Laboratory, AARON OOSTRA, University of California at Irvine, YONGKANG LUO, NICHOLAS WAKEHAM, FILIP RONNING, ERIC BAUER, Los Alamos National Laboratory, ZACHARY FISK, University of California at Irvine, JOE THOMPSON, Los Alamos National Laboratory — Unconventional superconductivity is often found in heavy fermion compounds close to a magnetic instability. Although magnetism and superconductivity may coexist when  $T_N > T_c$ , evidence for magnetism is usually suddenly lost when  $T_N < T_c$ . Here we study the heavy-fermion compound  $\text{Ce}_{0.95}\text{Nd}_{0.05}\text{RhIn}_5$  under pressure by means of electrical resistivity and AC calorimetry measurements. Our results show that, even at zero applied magnetic field, Nd substitution unveils a hidden magnetic instability below the superconducting dome. We examine the similarities and differences between our results and those on Nd-doped  $\text{CeCoIn}_5$  as well as pure  $\text{CeRhIn}_5$  under applied field and pressure. We discuss our results in light of recent calculations that include  $d$ -wave superconductivity and underlying magnetic correlations.

<sup>1</sup>Work at Los Alamos was performed under the auspices of the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering. P. F. S. Rosa acknowledges a Directors Postdoctoral Fellowship through the LDRD program.

### 10:12AM E27.00012 Hybrid heavy-fermion superlattices of $\text{CeCoIn}_5/\text{CeRhIn}_5$

MASAHIRO NARITSUKA, TOMOHIRO ISHII, RINTARO TODA, SHIGERU KASAHARA, YUICHI KASAHARA, YOSHI TOKIWA, TAKAHITO TERASHIMA, YUJI MATSUDA, Kyoto University — Interplay between superconductivity and magnetism continues to provide central topics in condensed matter physics. Among others,  $\text{CeTIn}_5$  ( $T = \text{Co, Rh}$ ) compounds offer one of the suitable platforms for the study of this important issue —  $\text{CeCoIn}_5$  undergoes superconducting transition at  $T_c = 2.3$  K while  $\text{CeRhIn}_5$  orders antiferromagnetically below  $T_N = 3.8$  K at ambient pressure. An intriguing issue concerns coexistence of superconductivity and antiferromagnetism which could be realized at an artificial interface of different materials, but it is not clear how the two different states are affected each other at the interface. Here, by using atomic layer-by-layer molecular beam epitaxy, we fabricate superconducting-antiferromagnetic hybrid superlattices consisting of alternating layers of  $\text{CeCoIn}_5$  and  $\text{CeRhIn}_5$ . Transport measurements confirm the presence of both superconducting and antiferromagnetic phases. The coexistence of superconductivity and antiferromagnetism in a hybrid system is discussed based on the proximity effect at the interface.

**10:24AM E27.00013 Switching of the Spin-Density-Wave in CeCoIn<sub>5</sub> probed by Thermal Conductivity<sup>1</sup>**, DUK Y. KIM, SHI-ZENG LIN, FRANZISKA WEICKERT, ERIC D. BAUER, FILIP RONNING, JOE D. THOMPSON, ROMAN MOVSHOVICH, Los Alamos National Laboratory — Unconventional superconductor CeCoIn<sub>5</sub> orders magnetically in a spin-density-wave (SDW) in the low-temperature and high-field corner of the superconducting phase. Recent neutron scattering experiment revealed that the single-domain SDW's ordering vector  $Q$  depends strongly on the direction of the magnetic field, switching sharply as the field is rotated through the anti-nodal direction. This switching may be manifestation of a pair-density-wave (PDW)  $p$ -wave order parameter, which develops in addition to the well-established  $d$ -wave order parameter due to the SDW formation. We have investigated the hypersensitivity of the magnetic domain with a thermal conductivity measurement. The heat current ( $J$ ) was applied along the [110] direction such that the  $Q$  vector is either perpendicular or parallel to  $J$ , depending on the magnetic field direction. A discontinuous change of the thermal conductivity was observed when the magnetic field is rotated around the [100] direction within  $0.2^\circ$ . The thermal conductivity with the  $Q$  parallel to the heat current ( $J||Q$ ) is approximately 15% larger than that with the  $Q$  perpendicular to the heat current ( $J\perp Q$ ). This result is consistent with additional gapping of the nodal quasiparticle by the  $p$ -wave PDW coupled to SDW.

<sup>1</sup>Work at Los Alamos was performed under the auspices of the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering.

**10:36AM E27.00014 Entanglement and exotic superfluidity in one-dimensional spin-imbalanced lattices<sup>1</sup>**, VIVIAN FRANÇA, Institute of Chemistry, São Paulo State University — The exotic coexistence of superfluidity and magnetism has been investigated theoretical and experimentally since decades. Among the several ideas and models to describe exotic superconductors the so-called Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phase stands out. In strongly correlated systems at low temperatures the FFLO state might emerges by the presence of external magnetic fields or by internal polarization as produced by spin-imbalanced populations. Although the FFLO papers are in their 50th birthday and state-of-the-art experiments have been addressed this matter, there have been no unequivocal observations of FFLO superconductivity. We investigate the FFLO superfluid regime in one-dimensional fermionic lattices from a quantum information theory perspective: studying the properties of entanglement. We find that entanglement is non-monotonic with the polarization whenever the lattice is predicted to be an exotic superfluid. We thus propose a simple model for the spin-flip channels involved in the process. Our model is found to allow a very good description of exotic superfluids, while beyond the FFLO regime it reveals a breaking pairs avalanche. Our findings are supported by both density functional theory and density matrix renormalization group calculations.

<sup>1</sup>This work was supported by FAPESP and CNPq.

**10:48AM E27.00015 Microscopic investigation of electronic inhomogeneity induced by substitutions in quantum critical CeCoIn<sub>5</sub>.**, FILIP RONNING, Los Alamos National Lab, HIRONORI SAKAI, Japanese Atomic Energy Agency, JIANXIN ZHU, NICHOLAS WAKEHAM, HIROSHI YASUOKA, Los Alamos National Lab, YO TOKUNAGA, SHIN KAMBE, Japanese Atomic Energy Agency, ERIC BAUER, JOE THOMPSON, Los Alamos National Lab — In Cd-doped CeCoIn<sub>5</sub> magnetic order can be suppressed by pressure giving rise to a dome of superconductivity surrounding a quantum critical point (QCP). However, the typical non-Fermi liquid (NFL) signatures expected at this QCP are absent. In contrast, in Sn-doped CeRhIn<sub>5</sub>, pressure also suppresses magnetism giving rise to a dome of superconductivity, but in this case, the NFL signatures ARE observed at the QCP. We presents results using nuclear quadrupole resonance to probe microscopically the response of the prototypical quantum-critical metal CeCoIn<sub>5</sub> to substitutions of small amounts of Sn and Cd for In. These substituents induce very different local electronic environments as observed by site dependent spin lattice relaxation rates  $1/T_1$ . Cd-doped samples generate a much more inhomogeneous spin environment than observed in Sn-doped samples. This difference naturally explains the presence and absence of NFL signatures at the respective QCPs mentioned above. The effects found here illustrate the need for care in general when interpreting NFL properties determined by macroscopic measurements achieved by chemical substitutions.

## Tuesday, March 15, 2016 8:00AM - 11:00AM – Session E28 DMP: Topological Superconductivity 327 - Abhay Pasupathy, Columbia University

**8:00AM E28.00001 Emergent surface superconductivity in a 3D topological insulator.<sup>1</sup>**, LIA KRUSIN-ELBAUM, Department of Physics, The City College of New York CUNY — Surfaces of three-dimensional topological insulators have emerged as one of the most remarkable states of condensed quantum matter where exotic charge and spin phases of Dirac particles could form. This work reports on novel mesoscopic superconductivity in the topological insulator Sb<sub>2</sub>Te<sub>3</sub> with transition to zero resistance induced through a minor tuning of growth chemistry that depletes bulk conduction channels [1]. The depletion shifts Fermi energy towards the Dirac point as witnessed by a factor of 300 reduction of bulk carrier density and by the largest carrier mobility ( $>25,000\text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ ) found in any topological material of this class. Direct evidence from transport, the unprecedentedly large diamagnetic screening, and the presence of  $\sim 25\text{ meV}$  gaps detected by scanning tunneling spectroscopy reveal the superconducting condensate to emerge first in surface puddles at unexpectedly high temperature of  $\sim 50\text{ K}$ , with the onset of global phase coherence at  $\sim 9\text{ K}$ . The unconventional spin response of Sb<sub>2</sub>Te<sub>3</sub> [2] and the presence of subsurface 2DEG quantum well states arising from charge transfer to the surface [3] are likely to play a role in the emergent superconducting state. The rich structure of this state lends itself to manipulation via growth conditions and the material parameters such as Fermi velocity and mean free path. [1] Emergent surface superconductivity in the topological insulator Sb<sub>2</sub>Te<sub>3</sub>, L. Zhao, H. Deng, I. Korzhovska, J. Secor, M. Begliarbekov, Z. Chen, E. Andrade, E. Rosenthal, A. Pasupathy, V. Oganessian, and Lia Krusin-Elbaum, *Nature Comm.* **6**, 8279 (2015); DOI:10.1038/ncomms9279. [2] Singular robust room-temperature spin response from topological Dirac fermions, L. Zhao, H. Deng, I. Korzhovska, Z. Chen, M. Konczykowski, A. Hruban, V. Oganessian and Lia Krusin-Elbaum, *Nature Mat.* **13**, 580 (2014); DOI: 10.1038/nmat3962. [3] Robust topological interfaces and charge transfer in epitaxial Bi<sub>2</sub>Se<sub>3</sub>/II-VI semiconductor superlattices, Z. Chen, L. Zhao, K. Park, T. A. Garcia, M. C. Tamargo, and Lia Krusin-Elbaum, *Nano Lett.* **15** (10), 6289 (2015); DOI:10.1021/acs.nanolett.5b01358.

<sup>1</sup>This work was supported by NSF DMR-1122594, DMR-1420634, DMR-1322483, and DOD-W911NF-13-1-0159.

**8:36AM E28.00002 Superconducting Proximity Effect in the Weyl Semimetal WTe<sub>2</sub> and MoTe<sub>2</sub>**, WUDI WANG, MINHAO LIU, Department of Physics, Princeton University, Princeton, NJ 08544, QUINN GIBSON, R. J. CAVA, Department of Chemistry, Princeton University, Princeton, NJ 08544, N. P. ONG, Department of Physics, Princeton University, Princeton, NJ 08544 — WTe<sub>2</sub> and MoTe<sub>2</sub> are predicted to have type-II Weyl nodes and many novel transport properties have been studied. We investigated the transport of cooper pairs and Andreev reflection in Weyl semimetals by proximitizing WTe<sub>2</sub> and MoTe<sub>2</sub> nanoflakes with superconducting pads (Nb and Al). We have fabricated superconductor-nanoflakes-superconductor structure with different length. Supercurrent were observed in both materials with junction length up to 700nm. We conducted dc IV curve measurements and got exotic Fraunhofer patterns. We also measured the current-phase relation with a radio frequency-based CPR measurement technique.

**8:48AM E28.00003 Superconducting proximity effect and the Fermi velocity in the surface-state of  $\text{SmB}_6$  thin films<sup>1</sup>**, SEUNGHUN LEE, XIAOHANG ZHANG, RICHARD L. GREENE, ICHIRO TAKEUCHI, CNAM, MSE, and Physics, University of Maryland —  $\text{SmB}_6$  recently has been predicted to be topological Kondo insulator. Here, we investigate the Fermi velocity ( $v_F$ ) of  $\text{SmB}_6$  using transport measurements and a study on the superconducting proximity effect, independently. In the transport measurement,  $\text{SmB}_6$  thin films show thickness-independent transport characteristics at low temperatures, which is a strong evidence for the presence of the surface conducting channel as well as the insulating bulk state as the nature of Kondo insulator. We estimate the thickness of the surface-state to be  $\approx 7$  nm and the  $v_F$  to be  $\sim 10^5$  m/s. In order to carry out the proximity effect investigation, we fabricated superconducting Nb/ $\text{SmB}_6$  bilayers *in-situ*. We performed Usadel fitting to the variation of critical temperatures of the Nb layers due to the proximity effect. Interestingly, only the fitting regarding a 2D surface model yielded the consistent value of the  $v_F$  with the value obtained from the transport measurement as well as the reported value from the quantum oscillation measurement. These results indicate that  $\text{SmB}_6$  has a true 2D surface-channel responsible for the observed proximity effect.

<sup>1</sup>This work is supported by NSF under grant No. DMR-1410665 and conducted at Center for Nanophysics and Advanced Materials (CNAM)

**9:00AM E28.00004 Probing the Superconducting Proximity Effect of Topological Insulator  $\text{Bi}_2\text{Se}_3$  Using Scanning Tunneling Microscopy**, IAN DAYTON, NICHOLAS SEDLMAYR, VICTOR RAMIREZ, Michigan State University Department of Physics and Astronomy, THOMAS CHASAPIS, Northwestern University Department of Chemistry, REZA LOLOEE, Michigan State University Department of Physics and Astronomy, ALEX LEVCHENKO, University of Wisconsin-Madison Department of Physics, MERCOURI KANATZIDIS, Northwestern University Department of Chemistry, STUART TESSMER, Michigan State University Department of Physics and Astronomy — Placing a 3D topological insulator (TI) in proximity to an s-wave superconductor is theoretically predicted to induce 2D p-wave superconductivity into the topologically protected surface state (TSS). In this talk, we will present cryogenic scanning tunneling microscopy measurements of a large  $\text{Bi}_2\text{Se}_3$  crystal with nanometer scale islands of PbBi deposited on the surface. Local density of states measurements are consistent with p-wave superconductivity in the top  $\text{Bi}_2\text{Se}_3$  quintuple layer, with coherence length of  $540 \pm 50$  nm in the direction parallel to the layer. We see indications of a reverse proximity effect as well, where the TSS from the TI leaks back into local density of states measured on the superconducting islands. The density of states curves also exhibit structure which we interpret as McMillan-Rowell oscillations due to Andreev confinement perpendicular to the layer.

**9:12AM E28.00005 Experimental consequences of candidate pairings for superconducting topological insulators.**, LEI HAO, Department of Physics and Texas Center for Superconductivity, University of Houston, TING-KUO LEE, Institute of Physics, Academia Sinica, WEI-FENG TSAI, Department of Physics, National Sun Yat-sen University, JUN WANG, Department of Physics, Southeast University, CHIN-SEN TING, Department of Physics and Texas Center for Superconductivity, University of Houston — Genuine pairing symmetry of the superconducting topological insulators, including  $\text{Cu}_x\text{Bi}_2\text{Se}_3$ ,  $\text{Bi}_2\text{Se}_3$ , and  $\text{Bi}_2\text{Te}_3$ , are under debate. In this work, we make an extensive comparison on the experimental consequences of several candidate pairings. The physical quantities studied include the surface spectral functions, the surface local density of states, and the electronic thermal conductivities. Apparent differences in the results are found and can be used to identify the actual pairing symmetry. In particular, for model and parameters used in this work which are obtained by fitting first-principles calculations, we get interesting new results such as a segmental flat band of surface Andreev bound states for a spin-singlet pairing. A combination of several experimental techniques should be able to identify the genuine pairing symmetry.

**9:24AM E28.00006 Stability of Majorana vortex bound states on the surface of superconducting topological insulators**, JUNYI ZHANG, Department of Physics, Princeton University, JENNIFER CANO, TITUS NEUPERT, PCTS, Princeton University — Fu and Kane showed that superconductivity induced on the surface of a 3D topological insulator results in isolated Majorana bound states that appear in the cores of vortices. Many efforts to realize this idea are based on proximity-induced superconducting order in a heterostructure. Recently, superconductivity has been observed in  $\text{PbTaSe}_2$ , which has the band topology of a topological insulator with Dirac cone surface states. Hence, it nourishes the vision of realizing the Fu and Kane proposal in a stoichiometric material without the need for doping or fabricating heterostructures. Motivated by this possibility, we give a comprehensive analysis of stability and localization properties of the vortex Majorana modes in such a topological superconducting material. In particular, we address the experimentally relevant questions regarding (i) the energy separation between the vortex bound and excited states, (ii) the dependence of the hybridization between Majorana modes from opposite surfaces on the thickness of a thin-film sample, (iii) the influence of the bulk superconducting pockets on the Majorana states.

**9:36AM E28.00007 Magnetic Ordering In Superconducting Nb-doped  $\text{Bi}_2\text{Se}_3$** , PAUL CORBAE, BENJAMIN LAWSON, GANG LI, FAN YU, TOMOYA ASABA, COLIN TINSMAN, Univ of Michigan - Ann Arbor, YUSHENG QUI, YEW SAN HOR, Missouri University of Science and Technology, LU LI, Univ of Michigan - Ann Arbor — Coexistence of superconductivity and magnetic order has been suggested by early studies of topological superconductor candidate, niobium doped  $\text{Bi}_2\text{Se}_3$ . In order to elucidate the interesting physics of this coexistence, we performed highly sensitive torque magnetometry to study the materials magnetization. We observed a bump feature in the magnetization around 8 Tesla in both the superconducting and non-superconducting samples. This is distinct from the paramagnetic torque response of the parent compound,  $\text{Bi}_2\text{Se}_3$ , suggesting some interesting magnetic order in Nb-doped  $\text{Bi}_2\text{Se}_3$ .

**9:48AM E28.00008 Multi-orbits observed in superconducting Nb-doped  $\text{Bi}_2\text{Se}_3$** , BENJAMIN LAWSON, PAUL CORBAE, GANG LI, FAN YU, TOMOYA ASABA, COLIN TINSMAN, Univ of Michigan - Ann Arbor, YUNSHENG QIU, YEW SAN HOR, Missouri University of Science and Technology, LU LI, Univ of Michigan - Ann Arbor — Recently discovered superconducting niobium doped  $\text{Bi}_2\text{Se}_3$  shows promise to realize new physical phenomenon including the coexistence of superconductivity and magnetic ordering and possibly topological superconductivity. To understand the new physics showcased in this system, a detailed knowledge of the electronic structure is needed. We present the first observation of quantum oscillations in the magnetization (the de Haas-van Alphen effect) of Nb-doped  $\text{Bi}_2\text{Se}_3$ . In the fully superconducting crystal, two distinct orbits are observed, in sharp contrast to  $\text{Bi}_2\text{Se}_3$ , Cu-doped  $\text{Bi}_2\text{Se}_3$ , and Sr-doped  $\text{Bi}_2\text{Se}_3$ . The multiple frequencies observed in our quantum oscillations, combined with our electrical transport studies, indicate the multi-orbit nature of the electronic state of Nb-doped  $\text{Bi}_2\text{Se}_3$ .

**10:00AM E28.00009 Lattice melting and surface Topological order in 3D Time reversal invariant topological superconductor**, YIZHI YOU, KITP — In this talk, we start from the eight copies of 3D Time reversal invariant topological superconductor on a crystal. By proliferating and condensing the disclinations, we can therefore restore the spatial rotation symmetry of the lattice crystal. During the procedure of lattice melting, the fermion acquires a  $\pi$  Berry Phase when winding around the  $2\pi$  disclination and therefore the fermions get confined when disclination loop proliferates. After the disclination condensed, we obtained a 3D bosonic SPT phase with by  $T$  and spatial rotation symmetry. In addition, we investigate the surface state of this Bosonic SPT. If we break the  $T$  symmetry on the surface, the 8 majorana cones are gapped and the  $2\pi$  disclination has semion statistics. To obtain a  $T$  and rotation invariant gapped surface state, we first turn on Fulde-Ferrell superfluid order of the surface to gap the surface fermion and then condensed the vortex/disclination of the superfluid to restore the  $T$  and rotation symmetry. The disclination dipole and vortex exhibit fractional statistics and therefore vortex condensation and lattice melting give rise to new surface topological order.

**10:12AM E28.00010 Topological Superconductivity in Dirac Semimetals** , MASATOSHI SATO, Kyoto Univ, SHINGO KOBAYASHI, Nagoya Univ — Dirac semimetals host bulk band-touching Dirac points and a surface Fermi loop. We develop a theory of superconducting Dirac semimetals. Establishing a relation between the Dirac points and the surface Fermi loop, we clarify how the nontrivial topology of Dirac semimetals affects their superconducting state. We note that the unique orbital texture of Dirac points and a structural phase transition of the crystal favor symmetry-protected topological superconductivity with a quartet of surface Majorana fermions. We suggest the possible application of our theory to recently discovered superconducting states in  $\text{Cd}_3\text{As}_2$ .

**10:24AM E28.00011 Superconducting states of topological surface states in  $\beta\text{-PdBi}_2$  investigated by STM/STS** , KATSUYA IWAYA, RIKEN-CEMS, KENJIRO OKAWA, Tokyo Institute of Technology, TETSUO HANAGURI, YUHKI KOHSAKA, TADASHI MACHIDA, RIKEN-CEMS, TAKAO SASAGAWA, Tokyo Institute of Technology — We investigate superconducting (SC) states of topological surface states in  $\beta\text{-PdBi}_2$  using very low temperature STM. Characteristic quasiparticle interference patterns strongly support the existence of the spin-polarized surface states at the Fermi level in the normal state. A fully-opened SC gap well described by the conventional BCS model is observed, indicating the SC gap opening at the spin-polarized Fermi surfaces. Considering a possible mixing of odd- and even parity orbital functions in  $C_{4v}$  group symmetry lowered from  $D_{4h}$  near the surface, we suggest that the SC gap consists of the mixture of  $s$ - and  $p$ -wave SC gap functions in the two-dimensional state.

**10:36AM E28.00012 Superconductivity in Weyl metals** , GRIGORY BEDNIK, ANTON BURKOV, University of Waterloo, ALEXANDER ZYUZIN, University of Basel — We report on a study of intrinsic superconductivity in a Weyl metal. We show that two distinct superconducting states are possible in this system in principle: a zero-momentum pairing BCS state, with point nodes in the gap function; and a finite-momentum FFLO-like state, with a full nodeless gap. We find that, in an inversion-symmetric Weyl metal the odd-parity BCS state has a lower energy than the FFLO state, despite the nodes in the gap. The FFLO state, on the other hand, may have a lower energy in a noncentrosymmetric Weyl metal, in which Weyl nodes of opposite chirality have different energy. We also discuss the anomalous Hall effect in a superconducting Weyl metal and show that it is not affected by the presence of superconductivity at low enough energies, i.e. when the Fermi surfaces is close enough to the nodes.

**10:48AM E28.00013 Topological nodal Cooper pairing in doped Weyl metals<sup>1</sup>** , YI LI, F. D. M. HALDANE, Princeton University — We generalize the concept of Berry connection of the single-electron band structure to the two-particle Cooper pair states between two Fermi surfaces with opposite Chern numbers. Because of underlying Fermi surface topology, the pairing Berry phase acquires non-trivial monopole structure. Consequently, pairing gap functions have the topologically-protected nodal structure as vortices in the momentum space with the total vorticity solely determined by the monopole charge  $q_p$ . The pairing nodes behave as the Weyl-Majorana points of the Bogoliubov-de Gennes pairing Hamiltonian. Their relation with the connection patterns of the surface modes from the Weyl band structure and the Majorana surface modes inside the pairing gap is also discussed. Under the approximation of spherical Fermi surfaces, the pairing symmetry are represented by monopole harmonic functions. The lowest possible pairing channel carries angular momentum number  $j=|q_p|$ , and the corresponding gap functions are holomorphic or anti-holomorphic functions on Fermi surfaces.

<sup>1</sup>F.D.M.H. acknowledges the support from MRSEC NSF-DMR-1420541 and the W. M. Keck Foundation.

## Tuesday, March 15, 2016 8:00AM - 11:00AM —

Session E29 DCMP: Majorana Fermions 328 - Sergey Frolov, University of Pittsburgh

**8:00AM E29.00001 Spinon Majorana fermion** , RUI WANG, HONG-YAN LU, Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, Texas 77204, USA, BAIGENG WANG, National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, Nanjing 210093, China, CHIN-SEN TING, Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, Texas 77204, USA — A new realization of Majorana fermions is proposed in the frustrated magnets via the topological proximity effect. Specifically, we consider the interface between a topological insulator and a frustrated magnetic material. Using the renormalization group-based mean-field theory, and calculating the self-energy correction due to the topological insulator, we find that the spin texture and the spin-momentum locking of the Dirac cone will be inherited by the spinons in the nearby frustrated magnets. This leads to a particular topological state of matter that supports the Majorana excitation. Unlike the conventional ones, these Majorana fermions are the composite states of spinons and anti-spinons, rather than electrons and holes. They can also participate in the transport of spinons, resulting in nontrivial spin current, while the charge current is completely frozen.

**8:12AM E29.00002 Chiral Majorana Interference in Quantum Anomalous Hall-Superconductor Junctions** , BIAO LIAN, JING WANG, SHOUCHENG ZHANG, Stanford University — We study the interference of the edge chiral Majorana fermions in junctions of quantum anomalous Hall (QAH) insulators and superconductors (SCs). We show the two chiral Majorana fermions on a QAH edge in contact with an SC generically have a momentum difference  $\Delta k$  that depends on the chemical potentials of both the QAH insulator and the SC. Due to the spacial interference induced by  $\Delta k$ , the longitudinal conductance of normal SC/QAH junctions exhibits an oscillation with respect to the edge lengths and the chemical potentials, which can be measured in transport experiments. Further, we show for QAH/chiral topological SC junctions where there is only one edge chiral Majorana fermion, the dynamical fluctuation of the SC phase yields a geometrical correction to the longitudinal conductance usually derived.

**8:24AM E29.00003 Majorana Fermions at the End of Topological Insulator Nanoribbon** , XIONGJUN LIU, YUQIN CHEN, Peking Univ — Majorana zero modes can exist at the end of a 1D  $p$ -wave SC. 1D semiconductor nanowire approximated a  $s$ -wave superconductor is a famous one of those proposals. In which, strong Zeeman field is required to have a large topological region, but unfortunately suppresses superconducting pairing and makes the system more sensitive to disorder. Here we propose a Nanoribbon system made of 2D topological insulator where finite size effect due to the narrow width between two edges plays an important role. A ferromagnetic insulator and an  $s$ -wave superconductor are attached at each edge, respectively. We introduce a low energy effective model to investigate the superconducting phase diagram. And, the disorder effect is studied analytically by using the self-consistent Born approximation (SCBA). Furthermore, realistic numerical calculation is carried out with a tight-binding model. We demonstrate that, strong Zeeman field generates a large topological region, and at the same time enhances superconducting pairing and makes the system more immune to disorder.

**8:36AM E29.00004 Molecular Andreev bound states and Majorana modes in a double dot system**<sup>1</sup>, EDSON VERNEK, JOELSON F. SILVA, Federal University of Uberlândia — Nanostructured systems such as quantum dots (QD) connected to superconductors have attracted a lot of attention in the recent years. One of the well known phenomena in such a system is the formation of a pair of bound states called Andreev bound states (ABS)<sup>2</sup>. Recently, it has been shown that when a QD is coupled to a topological superconductor wire, a Majorana bound state (MBS) leaks from the end of the wire into the dot<sup>3</sup>. The character of these bound states is much richer in structures like molecules and is far from being completely understood. In this work we study a system composed by a two inter-connected QDs in which one of them is coupled to a normal superconductor and to a normal lead while the other is coupled to a topological superconductor and to a distinct normal metallic lead. We show that in the atomic limit (for small interdot coupling), one of the dots has a pair of ABS whereas the other has a single MBS. More interestingly, in the molecular regime (large inter-dot coupling) we observe a localized Majorana mode coexisting with a delocalized molecular ABS.

<sup>1</sup>We would like to thank financial support from the Brazilian agencies CNPq, CAPES and FAPEMIG.

<sup>2</sup>T. Meng, S. Florens, and P. Simon, Phys. Rev. B **79**, 224521 (2009).

<sup>3</sup>E. Vernek, P. H. Penteado, A. C. Seridonio, and J. C. Egues, Phys. Rev. B **89**, 165314 (2014).

**8:48AM E29.00005 Coupled wire model of symmetric Majorana surfaces of topological superconductors I: 4-fermion gapping interactions**, SHARMISTHA SAHOO, ZHAO ZHANG, JEFFREY TEO, Univ of Virginia — Time reversal symmetric topological superconductors in three spatial dimensions carry gapless surface Majorana fermions. They are robust against any time reversal symmetric single-body perturbation weaker than the bulk energy gap. We mimic the massless surface Majorana's by coupled wire models in two spatial dimensions. We introduce explicit many-body interwire interactions that preserve time reversal symmetry and give energy gaps to all low energy degrees of freedom. The gapping 4-fermion interactions are constructed by interwire Kac-Moody current backscattering and rely on the fractionalization or conformal embedding of the Majorana wires.

**9:00AM E29.00006 Coupled wire model of symmetric Majorana surfaces of topological superconductors II: 32-fold periodic topological orders**, ZHAO ZHANG, SHARMISTHA SAHOO, JEFFREY TEO, University of Virginia — We mimic the massless surface Majorana's of topological superconductors by coupled wire models in two spatial dimensions, and introduce many-body gapping interactions that preserve time reversal symmetry. Coupling with a  $Z_2$  gauge theory, the symmetric gapped surface generically carries a non-trivial  $G_N$  topological order, where  $N$  is the number of Majorana species and  $G_N$  is some  $SO(r)_1$  or  $SO(3)_3$ -like topological state. These form a 32-fold periodic class  $G_N \cong G_{N+32}$ , and a  $Z_{32}$  relative tensor product structure  $G_{N_1} \otimes_b G_{N_2} \cong G_{N_1+N_2}$  by anyon condensation. We present the anyon structures of these topological states, and understand the topological orders through bulk-boundary correspondence and the Wilson structures on a torus geometry.

**9:12AM E29.00007 Topological Massive Dirac Edge Modes and Long-Range Superconducting Hamiltonians**, OSCAR VIYUELA, Universidad Complutense de Madrid, DAVIDE VODOLA, GUIDO PUPILLO, Universite de Strasbourg and CNRS, MIGUEL ANGEL MARTIN-DELGADO, Universidad Complutense de Madrid — We discover novel topological effects in the one-dimensional Kitaev chain modified by long-range Hamiltonian deformations in the hopping and pairing terms. This class of models display symmetry-protected topological order measured by the Berry phase of the ground state and the winding number of the Hamiltonians. For exponentially-decaying hopping amplitudes, the topological sector can be significantly augmented as the penetration length increases, something experimentally achievable. For power-law decaying superconducting pairings, the massless Majorana modes at the edges get paired together into a massive non-local Dirac fermion localised at both edges of the chain: a new topological quasiparticle that we call topological massive Dirac fermion. This topological phase has fractional topological numbers as a consequence of the long-range couplings. Possible applications to current experimental setups and topological quantum computation are also discussed.

**9:24AM E29.00008 Local and non-local conductance of one-dimensional topological superconductor with Majorana bound states**, ZHI-QIANG BAO, FAN ZHANG, The University of Texas at Dallas — A one-dimensional topological superconductor has a full pairing gap in the bulk and Majorana bound states on the boundary. It is well known that the existence of Majorana bound states enables a quantized resonant local Andreev reflection. Here we find that non-local topological signatures can also be induced by the Majorana bound states in a simple setup, even though the bulk is fully gapped. The non-local conductance, which can even be quantized, depends crucially on the symmetries, the topological index, and the mesoscopic properties of the bulk. Coulomb interactions can further drive the hybrid system into a novel phase, which can be understood by a set of renormalization-group flow equations.

**9:36AM E29.00009 Phase diagrams and transport signatures of Luttinger liquid - Majorana Kramers pair junction.**<sup>1</sup>, ERIKAS GAIDAMAUSKAS, Niels Bohr Institute, University of Copenhagen, DONG E. LIU, Microsoft Research Station Q, YOUNGHYUN KIM, UC Santa Barbara, JENS PAASKE, KARSTEN FLENSBERG, Niels Bohr Institute, University of Copenhagen, ROMAN M. LUTCHYN, Microsoft Research Station Q — Majorana Kramers pairs appearing at the ends of a time reversal invariant topological superconductor lead to a quantized conductance of  $4e^2/2h$  due to perfect Andreev reflection. We study the stability of Andreev reflection fixed point with respect to electron-electron interactions present in the nanowire and calculate the phase diagram for the system. We find that the low energy properties are determined by local or crossed Andreev reflection fixed points. We analyze transport properties of the junction at these fixed points.

<sup>1</sup>Phase diagrams and transport signatures of Luttinger liquid - Majorana Kramers pair junction

**9:48AM E29.00010 A New Infinite-Randomness Fixed Point in an Interacting Majorana Chain**, S VIJAY, LIANG FU, Massachusetts Inst of Tech-MIT — We perform a real-space renormalization group (RG) study of an interacting chain of Majorana fermions with strong randomness. Our theory naturally describes the interacting, disordered edge of a weak topological superconductor in the BDI symmetry class of fermion topological phases. Our RG scheme reveals a new infinite-randomness fixed-point, governed by flow equations for the probability distribution of couplings. A numerical implementation of our real-space RG yields critical exponents governing susceptibilities and correlation functions near the fixed-point.

**10:00AM E29.00011 Topological Phases of Inhomogeneous Superconductivity**, SILAS HOFFMAN, JELENA KLINOVAJA, DANIEL LOSS, University of Basel — We theoretically consider the effect of a spatially periodic modulation of the superconducting order parameter on the formation of Majorana fermions induced by a one-dimensional system with magnetic impurities brought into close proximity to an  $s$ -wave superconductor. When the magnetic exchange energy is larger than the inter-impurity electron hopping we model the effective system as a chain of coupled Shiba states. While in the opposite regime, the effective system is accurately described by a quantum wire model. Upon including a spatially modulated superconducting pairing, we find, for sufficiently large magnetic exchange energy, the system is able to support a single pair of Majorana fermions with one Majorana fermion on the left end of the system and one on the right end. When the modulation of superconductivity is large compared to the magnetic exchange energy, the Shiba chain returns to a trivially gapped regime while the quantum wire enters a new topological phase capable of supporting two pairs of Majorana fermions.

10:12AM E29.00012 ABSTRACT WITHDRAWN —

**10:24AM E29.00013 Kramers pair of Majoranas in contact with a Luttinger Liquid**, DMITRY PIKULIN, University of British Columbia, YASHAR KOMIJANI, University of British Columbia and Rutgers University, IAN AFFLECK, University of British Columbia — I will discuss the signatures of the Kramers pair of Majorana coupled to a quantum wire. I will start from the non-interacting case, showing perfect Andreev process at zero energy — either intrachannel, or interchannel. I will show that turning on the interactions will make one of the Andreev process stable, and another unstable. I will discuss the stability diagram of the fixed points as a function of interactions strength and show that strong enough interactions lead to a non-trivial fixed point.

**10:36AM E29.00014 Superconductor disorder and strong proximity coupling effects in Majorana nanowires<sup>1</sup>**, WILLIAM COLE, JAY SAU, CMTc and JQI, University of Maryland, College Park — Topological superconductivity induced by proximity to a conventional superconductor is only robust against moderate disorder in the parent superconductor, and only when the energy scale of the interface coupling is much smaller than the parent gap. I present detailed calculations of proximity-induced superconductivity in one-dimensional, spin-orbit coupled, semiconductor nanowires when the parent superconductor disorder and interface coupling exceed this limit. This parameter regime is characterized by unique spectroscopic signatures on both sides of the external field tuned topological phase transition.

<sup>1</sup>This work is supported by LPS-MPO-CMTC, Microsoft Q, and JQI-NSF-PFC

**10:48AM E29.00015 Disorder-induced topological transitions in multichannel Majorana wires<sup>1</sup>**, INANC ADAGIDELI, BARIS PEKERTEN, AYKUT TEKER, Sabanci University, MICHAEL WIMMER, Delft University of Technology, OZGUR BOZAT, Sabanci University — In this work, we investigate the effect of disorder on the topological properties of multichannel superconductor nanowires. While the standard expectation is that the spectral gap is closed and opened at transitions changing the topological property of the ground state, we show that the closing and opening of a *transport* gap can also cause topological transitions, even in the presence of (localized) states at both sides of the transition. Such transport gaps, induced by disorder, can thus change the topological index, driving a topologically trivial wire into a nontrivial state. We focus on nanowires exhibiting *p*-wave superconductivity as well as Rashba semiconductor nanowires in proximity to a conventional superconductor, and obtain analytical formulas for topological transitions in these wires, valid for generic realizations of disorder, generalizing earlier results. Full tight-binding simulations show excellent agreement with our analytical results without any fitting parameters.

<sup>1</sup>Work supported by TUBITAK under grant No. 110T841

**Tuesday, March 15, 2016 8:00AM - 11:00AM —**

**Session E30 DMP: Topological and Correlation Effects in Oxide Heterostructures** 329 - James Rondinelli, Northwestern University

**8:00AM E30.00001 Design of Mott and topological phases on buckled 3d-oxide honeycomb lattices<sup>1</sup>**, ROSSITZA PENTCHEVA, University Duisburg-Essen — The honeycomb lattice, as realized e.g. in graphene, has rendered a robust platform for innovative science and potential applications. A much richer generalization of this lattice arises in (111)-oriented bilayers of perovskites, adding the complexity of the strongly correlated, multiorbital nature of electrons in transition metal oxides. Based on first principles calculations with an on-site Coulomb repulsion, here we provide trends in the evolution of ground states versus band filling in (111)-oriented  $(\text{LaXO}_3)_2/(\text{LaAlO}_3)_4$  superlattices, with *X* spanning the entire 3d transition metal series. The competition between local quasi-cubic and global triangular symmetry triggers unanticipated broken symmetry phases, with mechanisms ranging from Jahn-Teller distortion, to charge-, spin-, and orbital-ordering.  $\text{LaMnO}_3$  and  $\text{LaCoO}_3$  bilayers, where spin-orbit coupling opens a sizable gap in the Dirac-point Fermi surface, emerge as much desired oxide-based Chern insulators, the latter displaying a gap capable of supporting room-temperature applications [1] Further realizations of the honeycomb lattice and geometry patterns beyond the perovskite structure will be addressed. [1] D. Doennig, S. Baidya, W.E. Pickett and R. Pentcheva, arXiv: 1510.09177.

<sup>1</sup>Research supported by the DFG, SFB/TR80.

**8:36AM E30.00002 Topological magnetic phase in  $\text{LaMnO}_3$  (111) bilayer**, YAKUI WENG, XIN HUANG, Southeast University, YUGUI YAO, Beijing Institute of Technology, SHUAI DONG, Southeast University — Candidates for correlated topological insulators, originated from the spin-orbit coupling as well as Hubbard type correlation, are expected in the (111) bilayer of perovskite-structural transition-metal oxides. Based on the first-principles calculation and tight-binding model, the electronic structure of a  $\text{LaMnO}_3$  (111) bilayer sandwiched in  $\text{LaScO}_3$  barriers has been investigated. For the ideal undistorted perovskite structure, the Fermi energy of  $\text{LaMnO}_3$  (111) bilayer just stays at the Dirac point, rendering a semi-metal (graphene-like) which is also a half-metal (different from graphene nor previous studied  $\text{LaNiO}_3$  (111) bilayer). The Dirac cone can be opened by the spin-orbit coupling, giving rise to nontrivial topological bands corresponding to the (quantized) anomalous Hall effect. For the realistic orthorhombic distorted lattice, the Dirac point moves with increasing Hubbard repulsion (or equivalent Jahn-Teller distortion). Finally, a Mott gap opens, establishing a phase boundary between the Mott insulator and topological magnetic insulator. Our calculation finds that the gap opened by spin-orbit coupling is much smaller in the orthorhombic distorted lattice ( $\sim 1.7$  meV) than the undistorted one ( $\sim 11$  meV).

**8:48AM E30.00003 Electronic structure of two dimensional electron gases at the (111) - surface of  $\text{KTaO}_3$  and  $\text{SrTiO}_3$ <sup>1</sup>**, FLAVIO BRUNO, S. MCKEOWN WALKER, A. DE LA TORRE, S. RICCO, A. TAMAI, University of Geneva (Switzerland), Z. WANG, M. SHI, Swiss Light Source, PSI (Switzerland), T. K. KIM, M. HOESCH, Diamond Light Source (United Kingdom), M.S. BAHRAMY, University of Tokyo (Japan), P. D. C. KING, University of St Andrews (United Kingdom), F. BAUMBERGER, University of Geneva (Switzerland) — Doping the band insulators  $\text{KTaO}_3$  (KTO) and  $\text{SrTiO}_3$  (STO) by chemical substitution or by the creation of oxygen defects induces metallicity and even superconductivity at exceptionally low carrier densities. A promising strongly correlated model system emerged when it was discovered that a 2D electron gas (2DEG) can be stabilized in KTO by field effect, and in STO by interfacing with other oxides. These materials also support a similar 2DEG formed by an electron accumulation layer screening positively charged oxygen vacancy defects that are created in the surface by irradiating the samples with photons of appropriate energy. [Adv. Mat. 27, 3894 (2015)] Here, we will report on direct measurements of the 2DEG band structure stabilized on the (111) – surface of KTO and STO using high resolution angle-resolved photoemission (ARPES) [Phys. Rev. Lett. 113, 177601 (2014)]. The differences and similarities between the electronic structure of these two systems in terms of the strong and weak spin orbit coupling found in KTO and STO respectively will be discussed.

<sup>1</sup>FYB acknowledge support from the Swiss National Science Foundation (Ambizione Grant PZ00P2\_161327/1)

**9:00AM E30.00004 Nitride Multilayers as a Platform for Parallel Two-Dimensional Electron-Hole Gases: MgO/ScN(111)** , ANTIA S. BOTANA, Argonne National Lab, VICTOR PARDO, Universidade de Santiago de Compostela, WARREN E. PICKETT, University of California Davis — At interfaces between insulating oxides  $\text{LaAlO}_3$  and  $\text{SrTiO}_3$ , a two dimensional electron gas has been observed and well studied, while the predicted hole gas has not been realized due to the strong tendency of holes in O-2p orbitals to localize. Here we propose, via ab initio calculations, an unexplored class of materials for the realization of parallel two dimensional (2D), two carrier (electron+hole) gases: nitride-oxide heterostructures, with (111)-oriented ScN and MgO as the specific example. Beyond a critical thickness of five ScN layers, this interface hosts spatially separated conducting Sc-3d electrons and N-2p holes, each confined to about two atomic layers— the transition metal nitride provides both gases. A guiding concept is that the  $\text{N}^{3-}$  anion should promote robust two carrier 2D hole conduction compared to that of  $\text{O}^{2-}$ : metal mononitrides are mostly metallic and even superconducting while most metal monoxides are insulating. Our results, provide guidance for new exploration, both experimental and theoretical, on nitride-based conducting gases that should promote study of long sought exotic states viz. new excitonic phases and distinct, nanoscale parallel superconducting nanolayers<sup>[1]</sup>.  
[1]A.S. Botana, V. Pardo, W.E. Pickett, arXiv/1509.08518(2015)

**9:12AM E30.00005 Low temperature transport at the {111}  $\text{LaAlO}_3/\text{SrTiO}_3$  interface.**<sup>1</sup> , S. DAVIS, Applied Physics Program, Northwestern University, V. CHANDRASEKHAR, Department of Physics and Astronomy, Northwestern University, Z. HUANG, K. HAN, ARIANDO ., T. VENKATESAN, Department of Physics, National University of Singapore — For the last ten years the interface between epitaxially grown {001}  $\text{LaAlO}_3$  (LAO) and  $\text{SrTiO}_3$  (STO) has provided a rich playground for exotic physics, including a gate-tuned metal to insulator transition, a gate-tuned superconductor-insulator transition, and the coexistence of 2-D superconductivity and magnetism. Recently the interfaces in other orientations of LAO-STO, namely the {110} and {111} orientations, have received increased attention after they were shown to become conducting. The {111} interface is particularly interesting due to its potential for topological effects as well as its complex Fermi surface. Here we present the results of low temperature electrical transport studies along two crystal directions of a {111} LAO-STO interface grown in intermediate oxygen partial pressures via PLD. More specifically we measure the longitudinal resistance as well as the transverse (Hall) resistance to elucidate the difference between the {111} and {001} LAO/STO interfaces.

<sup>1</sup>Supported by DOE Grant DE-FG02-06ER46346.

**9:24AM E30.00006 Anisotropic superconducting properties of nanowires at the  $\text{LaAlO}_3/\text{SrTiO}_3$  (110) interface**<sup>1</sup> , MENGCHEN HUANG, ANIL ANNADI, Univ of Pittsburgh, KALON GOPINADHAN, THIRU-MALAI VENKATESAN, ARIANDO ARIANDO, National University of Singapore, GUANGLEI CHENG, PATRICK IRVIN, JEREMY LEVY, Univ of Pittsburgh — Quasi-1D nanowires are created using conductive AFM (c-AFM) lithography<sup>2</sup> at the  $\text{LaAlO}_3/\text{SrTiO}_3$  (110) interface along the (001) and (110) crystallographic directions. The superconducting properties of nanowires were investigated under transport measurements with respect to the crystallography and orbital hierarchy. We observe anisotropic superconductivity where the upper critical magnetic field along the (001) and (110) directions are markedly different with a superconducting dome that is shifted for the two orientations as a function of gate voltages. The superconducting dome shift can be explained by anisotropic band structures along the two different directions combined with the Lifshitz transition<sup>3</sup>.

<sup>1</sup>We gratefully acknowledge support for this work from NSF DMR-1124131 and DMR-1104191 (JL), AFOSR FA9550-12-1-0057 and FA9550-12-1-0268 (JL), ONR N00014-15-1-2847 (JL), CRP Award NRF-CRP 8-2011-06 and 10-2012-02 (TV, A) and NUS FRC R-144-000-346-11 (TV, A)

<sup>2</sup>C. Cen *et al.*, Nat. Mater. **7**, 298 (2008)

<sup>3</sup>A. Joshua *et al.*, Nat. Commun. **3**, 1129 (2012)

**9:36AM E30.00007 Heteroepitaxially lifting Dirac degeneracy in topological semimetallic perovskite  $\text{SrIrO}_3$**  , JIAN LIU, University of Tennessee - Knoxville — Crystal symmetry-breaking and time-reversal symmetry breaking in epitaxial thin films and heterostructures of the topological semimetallic perovskite  $\text{SrIrO}_3$  were investigated by experimental growth, characterizations and theoretical calculations. Structure refinement on ultrathin films and first-principles calculations show that the symmetry-protected Dirac line nodes in the topological semimetallic perovskite  $\text{SrIrO}_3$  can be lifted simply by applying epitaxial constraints. In particular, the Dirac nodal ring is found to be gapped in epitaxial film structure where the n-glide symmetry of the bulk Pbnm space group is removed while the mirror symmetry is preserved. Our symmetry-breaking analysis shows that the n-glide operation protects the nodal ring and the b-glide operation provides additional protection for a pair of high-symmetry Dirac points of the nodal ring. These symmetry operations can be selectively broken by different epitaxially strained structures, leading to different semimetallic band crossing. Time-reversal symmetry is further investigated under epitaxial confinement by ferromagnetic  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$ . The resulted control over the magnetic anisotropy and spin-orbit coupling will be discussed. The results highlight the vital role of symmetry in spin-orbit-coupled correlated oxides.

**9:48AM E30.00008 Tunneling Spectroscopy of Strongly Correlated Electron Liquids in  $\text{SrTiO}_3$**  , PATRICK MARSHALL, EVGENY MIKHEEV, SANTOSH RAGHAVAN, SUSANNE STEMMER, University of California, Santa Barbara — Tunneling spectroscopy is used to probe the electronic structure of the two-dimensional electron liquid confined in  $\text{RTiO}_3/\text{SrTiO}_3/\text{RTiO}_3$  quantum wells ( $R = \text{Gd, Sm}$ ). The conductance spectra of metallic quantum wells exhibit power law behavior at high energies, reflecting the influence of disorder on the density of states. At low energies a pseudogap is observed in quantum wells containing 5 SrO layers and fewer, coinciding with the quantum phase transition in this system. As the quantum well thickness is reduced the DOS around the Fermi level vanishes in quantum wells embedded in  $\text{GdTiO}_3$ , consistent with the metal-insulator transition occurring at thicknesses of 2 SrO layers and fewer. In  $\text{SmTiO}_3$ -embedded quantum wells the metallic state persists down to the lowest thickness and temperature, with the emergence of coherence peaks indicating the onset of an ordered phase in the itinerant state with possible density wave order. The results shed light on the interplay of disorder, electron-electron interactions, and electron-lattice coupling in strongly correlated systems.

**10:00AM E30.00009 Internal Charge Transfer and Quasi-Two Dimensional Electron Gases at  $\text{NdTiO}_3/\text{SrTiO}_3$  interfaces**<sup>1</sup> , PENG XU, Univ of Minnesota - Twin Cities, TIMOTHY C. DROUBAY, Pacific Northwest National Laboratory, JONG SEOK JEONG, K. ANDRE MKHOYAN, Univ of Minnesota - Twin Cities, PETER V. SUSHKO, SCOTT A. CHAMBERS, Pacific Northwest National Laboratory, BHARAT JALAN, Univ of Minnesota - Twin Cities — Two-dimensional (2D) ultra-high carrier densities are of considerable current research interest for novel plasmonic and high charge-gain devices. However, the highest 2D electron density obtained is thus far limited to  $3 \times 10^{14} \text{ cm}^{-2}$  (electron/unit cell/interface) at  $\text{GdTiO}_3/\text{SrTiO}_3$  interfaces, and is typically an order of magnitude lower at  $\text{LaAlO}_3/\text{SrTiO}_3$  interfaces. In this work, we will present detailed study that carrier densities much higher than expected based on resolution of the polar discontinuity at perovskite oxide heterojunctions can be achieved via band engineering and internal charge<sup>[1]</sup>. The  $\text{SrTiO}_3(8 \text{ u.c.})/\text{NdTiO}_3(2 \text{ u.c.})/\text{SrTiO}_3(8 \text{ u.c.})/\text{LSAT}(001)$  heterostructure shows the expected electronic reconstruction behavior starting at  $t = 2 \text{ u.c.}$ , but then exhibits a higher carrier density regime at  $t \geq 6 \text{ u.c.}$  due to additional charge transfer from band alignment. Combining DFT modeling and experiments using x-ray photoelectron spectroscopy, scanning transmission electron microscopy, electron energy loss spectroscopy, energy dispersive x-ray spectroscopy and electronic transport measurements, we will discuss the origin of these carriers, dimensionality and transport mechanisms. [1] Peng Xu, et al. Advanced Material Interface (2015), in press.

<sup>1</sup>This work at UMN is supported primarily by NSF through the MRSEC.

**10:12AM E30.00010 One-dimensional Electron Gases at Oxide Interfaces<sup>1</sup>**, YANWEI CAO, Department of Physics, University of Arkansas, Fayetteville, AR 72701, USA, ZHICHENG ZHONG, Institute for Theoretical and Astrophysics, University of Wurzburg, Am Hubland 9704, Wurzburg, Germany, P. SHAFER, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA, XIAORAN LIU, M. KAREEV, S. MIDDEY, D. MEYERS, Department of Physics, University of Arkansas, Fayetteville, AR 72701, USA, E. ARENHOLZ, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA, JAK CHAKHALIAN, Department of Physics, University of Arkansas, Fayetteville, AR 72701, USA — Emergence of two-dimensional electron gases (2DEG) at the oxide interfaces of two dissimilar insulators is a remarkable manifestation of interface engineering. With continuously reduced dimensionality, it arises an interesting question: could one-dimensional electron gases (1DEG) be designed at oxide interfaces? So far there is no report on this. Here, we report on the formation of 1DEG at the carefully engineered titanate heterostructures. Combined resonant soft X-ray linear dichroism with electrical transport and the first-principles calculations have confirmed the formation of 1DEG driven by the interfacial symmetry breaking. Our findings provide a route to engineer new electronic and magnetic states.

<sup>1</sup>This work was supported by Gordon and Betty Moore Foundation, DODARO, DOE, and the Director, Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy.

**10:24AM E30.00011 Controlled Confinement of Half-metallic 2D Electron Gas in BaTiO<sub>3</sub>/Ba<sub>2</sub>FeReO<sub>6</sub>/BaTiO<sub>3</sub> Heterostructures: A First-principles Study<sup>1</sup>**, TANUSRI SAHA-DASGUPTA, S.N.Bose National Centre for Basic Sciences, Kolkata, SANTU BAIDYA, University of Duisburg-Essen, Duisburg, UMESH WAGHMARE, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bangalore, ARUN PARAMAKANTI, Canadian Institute for Advanced Research, Toronto, Ontario — Using density functional theory calculations, we establish that the half-metallicity of bulk Ba<sub>2</sub>FeReO<sub>6</sub> survives down to 1 nm thickness in BaTiO<sub>3</sub>/Ba<sub>2</sub>FeReO<sub>6</sub>/BaTiO<sub>3</sub> heterostructures grown along the (001) and (111) directions. The confinement of the two-dimensional (2D) electron gas in this quantum well structure arises from the suppressed hybridization between Re/Fe *d* states and unoccupied Ti *d* states, and it is further strengthened by polar fields for the (111) direction. This mechanism, distinct from the polar catastrophe, leads to an order of magnitude stronger confinement of the 2D electron gas than that at the LaAlO<sub>3</sub>/SrTiO<sub>3</sub> interface. We further show low-energy bands of (111) heterostructure display nontrivial topological character. Our work opens up the possibility of realizing ultra-thin spintronic devices.

Journal Ref: Phys. Rev. B 92, 161106(R) (2015)

<sup>1</sup>S.B. and T.S.D thank Department of Science and Technology, India for the support through Thematic Unit of Excellence. AP was supported by NSERC (Canada)

**10:36AM E30.00012 Electronic and magnetic phenomena at the interface of LaAlO<sub>3</sub> and Ru-doped SrTiO<sub>3</sub>**, MATTHEW GRAY, TED SANDERS, Stanford University, CATHERINE JENKINS, PADRIAC SHAFER, ELKE ARENHOLZ, Lawrence Berkeley National Laboratory, YURI SUZUKI, Stanford University — The emergence of a quasi-two dimensional electron gas with hints of magnetic order at the interface between bulk diamagnetic, band gap insulators LaAlO<sub>3</sub> (LAO) and SrTiO<sub>3</sub> (STO) has led to intensive research of this interface. We doped magnetic, isovalent Ru onto the Ti site of the STO side of the interface. 0-10 nm of SrTi<sub>0.98</sub>Ru<sub>0.02</sub>O<sub>3</sub> were deposited on TiO<sub>2</sub> terminated (001) STO single-crystal substrates and then capped with 1-17 nm of LAO. Insertion of more than 7 unit cells of Ru-doped STO at the interface suppresses metallic conductivity with a surprisingly sharp metal-insulator transition. A similar metal-insulator transition is observed when a homoepitaxial STO film is grown before LAO deposition. X-ray Magnetic Circular Dichroism indicated no magnetic ordering of Ti down to 10 K, and electric transport was indistinguishable from that of undoped LAO/STO interfaces. Together our results indicate that ferromagnetism is not intrinsic to the interface, magnetic Ru dopants are not significant sources of scattering, and that cation vacancy formation alone cannot explain the insulating behavior observed in thick homoepitaxial LAO/STO/STO trilayers.

**10:48AM E30.00013 The Superconducting Phase Diagram of LaAlO<sub>3</sub>/SrTiO<sub>3</sub> Interfaces**, STEFANO GARIGLIO, ALEXANDRE FTE, DANFENG LI, WEI LIU, MARGHERITA BOSELLI, DQMP, Univ of Geneva, MARC GABAY, LPS, Univ Paris-Sud, JEAN-MARC TRISCONI, DQMP, Univ of Geneva — The discovery of a two-dimensional electron liquid (2DEL), formed at the interface between the two band insulators LaAlO<sub>3</sub> (LAO) and SrTiO<sub>3</sub> (STO), has generated significant interest. The 2DEL has indeed intriguing electronic properties including superconductivity and spin-orbit interaction which can be tuned both by field-effect. In this talk I will discuss in detail the superconducting phase diagram revealed by field-effect experiments and the consequences of the electric field on the conducting layer extension. I will then compare the superconducting behaviour of this 2D system with the 3D one of doped STO crystals.

**Tuesday, March 15, 2016 8:00AM - 10:48AM —**

Session E31 DCP: Advances in Density Functional Theory III 331 - Neepa Maitra, Hunter College-CUNY

**8:00AM E31.00001 Orbitals and orbital energies in DFT and TDDFT**, EVERT JAN BAERENDS, Vrije Universiteit Amsterdam — The status and meaning of orbitals and orbital energies in the Kohn-Sham one-electron model of DFT has been controversial, in contrast to Hartree-Fock orbitals and orbital energies. We will argue the opposite: the exact Kohn-Sham orbitals of DFT are "better" than HF orbitals and their orbital energies are much closer to ionization energies than HF orbital energies are. This follows from the relation between the KS potential and the wavefunction, which can be cast in the form  $v_s = v_{c,kin} + v_H + v_{xc}^{hole} + v^{resp}$ <sup>1</sup>, where each term depends on the KS orbitals and the wavefunction (the one- or two-particle density matrices). The response potential

$$v^{resp}(r) = \sum_j \frac{|d_j(r)|^2}{\rho(r)} I_j - \sum_i^H \frac{|\psi_{s,i}(r)|^2}{\rho(r)} (-\epsilon_i) \quad (1)$$

( $d_j$  is the Dyson orbital corresponding to ion state  $\Psi_j^{N-1}$ ,  $\psi_{s,i}$  is a Kohn-Sham orbital) enables the connection between ionization energies  $I_i$  and orbital energies  $\epsilon_i$  to be made<sup>2</sup>. For virtual orbitals and orbital energies similar statements can be made: the shapes and energies of the (exact) KS orbitals are much more realistic than those of the Hartree-Fock model or hybrid functionals<sup>3</sup>. The HOMO-LUMO gap in molecules is very close to the optical gap, and very different from the fundamental gap. In solids the situation is very different, which is the well-known "KS gap problem". Again the response potential  $v^{resp}$  (a good approximation to it) helps to solve this problem, affording a straightforward correction method of the KS gap to the fundamental gap<sup>4</sup>.

<sup>1</sup>M. A. Buijse, E. J. Baerends, J. G. Snijders, **Phys. Rev. A** 40 (1989) 4190

<sup>2</sup>D. P. Chong, O. V. Gritsenko, E. J. Baerends, **J. Chem. Phys.** 116 (2002) 1760; O. V. Gritsenko, B. Braïda, E. J. Baerends, **J. Chem. Phys.** 119 (2003) 1937

<sup>3</sup>R. van Meer, O. V. Gritsenko and E. J. Baerends, **J. Chem. Theor. Comp.** 10 (2014) 4432

<sup>4</sup>O. Gritsenko, R. van Leeuwen, E. van Lenthe, E. J. Baerends, **Phys. Rev. A** 51 (1995) 1944; M. Kuisma, J. Ojanen, J. Enkovaara, T. T. Rantala, **Phys. Rev. B** 82 (2010) 115106

**8:36AM E31.00002 Revealing Open Quantum Systems with Subsystem DFT**, ALISA KRISHTAL, MICHELE PAVANELLO, Rutgers University - Newark — The traditional quantum chemical methods, wave function or density based, are designed to solve for a closed system, where the Hamiltonian contains all relevant interactions. The closed system is, however, not realistic, as in real life the system is embedded in an environment with which it interacts to some degree. Including the description of the environment at the full quantum mechanical level leads to the Open Quantum Systems (OQS) theory: the only theory which can describe non-Markovian dynamics between the system and the environment. By allowing the flow of information in both directions phenomena such as quantum entanglement, relevant for the design of quantum computers, become available. While most OQS theories rely on the density matrix to describe the system-bath interaction, time-dependent subsystem DFT[1,2] allows to approach the problem using the electron density. Through Dyson-like equations connecting the density-density response kernels of the OQS and its environment, the extent to which non-Markovian dynamics is present can be revealed. We illustrate this for the process of excitation energy transfer in coupled chromophores embedded in explicit solvent. [1] M. Pavanello, *J. Chem. Phys.* 138, 204118 (2013). [2] A. Krishtal et al. *J. Chem Phys.* 142, 154116 (2015).

**8:48AM E31.00003 An Open Source Embedding Code for the Condensed Phase**, ALESSANDRO GENOVA, Rutgers University - Newark, DAVIDE CERESOLI, CNR, ISTM, ALISA KRISHTAL, Rutgers University - Newark, OLIVIERO ANDREUSSI, EPFL, ROBERT DISTASIO, Cornell University, MICHELE PAVANELLO, Rutgers University - Newark — Work from our group [1,2] as well as others [3,4] has shown that for many systems such as molecular aggregates, liquids, and complex layered materials, subsystem Density-Functional Theory (DFT) is capable of immensely reducing the computational cost while providing a better and more intuitive insight into the underlying physics. We developed a massively parallel implementation of Subsystem DFT for the condensed phase [1] into the open-source Quantum ESPRESSO software package. In this talk, we will discuss how we: (1) implemented such a flexible parallel framework aiming at the optimal load balancing; (2) simplified the solution of the electronic structure problem by allowing a fragment specific sampling of the first Brillouin Zone [2]; (3) achieve enormous speedups by solving the electronic structure of each fragment in a unit cell smaller than the supersystem simulation cell, effectively introducing a fragment specific basis set, with no deterioration of the fully periodic simulation. As of March 14, 2016, the code has been released and is available to the public. [1] A. Genova et al., *JCP* 2014, 141, 174101 [2] A. Genova et al., *JPCM* 2015, Accepted [3] S. Lubert, *JCP* 2014, 141, 234110 [4] C. Jacob, et al., *WIREs* 2014, 4, 325

**9:00AM E31.00004 Scaling properties of the kinetic energy density of atoms – towards an orbital-free meta-GGA.**, ANTONIO CANCIO, JEREMY REDD, Ball State University — The scaling properties of atoms, combining periodicity with gradual increase in density, make a fruitful probe of relationships in density functional theory, and have driven advances in understanding the exchange and correlation energy. Although focus is normally upon the properties of integrated energies, insights can be generated from studying energy density functions as well. We visualize the behavior of the positive-definite kinetic energy density (KED) in closed-shell atoms, in comparison to invariant quantities based upon the gradient and Laplacian of the density. The latter are potential variables for constructing orbital-free functionals for the KE and can be used for analyzing the electronic structure of atoms and molecules. We notice a striking fit of the KED within the core of any atom to a gradient expansion model using both the gradient and the Laplacian, but one different from that derived from first principles for a slowly-varying electron gas. Correlated with this feature, we notice unexpected structure to the KED near the nucleus that cannot be explained simply by the von Weizsäcker model, as is often presumed. These unexpected features provide potential insights for developing better orbital-free meta-GGA models for the kinetic energy.

**9:12AM E31.00005 On the transferability of a parametrized kinetic functional for orbital-free density functional theory calculations**, ALEXANDER KARPENKO, LEONARDO ESPINOSA LEAL, MIGUEL CARO, JOUKO LEHTOMAKI, OLGA LOPEZ-ACEVEDO, Aalto Univ — Because of issues with accuracy and transferability of existing orbital-free (OF) density functionals, OF functional development remains an active research area. Due to numerical difficulties, all-electron self-consistent assessment of OF functionals is limited. Using the projector augmented wave method we compute OFDFT all-electron values<sup>1</sup> and we evaluate the performance of a parametrized OF functional for atoms and molecules. We combine the parametrized Thomas-Fermi-Weizsäcker (TF-W) kinetic model  $\lambda$  and  $\gamma$  for the fractions of Weizsäcker and TF functionals, respectively, with LDA for atoms<sup>2</sup>. We found that one-to-one relation between  $\lambda$  and  $\gamma$  values defines a region in parameter space that allows the atomic energies and eigenvalues to be approximated with a small average error with respect to the Kohn-Sham values. The optimum values is however different for every property and for every atom. Recently, these results have been combined to test parameter transferability from atoms to molecules<sup>3</sup> and we expect will help for further systematic improvement of OF density functionals.

<sup>1</sup>Lehtomaki *et al.*, *JCP.*, 141, 234102 (2014).

<sup>2</sup>Espinosa *et al.*, *PCCP.*, (2015).

<sup>3</sup>Karpenko *et al.*, in preparation.

**9:24AM E31.00006 Exact Expressions for Exchange-Correlation Potentials** , VIKTOR STAROVEROV, Department of Chemistry, The University of Western Ontario, London, Ontario N6A 5B7 — The Baerends and Staroverov groups have devised various exact expressions for the exchange-correlation potential in terms of wave-function and Kohn–Sham ingredients. We show that all these expressions can be obtained as special cases of one general approach. One particular expression derived by us involves at most the two-electron reduced density matrix and is ideally suited for practical calculations of exchange-correlation potentials from many-electron wave functions, as demonstrated by numerical examples. Interesting identities emerging from our derivation are also presented and discussed.

**10:00AM E31.00007 Stringent test for non-additive, non-interacting, kinetic energy functionals** , KAILI JIANG, JONATHAN NAFZIGER, Department of Physics and Astronomy, Purdue University, ADAM WASSERMAN, Department of Chemistry, Purdue University — Partition Density Functional Theory (PDFT) provides an ideal framework for testing and developing new approximations to the non-additive and non-interacting kinetic energy functional ( $T_s^{nadd}[\{n_\alpha\}]$ ), understood as a functional of the set of fragment ground-state densities. We present our progress on both of these fronts: (1) Systematic comparison of the performance of various existing approximations to  $T_s^{nadd}[\{n_\alpha\}]$ ; and (2) Development of new approximations. We find that a re-parametrization of the GGA enhancement factor employed for the construction of  $T_s^{nadd}[\{n_\alpha\}]$  through the conjointness conjecture captures essential features of the functional derivatives of  $T_s^{nadd}[\{n_\alpha\}]$ . A physically-motivated two-orbital approximation for  $T_s^{nadd}[\{n_\alpha\}]$  is shown to outperform most other approximations for the case of He<sub>2</sub>, and an intriguing one-parameter formula makes this approximation accurate for all noble-gas diatomics.

**10:12AM E31.00008 Partition Theory for Periodic and Semi-Infinite Systems** , KELSIE NIFFENEGGER, ADAM WASSERMAN, Purdue University — Standard approximations to the exchange-correlation (XC) functional of Kohn-Sham Density-Functional Theory are insufficiently accurate to describe charge transfer at metal-atom interfaces and other systems requiring proper treatment of fractional electron charges. The root of the problem is connected to the lack of derivative discontinuities in the approximate XC functionals at integer numbers of electrons. Partition Theory (PT) is a promising, formally exact method to correct this issue. We study the simplest model for an atom adsorbed at a metal surface: A one-dimensional step potential separated a fixed distance from an attractive well that admits only one bound state when isolated. The semi-infinite metal is populated with non-interacting electrons up to the Fermi energy. We derive the PT-equations for this problem and indicate how the associated partition potential can be calculated. PT is also a promising method for improving the computational scaling of other large and/or periodic systems. We study the partition potential for periodic 1-D chains of identical attractive wells and comment on the uniqueness of the partition potential when going from finite to periodic systems.

**10:24AM E31.00009 Petascale orbital-free density functional theory enabled by small-box techniques** , MOHAN CHEN, MAE, Princeton University, Princeton, NJ, 08544, USA, XIANG-WEI JIANG, Institute of Semiconductors, Chinese Academy of Sciences, Beijing, China, HOULONG ZHUANG, MAE, Princeton University, NJ, 08544, USA, LIN-WANG WANG, Materials Science Division, LBNL, CA, 94720, USA, EMILY CARTER, MAE, Program in Applied and Computational Mathematics, and the Andlinger Center for Energy and the Environment, Princeton University, NJ, 08544, USA — Orbital-free density functional theory (OFDFT) is a quantum-mechanics-based method that utilizes electron density as its sole variable. The main computational cost in OFDFT is use of the ubiquitous fast Fourier transform (FFT), which is mainly used to evaluate the kinetic energy density functional (KEDF) and electron-electron Coulomb interaction terms. We design and implement a small-box FFT (SBFFT) algorithm to overcome the parallelization limitations of traditional FFT algorithms. In addition, a real-space truncation of the non-local Wang-Teter KEDF kernel is proposed. The scalability of SBFFT is demonstrated by efficiently simulating one full optimization step (electron density, forces, and stresses) of 1,024,000 lithium (Li) atoms on up to 131,072 cores. Other tests include calculations of physical properties of different phases of bulk Li, geometry optimizations of nanocrystalline Li, and molecular dynamics simulations of liquid Li samples. All of the tests yield excellent accuracy compared to the original OFDFT calculations, suggesting that the OFDFT-SBFFT algorithm opens the door to first-principles simulations of materials containing millions of atoms.

**10:36AM E31.00010 Degenerate Open Shell Density Perturbation Theory** , MARK PALENIK, BRETT DUNLAP, Naval Research Lab — The density perturbation theory (DPT) methodology we have developed applies the Hohenberg-Kohn theorem to perturbations in density functional theory. At each order, the energy is directly minimized with respect to the density at all lower orders. The difference between the perturbed and unperturbed densities is expanded in terms of a finite number of basis functions, and a single matrix inversion in this space reduces the complexity of the problem to that of non-interacting perturbation theory. For open-shell systems with symmetry, however, the situation becomes more complex. Typically, the perturbation will break the symmetry leading to a zeroth-order shift in the Kohn-Sham potential. Because the symmetry breaking is independent of the strength of the perturbation, the mapping from the initial to the perturbed KS potential is discontinuous and techniques from perturbation theory for noninteracting particles fail. We describe a rigorous formulation of DPT for use in systems that display an initial degeneracy, such as atoms and Fe<sub>55</sub>Cp\*<sub>12</sub> clusters and present initial calculations on these systems.

**Tuesday, March 15, 2016 8:00AM - 10:48AM —**

**Session E32 DCP GERA: Emerging Nanomaterials for Solar Energy Conversion II** 332 - Arthur Nozik, NREL

**8:00AM E32.00001 The engineering of quantum dots for efficient solar energy capture<sup>1</sup>** , JEFFREY PIETRYGA, Los Alamos National Laboratory — Over the past decade, exciting advances have been made in the use of semiconductor nanocrystal quantum dots (QDs) for capture of solar energy, including efficient and inexpensive solar cells based on simple, single-component lead chalcogenide QDs. Such devices take advantage of key advantages offered by QDs, including the ability to control bandgap with particle size, and to alter carrier concentrations using surface modification. Remaining essentially untapped, however, is the much larger potential offered by heterostructured QDs to exhibit new functionality that will enable truly unprecedented device performance. In this talk, I will present recent results from our efforts in application-inspired band-structure engineering of heterostructured QDs. Specifically, I will examine how the selective combination of semiconductor materials in a simple core/shell geometry can result in QDs with radically altered properties optimized for use in applications such as carrier-multiplication-enhanced solar cells, and highly efficient luminescent solar concentrators. I will use these examples to demonstrate the general ability of solution-synthesized nanomaterials to contribute to the overall goal of efficient solar energy capture and conversion in a variety of roles.

<sup>1</sup>This work was performed within the Center for Advanced Solar Photophysics, a DOE Energy Frontier Research Center

**8:36AM E32.00002 Are quantum dots spiky balls?** , JAMES SHEPHERD, NADAV GEVA, TROY VAN VOORHIS, Massachusetts Institute of Technology — We here propose an alternative view to the spiky ball picture of passivated quantum dots. By studying the realistic surface morphology of a dot using atomistic molecular dynamics simulations, paying particular attention to the ligand structure, we find that the ligand shell thickness is substantially reduced by van der Waals packing. This affects the ability of the dot ligands to interdigitate. This is discussed in terms of the available experimental data for the superstructure of quantum dot layers, and related back to the electronic properties of quantum dots.

**8:48AM E32.00003 TBA** , ART NOZIK, National Renewable Energy Laboratory — No abstract available.

**9:24AM E32.00004 Photocatalytic Water-Splitting Characteristic of Electric Reduced Black TiO<sub>2</sub> Nanorods<sup>1</sup>**, JONG-WON YUN, Department of Physics and Energy, Univ. of Ulsan, KI YEON RYU, SUNHO KIM, SE-JUNG JANG, Department of Physics, Univ. of Ulsan, YONG SOO KIM, Department of Physics and Energy, Univ. of Ulsan — In various reduction methods of TiO<sub>2</sub>, the electric reduction could apply to anodized TiO<sub>2</sub> nanotube. However, it is not suitable to reduce TiO<sub>2</sub> nanorods(NRs) grown on fluorine doped tin oxide (FTO) substrate using hydrothermal method, because those are easily peeled off due to lattice mismatching between FTO and TiO<sub>2</sub> NRs. In this talk, we will demonstrate electric reduced-black TiO<sub>2</sub> NRs with strong adhesion on FTO substrate for an effective visible photocatalyst. To fabricate the reduced-black TiO<sub>2</sub> NRs, we firstly deposited TiO<sub>2</sub> seed layer on FTO glass using RF-sputtering for mitigating the exfoliation, then grow TiO<sub>2</sub> NRs with hydrothermal method. Finally, TiO<sub>2</sub> NRs were reduced with electric bias. The final reduced-black TiO<sub>2</sub> NRs exhibit a higher photocurrent density, 0.9 mA/cm<sup>2</sup> in comparison with pure-TiO<sub>2</sub> NRs. This result indicates that our reduced-black TiO<sub>2</sub> NRs has lower bandgap with modified valence band position and enhance the surface reactivity with oxygen defect generation.

<sup>1</sup>This research was supported by Priority Research Centers Program (2009-0093818), the Basic Science Research Program(2015-019609) and Basic Research Lab Program(2014-071686) through National Research Foundation of Korea(NRF) funded by the Korean government

**9:36AM E32.00005 TBA**, XIAOGANG PENG, Zhejiang University — No abstract available.

**10:12AM E32.00006 High Pressure Synthesis of Rhombohedral Delafossite Structured  $\alpha$ -AgGaO<sub>2</sub>**, MEYSAM AKHTAR, Department of Physics, University of Louisville, MADHU MENON, Center for Computational Sciences, University of Kentucky, MAHENDRA SUNKARA, Conn Center for Renewable Energy Research, University of Louisville, GAMINI SUMANASEKERA, Department of Physics, University of Louisville, ANDRIY DURYGIN, Center for the Study of Matter at Extreme Conditions, Florida International University, JACEK JASINSKI, Conn Center for Renewable Energy Research, University of Louisville — In this work, we demonstrate for the first time the high pressure synthesis of  $\alpha$ -AgGaO<sub>2</sub> via a solid state reaction of Ag<sub>2</sub>O and Ga<sub>2</sub>O<sub>3</sub>. Synthesis experiments were carried out at pressures and temperatures up to 10 GPa and 600 C, respectively, using a resistively-heated diamond anvil cell. Electron diffraction confirmed the rhombohedral delafossite crystal structure of the synthesized AgGaO<sub>2</sub> and its corresponding lattice parameters of  $a = 2.99$  Å and  $c = 18.43$  Å. The vibrational modes analysis was also conducted using a combination of ab initio density functional theory (DFT) and Raman spectroscopy. This analysis yielded good agreement between the calculated Raman-active modes and experimental Raman data. Finally, the application of the GGA +  $U$  formalism-based on DFT to calculate the electronic band structure of  $\alpha$ -AgGaO<sub>2</sub> provided a more realistic theoretical band gap value than those reported previously.

**10:24AM E32.00007 Competitive Adsorption of Carbon Dioxide/Methane in Coal: First-Principles Quantum Mechanical Investigations<sup>1</sup>**, YINGDI LIU, SANWU WANG, Univ of Tulsa — Sequestration of CO<sub>2</sub> into geological formations has been suggested to mitigate the effect of the increasing of the atmospheric CO<sub>2</sub> concentration on global warming. Coalbeds are investigated as one of the attractive storage sites since the cost of CO<sub>2</sub> sequestration can be offset by the enhanced coalbed methane (ECBM) recovery. Extensive experimental studies have been performed for the competitive adsorption of CO<sub>2</sub>/CH<sub>4</sub> into coalbeds. However, the atomic-level understanding for the interaction between the adsorbate (CO<sub>2</sub>/CH<sub>4</sub>) and the adsorbent (coal) has not been fully explored. We report first-principles density-functional calculations for the competitive adsorption between CO<sub>2</sub>/CH<sub>4</sub> in the coal network. In particular, we report results of atomic structures, bonding characteristics, energetics, as well as electronic structures of the CO<sub>2</sub>/CH<sub>4</sub>-coal systems.

<sup>1</sup>This research used the supercomputer resources at NERSC, of XSEDE, at TACC, and at the Tandy Supercomputing Center.

**10:36AM E32.00008 Gentlest Ascent Dynamics for Calculating First Excited State and Exploring Energy Landscape of Kohn-Sham Density Functionals**, CHEN LI, JIANFENG LU, WEITAO YANG, Duke University — We develop the gentlest ascent dynamics (GAD) for Kohn-Sham density functional theory to search for the index-1 saddle points (i.e., the stationary points with one and only one energy descending direction) on the energy landscape of the Kohn-Sham density functionals. These stationary solutions correspond to excited states in the ground state functionals. As shown by various examples, the first excited states of many chemical systems are given by these index-1 saddle points. Our novel approach provides an alternative, more robust way to obtain these excited states, compared with the widely used  $\Delta$ SCF approach. The method can be easily generalized to target higher index saddle points. Our results also reveal the physical interest and relevance of studying the Kohn-Sham energy landscape.

**Tuesday, March 15, 2016 8:00AM - 11:00AM —**

**Session E33 DPOLY: Polymer Glass Formation and Stability** 336 - Connie Roth, Emory University

**8:00AM E33.00001 DPOLY SESSION BREAK —**

**8:36AM E33.00002 Theoretical Insights from Facile Microsecond Simulation of the Glass Transition<sup>1</sup>**, JUI-HSIANG HUNG, TARAK PATRA, DAVID SIMMONS, Univ of Akron — Despite more than half a century of research, the fundamental nature of the glass transition remains one of the major open questions in polymer science and condensed matter physics. Molecular dynamics simulations have provided key insights into this problem, but their ability to firmly establish the underlying nature of glass formation have been limited by the extreme computational difficulty of directly probing the deeply supercooled regime most relevant to this process. Here we describe a new protocol for simulation of the glass transition enabling facile access to in-equilibrium segmental relaxation times approaching and exceeding one microsecond — well into the deeply supercooled regime of most glass-forming liquids. Coupled with a well-validated strategy for extrapolation to experimental timescales, this approach provides vastly improved prediction of experimental glass transition temperatures. Here we combine data acquired through this protocol for the deeply supercooled regime of polymeric, inorganic, organic, and metallic glass formers to robustly test several theories of glass formation and identify microscopic phenomenological features shared across all classes of glass-forming liquid in the deeply supercooled regime.

<sup>1</sup>We acknowledge the W. M. Keck Foundation for financial support of this research

**8:48AM E33.00003 Will it form a stable glass? How the stability of vapor deposited glasses depends on molecular structure**, MICHAEL TYLINSKI, MADELEINE BEASLEY, Univ of Wisconsin, Madison, YEONG ZEN CHUA, CHRISTOPH SCHICK, University of Rostock, Germany, MARK EDIGER, Univ of Wisconsin, Madison — Over the past nine years physical vapor deposition has been used to prepare molecular glasses with exceptional properties. When heated, transformation of these highly stable glasses takes orders of magnitude longer than the transformation of liquid-cooled glasses. Until recently, it appeared that most organic molecules could form stable glasses when vapor deposited. We test the generality of stable glass formation by vapor-depositing a wide range of small organic molecules, including hydroxyl, carbonyl, phosphate, aromatic, and aliphatic functional groups. When prepared under conditions expected to yield highly stable glasses, we observe glasses with a wide range of kinetic stabilities, depending on the functional groups in the molecule. In general, alcohols and molecules with long aliphatic chains do not form highly stable glasses while aromatic molecules do. We also test the hypothesis that the surface mobility during deposition determines if a molecule is able to create highly stable glasses.

**9:00AM E33.00004 Kinetics of Dewetting of Ultra-Thin Films of Organic Glasses**, ZAHRA FAKHRAAI, YUE ZHANG, ROBERT RIGGLEMAN, University of Pennsylvania — Physical vapor deposition (PVD) is widely used in manufacturing ultra-thin layers of amorphous organic solids. It is generally assumed that the properties of these ultra-thin films are the same as bulk dynamics. In this work, we demonstrate that these films exhibit a sharp transition from glassy solid to liquid-like behavior with thickness below 30 nm. This liquid-like behavior persists even at temperatures well below the glass transition temperature,  $T_g$ , where bulk properties suggest that the film should be vitrified. The enhanced dynamics in these films can produce large scale morphological features during PVD and lead to dewetting instability in films held at temperatures as low as  $T_g - 35$  K. We measure an effective viscosity of organic glass films by monitoring the dewetting kinetics. These measurements combined with cooling rate-dependent  $T_g$  measurements show that the apparent activation barrier for rearrangement decreases sharply in films thinner than 30 nm. These observations suggest long-range facilitation of dynamics induced by the free surface. These observations can help understand correlated dynamics in glassy systems and elucidate the processes that lead to the formation of exceptionally stable glasses.

**9:12AM E33.00005 Dynamics of Vapor-Deposited Polymer Glasses from Simulation<sup>1</sup>**, WENGANG ZHANG, FRANCIS STARR, Wesleyan University, JACK DOUGLAS, National Institute of Standards and Technology — We use molecular dynamics simulations to mimic the physical vapor deposition of glassy polymer films. Like experiments, the deposition results in "ultrastable glasses" that have lower energies, and greater kinetic stability than ordinary glasses. It has been suggested that these ultrastable glasses may be equivalent to very highly aged ordinary glasses. To explore this possibility, we contrast both the structure and dynamics of deposited and ordinary glasses. Our modeling indicates that the deposited polymer glass is structurally distinct from the ordinary glass due to anisotropy of chain packing. If the deposited glasses correspond to highly aged ordinary glasses, we would expect vastly larger relaxation times for the deposited glass. Instead, we find that relaxation times of the vapor-deposited glass are nearly the same as that of the ordinary glass. These findings do not support the view that vapor-deposited glassy polymer films are equivalent to highly-aged ordinary glassy polymer films. We further study the dynamical heterogeneity of highly out-of-equilibrium polymer films.

<sup>1</sup> Computer time was provided by Wesleyan University. This work was supported in part by NIST award 70NANB13H202 and ACS-PRF grant 51983-ND7.

**9:24AM E33.00006 Molecular Orientation in Two Component Vapor-Deposited Glasses: Effect of Substrate Temperature and Molecular Shape**, CHARLES POWELL, Department of Chemistry, University of Wisconsin-Madison, JING JIANG, Department of Polymer Science and Engineering, School of Chemistry and Chemical Engineering, Nanjing University, DIANE WALTERS, MARK EDIGER, Department of Chemistry, University of Wisconsin-Madison — Vapor-deposited glasses are widely investigated for use in organic electronics including the emitting layers of OLED devices. These materials, while macroscopically homogenous, have anisotropic packing and molecular orientation. By controlling this orientation, outcoupling efficiency can be increased by aligning the transition dipole moment of the light-emitting molecules parallel to the substrate. Light-emitting molecules are typically dispersed in a host matrix, as such, it is imperative to understand molecular orientation in two-component systems. In this study we examine two-component vapor-deposited films and the orientations of the constituent molecules using spectroscopic ellipsometry, UV-vis and IR spectroscopy. The role of temperature, composition and molecular shape as it effects molecular orientation is examined for mixtures of DSA-Ph in Alq<sub>3</sub> and in TPD. Deposition temperature relative to the glass transition temperature of the two-component mixture is the primary controlling factor for molecular orientation. In mixtures of DSA-Ph in Alq<sub>3</sub>, the linear DSA-Ph has a horizontal orientation at low temperatures and slight vertical orientation maximized at  $0.96T_{g,mixture}$ , analogous to one-component films.

**9:36AM E33.00007 Measuring Surface Diffusion of Organic Glasses Using Tobacco Mosaic Virus as Probe Nanoparticles<sup>1</sup>**, YUE ZHANG, RICHARD POTTER, ZAHRA FAKHRAAI, Department of Chemistry, University of Pennsylvania — Recent studies have shown that diffusion on the surface of organic glasses can be many orders of magnitude faster than bulk diffusion, with lower activation barrier. Developing new probes that can readily measure the diffusion at the surface of an organic glass can help study the effect of chemical structure and molecule's size on the enhanced surface diffusion. In this study, surface diffusion coefficient of molecular glass (TPD) is measured using tobacco mosaic virus (TMV) as probe particles. TMV is placed on the surface of bulk TPD films. The evolution of the meniscus formed around TMV, driven by curvature gradient, is probed at various temperatures. TMV has a well-defined cylindrical shape, with a large aspect ratio (18 nm wide, 300 nm long). As such, the shape of the meniscus around the center of TMV is semi-one dimensional. Based on the self-similarity nature of surface diffusion flow in one dimension, the surface diffusion coefficient and its temperature dependence are measured. It is found that the surface diffusion is greatly enhanced and has weak temperature dependence compared to bulk counterpart, consistent with previous studies, showing that TMV probes serve as an efficient method of measuring surface diffusion.

<sup>1</sup> NSF-CAREER DMR-1350044

**9:48AM E33.00008 Relationship between Fragility and  $T_g$  Changes on Confinement for Three Cyanurates**, EVELYN LOPEZ, SINDEE L. SIMON, Texas Tech University — The glass transition temperature ( $T_g$ ) is known to deviate from the bulk when subjected to both thin film and nanopore confinement. Previous work from our laboratory has analyzed the effect of nanopore confinement on the  $T_g$  of three materials: a cyanurate trimer, an uncrosslinked polycyanurate, and a polycyanurate network. The results showed that the  $T_g$ s of the three materials decreased under confinement and that with increasing molecular weight and molecular stiffness, the  $T_g$  depression increased. However, recent studies have pointed to fragility, and not stiffness, as a key factor in determining how the materials  $T_g$  will be affected by confinement, with fragile polymers showing greater confinement effects. In this work, we analyze the effect of both nanopore and thin film confinement on  $T_g$  and calculate the fragilities of the three materials to determine the relationship between the two properties. Fragility is calculated from the dependence of  $T_g$  on the cooling rate, with a fast-scanning calorimeter used to extend the range of cooling rates.

**10:00AM E33.00009 Liquid and Glassy Specific Volume Variations in Thin Supported Polystyrene Films**, XINRU HUANG, CONNIE ROTH, Emory University — Studies of density or specific volume in thin films have been previously studied as a possible means of understanding changes in the glass transition temperature  $T_g(h)$  with decreasing film thickness. In the late 1990s, studies reported no change in the glassy, room temperature density of thin films outside of the plus or minus 1 percent experimental error, while more recent studies have claimed large 25-30 percent increases in film density below about 40 nm. In addition, recent theoretical efforts have suggested that  $T_g(h)$  decreases may be associated with small less than 1 percent increases in specific volume of the equilibrium liquid-line. We use ellipsometry to investigate variations in the liquid and glassy specific volume lines for polystyrene films supported on silicon. We observe small, reproducible increases in specific volume of 0.4 plus or minus 0.2 percent for both the liquid and glassy regimes that are uncorrelated with the observed  $T_g(h)$  decrease. Below 20-30 nm, we also observe what appears to be large increases in density that we attribute to breakdown of the assumptions used to derive the Lorentz-Lorenz formula.

**10:12AM E33.00010 Polymer thin films as a route to access low energy glassy states**, DANIELE CANGIALOSI, CSIC, VIRGINIE M BOUCHER, None, ANGEL ALEGRIA, JUAN COLMENERO, UPV — We investigate the enthalpy recovery in the glassy state of stacked polystyrene films with thickness 30 nm. We first show how the equilibrium dynamics and thermodynamics of such films is mainly bulk-like. When studying enthalpy recovery, we find two mechanisms of equilibration: one showing up below 348 K, that is, the films  $T_g$ ; and the second active below 308 K. The latter mechanism appear to have low activation energy and, as a result, gives rise to dramatic decrease of the fictive temperature  $T_f$  within relatively short aging times. This allows to achieve low energy glasses, in particular approaching the Kauzmann temperature ( $T_k$ ), that is, the temperature at which the entropy of the glass equals that of the crystal. The implications of our results are discussed.

**10:24AM E33.00011 Are polymers glassier upon confinement?**, SIMONE NAPOLITANO, JEAN SPIECE, DANIEL E. MARTINEZ-TONG, MICHELE SFERRAZZA, Universite' Libre de Bruxelles (ULB), AURORA NOGALES, Instituto de Estructura de la Materia, CSIC Madrid — Glass forming systems are characterized by a stability against crystallization upon heating and by the easiness with which their liquid phase can be transformed into a solid lacking of long-range order upon cooling (glass forming ability). Here, we discuss on the the thickness dependence of the thermal phase transition temperatures of poly(L-lactide acid) thin films supported onto solid substrates [1]. The determination of the glass transition ( $T_g$ ), cold crystallization ( $T_{CC}$ ) and melting ( $T_m$ ) temperatures down to a thickness of 6 nm via ellipsometry, permitted us to build up parameters describing glass stability and glass forming ability. We observed a strong influence of the film thickness on the latter, while the former is not affected by 1D confinement. Remarkably, the increase in  $T_g/T_m$  ratio, a parameter related to glass forming ability, is not accompanied by an increase in  $T_{CC}-T_g$ , as observed on the contrary, in bulk metallic glasses. We explained this peculiar behavior of soft matter in confinement considering the impact of irreversible adsorption on local free volume content [2]. [1] J. Spiece et al. Soft Matter, 2015,11, 6179-6186 [2] Non-equilibrium Phenomena in Confined Soft Matter, S Napolitano (ed.) Springer, 2015

**10:36AM E33.00012 ENGINEERING THE CRYSTALLINE MORPHOLOGY OF POLYMER THIN FILMS VIA PHYSICAL VAPOR DEPOSITION**, HYUNCHEOL JEONG, CRAIG ARNOLD, RODNEY PRIESTLEY, Princeton University — Thin-film growth via physical vapor deposition (PVD) has been successfully exploited for the delicate control of film structure for molecular and atomic systems. The application of such a high-energetic process to polymeric film growth has been challenged by chemical degradation. However, recent development of Matrix Assisted Pulsed Laser Evaporation (MAPLE) technique opened up a way to deposit a variety of macromolecules in a PVD manner. Here, employing MAPLE technique to the growth of semicrystalline polymer thin films, we show the engineering of crystalline film morphology can be achieved via manipulation of substrate temperature. This is accomplished by exploiting temperature effect on crystallization kinetics of polymers. During the slow film growth crystallization can either be permitted or suppressed, and crystal thickness can be tuned via temperature modulation. In addition, we report that the crystallinity of polymer thin films may be significantly altered with deposition temperature in MAPLE processing. We expect that this ability to manipulate crystallization kinetics during polymeric film growth will open the possibility to engineer structure in thin film polymeric-based devices in ways that are difficult by other means.

**10:48AM E33.00013 Comparing the Bending Stiffness Measurements of Brittle Paper<sup>1</sup>**, ANDREA HALL, MOLLY MCGATH, PATRICIA MCGUIGGAN, Johns Hopkins University — It has been estimated that one third of the paper materials in libraries are too brittle to handle. A typical paper sheet is comprised of semi-rigid cellulose fibers that are more than ten times longer than the sheet thickness and can be considered a two dimensional random fiber network. The main pathways of degradation, acid-catalyzed hydrolysis and oxidation, cause depolymerization of the cellulose chains and breaking of the intrafiber bonds. Conventional mechanical measurements of aged paper are destructive and often too severe to understand the true extent of deterioration. By comparing the roll test, folding endurance tests, tensile tests and stiffness tests of naturally aged papers with varying amounts of brittleness, we intend to show the limits of each test and relate the state of the paper degradation to the mechanical test results.

<sup>1</sup>We thank the Andrew W. Mellon Foundation for funding this research.

**Tuesday, March 15, 2016 8:00AM - 11:00AM —**

**Session E34 GSNP GSOF: Continuum Descriptions of Discrete Materials I** 337 - Ken Kamrin, Massachusetts Institute of Technology

**8:00AM E34.00001 Fabric variables in dense sheared suspensions**, FARHANG RADJAI, UMI CNRS-MIT, MIT Energy Initiative, Cambridge, MA / LMGC, University of Montpellier, France, LHAASSAN AMARSID, LMGC, University of Montpellier, France, JEAN-YVES DELENNE, IATE, INRA, University of Montpellier, France — The rheology of granular flows and dense suspensions can be described in terms of their effective shear and bulk viscosities as a function of packing fraction. Using stress partition and equivalence between frictional and viscous descriptions in the dense state, we show that the effective viscosities can be expressed in terms of the force-network anisotropy. This is supported by our extensive DEM-LBM simulations for a broad range of inertial and viscous parameters.

**8:36AM E34.00002 Jammed granular cones affect frictional resistive forces at the onset of intrusion<sup>1</sup>**, JEFFREY AGUILAR, School of Mechanical Engineering, Georgia Institute of Technology, DANIEL GOLDMAN, School of Physics, Georgia Institute of Technology — Characterizing the functional form of granular resistive forces has allowed for analysis of the locomotion of animals and robots on and within dry granular media. Resistive force theory (RFT) has been an effective tool in predicting these forces for various locomotive gaits within the "frictional fluid" regime, where intrusions are sufficiently slow such that granular inertial effects are negligible. These forces have been typically described by a linear dependence to submersion depth. However, recent experiments on robotic jumping [Aguilar & Goldman, Nature Physics, 2015] have revealed the importance of considering the nonlinear effects at the onset of intrusion to accurately predict robot kinematics. Particle image velocimetry (PIV) analysis of sidewall grain flow during foot intrusion reveals a jammed granular cone that develops beneath the foot at the onset of intrusion. A geometric model of cone development combined with empirical RFT forces on angled conical surfaces was able to predict the non-linear force trajectory vs. depth for experimental intrusions of various foot sizes, suggesting that intruders experience non-linear frictional forces according to the shape of the granular jamming fronts that form at the onset of movement.

<sup>1</sup>This work was supported by NSF Physics of Living Systems, Burroughs Wellcome Fund, and the Army Research Office

**8:48AM E34.00003 Jammed Clusters and Non-locality in Dense Granular Flows** , PRASHIDHA KHAREL, PIERRE ROGNON<sup>1</sup>, University of Sydney — We investigate the micro-mechanisms underpinning dense granular flow behaviour from a series of DEM simulations of pure shear flows of dry grains. We observe the development of transient clusters of jammed particles within the flow. Typical size of such clusters is found to scale with the inertial number with a power law that is similar to the scaling of shear-rate profile relaxation lengths observed previously<sup>2</sup>. Based on the simple argument that transient clusters of size  $\ell$  exist in the dense flow regime, the formulation of steady state condition for non-homogeneous shear flow results in a general non-local relation, which is similar in form to the non-local relation conjectured for soft glassy flows<sup>3</sup>. These findings suggest the formation of jammed clusters to be the key micro-mechanism underpinning non-local behaviour in dense granular flows.

<sup>1</sup>Particles and Grains Laboratory, School of Civil Engineering, The University of Sydney, Sydney, NSW 2006, Australia

<sup>2</sup>K. Kamrin and G. Koval, Physical Review Letters 108, (2012); M. Bouzid, et al., Physical Review Letters 111, (2013); P. G. Rognon, et al., Journal of Fluid Mechanics 764, 171 (2015)

<sup>3</sup>Goyon, et al., Nature 454, 84 (2008)

**9:00AM E34.00004 Velocity profiles and rheology of a granular bed sheared by a fluid flow**<sup>1</sup> , BENJAMIN ALLEN, ARSHAD KUDROLI, Clark University — We discuss an experimental investigation of motion of a granular bed driven by a laminar fluid flow as a function of applied shear rate. This is a model system to investigate a variety of examples where such a situation arises including wind blowing over sand, sediment transport in rivers, slurries, and turbidity currents. We have developed an experimental apparatus which allows examination of the fluid as well as the grain dynamics both at the surface as well as deep into the bed under steady state conditions with refractive index matching technique. This allows us to obtain both the applied local shear stress by the fluid as well as the local strain rate inside the bed. We find that the granular flux as a function of depth decays exponentially into the bed. Further, the velocity profile is observed to exhibit a crossover from a regime where particles are fully suspended to where there is bed load transport. We will discuss the observed velocity and density profiles in light of various models of granular suspensions.

<sup>1</sup>Supported by NSF CBET - 1335928

**9:12AM E34.00005 Modeling Shear Banding in Amorphous Solids, from Atomistic to Continuum**<sup>1</sup> , DARIUS ALIX-WILLIAMS, MICHAEL FALK, Johns Hopkins University — Molecular dynamics simulations of strain localization are carried out using different materials systems and interatomic potentials including CuZr modeled via the embedded-atom method (EAM), amorphous Si modeled using Stillinger-Weber (SW) and a binary Lennard-Jones (LJ) system. Quench schedules and strain rates are varied. Different systems exhibit marked similarities in plastic behavior. Systematic differences between systems are analyzed in the context of Shear Transformation Zone (STZ) theory in the effort to develop a generalized constitutive framework for plasticity in glasses. Effective temperature inferred from the potential energy is explored as a local coarse-grained measure of the degree of disorder.

<sup>1</sup>This research is supported by National Science Foundation award 1408685.

**9:24AM E34.00006 Identifying shear transformation zones in amorphous solids via a virtual strain method** , MICHAEL FALK, Johns Hopkins University, SYLVAIN PATINET, ESPCI, Paris, France — One outstanding problem in the mechanical response of amorphous solids is the identification of flow defect sites, so called shear transformation zones (STZs), a priori in the structure. Many methods have been utilized in order to predict local STZ sites including short-range order, soft-mode analysis and machine learning. Here we directly probe local regions of the material via shear in order to detect nearby saddle points that can result in transformations. This non-perturbative method gives excellent correlation with global shear of the system. It also provides a means to cross-correlate the existence of such local transition pathways with other proposed diagnostics such as the soft-spot method of Manning and Liu. We use the information gained by this method to consider the coarse-graining necessary to connect atomistic methods to continuum theories.

**9:36AM E34.00007 Stick-slip instabilities in sheared granular flow: The role of friction and acoustic vibrations** , CHARLES K. C. LIEOU, Los Alamos National Laboratory and University of California, Santa Barbara, AHMED E. ELBANNA, University of Illinois at Urbana-Champaign, JAMES S. LANGER, JEAN M. CARLSON, University of California, Santa Barbara — We propose a theory of shear flow in dense granular materials. A key ingredient of the theory is an effective temperature that determines how the material responds to external driving forces such as shear stresses and vibrations. We show that, within our model, friction between grains produces stick-slip behavior at intermediate shear rates, even if the material is rate strengthening at larger rates. In addition, externally generated acoustic vibrations alter the stick-slip amplitude, or suppress stick-slip altogether, depending on the pressure and shear rate. We construct a phase diagram that indicates the parameter regimes for which stick-slip occurs in the presence and absence of acoustic vibrations of a fixed amplitude and frequency. These results connect the microscopic physics to macroscopic dynamics and thus produce useful information about a variety of granular phenomena, including rupture and slip along earthquake faults, the remote triggering of instabilities, and the control of friction in material processing.

**9:48AM E34.00008 A microstructural description of shear thickening in dense suspensions.** , ABHINENDRA SINGH, Levich Institute, City College of New York, ROMAIN MARI, DAMTP, University of Cambridge, RYOHEI SETO, Mathematical Soft Matter Unit, Okinawa Institute of Science and Technology, JEFF MORRIS, MORTON DENN, Chemical Engineering Department, City College of New York — The mechanism of shear thickening in dense suspensions has been recently linked to a transition from a lubricated “frictionless” to an unlubricated “frictional” rheology. Recent particle simulations have been successful to quantitatively reproduce both the continuous and discontinuous shear thickening as observed experimentally. However, a microstructural description of these suspensions is still lacking, which would aid in understanding and predicting the flow behavior of shear thickening suspensions. To tackle this challenging issue, we explore various microscopic properties, like the inter-particle force distribution, the particle motion correlations, and the anisotropy (in both contact and force network). Further, we also attempt to link the observed rheological behavior observed at the macro scale to mean displacement and fluctuations at the particle scale.

**10:00AM E34.00009 Deformation in Metallic Glass: Connecting Atoms to Continua**<sup>1</sup> , ADAM R. HINKLE<sup>2</sup>, MICHAEL L. FALK, Johns Hopkins University, CHRIS H. RYCROFT, Harvard University, MICHAEL D. SHIELDS, Johns Hopkins University — Metallic glasses like other amorphous solids experience strain localization as the primary mode of failure. However, the development of continuum constitutive laws which provide a quantitative description of disorder and mechanical deformation remains an open challenge. Recent progress has shown the necessity of accurately capturing fluctuations in material structure, in particular the statistical changes in potential energy of the atomic constituents during the non-equilibrium process of applied shear. Here we directly cross-compare molecular dynamics shear simulations of a ZrCu glass with continuum shear transformation zone (STZ) theory representations. We present preliminary results for a methodology to coarse-grain detailed molecular dynamics data with the goal of initializing a continuum representation in the STZ theory.

<sup>1</sup>NSF Grants Awards 1107838, 1408685, and 0801471

<sup>2</sup>NSF IGERT Fellowship Award Number 0801471

**10:12AM E34.00010 Size effects and internal length scales in the elasticity of random fiber networks.** , CATALIN PICU, Rensselaer Polytechnic Institute, KAMEL BERKACHE, EPSTA Alger, Algeria, ALI SHAHSAVARI, Rensselaer Polytechnic Institute, JEAN-FRANCOIS GANGHOFFER, Universite de Lorraine, Nancy, France — Random fiber networks are the structural element of many biological and man-made materials, including connective tissue, various consumer products and packaging materials. In all cases of practical interest the scale at which the material is used and the scale of the fiber diameter or the mean segment length of the network are separated by several orders of magnitude. This precludes solving boundary value problems defined on the scale of the application while resolving every fiber in the system, and mandates the development of continuum equivalent models. To this end, we study the intrinsic geometric and mechanical length scales of the network and the size effect associated with them. We consider both Cauchy and micropolar continuum models and calibrate them based on the discrete network behavior. We develop a method to predict the characteristic length scales of the problem and the minimum size of a representative element of the network based on network structural parameters and on fiber properties.

**10:24AM E34.00011 Is the microscopic stress computed from molecular simulations in mechanical equilibrium?** , ALEJANDRO TORRES-SANCHEZ, Universitat Politcnica de Catalunya, JUAN M. VANEGAS, Sandia National Laboratories, MARINO ARROYO, Universitat Politcnica de Catalunya — The microscopic stress field connects atomistic simulations with the mechanics of materials at the nano-scale through statistical mechanics. However, its definition remains ambiguous. In a recent work [1,2] we showed that this is not only a theoretical problem, but rather that it greatly affects local stress calculations from molecular simulations. We find that popular definitions of the local stress, which are continuously being employed to understand the mechanics of various systems at the nanoscale, violate the continuum statements of mechanical equilibrium. We exemplify these facts in local stress calculations of defective graphene, lipid bilayers, and fibrous proteins. Furthermore, we propose [1,3] a new physical and sound definition of the microscopic stress that satisfies the continuum equations of balance, irrespective of the many-body nature of the inter-atomic potential. Thus, our proposal provides an unambiguous link between discrete-particle models and continuum mechanics at the nanoscale. [1] Torres-Sanchez, A; Vanegas, J. M.; Arroyo, M.; Phys. Rev. Lett. 114, 258102 (2015). [2] Vanegas, J. M.; Torres-Sanchez, A; Arroyo, M.; J. Chem. Theor. Comput., 10 (2), 691702 (2014). [3] Torres-Sanchez, A; Vanegas, J. M.; Arroyo, M.; Submitted to J. Mech. Phys. Solid

**10:36AM E34.00012 Extending two-phase theories of soft composite solids to the non-dilute regime<sup>1</sup>** , FRANCESCO MANCARELLA, Nordic Institute of Theoretical Physics (NORDITA), ROBERT STYLE, University of Oxford, JOHN WETT-LAUFER, Yale University and Nordic Institute of Theoretical Physics (NORDITA) — Composite materials are ubiquitous in the natural environment and in engineered materials and hence capture the interest of a wide audience. Eshelby's 1957 theory treats the interaction of macroscopic stress fields with isolated inclusions within an elastic solid, and it has been widely used to treat the mechanics of composite materials. However, due to its neglect of interface stress, which is a particularly key effect in soft materials, the theory breaks down whenever the typical inclusion size  $R$  is of order or less than the elastocapillary lengthscale  $L$ . In this regime, under external stress, the effect of inclusion shape becomes strongly size-dependent. Here, we develop two new non-dilute theories, estimate the elastic moduli of composites comprised of an isotropic, compressible, linear-elastic compliant solid hosting a non-dilute spatially-random distribution of identical liquid droplets. The composite stiffness depends on a single dimensionless parameter  $L/R$ , and we find significant elastic moduli corrections for inclusions sizes  $R$  as large as  $100 L$ . By generalizing the exact theory recently developed for the corresponding dilute case, we find that when  $R < 3L/2$  ( $R = 3L/2$ ) liquid inclusions stiffen (cloak the far-field signature of) of the host solid.

<sup>1</sup>Swedish Research Council Grant No. 638-2013-9243.

**10:48AM E34.00013 Continuum modeling of dense granular flow down heaps** , DAVID HENANN, DAREN LIU, Brown University — Dense, dry granular flows display many manifestations of grain-size dependence, or nonlocality, in which the finite-size of grains has an observable impact on flow phenomenology. Such behaviors make the formulation of an accurate continuum model for dense granular flow particularly difficult, since local continuum models are not equipped to describe size-effects. One example of grain-size dependence is seen when avalanches occur on a granular heap – a situation which is frequently encountered in industry, as in rotating drums, as well as in nature, such as in landslides. In this case, flow separates into a thin, quickly flowing surface layer and a slowly creeping bulk. While existing local granular flow models are capable of capturing aspects of the flowing surface layer, they fail to even predict the existence of creeping flow beneath, much less being able to quantitatively describe the flow fields. Recently, we have proposed a new, scale-dependent continuum model – the nonlocal granular fluidity (NGF) model – that successfully predicted steady, slow granular flow fields, including grain-size-dependent shear-band widths in a variety of flow configurations. In this talk, we extend our model to the rapid flow regime and show that the model is capable of quantitatively predicting all aspects of gravity-driven heap flow. In particular, the model predicts the coexistence of a rapidly flowing, rate-dependent top surface layer and a rate-independent, slowly creeping bulk – a feature which is beyond local continuum approaches.

**Tuesday, March 15, 2016 8:00AM - 11:00AM –**

**Session E35 DBIO GSNP: Population and Evolutionary Dynamics I** 338 - Michael Pleimling, Virginia Tech

**8:00AM E35.00001 A non-classical phase diagram for virus-bacterial co-evolution mediated by CRISPR.** , PU HAN, MICHAEL DEEM, Rice University — CRISPR is a newly discovered prokaryotic immune system. Bacteria and archaea with this system incorporate genetic material from invading viruses into their genomes, providing protection against future infection by similar viruses. Due to the cost of CRISPR, bacteria can lose the acquired immunity. We will show an intriguing phase diagram of the virus extinction probability, which when the rate of losing the acquired immunity is small, is more complex than that of the classic predator-prey model. As the CRISPR incorporates genetic material, viruses are under pressure to evolve to escape the recognition by CRISPR, and this co-evolution leads to a non-trivial phase structure that cannot be explained by the classical predator-prey model.

**8:12AM E35.00002 Bacterial Invasion Dynamics in Zebrafish Gut Microbial Communities** , SAVANNAH LOGAN, MATTHEW JEMIELITA, Department of Physics, University of Oregon, TRAVIS WILES, Institute of Molecular Biology, University of Oregon, BRANDON SCHLOMANN, Department of Physics, University of Oregon, BRIAN HAMMER, School of Biology, Georgia Institute of Technology, KAREN GUILLEMIN, Institute of Molecular Biology, University of Oregon, RAGHUVeer PARTHASARATHY, Department of Physics, University of Oregon — Microbial communities residing in the vertebrate intestine play an important role in host development and health. These communities must be in part shaped by interactions between microbial species as they compete for resources in a physically constrained system. To better understand these interactions, we use light sheet microscopy and zebrafish as a model organism to image established gut microbial communities as they are invaded by robustly-colonizing challengers. We demonstrate that features of the challenger, including motility and spatial distribution, impact success in invasion and in outcompeting the original community. We also show that physical characteristics of the host, such as the motility of the gut, play important roles in mediating inter-species competition. Finally, we examine the influence of the contact-dependent type VI secretion system (T6SS), which is used by specific bacteria to cause cell lysis by injecting toxic effector proteins into competitors. Our findings provide insights into the determinants of microbial success in the complex ecosystems found in the gut.

**8:24AM E35.00003 Multiple Cancer Cell Population Dynamics in a Complex Ecology** , KE-CHIH LIN, Princeton University, GONZALO TARGA, KENNETH PIENTA, Johns Hopkins Medical Institute, JAMES STURM, ROBERT AUSTIN, Princeton University — We have developed a technology for study of complex ecology cancer population dynamics. The technology includes complex drug gradients, full bright field/dark field/fluorescence imaging of areas of several square millimeters and thin gas-permeable membranes which allow single cell extraction and analysis. We will present results of studies of prostate cancer cell dynamics.

**8:36AM E35.00004 Migration in asymmetric, random environments** , MICHAEL DEEM, DONG WANG, Rice University — Migration is a key mechanism for expansion of communities. As a population migrates, it experiences a changing environment. In heterogeneous environments, rapid adaption is key to the evolutionary success of the population. In the case of human migration, environmental heterogeneity is naturally asymmetric in the North-South and East-West directions. We here consider migration in random, asymmetric, modularly correlated environments. Knowledge about the environment determines the fitness of each individual. We find that the speed of migration is proportional to the inverse of environmental change, and in particular we find that North-South migration rates are lower than East-West migration rates. Fast communication within the population of pieces of knowledge between individuals, similar to horizontal gene transfer in genetic systems, can help to spread beneficial knowledge among individuals. We show that increased modularity of the relation between knowledge and fitness enhances the rate of evolution. We investigate the relation between optimal information exchange rate and modularity of the dependence of fitness on knowledge. These results for the dependence of migration rate on heterogeneity, asymmetry, and modularity are consistent with existing archaeological facts.

**8:48AM E35.00005 Velocity locking and pulsed invasions of fragmented habitats with seasonal growth** , KIRILL KOROLEV, CHING-HAO WANG, Boston University — From crystal growth to epidemics, spatial spreading is a common mechanism of change in nature. Typically, spreading results from two processes: growth and dispersal in ecology or chemical reactions and diffusion in physics. These two processes combine to produce a reaction-diffusion wave, an invasion front advancing at a constant velocity. We show that the properties of these waves are remarkably different depending whether space and time are continuous, as they are for a chemical reaction, or discrete, as they are for a pest invading a patchy habitat in seasonal climates. For discrete space and time, we report a new type of expansions with velocities that can lock into specific values and become insensitive to changes in dispersal and growth, i.e. the dependence of the velocity on model parameters exhibits plateaus or pauses. As a result, the evolution and response to perturbations in locked expansions can be markedly different compared to the expectations based on continuous models. The phenomenon of velocity locking requires cooperative growth and does not occur when per capita growth rate decline monotonically with population density. We obtain both numerical and analytical results describing highly non-analytic properties of locked expansions.

**9:00AM E35.00006 Spatial organization of cooperation.** , NICOLAS DESPRAT, LPS - Ecole Normale Supérieure (Paris) — The structure of the environment spatially confines bacteria inside groups where they live and evolve with their siblings. This population structure may not only select for individual abilities but also for group properties that would eventually enhance the fitness of the colony. In poor media, we might think that maximizing the contact with the environment would maximize the fitness of individual cells. However, we will show that the microcolony of *P. aeruginosa* adapts its morphogenesis to maximize cell-cell contacts rather than cell-environment interactions when iron becomes scarce in the environment. In this case, reducing the surface of exchange with the environment allows to limit the loss of secreted molecules required to efficiently fetch extracellular iron at very low concentration.

**9:36AM E35.00007 Non-equilibrium relaxation in a two-dimensional stochastic lattice Lotka-Volterra model<sup>1</sup>** , SHENG CHEN, UWE C. TÄUBER, Department of Physics, Virginia Tech — We employ Monte Carlo simulations to study a stochastic Lotka-Volterra model on a two-dimensional square lattice with periodic boundary conditions. There are stable states when the predators and prey coexist. If the local prey carrying capacity is finite, there emerges an extinction threshold for the predator population at a critical value of the predation rate. We investigate the non-equilibrium relaxation of the predator density in the vicinity of this critical point. The expected power law dependence between the relaxation time and predation rate is observed (critical slowing down). The numerically determined associated critical exponents are in accord with the directed percolation universality class. Following a sudden predation rate change to its critical value, one observes critical aging for the predator density autocorrelation function with a universal scaling exponent. This aging scaling signature of the absorbing state phase transition emerges at significantly earlier times than stationary critical power laws, and could thus serve as an advanced indicator of the population's proximity to its extinction threshold.

<sup>1</sup>This research is supported by the U. S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering under Award DE-FG02-09ER46613.

**9:48AM E35.00008 The effects of sudden changes in environmental conditions on the non-equilibrium relaxation of ecological systems<sup>1</sup>** , SHADI ESMAEILI, MICHEL PLEIMLING, Virginia Tech — We study the responses of predator-prey systems to temporary changes in environmental conditions. Such changes can cause a variation in species' predatory preferences which in our model appears as a perturbation in a many-species system. The type of perturbation that we consider in this study is a sudden change in the interaction scheme. We focus on systems evolving on a two-dimensional lattice and discuss the way the systems transition from one steady state to another. Using Monte Carlo simulations we monitor these transitions via the space-time correlation function and the derived correlation length.

<sup>1</sup>This work is supported by the US National Science Foundation through grant DMR-1205309.

**10:00AM E35.00009 Effect of flow and active mixing on bacterial growth in a colon-like geometry** , JONAS CREMER, IGOR SEGOTA, MARKUS ARNOLDINI, ALEX GROISMAN, TERENCE HWA, Department of Physics, U.C. San Diego — The large intestine harbors bacteria from hundreds of species, with bacterial densities reaching up to  $10^{12}$  cells per gram. Many different factors influence bacterial growth dynamics and thus bacterial density and microbiota composition. One dominant force is flow which can in principle lead to a washout of bacteria from the proximal colon. Active mixing by contractions of the colonic wall together with bacterial growth might counteract such flow-forces and allow high bacterial densities to occur. As a step towards understanding bacterial growth in the presence of mixing and flow, we constructed an in-vitro setup where controlled wall-deformations of a channel emulate contractions. We investigate growth along the channel under a steady nutrient inflow. In the limits of no or very frequent contractions, the device behaves like a plug-flow reactor and a chemostat respectively. Depending on mixing and flow, we observe varying spatial gradients in bacterial density along the channel. Active mixing by deformations of the channel wall is shown to be crucial in maintaining a steady-state bacterial population in the presence of flow. The growth-dynamics is quantitatively captured by a simple mathematical model, with the effect of mixing described by an effective diffusion term.

**10:12AM E35.00010 Predicting community composition from pairwise interactions**, JONATHAN FRIEDMAN, Physics, MIT, LOGAN HIGGINS, Microbiology, MIT, JEFF GORE, Physics, MIT — The ability to predict the structure of complex, multispecies communities is crucial for understanding the impact of species extinction and invasion on natural communities, as well as for engineering novel, synthetic communities. Communities are often modeled using phenomenological models, such as the classical generalized Lotka-Volterra (gLV) model. While a lot of our intuition comes from such models, their predictive power has rarely been tested experimentally. To directly assess the predictive power of this approach, we constructed synthetic communities comprised of up to 8 soil bacteria. We measured the outcome of competition between all species pairs, and used these measurements to predict the composition of communities composed of more than 2 species. The pairwise competitions resulted in a diverse set of outcomes, including coexistence, exclusion, and bistability, and displayed evidence for both interference and facilitation. Most pair outcomes could be captured by the gLV framework, and the composition of multispecies communities could be predicted for communities composed solely of such pairs. Our results demonstrate the predictive ability and utility of simple phenomenology, which enables accurate predictions in the absence of mechanistic details.

**10:24AM E35.00011 A field-theoretic approach to the May-Leonard cyclic population dynamics model**, SHANNON SERRAO, UWE TÄUBER, Virginia Tech — Spatially extended stochastic population dynamics models with cyclic predation interactions display intriguing time evolution and spontaneous structure formation. We study a version of the May-Leonard cyclic competition model in  $d$  dimensions with diffusive particle propagation. We use the second-quantized Doi-Peliti formalism and ensuing coherent-state path integral representation to construct its continuum representation and explore its collective dynamics. Expanding the resulting action about the mean-field species concentrations enables us to compute the diagonalized harmonic propagators and hence 'masses', i.e., relaxation rates and eigenfrequencies of the fundamental modes. Furthermore, operating near the Hopf bifurcation point, we identify the validity range for the necessary time scale separation that allows us to project out the purely relaxing eigenmode. The remaining oscillating fields obey the complex Ginzburg-Landau equation, which is consistent with spiral pattern formation.

**10:36AM E35.00012 Range expansions transition from pulled to pushed waves with increasing cooperativity in an experimental microbial population**, SAURABH GANDHI, EUGENE YURTSEV, Massachusetts Inst of Tech-MIT, KIRILL KOROLEV, Boston University, JEFF GORE, Massachusetts Inst of Tech-MIT — Range expansions are becoming more frequent due to environmental changes and rare long distance dispersal, often facilitated by anthropogenic activities. Simple models in theoretical ecology explain many emergent properties of range expansions, such as a constant expansion velocity, in terms of organism-level properties such as growth and dispersal rates. Testing these quantitative predictions in natural populations is difficult because of large environmental variability. Here, we used a controlled microbial model system to study range expansions of populations with and without intra-specific cooperativity. For non-cooperative growth, the expansion dynamics were dominated by population growth at the low-density front, which pulled the expansion forward. We found these expansions to be in close quantitative agreement with the classical theory of pulled waves by Fisher and Skellam, suitably adapted to our experimental system. However, as cooperativity increased, the expansions transitioned to being pushed, i.e. controlled by growth in the bulk as well as in the front. Although both pulled and pushed waves expand at a constant velocity and appear otherwise similar, their distinct dynamics leads to very different evolutionary consequences. Given the prevalence of cooperative growth in nature, understanding the effects of cooperativity is essential to managing invading species and understanding their evolution.

**10:48AM E35.00013 Selection of Cooperation in Spatially Structured Populations**, HYUNMO YANG, Ulsan National Institute of Science and Technology, CHEOL-MIN GHIM, Biomedical Engineering, Ulsan National Institute of Science and Technology — The social dilemma games give rise to an emergence of cooperation in which altruistic individuals survive the natural selection at higher rate than random chance. We try to extend our understanding of this spatial reciprocity by including the impact of degree-degree correlation on the propensity toward prosocial behaviour in an otherwise well-mixed population. In a stochastic death-birth process with weak selection, we find that the disassortative degree mixing, or negative correlation between the degrees of neighbouring nodes significantly promotes the fixation of cooperators whereas the assortative mixing acts to suppress it. This is consistent with the fact that the spatial heterogeneity weakens the average tendency of a population to cooperate, which we describe in a unified scheme of the effective isothermality in coarse-grained networks. We also discuss the individual-level incentives that indirectly foster restructuring the social networks toward the more cooperative topologies.

## **Tuesday, March 15, 2016 8:00AM - 11:00AM —**

**Session E36 GSOF: Colloids: Assembly, Mechanics and Techniques** 339 - Daniel Blair, Georgetown University

**8:00AM E36.00001 Fluid to solid transition of hard regular polygons**, JOSHUA ANDERSON, Univ of Michigan - Ann Arbor, MICHAEL ENGEL, JAMES ANTONAGLIA, ANDRES MILLAN, SHARON GLOTZER, University of Michigan — We perform simulations of hard regular polygons and determine the nature of the fluid to solid transition. Hard disks have a first order phase transition from fluid to hexatic and a continuous transition from hexatic to solid [1,2]. Hard polygons have shape and an additional degree of freedom. Directional entropic forces cause the polygons to attract edge to edge, which alters the phase transition. Polygons with enough edges have phase behavior similar to hard disks, with the density of the transition shifted lower. Polygons with few edges show a range of different behaviors. We develop and use HPMC [3] to run these simulations on the Titan supercomputer at the OLCF. HPMC is a scalable GPU-accelerated hard particle Monte Carlo simulation engine built on top of HOOMD-blue. [1] E. P. Bernard, W. Krauth, PRL 107, 155704 (2011). [2] M. Engel, J. A. Anderson, S. C. Glotzer, M. Isobe, E. P. Bernard, W. Krauth, PRE 87, 042134 (2013). [3] J. A. Anderson, M. E. J. L. Rrgang, S. C. Glotzer, arxiv:1509.04692

**8:12AM E36.00002 Shape Sensitive Assembly and Colloidal Superball Phase Transitions**, VISHAL SONI, University of Chicago, LAURA ROSSI, DOUGLAS J. ASHTON, Utrecht University, DAVID J. PINE, New York University, ALBERT P. PHILIPSE, Utrecht University, PAUL M. CHAIKIN, New York University, MARJOLEIN DIJKSTRA, Utrecht University, STEFANO SACANNA, New York University, WILLIAM T. M. IRVINE, University of Chicago — Guiding the self-assembly of materials by controlling the shape of the individual particle constituents is a powerful approach to material design. In particular the assembly of colloidal particles driven by depletants is a versatile playground for investigating this potential. We find that colloidal superballs may assemble into distinct phases that depend on both their shape and the size of the depletants. By using a mixture of depletants, one of which is size-tunable, we can explore reversible transitions between these phases.

**8:24AM E36.00003 Heaps of Shapes: Flow-Stabilized Solids with Non-Spherical Colloids**, SCOTT LINDAUER, North Carolina State University, C. WYATT SHIELDS IV, GABRIEL P. LOPEZ, Duke University, KAREN E. DANIELS, ROBERT RIEHN, North Carolina State University — Flow-stabilized solids are a class of fragile matter that are formed when a dense suspension of hard colloids is accumulated against a semipermeable barrier. We build a microfluidic device to confine Brownian particles in a quasi-2D channel; a controlled flow rate above a critical value forms flow-stabilized solids against the barrier. We extend prior work on submicron spherical particles, to particles of size 2-5 microns, and of various shapes: circular, rectangular, hexagonal, and triangular prisms. We perform experiments on these flow-stabilized solids to observe the angle of repose, packing fraction, and orientational order as a function of flow rate. We vary the flow rate quasi-statically in order to conduct the experiment at steady state. We find a critical flow rate below which no pile forms. In general, particles with less-circular shape form more stable heaps.

**8:36AM E36.00004 Digital Alchemy for Materials Design: Colloids and Beyond**, GREG VAN ANDERS, DAPHNE KLOTSAS, ANDREW KARAS, PAUL DODD, SHARON GLOTZER, University of Michigan — Starting with the early alchemists, a holy grail of science has been to make desired materials by manipulating basic building blocks. Building blocks that show promise for assembling new complex materials can be synthesized at the nanoscale with attributes that would astonish the ancient alchemists in their versatility. However, this versatility means that connecting building-block attributes to bulk structure is both necessary for rationally engineering materials and difficult because building block attributes can be altered in many ways. We show how to exploit the malleability of colloidal nanoparticle elements to quantitatively link building-block attributes to bulk structure through a statistical thermodynamic framework we term digital alchemy. We use this framework to optimize building blocks for a given target structure and to determine which building-block attributes are most important to control for self-assembly, through a set of novel thermodynamic response functions. We thereby establish direct links between the attributes of colloidal building blocks and the bulk structures they form. Moreover, our results give concrete solutions to the more general conceptual challenge of optimizing emergent behaviors in nature and can be applied to other types of matter.

**8:48AM E36.00005 Shaping Crystal-Crystal Phase Transitions**, XIYU DU, GREG VAN ANDERS, JULIA DSHE-MUCHADSE, SHARON GLOTZER, Univ of Michigan - Ann Arbor — Previous computational and experimental studies have shown self-assembled structure depends strongly on building block shape. New synthesis techniques have led to building blocks with reconfigurable shape and it has been demonstrated that building block reconfiguration can induce bulk structural reconfiguration. However, we do not understand systematically how this transition happens as a function of building block shape. Using a recently developed digital alchemy[1] framework, we study the thermodynamics of shape-driven crystal-crystal transitions. We find examples of shape-driven bulk reconfiguration that are accompanied by first-order phase transitions, and bulk reconfiguration that occurs without any thermodynamic phase transition. Our results suggest that for well-chosen shapes and structures, there exist facile means of bulk reconfiguration, and that shape-driven bulk reconfiguration provides a viable mechanism for developing functional materials. [1] G. van Anders, D. Klotsa, A. S. Karas, P. M. Dodd, and S. C. Glotzer, ACS Nano, 9, 9542 (2015).

**9:00AM E36.00006 Discontinuous Shear Thickening using Boundary Stress Microscopy**, VIKRAM RATHEE, DANIEL BLAIR, JEFFERY URBACH, Georgetown Univ — The microscopic picture of particle chain formation in discontinuous shear thickening suspensions remains unclear. In order to identify the role of localized stresses arising from particle chains we have applied the technique of Boundary Stress Microscopy to shear thickening suspension. By imaging deformations of an elastic boundary of the sheared suspension, we observe the appearance of localized forces on elastic substrate above critical stress value. These forces possibly arise from particles forming local network under shear. At the onset of thickening, we observe a change in first normal stress difference from negative to positive, inferring frictional contacts. However, the localized forces are only evident when the viscosity increases by an order of magnitude.

**9:12AM E36.00007 Viscosity of Sheared Helical filament Suspensions**, MATTHEW SARTUCCI, JEFF URBACH, DAN BLAIR, Georgetown University, WALTER SCHWENGER, Brandeis University — The viscosity of suspensions can be dramatically affected by high aspect ratio particles. Understanding these systems provides insight into key biological functions and can be manipulated for many technological applications. In this talk, the viscosity as a function of shear rate of suspensions of helical filaments is compared to that of suspensions of straight rod-like filaments. Our goal is to determine the impact of filament geometry on low volume fraction colloidal suspensions in order to identify strategies for altering viscosity with minimal volume fraction. In this research, the detached flagella of the bacteria *Salmonella Typhimurium* are used as a model system of helical filaments and compared to mutated straight flagella of the *Salmonella*. We compare rheological measurements of the suspension viscosity in response to shear flow and use a combination of the rheology and fluorescence microscopy to identify the microstructural changes responsible for the observed rheological response.

**9:24AM E36.00008 Holographic Characterization of Imperfect Spheres**, MARK HANNEL, CHRISTINE MIDDLETON, DAVID GRIER, New York University — Holographic snapshots of colloidal spheres can be fit to Lorenz-Mie theory, yielding the radius, refractive index and position of individual colloids in situ. This procedure assumes that the scatterer is a uniformly dense ideal sphere. Via experimentation and simulation, we demonstrate that small deviations from ideal sphericity produce palatable errors (approximately 1%) in our estimation of the particle's physical properties.

**9:36AM E36.00009 Thermo-responsive cross-linked liquid crystal bowl-shaped colloids<sup>1</sup>**, WEI-SHAO WEI, University of Pennsylvania, Department of Physics and Astronomy, YU XIA, SHU YANG, University of Pennsylvania, Department of Materials Science and Engineering, A. G. YODH, University of Pennsylvania, Department of Physics and Astronomy — In this work we create and investigate cross-linked bowl-shaped nematic liquid crystal (NLC) colloidal particles. Janus colloids are first formed via solvent-induced phase separation in emulsions consisting of NLC monomers and isotropic polymers. This scheme enables us to realize different particle morphologies such as bowl-shape by fine-tuning the confinement of NLCs within the droplets, e.g. by varying the size of droplets, the volume ratio between NLC and polymer, and the type/concentration of surfactants in aqueous background phase. The NLC compartment is composed of RM82 (1,4-Bis-[4-(6-acryloyloxyhexyloxy)benzoyloxy]-2-methylbenzene) monomers, which are then photocrosslinked by dithiol groups to form nematic liquid crystal elastomer. Finally, we remove the polymer parts of Janus colloids to obtain the target structures, which are temperature sensitive due to change of elasticity and molecular alignment of NLC near the isotropic to nematic phase transition temperature. We will explore novel mechanical and optical properties from the thermo-responsive structures as well as their applications, such as biomimic swimming behaviors and adjustable lensing effects.

<sup>1</sup>This work is supported by the foundation through NSF Grant DMR12-05463, NSF-MRSEC Grant DMR11-20901, and NASA Grant NNX08AO0G.

**9:48AM E36.00010 Simulating Electrophoresis with Discrete Charge and Drag<sup>1</sup>**, AARON J. MOWITZ, THOMAS A. WITTEN, University of Chicago — A charged asymmetric rigid cluster of colloidal particles in saline solution can respond in exotic ways to an electric field: it may spin or move transversely. These distinctive motions arise from the drag force of the neutralizing countercharge surrounding the cluster. Because of this drag, calculating the motion of arbitrary asymmetric objects with nonuniform charge is impractical by conventional methods. Here we present a new method of simulating electrophoresis, in which we replace the continuous object and the surrounding countercharge with discrete point-draggers, called Stokeslets. The balance of forces imposes a linear, self-consistent relation among the drag and Coulomb forces on the Stokeslets, which allows us to easily determine the object's motion via matrix inversion. By explicitly enforcing charge+countercharge neutrality, the simulation recovers the distinctive features of electrophoretic motion to few-percent accuracy using as few as 1000 Stokeslets. In particular, for uniformly charged objects, we observe the characteristic Smoluchowski independence of mobility on object size and shape. We then discuss electrophoretic motion of asymmetric objects, where our simulation method is particularly advantageous.

<sup>1</sup>This work is supported by a grant from the US-Israel Binational Science Foundation

**10:00AM E36.00011 Dielectrophoresis force of colloidal nanoparticles<sup>1</sup>**, HAO HUANG, Department of Chemical and Biomolecular Engineering, Lehigh University, DANIEL OU-YANG, Department of Physics, Lehigh University — Dielectrophoresis (DEP) is the motion of a polarizable colloidal particle in a nonuniform electric field. The magnitude of the DEP force is known to be proportional to the gradient of  $E^2$ . The DEP force also depends on the relative polarizability of the particle to that of the surrounding medium. Due to its ease of use, DEP has been proposed for a variety of applications to manipulate colloidal particles in a microfluidic setting. However, accurate measurements of the DEP force on colloidal nanoparticles are lacking. A new method is proposed to measure accurately the DEP potential force of colloidal nanoparticles by using confocal fluorescence imaging to determine the density distributions of dilute colloidal nanoparticle in a DEP potential force field. The DEP potential field can be calculated from the particle density distributions since the spatial distribution of the particle number density follows the Boltzmann distribution of the DEP potential energy. The validity of the measured DEP force is tested by examining the force as a function of the E field strength and particle size. The classic MaxwellWagnerOKonski is found to be inadequate to fully describe the frequency dependence of the DEP force.

<sup>1</sup>NSF 0928299, Emulsion Polymer Institute, Department of Physics of Lehigh University

**10:12AM E36.00012 Extremely Small and Incredibly Fast Microscopy: 1 nm and 10 us dynamics in concentrated colloidal suspensions**, BRIAN LEAHY, MATTHEW BIERBAUM, Cornell Univ, ALEXANDER ALEMI, Disney Research, ITAI COHEN, JAMES SETHNA, Cornell Univ — Recently we developed PERI, a technique for locating colloidal sphere's positions and radii to within 1 nm from ordinary light microscopy images. PERI provides unprecedented access to the physics of colloidal suspensions at small length scales. We use this for high precision measurements of the pair-correlation function  $g(r)$  and colloidal interactions at 1-nm distances. Finally, we couple PERI with high-speed brightfield light microscopy to examine fast dynamics of concentrated suspensions.

**10:24AM E36.00013 Confocal light microscopy at 1 nm: Locating colloids at maximum resolution**, MATTHEW BIERBAUM, BRIAN D. LEAHY, ALEXANDER A. ALEMI, ITAI COHEN, JAMES P. SETHNA, Cornell University — We present PERI, a method to locate colloidal spheres at the information theoretic limit using a generative model for confocal microscope images. Without modification to the microscope we resolve positions and radii to 1 nm, which we verify with experimental data. Employing Monte Carlo techniques, we recover the probability distributions for all particle positions and radii, microscope point spread function, laser intensity fluctuation, scan parameters, and signal to noise ratio in a single fit. Using this technique we explore precision measurements of dense colloidal suspensions including standard quantities such as mean squared displacement and the pair correlation function.

**10:36AM E36.00014 Dissecting diffusive and advective motion in colloidal sedimentation by multi-speckle Ultra-Small-Angle XPCS**, JOHANNES MLLER, THEYENCHERI NARAYANAN, ESRF - The European Synchrotron — In colloidal suspensions internal or external fields can induce directed motions of particles in addition to Brownian diffusion. Here, gradients in temperature or chemical potential, shear flow as well as gravity can act as an external field. Examples for internal motions can be found in synthetic self-propelling particles and microorganisms, generally coined as active matter. We present multi-speckle X-ray photon correlation spectroscopy measurements in the Ultra-Small-Angle scattering range which probes an expanded length scale comparable to DLS and optical microscopy. To demonstrate the advanced capabilities, we show measurements probing the motions within a settling suspension of sub-micron sized silica particles. A global fitting procedure has been applied to separate the diffusive and advective contributions to the particle dynamics. With this, macroscopic parameters such as the sedimentation velocity can be probed on a microscopic level in highly opaque and concentrated systems, which are in general difficult to access for optical investigations. This procedure may prove its value for investigating various kinds of non-equilibrium systems.

**10:48AM E36.00015 Enthalpy versus Entropy: the Thermodynamic Origin of Hard Particle Ordering<sup>1</sup>**, MITCHELL ANTHAMATTEN, SHAW CHEN, JANE OU, JEFFREY WEINFELD, University of Rochester, DEPARTMENT OF CHEMICAL ENGINEERING TEAM — The topic of hard particle ordering transitions is important in the development of molecular to mesoscale materials with potential applications in biomedicine, catalysis, optoelectronics, and renewable energy. The first step toward deterministic materials design rests on understanding the thermodynamic nature of ordering transitions involving two phases in equilibrium. We apply classical thermodynamics to show that (i) first-order, hard particle ordering transitions are forbidden at constant volume; and that (ii) hard-particle ordering is driven by a loss in enthalpy through volume reduction that outweighs a concomitant entropy loss upon ordering. The traditional approach considers minimization of Helmholtz energy, at constant volume, whereas the current study exclusively focuses on equilibrium phase transitions and, therefore, targets minimization of Gibbs energy at constant pressure. The Gibbs energy platform offers physically intuitive interpretations consistent with existing computation and experiments. The prevalent idea of entropy-driven ordering at constant V is restricted to transitions from non-equilibrium initial states that have yet to be properly defined for quantification.

<sup>1</sup>Laboratory of Laser Energetics, DE-FC52-08NA28302

**Tuesday, March 15, 2016 8:00AM - 11:00AM —**

**Session E37 GSOFD DPOLY: Self and Directed Assembly (Equilibrium and Non-Equilibrium)**

340 - Kazem Edmond, Oxford University

**8:00AM E37.00001 Phase Behavior of Thermodynamically Small Clusters of Colloidal Particles**, RAGHURAM THYAGARAJAN, DIMITRIOS MAROUDAS, DAVID FORD, Univ of Mass - Amherst — The self-assembly of finite clusters of colloidal particles into crystalline objects is a topic of technological interest, as a route to produce photonic crystals and other metamaterials. Such assembly problems also are fundamentally interesting because they involve thermodynamically small systems, with number of particles between 10 and 1000 that is far below the bulk limit. In contrast to bulk systems, these colloidal assemblies exhibit phase coexistence over a finite range of physical conditions. Here, we report the results of a computational study of phase behavior of small colloidal clusters interacting via the Asakura-Oosawa depletion pair potential. We conducted Monte Carlo simulations for various levels of the osmotic pressure that controls the strength of the interparticle interactions, using potential energy histograms to identify distinct phases. Over a narrow but finite range of the osmotic pressure, we find bimodal distributions in the potential energy space that are indicative of coexistence between fluid-like and crystalline configurations. We also report systematic quantitative comparisons of the phase behavior observed here with results from a Fokker-Planck order-parameter approach.

### 8:12AM E37.00002 Two-dimensional self-assembly of DNA-functionalized gold nanoparticles<sup>1</sup>

, WENJIE WANG, HONGHU ZHANG, NOAH HAGEN, Ames Laboratory and Iowa State University, IVAN KUZMENKO, Argonne National Laboratory, MUFIT AKINC, ALEX TRAVESSET, SURYA MALLAPRAGADA, DAVID VAKNIN, Ames Laboratory and Iowa State University — 2D superlattices of nanoparticles (NPs) are promising candidates for nano-devices. It is still challenging to develop a simple yet efficient protocol to assemble NPs in a controlled manner. Here, we report on formation of 2D Gibbs monolayers of single-stranded DNA-coated gold nanoparticles (ssDNA-AuNPs) at the air-water interface by manipulation of salts contents. MgCl<sub>2</sub> and CaCl<sub>2</sub> in solutions facilitate the accumulation of the non-complementary ssDNA-AuNPs on aqueous surfaces. Grazing-incidence small-angle X-ray scattering (GISAXS) and X-ray reflectivity show that the surface AuNPs assembly forms a mono-particle layer and undergoes a transformation from short-range to long-range (hexagonal) order above a threshold of [MgCl<sub>2</sub>] or [CaCl<sub>2</sub>]. For solutions that include two kinds of ssDNA-AuNPs with complementary base-pairing, the surface AuNPs form a thicker film and only in-plane short-range order is observed. By using other salts (NaCl or LaCl<sub>3</sub>) at concentrations of similar ionic strength to those of MgCl<sub>2</sub> or CaCl<sub>2</sub>, we find that surface adsorbed NPs lack any orders. X-ray fluorescence measurements provide direct evidence of surface enrichment of AuNPs and divalent ions (Ca<sup>2+</sup>).

<sup>1</sup>The work was supported by the Office of Basic Energy Sciences, USDOE under contract No. DE-AC02-07CH11358 and DE-AC02-06CH11357.

### 8:24AM E37.00003 Novel liquid crystal phase transition of linear defects in an epitaxial layer of DNA-nanoparticle superlattices<sup>1</sup>

, SAIJIE PAN, NIELS BOON, MONICA OLVERA DE LA CRUZ, Northwestern Univ — We use Monte Carlo simulations and mean-field theory to study a lattice model system in which DNA-coated nanoparticles form an epitaxial layer onto a patterned bcc (100) template. If nanoparticles only attach to the so-called “center” sites, each of which is the center of a unit cell in the square lattice template, it would result in a perfect bcc epitaxial layer. However, defects arise due to attachment to “edge” sites and “corner” sites. In simulation, we show that edge-binding defects prefer to form linear clusters in horizontal and vertical directions. These linear defects can undergo a second-order isotropic-nematic phase transition in some regimes. A mean-field approach is introduced to provide theoretical descriptions for the system in each of the phases and predict the critical phase transition conditions. Striking agreement is observed between the theory and simulation.

<sup>1</sup>This work was supported by the the Air Force Office of Scientific Research (AFOSR) Multidisciplinary University Research Initiative (MURI) FA9550-11-1-0275.

### 8:36AM E37.00004 Transformations and Reconstructions of DNA-directed colloidal crystals

, JOHN CROCKER, YIFAN WANG, IAN JENKINS, TALID SINNO, University of Pennsylvania — DNA is a versatile tool for directing the equilibrium self-assembly of nanoscopic and microscopic objects, but also for subsequently transforming them into new structures. In experiment, at high densities of long grafted DNA strands, and temperatures where the binding is reversible, these systems readily form colloidal crystals and colloidal clusters having a range of symmetries. For interactions that favor alloying between two differently-sized colloidal species, our experimental observations compare favorably to a simulation framework that predicts the equilibrium phase behavior, growth kinetics and solid-solid transitions. Overall, we find that this system recapitulates both ionic crystals and noble-metal alloys. We will discuss the crystallography of the alloy structures formed as well as the interesting Martensitic-type transformations and super-lattice reconstructions they undergo.

### 8:48AM E37.00005 Bioinspired Composites with Spatial and Orientational Control of Reinforcement<sup>1</sup>

, AHMET DEMIROERS, ANDRE STUDART, ETH Zurich, COMPLEX MATERIALS TEAM — Living organisms combine soft and hard components to fabricate composite materials with out-standing mechanical properties. The optimum design and assembly of the anisotropic components reinforce the material in specific directions against multidirectional external loads. Although nature does it quite readily, it is still a challenge for material scientists to control the orientation and position of the colloidal components in a matrix. Here, we use external electric and magnetic fields to achieve positional and orientational control over colloid-polymer composites to fabricate mechanically robust materials to capture some of the essential features of natural systems. We first investigated the assembly of spherical micron-sized colloids using dielectrophoresis, as these particles provided an easily accessible and instructive length scale for performing initial experiments. We used dielectrophoresis for spatial control of reinforcing anisotropic components and magnetic fields to provide control over the orientation of these reinforcing constituents. The obtained composites with different orientational and spatial reinforcement showed enhanced mechanical properties, such as wear resistance, which exhibits similarities to tooth enamel.

<sup>1</sup>SNSF Ambizione grant PZ00P2.148040

### 9:00AM E37.00006 Harmonic and Anharmonic Free Energies in Superlattices of Soft Particle Systems<sup>1</sup>

, ALEX TRAVESSET, Iowa State Univ and Ames lab, CARLES CALERO, Center for Polymer Studies and Department of Physics, Boston University, 590 Commonwealth Avenue, Boston, MA 02215, USA, CHRIS KNOROWSKI, Iowa State Univ and Ames lab — Many problems in self and directed assembly rely on the rigorous calculation of free energies. In systems of nanoparticles with capping ligands, for example, superlattices are found in closely competing structures, such as hcp/fcc, cubic/hexagonal diamond or those isomorphic between MgCu<sub>2</sub> and MgZn<sub>2</sub>. With this motivation, we investigate a general method to calculate free energy of crystalline solids by considering the harmonic approximation and quasistatically switching the anharmonic contribution. The advantage of the method is that the harmonic approximation provides an already very accurate estimate of the free energy, and therefore the anharmonic term is numerically very small and can be determined to very high accuracy. We further show that the anharmonic contribution to the free energy satisfies a number of exact inequalities that place constraints on its magnitude and allows approximate but fast and accurate estimates. We apply it to Lennard Jones systems where we demonstrate that hcp is the equilibrium phase at low temperature and pressure and obtain the coexistence curve with the fcc phase, which exhibits reentrant behavior and binary systems that model nanoparticle superlattices with hydrocarbon capping ligand.

<sup>1</sup>The research was performed at the Ames Laboratory, which is operated for the US DOE by Iowa State University under contract number DE-AC02-07CH11358

### 9:12AM E37.00007 Designing self-assembling 3D structures of microcapsules

, LIKE LI, HENRY SHUM, OLEG SHKLYAEV, VICTOR YASHIN, ANNA BALAZS, University of Pittsburgh — Self-assembly of complex, three-dimensional structures is commonly achieved by biological cells but difficult to realize in synthetic systems with micron-scale or larger components. Some previous modeling studies have considered only the planar self-assembly of microcapsules on a substrate. In this work, nanoparticles released from the capsules bind to the substrate and to the shells of nearby capsules. The non-uniform nanoparticle deposition on a capsule's surface leads to adhesion gradients, which drive the capsules to effectively “climb” on top of one another and self-organize in the vertical direction. We determine conditions that favor this structural organization. In particular, we study how the vertical structuring depends on the background fluid flow, the topography of the microcapsules and the underlying surface, the capsule-capsule interaction and that between the capsules and the substrate. The findings can provide design rules for the autonomous creation of novel nanocomposites, where the layers are formed from nanoparticle-containing and nanoparticle-decorated microcapsules.

**9:24AM E37.00008 Stripes or Checkerboards: Distinguishing Patterns of Self-Assembled Water Drops to Chiral Structures**, LAURA ADAMS, Harvard, SAM OCKO, Stanford University, DAVID WEITZ, Harvard — A robust route for the biased production of single-handed chiral structures has been found in generating non-spherical, multi-component double emulsions, drops within drops, using glass microfluidic devices. Driving the minimization of surface energy are capillary forces that cause linear chains of encapsulated water drops to self-assemble into three-dimensional configurations with a well-defined preference to one type of handedness; thus, breaking left-right symmetry. In two dimensions, the encapsulated drops form patterns of stripes or checkerboards that are captured with a high speed camera. We quantify the dynamics of the evolving structures by measuring the second moment of the mass distribution and their growth and evolution rates. These new self-assembled soft structures are highly stable and open the door for a wide range of exotic configurations.

**9:36AM E37.00009 Bias-free simulation of diffusion-limited aggregation on a square lattice**, YEN LEE LOH, Univ of North Dakota — We identify sources of systematic error in traditional simulations of the Witten-Sander model of diffusion-limited aggregation (DLA) on a square lattice. Based on semi-analytic solutions of the walk-to-line and walk-to-square first-passage problems, we develop an algorithm that reduces the simulation bias to below  $10^{-12}$ . We grow clusters of  $10^8$  particles on  $65536 \times 65536$  lattices. We verify that lattice DLA clusters inevitably grow into anisotropic shapes, dictated by the anisotropy of the aggregation process. We verify that the fractal dimension evolves from the continuum DLA value,  $D = 1.71$ , for small disk-shaped clusters, towards Kesten's bound of  $D = 3/2$  for highly anisotropic clusters with long protruding arms.

**9:48AM E37.00010 The role of symmetry for the orientational ordering of hard regular polygons**, WENBO SHEN, Department of Physics, University of Michigan - Ann Arbor, MICHAEL ENGEL, JOSHUA A. ANDERSON, Department of Chemical Engineering, University of Michigan - Ann Arbor, JAMES A. ANTONAGLIA, Department of Physics, University of Michigan - Ann Arbor, SHARON C. GLOTZER, Department of Chemical Engineering, University of Michigan - Ann Arbor, GLOTZER GROUP TEAM — Understanding the relationship between particle shape and structure is critical for targeted self-assembly. Hard particles, whose phase behavior is governed by geometry alone, spontaneously order when compressed to high enough packing density. Different routes of ordering have been suggested: a direct transition from fluid to crystal as well as the appearance of an intermediate liquid crystalline or a rotator phase. Here, we investigate a family of hard shapes in two dimensions that interpolate from highly anisotropy to highly circular. For this purpose, we determine the phase behavior of hard regular polygons from triangles to dodecagons at densities comprising the development of orientational order. In particular, we focus on the role of particle symmetry on rotational motion and the appearance of rotator phases.

**10:00AM E37.00011 Shape Allophiles Improve Entropic Assembly<sup>1</sup>**, ERIC HARPER, RYAN MARSON, JOSHUA ANDERSON, GREG VAN ANDERS, SHARON GLOTZER, Univ of Michigan - Ann Arbor — We investigate a class of “shape allophiles” that fit together like puzzle pieces as a method to access and stabilize desired structures by controlling directional entropic forces. Squares are cut into rectangular halves, which are shaped in an allophilic manner with the goal of re-assembling the squares while self-assembling the square lattice. We examine the assembly characteristics of this system via the potential of mean force and torque, and the fraction of particles that entropically bind. We generalize our findings and apply them to self-assemble triangles into a square lattice via allophilic shaping. Through these studies we show how shape allophiles can be useful in assembling and stabilizing desired phases with appropriate allophilic design. [1] Harper, et. al., Soft Matter, 2015, 11, 7250-7256. DOI: 10.1039/C5SM90160J. This work was featured on the cover of Soft Matter 07 October, 2015.

<sup>1</sup>NSF Grant ACI-1053575 (XSEDE award DMR 140129), U.S. Army Research Office Grant Award W911NF-10-1-0518, DOD/ASD(R&E) Award N00244-09-1-0062, NSF DGE 0903629 Open Data IGERT, NSF Division of Materials Research Award DMR 1409620

**10:12AM E37.00012 Molecular Dynamics Investigation of the Products of Alkoxysilane Condensation: Bulk Gels and Surface Coatings**, ROLAND FALLER, JOSHUA DEETZ, UC Davis — We characterize silica gels and organo-silicon surface coatings using reactive molecular dynamics simulations. To model the chemical reactions, we use a reactive force field (ReaxFF) which we have optimized in a novel parallelized semi-automatic way to model hydrolysis and condensation reactions. The morphologies of silica gels obtained from tetra- and tri-alkoxysilanes are determined by allowing the system to condense while simultaneously removing water and replacing it with precursor solution. It is found that the gels obtained from trialkoxysilanes are more loosely bonded, and that the chemistry of the headgroup is important to the gel morphology. We furthermore simulated the chemisorption of alkoxysilanes with organic headgroups to hydroxylated silica surfaces. We observe a competition between alkoxysilanes condensing with themselves or with the silica surface.

**10:24AM E37.00013 Multiscale Self-Assembly of Quantum-Dots into an Anisotropic Three-Dimensional Random Network**, SERIM ILDAY, Bilkent University & METU, FATIH ILDAY, Bilkent University, RENE HBNER, Helmholtz-Zentrum Dresden-Rossendorf, TY PROSA, ISABELLE MARTIN, CAMECA Instruments Inc, GIZEM NOGAY, METU, ISMAIL KABACELIK, Akdeniz University, ZOLTAN MICS, MISCHA BONN, DMITRY TURCHINOVICH, Max Planck Institute for Polymer Research, HANDE STNEL, METU, DANIELE TOFFOLI, Università di Trieste, DAVID FRIEDRICH, BERND SCHMIDT, KARL-HEINZ HEINIG, Helmholtz-Zentrum Dresden-Rossendorf, RASIT TURAN, METU — Multiscale self-assembly is ubiquitous in nature but its deliberate use to synthesise multifunctional materials remains rare, partly due to the notoriously difficult problem of controlling topology from atomic to macroscopic scales to obtain properties by design. Here, we demonstrate an anisotropic random network of silicon quantum-dots that hierarchically self-assembles from the atomic to the microscopic scales: First, quantum-dots form, to subsequently interconnect without inflating their diameters to form a random network. This network then grows in a preferential direction to form undulated and branching nanowire-like structures. This specific topology allows simultaneous good electrical conduction and a tuneable bandgap. These scale-dependent features were previously thought to be mutually exclusive. Furthermore, we show that the topology is designed and self-assembled following an inherently modular, material-independent methodology, so that the approach is applicable to achieve programmable properties in other materials.

**10:36AM E37.00014 Experimental Investigations of Ionic Self-Assembly of Silica Nanoparticles**, GILLENHAAL BECK, SABIN NISHIMYUMUKIZA, MOHAMMAD ABUDAYYEH, REBECCA MELKERSON, ESTEVAN HALL-MEJIA, IRINA MAZILU, DAN MAZILU, Washington & Lee University — We present a novel experimental method for determining the rate at which anionic silica nanoparticles in a colloidal suspension are adsorbed to a cationic polymer on a glass substrate. This method allows us to study particle self-assembly at time scales under one tenth of a second, two orders of magnitude smaller than previously reported in literature. We compare our experimental findings with a class of stochastic models for cooperative sequential adsorption of particles.

**10:48AM E37.00015 Programmable concatenation of conductively linked gold nanorods using molecular assembly and femtosecond irradiation**, JAKE FONTANA, STEVE FLOM, JAWAD NACIRI, BANAHALLI RATNA, Naval Research Laboratory — The ability to tune the resonant frequency in plasmonic nanostructures is fundamental to developing novel optical properties and ensuing materials. Recent theoretical insights show that the plasmon resonance can be exquisitely controlled through the conductive concatenation of plasmonic nanoparticles. Furthermore these charge transfer systems may mimic complex and hard to build nanostructures[1]. Here we experimentally demonstrate a directed molecular assembly approach to controllably concatenate gold nanorods end to end into discrete linear structures, bridged with gold nanojunctions, using femtosecond laser light. By utilizing high throughput and nanometer resolution this approach offers a pragmatic assembly strategy for charge transfer plasmonic systems. [1] J. Fontana and B. R. Ratna, Applied Physics Letters **105** (2014)

**Tuesday, March 15, 2016 8:00AM - 10:48AM —**

**Session E38 GSOFD DBIO GSNP/DFD: Active Matter III** 341 - Cynthia J. Reichardt, Los Alamos National Laboratory

**8:00AM E38.00001 Statistical Mechanics and Hydrodynamics of Self-Propelled Hard Disks**, BENJAMIN HANCOCK, APARNA BASKARAN, Brandeis University — Active particle fluids have constant energy production and dissipation at the level of its constituent particles. Yet, despite its out-of-equilibrium nature, analogies have been drawn between the steady state behavior of active fluids and their passive fluid counterparts. While most of the studies have been phenomenological or numerical, in this talk we present a first systematic derivation of the statistical mechanics and hydrodynamics of self propelled hard disks in particular we focus on two results. First, a dynamical instability signaling the onset of phase separation and cluster formation is derived and compared to existing phenomenological and kinetic estimates. Second, a leading order contribution to the pressure due to particle interactions is derived and compared with simulations of active brownian particles.

**8:12AM E38.00002 Reversible Ratchet Effects and Structural Ordering for Self-Propelled Disks on Quasi-One Dimensional Asymmetric Substrates**, DANIELLE MCDERMOTT, Wabash College, CYNTHIA REICHHARDT, CHARLES REICHHARDT, Los Alamos National Laboratory, Theoretical Division — When a particle is placed in an asymmetric periodic potential and an ac driving force is applied, it is possible to produce a net dc flow through a ratchet effect. When the particles are active, a net dc particle flow can arise even in the absence of external driving, creating an active ratchet effect as has been observed for bacteria in funnel geometries. Here we examine a 2D assembly of self-propelled disks interacting with an asymmetric 1D substrate. We find that at low density, with few particle collisions, this system exhibits a robust ratchet effect in which the particles undergo a net drift in the easy direction of the substrate asymmetry. At higher densities where particle-particle interactions become important, a reversed ratchet effect can arise with the net flow of particles in the hard direction. These reversals occur due to the formation of commensurate chain-like structures of disks. When there are two or more chains of particles in a one substrate well, the effective substrate potential is inverted. This reversible active ratchet effect could be used to separate different species of particles, cause the shepherding of passive particles, or control the migration of micro-organisms, and should be general to a wide class of self driven interacting particle systems.

**8:24AM E38.00003 Melting a crystal of self-propelled particles**, CHRISTOPHER OLSON, MICHAEL MULLER, LEE WALSH, NARAYANAN MENON, Univ. of Massachusetts Amherst — We experimentally study the kinetics of melting a two-dimensional non-cohesive crystal of hard, square-shaped millimeter-scale particles. Interactions between the square particles have four-fold rotational symmetry, but particles are designed with features such that when vibrated their predominant motion is polar along one body axis. We prepare the initial crystalline state with varying orientations of the particle polarity relative to the symmetry axes of the crystal. We then study the melting of this crystal when vertical vibrations are turned on. Orientational and translational order are initially strongly coupled, and during melting translational order is lost before orientational order. The spatial distribution of order parameters and the time scale for melting kinetics is strongly affected by compatibility between the polarity and the crystal axes in the initial condition.

**8:36AM E38.00004 Magnetic properties of self propelled particles**, MELISSA FERRARI, MICHELLE DRISCOLL, New York University, JEREMIE PALACCI, University of California, San Diego, STEFANO SACANNA, DAVID PINE, PAUL CHAIKIN, New York University — We study a class of synthetic light-activated colloidal swimmers which self propel osmotically/phoretically close to a surface and self organize into dynamic clusters. Swimming is activated by a photocatalytic hematite cube exposed from the colloidal surface. Hematite is a canted antiferromagnet, with a permanent magnetic moment; the magnetic moment is oriented in a discrete number of directions relative to the exposed hematite face. The permanent moment allows us to orient and direct the swimmers motion with an applied magnetic field, and different field configurations allow for a large range of directed motion. Furthermore, the various orientations of the magnetic moment give rise to distinct species of swimmers, which can simultaneously undergo clockwise and counterclockwise orbits in a rotating magnetic field.

**8:48AM E38.00005 Guiding catalytically active particles with chemically patterned surfaces**, WILLIAM USPAL, MIHAIL POPESCU, SIEGFRIED DIETRICH, MYKOLA TASINKEVYCH, Max-Planck-Institut für Intelligente Systeme and IV. Institut für Theoretische Physik, Universität Stuttgart — Catalytically active Janus particles in solution create gradients in the chemical composition of the solution along their surfaces, as well as along any nearby container walls. The former leads to self-phoresis, while the latter gives rise to chemi-osmosis, providing an additional contribution to self-motility. Chemi-osmosis strongly depends on the molecular interactions between the diffusing chemical species and the wall. We show analytically, using an approximate “point-particle” approach, that by chemically patterning a planar substrate (e.g., by adsorbing two different materials) one can direct the motion of Janus particles: the induced chemi-osmotic flows can cause particles to either “dock” at a chemical step between the two materials, or to follow a chemical stripe. These theoretical predictions are confirmed by full numerical calculations. Generically, docking occurs for particles which tend to move away from their catalytic caps, while stripe-following occurs in the opposite case. Our analysis reveals the physical mechanisms governing this behavior.

**9:00AM E38.00006 3-d Brownian dynamics simulations of the smallest units of an active biological material**, JUTTA LUETTNER-STRAHMANN, NABINA PAUDYAL, MARAL ADELI KOUDEHI, Department of Physics, The University of Akron — Motor proteins generate stress in a cytoskeletal network by walking on one strand of the network while being attached to another one. A protein walker in contact with two elements of the network may be considered the smallest unit of an active biological material. In vitro experiments, mathematical modeling and computer simulations have provided important insights into active matter on large and on very small length and time scales. However, it is still difficult to model the effects of local environment and interactions at intermediate scales. Recently, we developed a coarse-grained, three-dimensional model for a motor protein transporting cargo by walking on a substrate. In this work, we simulate a tethered motor protein pulling a substrate with elastic response. As the walker progresses, the retarding force due to the substrate tension increases until contact fails. We present simulation results for the effect of motor-protein activity on the tension in the substrate and the effect of the retarding force on the processivity of the molecular motor.

**9:12AM E38.00007 Smarticles: smart, active granular matter<sup>1</sup>**, WILL SAVOIE, Georgia Tech, ARMAN PAZOUKI, DAN NEGRUT, U. Wisconsin-Madison, DANIEL GOLDMAN, Georgia Tech — We investigate a granular medium composed of smart, active particles, or “smarticles”. Previously, we discovered that ensembles of “u”-shaped particles exhibited geometrically-induced cohesion by mechanically entangling via particle interpenetration [Gravish et al, PRL, 2012]; the strength and/or extent of entanglement could be varied by changing particle level entanglement by changes in arm-to-base length of the u-particle. Since changing this parameter on demand is inconvenient, we develop a power-autonomous programmable robot composed of two motors and three links with an on-board microcontroller. This smarticle can be activated to change its configuration (specified by its two joint angles) through audio communication. To complement these experiments, since study large ensembles of smarticles is cost and labor prohibitive, we also develop a simulated smarticle in the Chrono multibody simulation environment. We systematically study ensemble cohesiveness and compaction as a function of shape changes of the smarticles. We find that suitable activation of smarticles allows ensembles to become cohesive to “grip” rigid objects and lose cohesion to release on command.

<sup>1</sup>work supported by ARO

**9:24AM E38.00008 Active Brownian particles near straight or curved walls: Pressure and boundary layers<sup>1</sup>**, AYHAN DUZGUN, JONATHAN SELINGER, Kent State Univ - Kent — Unlike equilibrium systems, active matter is not governed by the conventional laws of thermodynamics. Through a series of Langevin dynamics simulations and analytic calculations, we explore how systems cross over from equilibrium to active behavior as the activity is increased. In particular, we calculate the profiles of density and orientational order near straight or circular walls, and show the characteristic width of the boundary layers. We find a simple relationship between the enhancements of density and pressure near a wall. Based on these results, we determine how the pressure depends on wall curvature, and hence make approximate analytic predictions for the motion of curved tracers, as well as the rectification of active particles around small openings in confined geometries.

<sup>1</sup>Supported by NSF Grant No. DMR-1409658.

**9:36AM E38.00009 Active particles on curved surfaces**, YAOUE FILY, APARNA BASKARAN, MICHAEL HAGAN, Brandeis University — Active systems have proved to be very sensitive to the geometry of their environment. This is often achieved by spending significant time at the boundary, probing its shape by gliding along it. I will discuss coarse graining the microscopic dynamics of self-propelled particles on a general curved surface to predict the way the density profile on the surface depends on its geometry. Beyond confined active particles, this formalism is a natural starting point to study objects that cannot leave the boundary at all, such as cells crawling on a curved substrate, animals running on uneven ground, or active colloids trapped at an interface.

**9:48AM E38.00010 Edge states in confined active fluids**, ANTON SOUSLOV, VINCENZO VITELLI, Leiden University — Recently, topologically protected edge modes have been proposed and realized in both mechanical and acoustic metamaterials. In one class of such metamaterials, Time-Reversal Symmetry is broken, and, to achieve this TRS breaking in mechanical and acoustic systems, an external energy input must be used. For example, motors provide a driving force that uses energy and, thus, explicitly break TRS. As a result, motors have been used as an essential component in the design of topological metamaterials. By contrast, we explore the design of topological metamaterials that use a class of far-from-equilibrium liquids, called polar active liquids, that spontaneously break TRS. We thus envision the confinement of a polar active liquid to a prescribed geometry in order to realize topological order with broken time-reversal symmetry. We address the design of the requisite geometries, for example a regular honeycomb lattice composed of annular channels, in which the active liquid may be confined. We also consider the physical character of the active liquid that, when introduced into the prescribed geometry, will spontaneously form the flow pattern of a metamaterial with topologically protected edge states. Finally, we comment on potential experimental realizations of such metamaterials.

**10:00AM E38.00011 Effect of micro-stirring on enzymatic reaction kinetics inside a biomimetic container**, IREP GOZEN, VIVA HOROWITZ, ZACHARY CHAMBERS, VINOTHAN MANOHARAN, Harvard University — The intracellular environment is dynamic, influenced by the motion of active machinery such as cytoskeleton filaments and molecular motors. To understand whether and how such activity affects the rates of diffusion-limited reactions, we construct a model system consisting of a phospholipid vesicle encapsulating a small number of micro- or nanoparticles, the active motion of which can be induced by chemical or magnetic cues. We aim to determine a relation between active motion of particles and rates of enzymatic reactions in the confined volume. Our findings might illuminate how active motion influences cytoplasmic reaction dynamics, or may have played a role in protocell genetics.

**10:12AM E38.00012 Correlated Rotational Noise in Active Brownian Systems**, CALEB WAGNER, APARNA BASKARAN, Brandeis Univ — We consider a system of self-propelled particles in a viscous medium for which the angle parametrizing the direction of particle propulsion is subject to correlated noise. The physics involved in the correlated noise is explored by deriving a modified Smoluchowski equation that governs the evolution of the probability distribution for particle positions and orientations. More precisely, given noise correlations that decay exponentially in time with decay constant  $\nu$ , we give the modified Smoluchowski equation as a perturbative expansion in  $\nu$ . While the physical origins of correlated noise may be diverse, we give one interpretation of the resulting dynamics in terms of inertial effects that are absent from the usual overdamped description of self-propelled particles in a viscous medium.

**10:24AM E38.00013 ABSTRACT WITHDRAWN —**

**10:36AM E38.00014 Dancing the night away: Improving the persistence of locomotion on the micron scale**, EMILY W. GEHRELS, W. BENJAMIN ROGERS, Harvard University, ZORANA ZERAVCIC, The Rockefeller University, VINOTHAN N. MANOHARAN, Harvard University — In recent years a range of nano and microscale walkers (motors that are able to move along a preformed track) have been developed. Many of these walkers bind to their tracks using a single binding site at each station along the track. A disadvantage of these systems is that any failure involving a single site becoming unbound leads to the walker falling off of the track and locomotion being prematurely terminated. For this reason, it has been difficult to develop a motor that can reliably take more than a few sequential steps. We present an experimental system of DNA-functionalized colloidal particles which exhibit directed motion along patterned substrates in response to temperature cycling. Many DNA bridges form between each pair of interacting particles, adding redundancy to the binding at each station to realize a system that should be able to consistently take many steps. We take advantage of toehold exchange in the design of the DNA sequences that mediate the colloidal interactions to produce broadened, flat, or even re-entrant binding and unbinding transitions between the particles and substrate. Using this new freedom of design, we devise systems where, by thermal ratcheting, we can externally control the direction of motion and sequence of steps of the colloidal motor.

**Tuesday, March 15, 2016 8:00AM - 11:00AM —**

**Session E39 DBIO GSOFT: Cell Motility: From Single Cell to Collective Dynamics I** 342 - Sima Setayeshgar

**8:00AM E39.00001 From single cells to fruiting bodies: Bridging scales in collective behavior**, ALLYSON SGRO, Department of Physics/Lewis-Sigler Institute for Integrative Genomics, Princet — No abstract available.

**8:36AM E39.00002 Superdiffusive cell motility on 2D substrates modeled as a persistent Levy walk** , GIUSEPPE PASSUCCI, MEGAN E. BRASCH, Syracuse University, NICHOLAS O. DEAKIN, CHRISTOPHER E. TURNER, SUNY Upstate Medical University, JAMES H. HENDERSON, M. LISA MANNING, Syracuse University — Cell motility is an essential part of many biological processes such as morphogenesis, wound healing and tumorigenesis. We quantified cell motility by tracking mouse fibroblast and human breast carcinoma nuclei to construct cell trajectories. The mean-squared displacement of these trajectories reveals that cell motion is super diffusive, where displacements scale faster than  $t^{1/2}$  in all directions. Existing self-propelled particle (SPP) models that do not explicitly incorporate ensemble heterogeneity are unable to predict this super-diffusive behavior. Therefore we developed a run-and-tumble SPP model with Levy distributed run times that captures observed super-diffusive behavior in the mean-squared displacement as well as scaling collapse exponents of displacement probability distributions which match those of mouse fibroblast and human breast carcinoma cell trajectories. We additionally introduced small fluctuations in particle orientation during runs, which generates a crossover from super-diffusive to diffusive dynamics at a very long times. This timescale can be extracted in experiments from the velocity auto-correlation function, allowing us to explicitly test this model prediction.

**8:48AM E39.00003 Modelling Rho GTPase biochemistry to predict collective cell migration** , BRIAN MERCHANT, JAMES FENG, Univ British Columbia — The collective migration of cells, due to individual cell polarization and intercellular contact inhibition of locomotion, features prominently in embryogenesis and metastatic cancers. Existing methods for modelling collectively migrating cells tend to rely either on highly abstracted agent-based models, or on continuum approximations of the group. Both of these frameworks represent intercellular interactions such as contact inhibition of locomotion as hard-coded rules defining model cells. In contrast, we present a vertex-dynamics framework which predicts polarization and contact inhibition of locomotion naturally from an underlying model of Rho GTPase biochemistry and cortical mechanics. We simulate the interaction between many such model cells, and study how modulating Rho GTPases affects migratory characteristics of the group, in the context of long-distance collective migration of neural crest cells during embryogenesis.

**9:00AM E39.00004 Two distinct actin networks mediate traction oscillations to confer mechanosensitivity of focal adhesions** , ZHANGHAN WU, Natl Inst of Health - NIH, SERGEY PLOTNIKOV, Univ of Toronto, CLARE WATERMAN, JIAN LIU, Natl Inst of Health - NIH — Cells sense the mechanical stiffness of their extracellular matrix (ECM) by exerting traction force through focal adhesions (FAs), which are integrin-based protein assemblies. Strikingly, FA-mediated traction forces oscillate in time and space and govern durotaxis – the tendency of most cell types to migrate toward stiffer ECM. The underlying mechanism of this intriguing oscillation of FA traction force is unknown. Combining theory and experiment, we develop a model of FA growth, which integrates coordinated contributions of a branched actin network and stress fibers in the process. We show that retrograde flux of branched actin network contributes to a traction peak near the FA distal tip and that stress fiber-mediated actomyosin contractility generates a second traction peak near the FA center. Formin-mediated stress fiber elongation negatively feeds back with actomyosin contractility, resulting in the central traction peak oscillation. This underpins observed spatio-temporal patterns of the FA traction, and broadens the ECM stiffness range, over which FAs could accurately adapt with traction force generation. Our findings shed light on the fundamental mechanism of FA mechanosensing and hence durotaxis.

**9:12AM E39.00005 Cell Shapes and Traction Forces Determine Stress in Motile Confluent Tissue** , XINGBO YANG, Northwestern University, DAPENG BI, Rockefeller University, MICHAEL CZAJKOWSKI, LISA MANNING, CRISTINA MARCHETTI, Syracuse University — Collective cell migration is a highly regulated process involved in wound healing, cancer metastasis and morphogenesis. The understanding of the regulatory mechanism requires the study of mechanical interactions among cells that coordinate their active motion. To this end, we develop a method that determines cellular forces and tissue stresses from experimentally accessible cell shapes and traction forces. This approach allows us for the first time to calculate membrane tensions and hydrostatic pressures at a cellular level in collective migrating cell layers out of equilibrium. It helps us understand the mechanical origin of tissue stresses as previous inferred using Traction Force Microscopy (TFM). We test this approach on a new model of motile confluent tissue, which we term Self-propelled Voronoi Model (SPV) that incorporates cell elasticity, contractility and motility. With the model, we explore the mechanical properties of confluent motile tissue as a function of cell activities and cell shapes in various geometries.

**9:24AM E39.00006 Elastic mismatch enhances cell motility** , YONY BRESLER, BENOIT PALMIERI, MARTIN GRANT, McGill University — In recent years, the study of physics phenomena in cancer has drawn considerable attention. In cancer metastasis, a soft cancer cell leaves the tumor, and must pass through the endothelium before reaching the bloodstream. Using a phase-field model we have shown [1] that the elasticity mismatch between cells alone is sufficient to enhance the motility of the softer cancer cell by means of bursty migration, in agreement with experiment [2]. We will present further characterization of these behaviour, as well as new possible applications for this model. [1] Palmieri, B. et al. Sci. Rep. 5, 11745; [2] Lee, M. et al. Biophys. J 102, 2731 (2012).

**9:36AM E39.00007 Two interacting active dimers on a rigid track** , DAVID MAYETT, Syracuse University, MOUMITA DAS, Rochester Institute of Technology, J. M. SCHWARZ, Syracuse University — Cell migration in morphogenesis and cancer metastasis typically involves an interplay between different cell types. The rules governing such interplay remain largely unknown; however, a recent experiment studying the interaction between neural crest (NC) cells and placodal cells reveals an example of such rules. The study found that NC cells chase the placodal cells by chemotaxis, while placodal cells run away from NC cells when contacted by them. Motivated by this observation, we construct and study a minimal one-dimensional cell-cell model comprised of two cells with each cell represented by two-beads-connected-by-an-active spring. The active spring for each moving cell models the stress fibers with their myosin-driven contractility (and alpha-actinin extensibility), while the friction coefficients of the beads describe the catch/slip bond behavior of the integrins in focal adhesions. We also include a dynamic contact interaction between the two cells to decipher the chase-and-run dynamics observed in the experiment. We then use our model to construct a "phase diagram" consisting of chase-and-run behavior, clumping (of the two cells) with repolarization behavior and clumping with no repolarization behavior that can be qualitatively compared to experiments.

**9:48AM E39.00008 Traction force and tension fluctuations in growing axons** , JEFFREY URBACH, JAMIE POLACKWICH, DANIEL KOCH, RYAN MCALLISTER, Georgetown University, HERBERT GELLER, NHLBI, NIH — Actively generated mechanical forces play a central role in axon growth and guidance during nervous system development. We describe the dynamics of traction stresses from growth cones of actively advancing axons from postnatal rat DRG neurons. By tracking the movement of the growth cone and analyzing the traction stresses in a co-moving reference frame, we show that there is a clear and consistent average stress field underlying the complex spatial stresses present at any one time. The average stress field has strong maxima on the sides of the growth cone, directed inward toward the growth cone neck. This pattern represents a contractile stress contained within the growth cone, and a net force that is balanced by the axon tension. In addition, using high time-resolution measurements, we show that the stress field is composed of fluctuating local stress peaks, with a population of peaks whose lifetime distribution follows an exponential decay, and a small number of very long-lived peaks. We also find that the tension appears to vary randomly over short time scales, roughly consistent with the lifetime of the stress peaks, suggesting that the tension fluctuations originate from stochastic adhesion dynamics.

**10:00AM E39.00009 Multiscale Modeling of Cell Interaction in Angiogenesis: From the Micro- to Macro-scale**, SAMARA PILLAY, PHILIP MAINI, HELEN BYRNE, University of Oxford — Solid tumors require a supply of nutrients to grow in size. To this end, tumors induce the growth of new blood vessels from existing vasculature through the process of angiogenesis. In this work, we use a discrete agent-based approach to model the behavior of individual endothelial cells during angiogenesis. We incorporate crowding effects through volume exclusion, motility of cells through biased random walks, and include birth and death processes. We use the transition probabilities associated with the discrete models to determine collective cell behavior, in terms of partial differential equations, using a Markov chain and master equation framework. We find that the cell-level dynamics gives rise to a migrating cell front in the form of a traveling wave on the macro-scale. The behavior of this front depends on the cell interactions that are included and the extent to which volume exclusion is taken into account in the discrete micro-scale model. We also find that well-established continuum models of angiogenesis cannot distinguish between certain types of cell behavior on the micro-scale. This may impact drug development strategies based on these models.

**10:12AM E39.00010 Cellular Polarization and Contractility in Collective Cell Migration<sup>1</sup>**, KAZAGE J CHRISTOPHE UTUJE, Syracuse University, JACOB NOTBOHM, University of Wisconsin-Madison, SHILADITYA BANERJEE, University of Chicago, BOMI GWEON, Hanyang University, HWANSEOK JANG, YONGDOO PARK, Korea University, JENNIFER SHIN, KAIST, JAMES P. BUTLER, JEFFREY J. FREDBERG, Harvard T.H. Chan School of Public Health, M. CRISTINA MARCHETTI, Syracuse University — Collective cell migration drives many biological processes such as metastasis, morphogenesis and wound healing. These coordinated motions are driven by active forces. The physical nature of these forces and the mechanisms by which they generate collective cell migration are still not fully understood. We have developed a minimum physical model of a cell monolayer as an elastic continuum whose deformation field is coupled to two internal degrees of freedom: the concentration of a chemical signal, controlling cell contractility, and the polarization field controlling the direction of local cell motion. By combining theory with experiments, we show that these two internal variables account for the sloshing waves and the systematic deviations of the direction of cell polarization from that of local cell velocity observed in confined cell monolayers.

<sup>1</sup>KJCU and MCM were supported by the Simons Foundation.

**10:24AM E39.00011 Analysis of Shape Dynamics and Actin Polymerization of Collectively Migrating Streams of Cells**, CHENLU WANG, Biophysics Program, University of Maryland, College Park, CAROLE A. PARENT, LCMB, National Cancer Institute, National Institutes of Health, WOLFGANG LOSERT, Department of Physics, University of Maryland, College Park — We use Principal Component Analysis (PCA) to investigate cell-cell coupling during collective cell migration of Dictyostelium discoideum, and explore the underlying mechanisms that regulate the coupling. From PCA of the cell boundary motion obtained from time-lapse images of multicellular streams, we find that cells in streams exhibit more localized anterior protrusions than individually migrating cells. We also find that traveling protrusion waves along cell boundaries connect from cell to cell with high correlation. Further analysis of actin polymerization indicates that actin polymerization is significantly enhanced at the leading edge of cells at cell-cell contacts. The coupling of waves disappears when reducing F-actin polymerization with Latrunculin A.

**10:36AM E39.00012 Connecting single cell to collective cell behavior in a unified theoretical framework**, MISHEL GEORGE, FRANCESCO BULLO, OTGER CAMPÀS, University of California - Santa Barbara — Collective cell behavior is an essential part of tissue and organ morphogenesis during embryonic development, as well as of various disease processes, such as cancer. In contrast to many *in vitro* studies of collective cell migration, most cases of *in vivo* collective cell migration involve rather small groups of cells, with large sheets of migrating cells being less common. The vast majority of theoretical descriptions of collective cell behavior focus on large numbers of cells, but fail to accurately capture the dynamics of small groups of cells. Here we introduce a low-dimensional theoretical description that successfully captures single cell migration, cell collisions, collective dynamics in small groups of cells, and force propagation during sheet expansion, all within a common theoretical framework. Our description is derived from first principles and also includes key phenomenological aspects of cell migration that control the dynamics of traction forces. Among other results, we explain the counter-intuitive observations that pairs of cells repel each other upon collision while they behave in a coordinated manner within larger clusters.

**10:48AM E39.00013 Emergence of oligarchy in collective cell migration.**, LINUS SCHUMACHER, PHILIP MAINI, RUTH BAKER, University of Oxford — Identifying the principles of collective cell migration has the potential to help prevent birth defects, improve regenerative therapies and develop model systems for cancer metastasis. In collaboration with experimental biologists, we use computational simulations of a hybrid model, comprising individual-based stochastic cell movement coupled to a reaction-diffusion equation for a chemoattractant, to explore the role of cell specialisation in the guidance of collective cell migration. In the neural crest, an important migratory cell population in vertebrate embryo development, we present evidence that just a few cells are guiding group migration in a cell-induced chemoattractant gradient that determines the switch between “leader” and “follower” behaviour in individual cells. This leads us to more generally consider under what conditions cell specialisation might become advantageous for collective migration. Alternatively, individual cell responses to locally different microenvironmental conditions could create the (artefactual) appearance of heterogeneity in a population of otherwise identical cellular agents. We explore these questions using a self-propelled particle model as a minimal description for collective cell migration in two and three dimensions.

**Tuesday, March 15, 2016 8:00AM - 11:00AM –**

**Session E40 GSNP GPC: Leo Kadanoff Session I** 343 - Sidney Nagel, University of Chicago

**8:00AM E40.00001 Droplet formation and neck rupture in granular streams and dense suspensions**, HEINRICH JAEGER, University of Chicago — When a pendant drop of liquid breaks off, the final stages of neck formation before the singular event of separation are well described by a power law with an exponent that characterizes the liquid. Specifically, a linear decrease of the neck width with time to breakup implies a highly viscous liquid, while sublinear behavior with exponent 2/3 signals the inviscid limit. It therefore has come as a complete surprise that droplet neck formation in dry granular streams as well as concentrated suspensions, both systems with high apparent viscosity, exhibits the same scaling as the inviscid case. I will discuss some of the experimental evidence for this behavior and attempt an explanation that explicitly considers an aspect unique to the presence of the particles: the feedback between the ability of a (nearly) jammed state to deform and the Gaussian curvature introduced by the neck

**8:12AM E40.00002 Particle Laden Flows from Theory to Experiment<sup>1</sup>**, ANDREA BERTOZZI, Univ of California - Los Angeles — Leo Kadanoff inspired a generation of collaboration across the boundaries of applied mathematics, theoretical physics, engineering, and experimental physics. His influence is seen in laboratories, classrooms, PhD theses, and even undergraduate research across the world. In this talk I review a body of research at UCLA spanning the past ten years in which we have worked to understand the basic physics of particle laden flow by comparing experiments with mathematical models. The project was inspired by some initial experiments and models developed by A. Hosoi's group at MIT. We derive and analyze systems of conservation laws with rich behavior that includes multiple shocks, rarefactions, and singular shocks - and study these along side laboratory experiments. Our work includes both basic physics problems and industrial applications such as spiral separators used in the mining industry.

<sup>1</sup>Supported by NSF grants DMS-1312543 and DMS-1045536

**8:24AM E40.00003 Surface tension models for particle laden thin films<sup>1</sup>**, JEFFREY WONG, LI WANG, ANDREA BERTOZZI, Univ of California - Los Angeles — We study viscous slurries on an incline, for which particles migrate in a fluid due to a combination of gravity-induced settling and shear-induced migration. The lubrication model for the bulk of the fluid is a hyperbolic system of conservation laws for the film height and particle concentration which exhibits interesting behavior, including singular shock solutions corresponding to accumulation of particles at the front. The addition of surface tension to the model produces a capillary ridge that is affected by the particle accumulation and in two dimensions leads to fingering instabilities. We compare this model to experimental results.

<sup>1</sup>This work is supported by NSF grants DMS-1312543 and DMS-1045536.

**8:36AM E40.00004 Plastic flow of polycrystalline materials**, JAMES LANGER<sup>1</sup>, University of California, Santa Barbara — Leo Kadanoff had a long interest in fluid flows, especially fingering instabilities. This interest was one example of his insatiable curiosity about simple, fundamentally important, and often multidisciplinary phenomena. Here is an example of another class of such phenomena that I had hoped to show him this year. The experts in polycrystalline solid mechanics have insisted for decades that their central problem – dislocation-mediated strain hardening – is intrinsically unsolvable. I think they're wrong. My colleagues and I have made progress recently in theories of both amorphous and polycrystalline plasticity by introducing an effective disorder temperature as a dynamical variable in our equations of motion. In this way, we have been able to describe how the densities of flow defects or dislocations evolve in response to external forcing, and thus to develop theories that promise to become as predictive, and full of surprises, as the laws of fluid flow.

<sup>1</sup>For Kadanoff session

**8:48AM E40.00005 Scaling theory of the jamming transition<sup>1</sup>**, ANDREA LIU, University of Pennsylvania, Department of Physics and Astronomy, CARL GOODRICH, SEAS, Harvard University, JAMES SETHNA, Cornell University, Department of Physics, SIDNEY NAGEL, University of Chicago, James Franck Institute — The concept of jamming was first introduced at the University of Chicago by Sid Nagel and Tom Witten. By now we know that there is a zero-temperature critical jamming transition that marks the onset of rigidity in packings of soft repulsive spheres. In contrast to the perfect fcc crystal state, which is the maximally stable state for such systems, the jammed state is only marginally stable mechanically, and thus represents an opposite extreme to the perfect crystal. This marginal stability gives rise to power law scalings and diverging length scales at the transition. Here I will discuss recent developments that put the jamming transition in the same place that the Ising transition was when Leo Kadanoff introduced the ideas of coarse-graining and rescaling into critical phenomena.

<sup>1</sup>Supported by DOE-DE-FG02-05ER46199

**9:00AM E40.00006 Thermal Boundary Layer Equation for Turbulent Rayleigh-Bénard Convection<sup>1</sup>**, EMILY SC CHING, Department of Physics, The Chinese University of Hong Kong, OLGA SHISHKINA, Max Planck Institute for Dynamics and Self-Organization, SUSANNE HORN, Department of Mathematics, Imperial College, SEBASTIAN WAGNER, Max Planck Institute for Dynamics and Self-Organization — Turbulent Rayleigh-Bénard convection, consisting of a fluid confined between two horizontal plates, heated from below and cooled from above, is a paradigm system for studying turbulent thermal convection, which is ubiquitous in nature. In turbulent Rayleigh-Bénard convection, there are viscous boundary layers near all rigid walls and two thermal boundary layers, one above the bottom plate and one below the top plate. The classical Prandtl-Blasius-Pohlhausen theory has often been used to describe the mean velocity and temperature boundary layer profiles but systematic deviations are known to exist. These deviations are due to turbulent fluctuations. In this talk, we report a new thermal boundary layer equation for turbulent Rayleigh-Bénard convection derived for Prandtl number (Pr) greater than 1, which takes into account the effects of turbulent fluctuations by using the idea of an eddy thermal diffusivity. Solving this equation, we have obtained two analytical mean temperature profiles for  $Pr \sim 1$  and  $Pr \gg 1$ . These two theoretical predictions are shown to be in excellent agreement with the results of our direct numerical simulations for  $Pr=4.38$  (water) and  $Pr=2547.9$  (glycerol).

<sup>1</sup>Work of ESCC was supported by the Hong Kong Research Grants Council under Grant No. CUHK-400311.

**9:12AM E40.00007 Leo Kadanoff's legacy for turbulent thermal convection**, DETLEF LOHSE<sup>1</sup>, University of Twente — Rayleigh-Bénard (RB) convection the buoyancy-driven flow of a fluid heated from below and cooled from above is a classical problem in fluid dynamics. It played a crucial role in the development of stability theory in hydrodynamics (Rayleigh, Chandrasekhar) and had been paradigmatic in pattern formation and in the study of spatial-temporal chaos (Ahlers, Libchaber, and many other). It was Leo Kadanoff and his associates in Chicago who, in the 1980s and 1990s, propagated the RB system as paradigmatic for the *physics* of fully developed turbulence and contributed tremendously to today's understanding of thermally driven turbulence. He and his experimental coworkers (Libchaber et al.) revealed the importance of the thermal plumes and the large-scale wind, and elucidated the interplay between thermal boundary layers and bulk. His scaling analysis laid the basis for our present understanding of turbulent convection, which I will review in this talk, highlighting Leo's trailblazing contributions.

<sup>1</sup>Kadanoff session

**9:24AM E40.00008 Control and large deformations of marginal disordered structures**, ARVIND MURUGAN, MATTHEW PINSON, University of Chicago, ELIZABETH CHEN, Harvard University — Designed deformations, such as origami patterns, provide a way to make easily controlled mechanical metamaterials with tailored responses to external forces. We focus on an often overlooked regime of origami - non-linear deformations of large disordered origami patterns with no symmetries. We find that practical questions of control in origami have counterintuitive answers, because of intimate connections to spin glasses and neural networks. For example, 1 degree of freedom origami structures are actually difficult to control about the flat state with a single actuator; the actuator is thrown off by an exponential number of 'red herring' zero modes for small deformations, all but one of which disappear at larger deformations. Conversely, structures with multiple programmed motions are much easier to control than expected - in fact, they are as easy to control as a dedicated single-motion structure if the number of programmed motions is below a threshold ('memory capacity').

**9:36AM E40.00009 Planarity of Force Tilings in Jammed Packings of Disks<sup>1</sup>**, KABIR RAMOLA, BULBUL CHAKRABORTY, Brandeis University — We propose a new order parameter for load induced jamming transitions in disk packings based on the planarity of force tilings. Contact forces between disks in mechanical equilibrium can be arranged in a dual space to form a network (tiling) represented by a set of vertices and edges  $\mathcal{G} = (V, E)$ . A Delaunay triangulation of these vertices then forms a related network  $\mathcal{G}_D = (V, E_D)$ . We define a planarity order parameter  $\psi$  as the overlap of these two graphs  $\psi = \langle \mathcal{G}_D | \mathcal{G} \rangle$ . We use this parameter to characterize jamming transitions in two dimensional granular systems. We find clear signatures of the existence of non-planar and planar phases as a function of external load. We study this behaviour using simulation data of frictionless soft disks and experimental data of frictional disk packings.

<sup>1</sup>This work has been supported by NSF-DMR 1409093 and the W. M. Keck Foundation.

**9:48AM E40.00010 Consolidation by lubrication at sedimentary jamming fronts**, DOUGLAS DURIAN, CARLOS ORTIZ, TED BRZINSKI, University of Pennsylvania — We formulate a nonlinear partial differential equation to describe changes in packing fraction for sedimenting particles at low Reynolds number. It is based on two key fluid-mediated forces. One is the viscous interaction of a particle with the surrounding suspension, which causes the settling speed to decrease with increasing packing fraction according to a hindered settling function; we constrain its form by a comprehensive data compilation. The other ingredient is a lubrication force that resists change in separation between neighboring particles; it diverges at contact and hence captures the accumulation of a close-packed sediment. These forces, plus gravity and mass conservation, lead to a new "sedimentation equation" that we propose for the evolution of packing fraction versus position and time. Asymptotic and numerical solutions are presented, and compared with experiment, for the shape of the stationary jamming front between sediment and suspension that moves upwards at constant shape and speed.

**10:00AM E40.00011 What are the microscopic origins of shear jamming?**<sup>1</sup>, BOB BEHRINGER, DONG WANG, Duke University, JIE REN, Merck & Co., JONATHAN BARES, Duke University, BULBUL CHAKRABORTY, Brandeis University, LENKA KOVALCINOVA, LOU KONDIC, NJIT — Granular materials can jam by shear: shear strain applied to a stress-free state in a packing fraction range  $\phi_S < \phi < \phi_J$ , leads to mechanically stable (jammed) anisotropic states (Bi et al. Nature, 2011).  $\phi_J$  is the lowest  $\phi$  for which an isotropic state is jammed, and shear jamming ceases below  $\phi_S$ . The process of shear jamming involves the formation of strong force networks that are initially highly anisotropic 'force chains', then become more isotropic with increasing shear. The mechanisms that lead to shear jamming are also presumably similar to those that lead to Reynolds dilatancy. What microscopic processes can account for shear jamming? Force chains, roughly linear sequences of particles experiencing average or above forces are not stable by themselves. Hence, force chain particles must form additional 'non-chain' contacts. Here, we propose micro-scale structures and their response to shear that serve as a basis to understand the formation of stable force networks and shear jamming. We identify these structures in experimental and numerical data, and track their response to shear.

<sup>1</sup>Work supported by NSF-DMR1206351, DMS1248071, NASA NNX15AD38G, and the W.M. Keck Foundation

**10:12AM E40.00012 Itokawa: a case for ballistic segregation**<sup>1</sup>, TROY SHINBROT, Rutgers University, TAPAN SABAWULA, Okinawa Institute for Science and Technology, THEO SIU, MIGUEL VIVAR LAZO, Rutgers University, PINAKI CHAKRABORTY, Okinawa Institute for Science and Technology — Recent photographs of the asteroid Itokawa have revealed strong separation between regions populated almost entirely by small pebbles and other regions consisting only of larger boulders. This size separation has been attributed to the Brazil Nut Effect (BNE), however we point out here that the BNE depends on conditions such as isotropic gravity, parallel sidewalls and periodic vertical shaking that are wholly absent on asteroids. On the other hand, surface areas of boulders and pebbles appear to be comparable on Itokawa, and in this situation it follows that the asteroid must have suffered many orders of magnitude more collisions with pebbles than with boulders. We observe that a pebble will tend to bounce off of a boulder but will sink into a sea of similar pebbles, and so we predict that seas of pebbles must grow on such asteroids. We carry out experiments and simulations to evaluate this and related predictions, and we demonstrate that this new mechanism of segregation based on simple counting of grains can produce the strong separation of sizes reported.

<sup>1</sup>Support provided by NSF grant 1404792

**10:24AM E40.00013 A trans-phase granular continuum relation and its use in simulation**, KEN KAMRIN, SACHITH DUNATUNGA, HESAM ASKARI, MIT — The ability to model a large granular system as a continuum would offer tremendous benefits in computation time compared to discrete particle methods. However, two infamous problems arise in the pursuit of this vision: (i) the constitutive relation for granular materials is still unclear and hotly debated, and (ii) a model and corresponding numerical method must wear "many hats" as, in general circumstances, it must be able to capture and accurately represent the material as it crosses through its collisional, dense-flowing, and solid-like states. Here we present a minimal trans-phase model, merging an elastic response beneath a fictional yield criterion, a  $\mu(I)$  rheology for liquid-like flow above the static yield criterion, and a disconnection rule to model separation of the grains into a low-temperature gas. We simulate our model with a meshless method (in high strain/mixing cases) and the finite-element method. It is able to match experimental data in many geometries, including collapsing columns, impact on granular beds, draining silos, and granular drag problems.

**10:36AM E40.00014 A Hierarchy of Dynamic Equilibria and a View of a Fly's Equilibrium Reflex**, Z. JANE WANG<sup>1</sup>, Cornell University — Understanding structures within a structure is a topic that has fascinated Leo throughout his life, and we are now benefiting from his fundamental insights when we think about living organisms. A living organism is far from statistical equilibrium and it does not have a single critical parameter. Nevertheless, each organism has a hierarchical structure within itself. Recently, asking how often a fly must sense its orientation in order to balance in air has led us to suggest one of the fly's 17 steering muscles, the first basalar muscle, is responsible for maintaining flight stability. Here I suggest that the chain of events associated with flight equilibrium reflex can be viewed as a succession of local linear transformation about a set of dynamic equilibria[1]. Each of the functionally different parts, the sensors, motor neurons, muscles, wing-hinges, flapping wings, and the thorax, operates near its own dynamic equilibrium, often close to the boundary between stability and instability. Locomotion rises as an organism responds to a small perturbation from these equilibria. [1] ZJ Wang, Ann. Rev. Cond. Matter Physics, Vol 7, 2016

<sup>1</sup>Kadanoff session

**10:48AM E40.00015 The life of vortex knots and the flow of helicity**, WILLIAM IRVINE, University of Chicago — What happens if you take a vortex loop - akin to a smoke ring in air - and tie it into a knot or a link? The knottiness (Helicity) of a fluid is a conserved quantity in many idealized situations (such as Euler fluids) offering the potential for fundamental insights into fluid flow. In real fluids, progress has been hindered by lack of accessible experimental systems. I will tell of how to make a vortex knot and link in water, in the wave function of a superfluid (on a computer) and of what happens thence, with an emphasis on universal aspects of the dynamics and the flow of helicity.

**Tuesday, March 15, 2016 8:00AM - 11:00AM —**

**Session E41 DBIO: Physics of Neural Systems 344 - Marc Howard, Boston University**

**8:00AM E41.00001 An objective function for Hebbian self-limiting synaptic plasticity rules**, CLAUDIUS GROS, SAMUEL ECKMANN, RODRIGO ECHEVESTE, Institute for Theoretical Physics, Goethe University Frankfurt — Objective functions, formulated in terms of information theoretical measures with respect to the input and output probability distributions, provide a useful framework for the formulation of guiding principles for information processing systems, such as neural networks. In the present work, a guiding principle for neural plasticity is formulated in terms of an objective function expressed as the Fisher information with respect to an operator that we denote as the synaptic flux <sup>1</sup>. By minimization of this objective function, we obtain Hebbian self-limiting synaptic plasticity rules, avoiding unbounded weight growth. Furthermore, we show how the rules are selective to directions of maximal negative excess kurtosis, making them suitable for independent component analysis. As an application, the non-linear bars problem <sup>2</sup> is studied, in which each neuron is presented with a non-linear superposition of horizontal and vertical bars. We show that, under the here presented rules, the neurons are able to find the independent components of the input.

<sup>1</sup>Echeveste & Gros, **Front. Robot. AI** 1, 2014

<sup>2</sup>Földiák, **Biol. Cybern.** 64: 165170, 1990

**8:12AM E41.00002 Calculation of correlation function of a spatially coupled spiking neural network**<sup>1</sup>, SIWEI QIU, CARSON CHOW, Lab of Biological Mathematics, NIDDK, National Institute of Health — The dynamics of a large but finite number of coupled spiking neurons is not well understood. We analyze finite size effects in a network of synaptically coupled theta neurons. We show how the system can be characterized by a functional integral from which finite size effects are calculated perturbatively. We discuss the implications of this technique for bump attractors.

<sup>1</sup>Thanks to support of the Intramural Research Program of the NIH, NIDDK

**8:24AM E41.00003 The role of symmetry in the regulation of brain dynamics.**, EVELYN TANG, CHAD GIUSTI, University of Pennsylvania, MATTHEW CIESLAK, SCOTT GRAFTON, University of California, Santa Barbara, DANIELLE BASSETT, University of Pennsylvania — Synchronous neural processes regulate a wide range of behaviors from attention to learning. Yet structural constraints on these processes are far from understood. We draw on new theoretical links between structural symmetries and the control of synchronous function, to offer a reconceptualization of the relationships between brain structure and function in human and non-human primates. By classifying 3-node motifs in macaque connectivity data, we find the most prevalent motifs can theoretically ensure a diversity of function including strict synchrony as well as control to arbitrary states. The least prevalent motifs are theoretically controllable to arbitrary states, which may not be desirable in a biological system. In humans, regions with high topological similarity of connections (a continuous notion related to symmetry) are most commonly found in fronto-parietal systems, which may account for their critical role in cognitive control. Collectively, our work underscores the role of symmetry and topological similarity in regulating dynamics of brain function.

**8:36AM E41.00004 Synchronization in a non-uniform network of excitatory spiking neurons.**, RODRIGO ECHEVESTE, CLAUDIUS GROS, Institute for Theoretical Physics, Goethe University Frankfurt — Spontaneous synchronization of pulse coupled elements is ubiquitous in nature and seems to be of vital importance for life <sup>1</sup>. Networks of pacemaker cells in the heart <sup>2</sup>, extended populations of southeast asian fireflies <sup>3</sup>, and neuronal oscillations in cortical networks <sup>4</sup>, are examples of this. In the present work, a rich repertoire of dynamical states with different degrees of synchronization are found in a network of excitatory-only spiking neurons connected in a non-uniform fashion. In particular, uncorrelated and partially correlated states are found without the need for inhibitory neurons or external currents. The phase transitions between these states, as well the robustness, stability, and response of the network to external stimulus are studied.

<sup>1</sup>Strogatz & Stewart, **Sci. Am.** 269(6): 102-109, 1993.

<sup>2</sup>Peskin, **Mathematical aspects of heart physiology**, Courant Institute of Mathematical Sciences, New York University, 1975.

<sup>3</sup>Buck, **Quarterly review of biology** 265-289, 1988.

<sup>4</sup>Buzsaki & Draguhn, **Science** 304(5679): 1926-1929, 2004.

**8:48AM E41.00005 Information Transmission and Anderson Localization in two-dimensional networks of firing-rate neurons**<sup>1</sup>, JOSEPH NATALE, GEORGE HENTSCHEL, Emory Univ — Firing-rate networks offer a coarse model of signal propagation in the brain. Here we analyze sparse, 2D planar firing-rate networks with no synapses beyond a certain cutoff distance. Additionally, we impose Dale's Principle to ensure that each neuron makes only or inhibitory outgoing connections. Using spectral methods, we find that the number of neurons participating in excitations of the network becomes insignificant whenever the connectivity cutoff is tuned to a value near or below the average interneuron separation. Further, neural activations exceeding a certain threshold stay confined to a small region of space. This behavior is an instance of Anderson localization, a disorder-induced phase transition by which an information channel is rendered unable to transmit signals. We discuss several potential implications of localization for both local and long-range computation in the brain.

<sup>1</sup>This work was supported in part by grants JSMF/ 220020321 and NSF/IOS/1208126

**9:00AM E41.00006 Controlling chaos in balanced neural circuits with input spike trains**, RAINER ENGELKEN, FRED WOLF, MPI for Dynamics and Self-Organization, Goettingen, Germany, BCCN Gttingen, Germany, University of Goettingen, Germany — The cerebral cortex can be seen as a system of neural circuits driving each other with spike trains. Here we study how the statistics of these spike trains affects chaos in balanced target circuits. Earlier studies of chaos in balanced neural circuits either used a fixed input [van Vreeswijk, Sompolinsky 1996, Monteforte, Wolf 2010] or white noise [Lajoie et al. 2014]. We study dynamical stability of balanced networks driven by input spike trains with variable statistics. The analytically obtained Jacobian enables us to calculate the complete Lyapunov spectrum. We solved the dynamics in event-based simulations and calculated Lyapunov spectra, entropy production rate and attractor dimension. We vary correlations, irregularity, coupling strength and spike rate of the input and action potential onset rapidness of recurrent neurons. We generally find a suppression of chaos by input spike trains. This is strengthened by bursty and correlated input spike trains and increased action potential onset rapidness. We find a link between response reliability and the Lyapunov spectrum. Our study extends findings in chaotic rate models [Molgedey et al. 1992] to spiking neuron models and opens a novel avenue to study the role of projections in shaping the dynamics of large neural circuits.

**9:12AM E41.00007 Simulation of dendritic growth reveals necessary and sufficient parameters to describe the shapes of dendritic trees.** , OLIVIER TROTTIER, SUJOY GANGULY, HUGO BOWNE-ANDERSON, Yale University, XIN LIANG, Tsinghua University, JONATHON HOWARD, Yale University — For the last 120 years, the development of neuronal shapes has been of great interest to the scientific community. Over the last 30 years, significant work has been done on the molecular processes responsible for dendritic development. In our ongoing research, we use the class IV sensory neurons of the *Drosophila melanogaster* larva as a model system to understand the growth of dendritic arbors. Our main goal is to elucidate the mechanisms that the neuron uses to determine the shape of its dendritic tree. We have observed the development of the class IV neuron's dendritic tree in the larval stage and have concluded that morphogenesis is defined by 3 distinct processes: 1) branch growth, 2) branching and 3) branch retraction. As the first step towards understanding dendritic growth, we have implemented these three processes in a computational model. Our simulations are able to reproduce the branch length distribution, number of branches and fractal dimension of the class IV neurons for a small range of parameters.

**9:24AM E41.00008 Partial Synchronization in Pulse-Coupled Oscillator Networks I: Theory<sup>1</sup>** , JAN ENGELBRECHT, BOLUN CHEN, RENATO MIROLLO, Boston College — We study  $N$  identical integrate and fire model neurons coupled in an all to all network through  $\alpha$ -function pulses, weighted by a parameter  $K$ . Studies of the dynamics of this system often focus on the stability of the fully synchronous and the fully asynchronous splay states, that naturally depend on the sign of  $K$ , i.e. excitation vs inhibition. We find that for finite  $N$  there is a rich set of other partially synchronized attractors, such as  $(N - 1, 1)$  fixed states and partially synchronized splay states. Our framework exploits the neutrality of the dynamics for  $K = 0$  which allows us to implement a dimensional reduction strategy that replaces the discrete pulses with a continuous flow, with the sign of  $K$  determining the flow direction. This framework naturally incorporates a hierarchy of partially synchronized subspaces in which the new states lie. For  $N = 2, 3, 4$ , we completely describe the sequence of bifurcations and the stability of all fixed points and limit cycles.

<sup>1</sup>Work Supported by NSF DMS 1413020

**9:36AM E41.00009 Partial Synchronization in Pulse-Coupled Oscillator Networks II: A Numerical Study<sup>1</sup>** , BOLUN CHEN, JAN R. ENGELBRECHT, RENATO MIROLLO, Boston College — We use high-precision numerical simulations, to compute the dynamics of  $N$  identical integrate and fire model neurons coupled in an all-to-all network through  $\alpha$ -function pulses. In particular, we determine the discrete evolution of the state of our system from spike to spike. In addition to traditional fully synchronous and splay states, we exhibit multiple competing partially synchronized ordered states, which are fixed points and limit cycles in the phase space. Close examinations reveal the bifurcations among different states. By varying the parameters, we map out the phase diagram of stable fixed points. Our results illustrate the power of dimensional reduction in complex dynamical systems, and shed light on the collective behaviors of neural networks.

<sup>1</sup>Work supported by NSF DMS 1413020.

**9:48AM E41.00010 Critical behavior of large maximally informative neural populations<sup>1</sup>** , JOHN BERKOWITZ, Univ of California - San Diego, TATYANA SHARPEE, Computational Neurobiology Laboratory, Salk Institute for Biological Studies, La Jolla, CA; Department of Physics, University of California, San Diego — We consider maximally informative encoding of scalar signals by neural populations. In a small time window, neural responses are binary, with spiking probability that follows a sigmoidal tuning curve. The width of the tuning curve represents effective noise in neural transmission. Previous analyses of this problem for relatively small numbers of neurons with identical noise parameters indicated the presence of multiple bifurcations that occurred with decreasing noise value. For very high noise values, maximal information is achieved when all neurons have the same threshold values. With decreasing noise, the threshold values split into two or more groups via a series of bifurcations, until finally each neuron has a different threshold. Analyzing this problem in the large  $N$  limit, we found instead that there is a single phase transition from redundant coding to coding based on distributed thresholds. The order parameter of this transition is the threshold standard deviation across the population; differences in noise parameter from the mean are analogous to local magnetic fields. Near the bifurcation point, information transmitted follows a Landau expansion. We use this expansion to quantify the scaling of the order parameter with noise and effective magnetic field.

<sup>1</sup>NSF CAREER award IIS-1254123, NSF Ideas Lab Collaborative Research IOS 1556388.

**10:00AM E41.00011 Spike frequency adaptation is a possible mechanism for control of attractor preference in auto-associative neural networks.<sup>1</sup>** , JAMES ROACH, LEONARD SANDER, MICHAL ZOCHOWSKI, Univ of Michigan - Ann Arbor — Auto-associative memory is the ability to retrieve a pattern from a small fraction of the pattern and is an important function of neural networks. Within this context, memories that are stored within the synaptic strengths of networks act as dynamical attractors for network firing patterns. In networks with many encoded memories, some attractors will be stronger than others. This presents the problem of how networks switch between attractors depending on the situation. We suggest that regulation of neuronal spike-frequency adaptation (SFA) provides a universal mechanism for network-wide attractor selectivity. Here we demonstrate in a Hopfield type attractor network that neurons minimal SFA will reliably activate in the pattern corresponding to a local attractor and that a moderate increase in SFA leads to the network to converge to the strongest attractor state. Furthermore, we show that on long time scales SFA allows for temporal sequences of activation to emerge. Finally, using a model of cholinergic modulation within the cortex we argue that dynamic regulation of attractor preference by SFA could be critical for the role of acetylcholine in attention or for arousal states in general.

<sup>1</sup>This work was supported by: NSF Graduate Research Fellowship Program under Grant No. DGE 1256260 (JPR), NSF CMMI 1029388 (MRZ) and NSF PoLS 1058034 (MRZ & LMS)

**10:12AM E41.00012 On the Emergent Properties of Recurrent Neural Networks at Criticality** , YAHYA KARIMIPANAH, ZHENGYU MA, RALF WESSEL, Washington University in St. Louis — Irregular spiking is a widespread phenomenon in neuronal activities in vivo. In addition, it has been shown that the firing rate variability decreases after the onset of external stimuli. Since these are known as two universal features of cortical activity, it is natural to ask whether there is a universal mechanism underlying such phenomena. Independently, there has been mounting evidence that superficial layers of cortex operate near a second-order phase transition (critical point), which is manifested in the form of scale free activity. However, despite the strong evidence for such a criticality hypothesis, it is still very little known on how it can be leveraged to facilitate neural coding. As the decline in response variability is regarded as an essential mechanism to enhance coding efficiency, we asked whether the criticality hypothesis could bridge between scale free activity and other ubiquitous features of cortical activity. Using a simple binary probabilistic model, we show that irregular spiking and decline in response variability, both arise as emergent properties of a recurrent network poised at criticality. Our results provide us with a unified explanation for the ubiquity of these two features, without a need to exploit any further mechanism.

**10:24AM E41.00013 Computing with scale-invariant neural representations<sup>1</sup>**, MARC HOWARD, KARTHIK SHANKAR, Boston Univ — The Weber-Fechner law is perhaps the oldest quantitative relationship in psychology. Consider the problem of the brain representing a function  $f(x)$ . Different neurons have receptive fields that support different parts of the range, such that the  $i$ th neuron has a receptive field at  $x_i$ . Weber-Fechner scaling refers to the finding that the width of the receptive field scales with  $x_i$  as does the difference between the centers of adjacent receptive fields. Weber-Fechner scaling is exponentially resource-conserving. Neurophysiological evidence suggests that neural representations obey Weber-Fechner scaling in the visual system and perhaps other systems as well. We describe an optimality constraint that is solved by Weber-Fechner scaling, providing an information-theoretic rationale for this principle of neural coding. Weber-Fechner scaling can be generated within a mathematical framework using the Laplace transform. Within this framework, simple computations such as translation, correlation and cross-correlation can be accomplished. This framework can in principle be extended to provide a general computational language for brain-inspired cognitive computation on scale-invariant representations.

<sup>1</sup>Supported by NSF PHY 1444389 and the BU Initiative for the Physics and Mathematics of Neural Systems,

**10:36AM E41.00014 ABSTRACT WITHDRAWN —**

**10:48AM E41.00015 Physics of Intrinsic and Extrinsic Factors that Cause the Onset of the Deadliest Illness of Mankind and are Important for Diagnostics and Treatment**, ARJUN SAXENA, retired — One of the most important topic of research in the field of Physics of Behavior is the deadliest illness of mankind which is the group of illnesses called mental illnesses. They are getting attention increasingly worldwide by the medical communities and their respective governments, because of the following fact. It is now well established that these illnesses cause more loss of human lives, destruction of families, businesses and overall economy than all the other illnesses combined. The purpose of this paper is to identify and provide solutions to two fundamental issues of such illnesses which still remain as problems. One is the stigma associated with them because of their name “mental”. The patients are regarded as less than normal because their illness is only “mental” in origin. The second is that it is still not widely recognized that they are caused by medical problems in their “brain” which afflict their “mind”. This paper explains this and gives an improved 3-D model using the physics of intrinsic and extrinsic factors of both “brain” and “mind”. It leads to an important new name, “BAMI” (Brain and Mind Illness), which eliminates the stigma and gives quantitative parameters to diagnose the illness and monitor medicines to treat such illnesses.

**Tuesday, March 15, 2016 8:00AM - 11:00AM —**

**Session E42 DPOLY: Bi-Component Systems: Composites and Blends** 345 - Debra Audus, NIST

**8:00AM E42.00001 DPOLY SESSION BREAK —**

**8:36AM E42.00002 Broader Understanding of Multiple Component Dynamic Processes in Miscible Polymer/Polymer Blends**, RAVI SHARMA, HENGXI YANG, PETER GREEN, University of Michigan — Utilizing two different experimental techniques, isothermal frequency sweeps and isochronal temperature sweeps, in broadband dielectric spectroscopy can allow for the identification of multiple processes derived from the same relaxation mechanism in certain polymer/polymer blends. A study of poly(vinyl methyl ether) (PVME) in bulk, miscible blends with polystyrene (PS) gives evidence of two separate relaxation processes associated exclusively with the segmental dynamics of PVME; the  $\alpha_0$  process from the temperature sweep, related to average segmental dynamics, and the  $\alpha'$  process from the frequency sweep, related to relaxations confined within “frozen” domains. The appearance of multiple processes is driven by compositional heterogeneity, mainly chain connectivity and concentration fluctuation effects. Analysis of the breadth and intensity of the dielectric loss curves gives insight into the structure and thermodynamics of the blend, which in turn can explain temperature and composition dependent dynamic trends. These results are contrasted with other miscible blend systems, polyisoprene (PI)/poly(4-tert-butylstyrene) (P4tBS) and polyisoprene (PI)/polyvinyl ether (PVE).

**8:48AM E42.00003 Thermal and Mechanical Properties of Poly(methyl methacrylate)/Poly(vinylidene fluoride-r-hexafluoro propylene) Blends<sup>1</sup>**, STEVEN LEE, Materials Science and Engineering, MAEVE CONWAY<sup>2</sup>, Mechanical, Aerospace and Nuclear Engineering, DENIZ RENDE, Center for Materials, Devices and Integrated Systems, RAHMI OZISIK, Materials Science and Engineering; Rensselaer Polytechnic Institute — Poly(vinylidene fluoride), PVDF, is a highly crystalline and rigid polymer, and is used in many applications where chemical inertness, resistance to various solvents and environmental degradation are required. Copolymerization of PVDF with hexafluoropropylene (HFP) tends to decrease the amount of crystallinity, thereby, resulting in a more flexible polymer, which provides new applications for PVDF. Various studies were undertaken to investigate the structure and properties of miscible blends of PVDF and poly(methyl methacrylate), PMMA; however, no studies were performed on the blends of P(VDFHFP) random copolymers and PMMA. In the current study, we investigate the miscibility, and thermal and mechanical properties of P(VDFHFP)/PMMA blends via differential scanning calorimetry, thermogravimetric analysis, and nanoindentation. Results indicate that increasing PMMA concentration leads to decreased crystallinity and shifting of the crystallization onset temperature during cooling to lower values.

<sup>1</sup>This material is based upon work supported by the National Science Foundation under Grant No. CMMI-1538730.

<sup>2</sup>Undergraduate Student

**9:00AM E42.00004 Engineering thermal conductivity in polymer blends<sup>1</sup>**, VAHID RASHIDI, ELEANOR COYLE, JOHN KIEFFER, KEVIN PIPE, Univ of Michigan - Ann Arbor — Weak inter-chain bonding in polymers is believed to be a bottleneck for both thermal conductivity and mechanical strength. Most polymers have low thermal conductivity (~0.1 W/mK), hindering their performance in applications for which thermal management is critical (e.g., electronics packaging). In this work, we use computational methods to study how hydrogen bonding between polymer chains as well as water content can be used to engineer thermal transport in bulk polymers. We examine how changes in the number of hydrogen bonds, chain elongation, density, and vibrational density of states correlate with changes in thermal conductivity for polymer blends composed of different relative constituent fractions. We also consider the effects of bond strength, tacticity, and polymer chain mass. For certain blend fractions, we observe large increases in thermal conductivity, and we analyze these increases in terms of modifications to chain chemistry (e.g., inter-chain bonding) and chain morphology (e.g., chain alignment and radius of gyration). We observe that increasing the number of hydrogen bonds in the system results in better packing as well as better chain alignment and elongation that contribute to enhanced thermal conductivity.

<sup>1</sup>The Air Force Office of Scientific Research, Grant No. FA9550-14-1-0010

**9:12AM E42.00005 Field-theoretic study on colloidal interaction in solutions of adsorbing homopolymers** , WEI LI, KRIS DELANEY, GLENN FREDRICKSON, Univ of California - Santa Barbara — Using self-consistent field theory, we study the free polymer induced (FPI) interaction between colloidal particles in a homopolymer solution. In the colloid limit, the Derjaguin approximation can be applied to relate the potential of mean force between two spherical objects to that between two parallel plates. A field-theoretic model is formulated in the grand canonical ensemble to compute the potential of mean force for the system consisting of two solid plates with polymer solution confined in between. The relationship between polymer-colloid affinity and FPI interaction is investigated through simulations. Three distinct regimes, including depletion interaction, steric repulsion and bridging interaction, are identified. A transition through these interaction regimes with increasing polymer-colloid affinity is shown as a consequence of competing entropic and enthalpic effects. We also study the impact of varying the degree of polymerization of the homopolymer, the solvent quality and the polymer concentration on the FPI interaction.

**9:24AM E42.00006 Entanglement Length in Miscible Blends of *cis*-Polyisoprene and Poly(*p*tert-butylstyrene)** , HIROSHI WATANABE, YUMI MATSUMIYA, Inst. Chem. Res., Kyoto Univ. — In miscible polymer blends, the entanglement length is common for the components, but its changes with the composition  $w$  remain unclear. For this problem, this study analyzed viscoelastic data for miscible blends of *cis*-polyisoprene (PI) and poly(*p*tert-butylstyrene) (PtBS), considering the basic feature that the local relaxation is determined only by  $w_{PI}$ . On the basis of this feature, a series of unentangled low- $M$  PI/PtBS blends having various  $M$  and a given  $w_{PI}$  were utilized as references for well-entangled high- $M$  PI/PtBS blends having the same  $w_{PI}$ , and the modulus data of the references were subtracted from the high- $M$  blend data. For an optimally chosen reference, the storage modulus  $G'_e$  of the high- $M$  blends obtained after the subtraction exhibited a clear entanglement plateau  $G'_N$  and the corresponding  $G''_e$  decreased in proportion to  $1/\omega$  at high frequencies  $\omega$ . Thus, the onset of entanglement relaxation was detected. The  $G'_N$  values were well described by a linear mixing rule of the entanglement length with the number fraction of Kuhn segments of the components being utilized as the averaging weight. This result, not explained by a mean-field picture of entanglement, is discussed in relation to local packing of bulky PtBS chains and skinny PI chains.

**9:36AM E42.00007 Effect of twist-orientation on mechanical properties of self-reinforced poly(lactic acid) screws in simulated body environment** , MASATO SAKAGUCHI, SATOSHI KOBAYASHI, tokyo metropolitan university, COMPOSITE ENGINEERING LAB TEAM — Poly(lactic acid) (PLA) attracts much attention as a typical biodegradable polymer, and has been applied as a bone fixation device. As one of the methods to improve mechanical properties of PLA bone fixation device, orientations of molecular chains have been investigated. However, conventional uniaxial drawing could not improve mechanical properties along the other loading direction than the drawing direction, such as torsion. In this study, screw is treated as a bone fixation device. In order to improve torsional strength of a bioabsorbable PLA screw, twist-orientation method has been developed. PLA screw is prepared through a series of routes including extrusion molding, extrusion drawing, twist-orientation and forging. This screw was immersed in the phosphate buffer solution for 0, 8, 16 and 24 weeks, then shear strength, orientation function, crystallinity and molecular weight were measured. As a result, twist-orientation improves the initial torsional strength of PLA screw without the decrease in initial shear strength. In addition, the shear strength on twist-oriented screw is equivalent that of non-twist oriented screw during immersion until 24 weeks. This result shown that the twist-orientation does not decrease shear strength after immersion.

**9:48AM E42.00008 PVC-OH Functionalized SWCNT Nanocomposites** , ANDRES SALGADO, ROBERT JONES, SAMANTHA RAMIREZ, IBRAHIM ELAMIN, JAMES HINTHORNE, MIRCEA CHIPARA, University of Texas Rio Grande Valley — Nanocomposites of polyvinylchloride loaded with various amounts of OH functionalized Single Walled Carbon Nanotubes (SWCNT-OH) have been obtained by melt mixing using a Haake Rheomixer. The polymeric matrix has been loaded by various amount of SWCNT-OH ranging between 0 and 15 % wt. The as obtained nanocomposites have been measured by Raman spectroscopy using a InVia Renishaw spectrometer. The Raman lines have been deconvoluted into a superposition of extended Breit-Wigner-Fano line shapes. The effect of nanofiller concentration on the stress transfer from the polymeric matrix to SWCNTs has been analyzed and the Radial Breathing Mode was investigated. Differential Scanning Calorimetry revealed modest shifts of the melting and crystallization temperatures upon loading with SWCNT-OH. Additional information has been obtained by X-Ray measurements. The as obtained nanocomposites have not a very good thermal stability due to the thermally induced dehydrochlorination process. The thermogravimetric data are analyzed in detail and related to Raman results. Preliminary data on the thermal stability of these nanocomposites are reported.

**10:00AM E42.00009 Bottlebrush Polymer Additives for Binary Polymer Blends** , HUI ZHEN MAH, PANTEA AFZALI, HANH PHAN, University of Houston, LUQING QI, STACY PESEK, RAFAEL VERDUZCO, Rice University, GILA STEIN, University of Houston — Bottlebrush polymers are highly branched polymers that have been used in applications such as self-assembling photonics, drug delivery and stimuli-responsive surface coatings. However, they have not been widely studied as compatibilizers for polymer blends. In this study, bottlebrush polymers with poly(styrene-*r*-methyl methacrylate) side chains were used as additives for thin film blends of polystyrene (PS) and poly(methyl methacrylate) (PMMA). The blends were heated above the glass transition temperature to drive phase separation, and the resulting morphology was characterized with atomic force microscopy and optical microscopy. Outcomes were compared with PS/PMMA blends that contain conventional compatibilizers such as linear random copolymers of poly(styrene-*r*-methyl methacrylate) and diblock PS-PMMA copolymers. The bottlebrush additive accumulates at the PS/PMMA interface and drives the formation of vesicle-like droplets that assemble into longer chains. The continuity of the chains depends on the blend composition, where a network structure is achieved close to the critical composition. This unusual microstructure was not observed with the other additives, and may be a consequence of preferential wetting of the bottlebrush by the PS phase.

**10:12AM E42.00010 Molecular Dynamics Simulations of Nanoparticles Coated with Charged Polymers** , CHENGYUAN WEN, SHENGFENG CHENG, Virginia Polytechnic Institute and State University — Polymer coating is frequently used to stabilize colloidal and nano-sized particles. We employ molecular dynamics simulations to study nanoparticles coated with polymer chains that contain ionizable groups. In a polar solvent, the chains become charged with counterions dissociated. In the computational model, we treat the solvent as a uniform dielectric background and use the bead-spring model for the polymer chains. Counterions are explicitly included as mobile beads. The nanoparticle is modeled as a layer of sites uniformly distributed on a spherical surface with a certain fraction of sites serving as the tether points of the grafted polymer brush. We vary the grafting density and calculate the distribution of polymer beads and counterions around the nanoparticle. Our results indicate that charged chains adopt extended conformations because of their mutual repulsions. We further study the interactions between two polymer-coated nanoparticles and obtain the potential of mean force. We also find an interesting transition of a confined single layer of such polymer-coated nanoparticles into two layers when the confinement is removed. Results show that the brush-brush contact has a nonuniform distribution and the nanoparticles tend to form dipole-like structures.

**10:24AM E42.00011 Raman Investigations of PVDF-BaTiO<sub>3</sub> Nanocomposites** , JULIO CANTU, Univ of Texas, Rio Grande Valley, CRISTIAN CHIPARA, PULLICKEL AJAYAN, Rice University, JAMES HINTHORNE, MIRCEA CHIPARA, Univ of Texas, Rio Grande Valley — BaTiO<sub>3</sub> nanoparticles (from Nanostructured & Amorphous Materials, Inc.) were dispersed within PVDF powder (from Sigma Aldrich) by melt mixing using a Haake Rheomix with two counter rotating screws. The mixing consisted of 3 segments first at 190 °C and 60 rotations per minute (rpm) for 30 minutes, second at 210 °C and 80 rpm for 15 minutes, and the last at 180 °C and 60 rpm for 30 minutes. Nanocomposites containing various fractions of nanofiller, ranging from 0 to 15 % wt. have been prepared. Raman investigations on the as obtained nanocomposites have been performed by using a Renishaw InVia spectrometer operating at 532 and 785 cm<sup>-1</sup>. Complementary Wide Angle X-Ray Scattering measurements on the same samples revealed that the as obtained nanocomposites have a dominant beta phase and provided additional information about the size of polymeric crystallites. The effect of the nanofiller on the Raman lines of the PVDF are analyzed in detail. The Raman spectra have been deconvoluted assuming a superposition distorted Lorentzian line shape. The changes of the Raman spectrum parameters (position, amplitude, width, and asymmetry factors) due to the loading with BaTiO<sub>3</sub> is discussed.

**10:36AM E42.00012 Coarse-grained explicit solvent simulation of the translational and rotational diffusion of a spherical particle in a polymer solution**, VICTOR PRYAMITSYN, Northwestern University, VENKAT GANESAN, University of Texas at Austin — We use an extension of DPD model to address the dynamical properties of a colloid particle in an unentangled semi-dilute polymer solution. Solvent and monomers are represented as DPD particles. The colloid particle is represented as a larger DPD particle with the rotational degrees of freedom and tangential component of the dissipative and random DPD interactions with the solvent and monomers. This allows us to model a finite slip length boundary condition at the particle fluid interface and study translational  $D_t$  and rotational  $D_r$  diffusivities of a spherical particle. For zero polymer concentration our results agree with the Stokes-Einstein (SE) theory. For dilute and semi-dilute polymer solutions we have found that polymer dynamic follow the Zimm model in a dilute regime and the Rouse model at high polymer concentration. For particles smaller than the polymer  $R_g$  observed  $D_t$  is much higher than SE prediction for  $R > R_g$  SE prediction recovers. We have found that increase of  $D_r$  relative to SE is rather correlated to the  $\frac{R}{R_g}$  ratio than  $\frac{R}{\xi}$ , where  $\xi$  is the thickness of a depletion shell around the particle.  $D_r$  is very sensitive to the slip length at the particle fluid interface and insensitive to  $\frac{R}{R_g}$ .

**10:48AM E42.00013 Characterization of the crosslinking reaction in high performance phenolic resins**, JIGNESHKUMAR PATEL, GUO XIANG ZOU, SHAW LING HSU, university of massachusetts, UNIVERSITY OF MASSACHUSETTS/POLYMER SCIENCE & ENGINEERING TEAM — In this study, a combination of thermal analysis, infrared spectroscopy (near and mid) in conjunction with low field NMR, was used to characterize the crosslinking reaction involving phenol formaldehyde resin and a crosslinking agent, Hexamethylenetetramine (HMTA). The strong hydrogen bonds in the resin and the completely crystalline HMTA ( $T_m = 280$  C) severely hamper the crosslinking process. Yet the addition of a small amount of plasticizer can induce a highly efficient crosslinking reaction to achieve the desired mechanical properties needed in a number of high performance organic-inorganic composites. The infrared spectroscopy clarifies the dissolution process of the crystalline crosslinker and the specific interactions needed to achieve miscibility of the reactants. The thermal analysis enabled us to follow the changing mobility of the system as a function of temperature. The low field NMR with the T1 inverse recovery technique allowed us to monitor the crosslinking process directly. For the first time, it is now possible to identify the functionality of the plasticizer and correlate the crosslinked structure achieved to the macroscopic performance needed for high performance organic-inorganic composites.

**Tuesday, March 15, 2016 8:00AM - 11:00AM —**  
**Session E43 GSNP GSOF: Jamming and the Glass Transition I** 346 - Ray Orbach

**8:00AM E43.00001 ABSTRACT WITHDRAWN —**

**8:12AM E43.00002 Jamming for a system of granular crosses<sup>1</sup>**, ZEGAN SHANG, Duke University, HU ZHENG, Hohai University, DONG WANG, JONATHAN BARES, ROBERT BEHRINGER, Duke University — A disordered stress-free granular packing can be turned into a rigid structure, which is called jammed state, by increasing the density of particles per unit volume or by applying shear deformation. The jamming behavior of systems made of 2D circular discs have been investigated in detail, but very little is known about the special geometry particles, particularly non-convex particles like crosses. Here, we perform an experimental study on the jamming of a system of quasi-2D granular crosses. In the present experiments, we measure the pressure, and coordinate number evolution of a 2D packing of photo-elastic cross discs. This talk will present results from a simple shear experiment for stresses and for the order parameter associated with the cross orientation and its correlation.

<sup>1</sup>We acknowledge support from NSF Grant No. DMR1206351, NASA Grant No. NNX15AD38G and the W.M. Keck Foundation

**8:24AM E43.00003 Experimental studies of contact networks in jammed colloidal systems**, ERU KYEYUNE-NYOMBI, LANE GILCHRIST, HERNN MAKSE, City College of New York — Recent theoretical advances in the statistical mechanics of jamming have provided a new outlook for thermodynamically characterizing packings of granular matter. Packing density, spatial ordering metrics, and the number of inter-particle contacts are a few fundamental parameters used in various theoretical models. However, experimental measurements of inter-particle forces have been illusive. Here, fluorescent molecular probes are used to identify inter-particle contacts in high resolution confocal images of jammed colloidal systems.

**8:36AM E43.00004 Experimental Study of Athermal Elastic Network Mechanics**, JONATHAN MICHEL, PETER YUNKER, Georgia Institute of Technology — Recently, significant theoretical effort has been directed towards understanding the mechanics of networks. Elastic networks are of inherent fundamental interest <sup>1</sup> and serve as useful analogs for describing other physical systems. Recent applications include modeling of collagen <sup>2</sup> and descriptions of jamming in granular media and glass formation <sup>3</sup>. I propose to discuss ongoing experimental efforts to study mechanical properties of elastic networks, such as Young's modulus and ultimate strength, in the athermal limit. I will begin with the simple case of regular, isostatic crystalline lattices and proceed to studies of random, connected elastic networks of varying bond number for a given number of lattice sites, including both isostatic and sub-isostatic networks.

<sup>1</sup>Mao, X., Stenull, O. and Lubensky, T.C., "Elasticity of a filamentous kagome lattice", Physical Review E, 87:042604

<sup>2</sup>Licup, J. et al., "Stress Controls the mechanics of collagen networks", PNAS, 2015, 112:9573-9578

<sup>3</sup>Liu, A and Nagel, S. R., "The Jamming Transition and the Marginally Jammed Solid", Annual Reviews of Condensed Matter Physics, 2010, 1:347-69

**8:48AM E43.00005 Interparticle contact networks of granular packings below jamming**, BHASKAR SEN GUPTA, THIBAUT BERTRAND, COREY S. O'HERN, Yale University, MARK D. SHATTUCK, City College of New York — We employ computer simulations to investigate the structural properties of interparticle contact networks in granular packings of bidisperse disks below jamming onset at which the system becomes solid-like. We show that the properties of the contact networks are highly sensitive to changes in the packing-generation protocol and its numerical implementation. Thus, we formulate an analytical method to implement steepest descent of hard, athermal particles undergoing isotropic compression, which allows us to calculate the number of contacts as a function of packing fraction. These results represent an important first step in developing a theoretical description of shear- and compression-induced jamming in frictional granular media.

**9:00AM E43.00006 Contact breaking in frictionless granular packings<sup>1</sup>**, QIKAI WU, THIBAUT BERTRAND, COREY O'HERN, Yale University, MARK SHATTUCK, City College of the City University of New York — We numerically study the breaking of interparticle contact networks in static granular packings of frictionless bidisperse disks that are subjected to vibrations. The packings are created using an isotropic compression protocol at different values of the total potential energy per particle  $E_p$ . We first add displacements along a single vibrational mode  $i$  of the dynamical matrix to a given packing and calculate the minimum amplitude  $A_i$  of the perturbation at which the first interparticle contact breaks. We then identify the minimum amplitude  $A_{\min}$  over all perturbations along each mode and study the distribution of  $A_{\min}$  from an ensemble of packings at each  $E_p$ . We then study two-, three-, and multi-mode excitations and determine the dependence of  $A_{\min}$  on the number of modes that are included in the perturbation.

<sup>1</sup>W. M. Keck Foundation Science and Engineering Grant

**9:12AM E43.00007 Echoes of the glass transition in athermal soft spheres** , PETER MORSE, ERIC CORWIN, University of Oregon — The glass transition and the athermal jamming transition are both transitions from one disordered state to another marked by a sudden increase in rigidity. Before the onset of rigidity, thermal hard spheres and athermal soft spheres both share the same configuration space. Is there a signature of the glass transition in the topology of the allowed configuration space, and is this same signature present for athermal spheres? I will answer these questions by introducing the concept of local rigidity, and in doing so, I will demonstrate the existence of a pre-jamming phase transition precisely at the glass transition density.

**9:24AM E43.00008 Structural Signatures of the glass transition** , CHI ZHANG, Department of Physics, Université de Fribourg, CH-1700 Fribourg, Switzerland., NICOLETTA GNAN, EMANUELA ZACCARELLI, CNR-ISC, UOS Sapienza, P.le A. Moro 2, Roma I-00185, Italy. Dipartimento di Fisica, Sapienza Università di Roma, P.le A. Moro 2, Roma I-00185, Ital, FRANK SCHEFFOLD, Department of Physics, Université de Fribourg, CH-1700 Fribourg, Switzerland. — The nature of colloidal glasses and the glass transition remains a topic of scientific interest. Scientists often focus on the study of dynamical properties since major structural changes have not been found to date in the vicinity of the glass transition. In this work we study both structural and dynamic signatures of the glass and jamming transition. Confocal microscopy measurements and molecular dynamic simulations are conducted on buoyancy and index matched microscale emulsion droplets with polydispersity of 12%, where crystallization is avoided. We find that the glass transition of such system is associated with detailed structural signatures on both global and local scales. At the global level, the peak amplitude of the radial distribution function shows a nonmonotonic evolution around a volume fraction of 59%. At the individual particle level, some local parameters such as the configuration of the nearest neighbors and the locally favoured structures also evolve differently across a volume fraction of about 59% whereas the jamming transition is clearly observed at higher densities 64.2%. Our results reveal clear structural signatures of the glass transition, which could help the further understanding of the underlying physical mechanism leading to dynamical arrest.

**9:36AM E43.00009 Casimir forces in systems near jamming<sup>1</sup>** , JUSTIN BURTON, JUAN-JOSÉ LIÉTOR-SANTOS, Department of Physics, Emory University — Casimir forces arise when long-ranged fluctuations are geometrically confined between two surfaces. In most cases these fluctuations are quantum or thermal in nature, such as those near a classical critical point, yet this is not a requirement. The  $T = 0$  jamming transition in frictionless, granular systems shares many properties with classical critical points, such as a diverging correlation length, although it has recently been identified as a unique example of a random first-order transition (RFOT). Here we show the existence of Casimir forces between two pinned particles immersed in systems near the frictionless jamming transition. We observe two components to the total force: a short-ranged, depletion force and a long-ranged, repulsive Casimir force. The Casimir force dominates when the pinned particles are much larger than the ambient jammed particles. In this case, we find that particles with the largest forces have the least number of contacts, and that these particles are clustered between the pinned particles, giving rise to a repulsive force which is independent of system preparation and inter-particle potential.

<sup>1</sup>We acknowledge support from NSF DMR-1455086

**9:48AM E43.00010 Rearrangements in Sheared Disordered Solids: Low and High Pressure Regimes** , SVEN WIJTMANS, Syracuse University, MERLIJN VAN DEEN, MARTIN VAN HECKE, Universiteit Leiden, M. LISA MANNING, Syracuse University — We study contact changes and rearrangements in quasistatic shear of disordered jammed packings at a range of pressures. We distinguish rearrangements where particle positions are discontinuous, leading to energy and stress discontinuities, from more frequent network events where contacts change but particle positions remain continuous. Moreover, we introduce two distinct protocols to unambiguously distinguish line reversible, loop reversible and irreversible events. The prevalence and spatial extension of five distinct event types (there are no loop reversible network events) evidence two distinct regimes: a low pressure regime dominated by irreversible extended events and a high pressure regime dominated by reversible localized ones. These trends indicate a crossover in the qualitative nature of plastic behavior in disordered solids near and far from jamming.

**10:00AM E43.00011 ABSTRACT WITHDRAWN —**

**10:12AM E43.00012 Rheological Transition of Sheared Frictionless Disks with Rotational Motion<sup>1</sup>** , PETER OLSSON, Ume University, STEVE TEITEL, University of Rochester — We consider the massive Durian bubble model for sheared bidisperse disks, but modified so as to include the rotational motion of particles due to dissipative collisional torques. In such a model, particles possess a viscous tangential dissipation, though no elastic tangential friction. As the packing fraction is increased, we find a discontinuous transition from Bagnoldian to Newtonian rheology, at a packing fraction that lies below the jamming transition. At this transition we find a region of coexisting shear bands of Bagnoldian and Newtonian rheology, and suggestions of discontinuous shear thickening upon increasing the shear strain rate.

<sup>1</sup>This work has been supported by NSF Grant No. DMR-1205800.

**10:24AM E43.00013 Critical Scaling of Bagnold Rheology at the Jamming Transition of Frictionless Disks<sup>1</sup>** , STEPHEN TEITEL, University of Rochester, DANIEL VÅGBERG, Delft Univ of Tech, PETER OLSSON, Umeå University — We simulate shear-driven, frictionless, bidisperse disks in two dimensions, as a function of applied shear strain rate and packing fraction, for a model with a normal viscous dissipation that results in Bagnoldian rheology for all control parameters. Carrying out a critical scaling analysis of the pressure and shear stress near the jamming transition we find values of the critical exponents that disagree with theoretical predictions of Otsuki and Hayakawa[1] but are closer to more recent theoretical results by DeGiuli et al[2], as well as earlier simulations by Peyneau and Roux[3]. We find that it is essential to include leading corrections-to-scaling to arrive at self-consistent results.

[1] M. Otsuki and H. Hayakawa, Prog. Theor. Phys. 121, 647 (2009) and Phys. Rev. E 80, 011308 (2009)

[2] E. DeGiuli, G. Duřing, E. Lerner, and M. Wyart, Phys. Rev. E 91, 062206 (2015)

[3] P.-E. Peyneau and J.-N. Roux, Phys. Rev. E 78, 011307 (2008)

<sup>1</sup>This work has been supported by NSF Grant No. DMR-1205800, Swedish Research Council Grant No. 2010-3725, and the Dutch Organization for Scientific Research (NWO).

**10:36AM E43.00014 Single Particle Jumps in Sheared SiO<sub>2</sub><sup>1</sup>** , SEAN MCMAHON, KATHARINA VOLLMAYR-LEE, Bucknell University, JONATHAN COOKMEYER, Haverford College, JUERGEN HORBACH, Heinrich-Heine-University Duesseldorf, Germany — We study the dynamics of a sheared glass via molecular dynamics simulations. Using the BKS potential we simulate the strong glass former SiO<sub>2</sub>. The system is initially well equilibrated at a high temperature, then quenched to a temperature below the glass transition, and, after a waiting time at the desired low temperature, sheared with constant strain rate. We present preliminary results of an analysis of single particle trajectories of the sheared glass.

<sup>1</sup>We acknowledge the support via NSF REU grant PHY-1156964, DoD ASSURE program, and NSF-MRI CHE-1229354 as part of the MERCURY high-performance computer consortium. We thank G.P. Shrivastav, Ch. Scherer and B. Temelso.

**10:48AM E43.00015 Increasing the maximally random jammed density with electric field to reduce the fat level in chocolate**, R. TAO<sup>1</sup>, H. TANG, Temple Univ — Chocolate is one of the most popular food types and flavors in the world. Unfortunately, at present, chocolate products contain too much fat, leading to obesity. For example, a typical molding chocolate has various fat up to 40% in total and chocolate for covering ice cream has fat 50 -60%. Especially, as children are the leading chocolate consumers, reducing the fat level in chocolate products to make them healthier is important and urgent. While this issue was called into attention and elaborated in articles and books decades ago and led to some patent applications, no actual solution was found unfortunately. Why is reducing fat in chocolate so difficult? What is the underlying physical mechanism? We have found that this issue is deeply related to the basic science of soft matters, especially to their viscosity and maximally random jammed (MRJ) density  $\varphi_x$ . All chocolate productions are handling liquid chocolate, a suspension with cocoa solid particles in melted fat, mainly cocoa butter. The fat level cannot be lower than  $1-\varphi_x$  in order to have liquid chocolate to flow. Here we show that that with application of an electric field to liquid chocolate, we can aggregate the suspended particles into prolate spheroids. This microstructure change reduces liquid chocolate's viscosity along the flow direction and increases its MRJ density significantly. Hence the fat level in chocolate can be effectively reduced. We are looking forward to a new class of healthier and tasteful chocolate coming to the market soon.

<sup>1</sup>Dept. of Physics, Temple Univ, Philadelphia, PA 19122

**Tuesday, March 15, 2016 8:00AM - 11:00AM –**  
**Session E44 GQI: Quantum Characterization, Verification and Validation II** 347 - Barry Sanders,  
University of Calgary

**8:00AM E44.00001 INVITED ABSTRACT WITHDRAWN –**

**8:36AM E44.00002 Entanglement verification with detection efficiency mismatch**, YANBAO ZHANG, NORBERT LÜTKENHAUS, Institute for Quantum Computing & Department of Physics and Astronomy, University of Waterloo — Entanglement is a necessary condition for secure quantum key distribution (QKD). When there is an efficiency mismatch between various detectors used in the QKD system, it is still an open problem how to verify entanglement. Here we present a method to address this problem, given that the detection efficiency mismatch is characterized and known. The method works without assuming an upper bound on the number of photons going to each threshold detector. Our results suggest that the efficiency mismatch affects the ability to verify entanglement: the larger the efficiency mismatch is, the smaller the set of entangled states that can be verified becomes. When there is no mismatch, our method can verify entanglement even if the method based on squashing maps [PRL 101, 093601 (2008)] fails.

**8:48AM E44.00003 Machine Learning for Quantum Metrology and Quantum Control<sup>1</sup>**, BARRY SANDERS<sup>2</sup>, EHSAN ZAHEDINEJAD, PANTITA PALITTAPONGARNPIM, University of Calgary — Generating quantum metrological procedures and quantum gate designs, subject to constraints such as temporal or particle-number bounds or limits on the number of control parameters, are typically hard computationally. Although greedy machine learning algorithms are ubiquitous for tackling these problems, the severe constraints listed above limit the efficacy of such approaches. Our aim is to devise heuristic machine learning techniques to generate tractable procedures for adaptive quantum metrology and quantum gate design. In particular we have modified differential evolution to generate adaptive interferometric-phase quantum metrology procedures for up to 100 photons including loss and noise, and we have generated policies for designing single-shot high-fidelity three-qubit gates in superconducting circuits by avoided level crossings. Although quantum metrology and quantum control are regarded as disparate, we have developed a unified framework for these two subjects, and this unification enables us to transfer insights and breakthroughs from one of the topics to the other.

<sup>1</sup>Thanks to NSERC, AITF and 1000 Talent Plan.

<sup>2</sup>Also Univ of Science and Technology of China and Canadian Inst for Advanced Research.

**9:00AM E44.00004 Ultimate precision limit and optimal probe states for quantum metrology**, HAIDONG YUAN, Chinese Univ of Hong Kong, CHI-HANG FRED FUNG, Huawei, Hong Kong Science Park — An important task in science and technology is to find out the highest achievable precision in measuring and estimating parameters of interest with given resources, and design schemes to reach it. Quantum metrology, which exploits quantum mechanical effects to achieve high precision, has gained increasing attention in recent years. Here we present a general framework for quantum metrology which relates the ultimate precision limit directly to the underlying dynamics, this framework provides efficient methods for computing the ultimate precision limit and optimal probe states. We further demonstrate the power of the framework by deriving a sufficient condition on when ancillary systems are not useful for improving the precision limit.

**9:12AM E44.00005 Improving the precision of weak measurement by nonclassical states**, SHENG-SHI PANG, University of Rochester, TODD A. BRUN, University of Southern California — Weak value amplification is a useful protocol to amplify tiny physical effects by postselecting the system in a weak measurement. However, there has been controversy over its precision advantage in parameter estimation recently, since it discards unselected results of the postselection measurement on the system, which may take away useful information. While it is now clear that retaining failed postselections can yield more Fisher information than discarding them, the advantage of postselection measurement itself still remains to be clarified. If a weak measurement with postselection measurement cannot not produce higher precision than without postselection measurement, it would be meaningless to discuss the use of postselection results. In this work, we address this problem by studying the optimal signal-to-noise ratio (SNR) of postselected weak measurement. We find a surprising result that when the probe is initially prepared in a proper squeezed coherent state, the postselected weak measurement can give a higher SNR than the standard weak measurement, while such an advantage vanishes when the probe is prepared in a normal coherent state. This suggests that raising the precision of weak measurement by postselection calls for the presence of nonclassicality in the probe state.

**9:24AM E44.00006 Robust Calibration of a Universal Single-Qubit Gate-Set via Robust Phase Estimation**, SHELBY KIMMEL, University of Maryland, QUICS, GUANG HAO LOW, THEODORE J. YODER, Massachusetts Institute of Technology — An important step in building a quantum computer is calibrating experimentally implemented quantum gates to produce operations that are close to ideal unitaries. The calibration step involves estimating the systematic errors in gates and then using controls to correct the implementation. Quantum process tomography is a standard technique for estimating these errors, but is both time consuming, (when one only wants to learn a few key parameters), and is usually inaccurate without resources like perfect state preparation and measurement, which might not be available. With the goal of efficiently and accurately estimating specific errors using minimal resources, we develop a parameter estimation technique, which can gauge key systematic parameters (specifically, amplitude and off-resonance errors) in a universal single-qubit gate-set with provable robustness and efficiency. In particular, our estimates achieve the optimal efficiency, Heisenberg scaling, and do so without entanglement and entirely within a single-qubit Hilbert space. Our main theorem making this possible is a robust version of the phase estimation procedure of Higgins et al. [B. L. Higgins et al., New J. Phys. 11 073023 (2009)].

**9:36AM E44.00007 Numerical Analysis of Robust Phase Estimation** , KENNETH RUDINGER, Center for Computing Research, Sandia National Laboratories, SHELBY KIMMEL, QuICS, University of Maryland — Robust phase estimation (RPE) is a new technique for estimating rotation angles and axes of single-qubit operations, steps necessary for developing useful quantum gates [arXiv:1502.02677]. As RPE only diagnoses a few parameters of a set of gate operations while at the same time achieving Heisenberg scaling, it requires relatively few resources compared to traditional tomographic procedures. In this talk, we present numerical simulations of RPE that show both Heisenberg scaling and robustness against state preparation and measurement errors, while also demonstrating numerical bounds on the procedure's efficacy. We additionally compare RPE to gate set tomography (GST), another Heisenberg-limited tomographic procedure. While GST provides a full gate set description, it is more resource-intensive than RPE, leading to potential tradeoffs between the procedures. We explore these tradeoffs and numerically establish criteria to guide experimentalists in deciding when to use RPE or GST to characterize their gate sets.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

**9:48AM E44.00008 Formal Computer Validation of the Quantum Phase Estimation Algorithm<sup>1</sup>** , WAYNE WITZEL, KENNETH RUDINGER, Sandia National Laboratories, Albuquerque, NM, MOHAN SAROVAR, Sandia National Laboratories, Livermore, CA, ROBERT CARR, University of New Mexico — While peer review and scientific consensus provide some assurance to the validity of ideas, people do make mistakes that can slip through the cracks. A plethora of formal methods tools exist and are in use in a variety of settings where high assurance is demanded. Existing tools, however, require a great deal of expertise and lack versatility, demanding a non-trivial translation between a high-level description of a problem and the formal system. Our software, called Prove-It, allows a nearly direct translation between human-recognizable formulations and the underlying formal system. While Prove-It is not designed for particularly efficient automation, a primary goal of other formal methods tools, it is extremely flexible in following a desired line of reasoning (proof structure). This approach is particularly valuable for validating proofs that are already known. We will demonstrate a validation of the Quantum Phase Estimation Algorithm using Prove-It. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

<sup>1</sup>This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories.

**10:00AM E44.00009 Efficient Bayesian Phase Estimation** , NATHAN WIEBE, Microsoft Research, CHRISTOPHER GRANADE, University of Sydney — We provide a new efficient adaptive algorithm for performing phase estimation that does not require that the user infer the bits of the eigenphase in reverse order; rather it directly infers the phase and estimates the uncertainty in the phase directly from experimental data. Our method is highly flexible, recovers from failures, and can be run in the presence of substantial decoherence and other experimental imperfections and is as fast or faster than existing algorithms.

**10:12AM E44.00010 Bounding quantum gate error rate based on reported average fidelity** , YUVAL SANDERS, JOEL WALLMAN, Univ of Waterloo, BARRY SANDERS, Univ of Calgary — Remarkable experimental advances in quantum computing are exemplified by recent announcements of impressive average gate fidelities exceeding 99.9% for single-qubit gates and 99% for two-qubit gates. Although these high numbers engender optimism that fault-tolerant quantum computing is within reach, the connection of average gate fidelity with fault-tolerance requirements is not direct. Here we use reported average gate fidelity to determine an upper bound on the quantum-gate error rate, which is the appropriate metric for assessing progress towards fault-tolerant quantum computation, and we demonstrate that this bound is asymptotically tight for general noise. Although this bound is unlikely to be saturated by experimental noise, we demonstrate using explicit examples that the bound indicates a realistic deviation between the true error rate and the reported average fidelity. We introduce the Pauli-distance as a measure of this deviation, and we show that knowledge of the Pauli-distance enables tighter estimates of the error rate of quantum gates.

**10:24AM E44.00011 Percolation bounds for decoding thresholds with correlated erasures in quantum LDPC codes<sup>1</sup>** , KATHLEEN HAMILTON, None, LEONID PRYADKO, University of California, Riverside — Correlations between errors can dramatically affect decoding thresholds, in some cases eliminating the threshold altogether. We analyze the existence of a threshold for quantum low-density parity-check (LDPC) codes in the case of correlated erasures. When erasures are positively correlated, the corresponding multi-variate Bernoulli distribution can be modeled in terms of cluster errors, where qubits in clusters of various size can be marked all at once. In a code family with distance scaling as a power law of the code length, erasures can be always corrected below percolation on a qubit adjacency graph associated with the code. We bound this correlated percolation transition by weighted (uncorrelated) percolation on a specially constructed cluster connectivity graph, and apply our recent results [1] to construct several bounds for the latter.

[1] K. E. Hamilton and L. P. Pryadko, "Algebraic bounds for weighted percolation on directed and undirected graphs," arXiv:1505.03963 (2015).

<sup>1</sup>This research was supported in part by the NSF grant PHY-1416578 and by the ARO grant W911NF-14-1-0272

**10:36AM E44.00012 Robustness and performance scaling of quantum information processors with respect to gate removal and defects** , YUNSEONG NAM, REINHOLD BLÜMEL, Wesleyan Univ — A single logical gate, when removed from a classical computer, can completely destroy its information processing capability. For a quantum processor, the story is quite different. We find that the processing capability of a quantum information processor is robust with respect to the removal of a large number of quantum logical gates. In fact, even when most of the quantum processor's gates are removed, quantum processors, such as the universally applicable quantum Fourier transform or the quantum adder, work with satisfactory performance. In this talk, we present our numerical and analytical results detailing the performance scaling of quantum processors with respect to gate pruning operations. We also present the performance scaling of pruned quantum processors subjected to gate defects in the remaining gates.

**10:48AM E44.00013 Assessing the performance of quantum repeaters for all phase-insensitive Gaussian bosonic channels** , KENNETH GOODENOUGH, DAVID ELKOUSS, STEPHANIE WEHNER, Delft Univ of Tech, QUTECH TEAM — One of the most sought-after goals in experimental quantum communication is the implementation of a quantum repeater. Quantum repeaters can be assessed by comparing their performance with the quantum- and private capacity of a direct transmission, assisted by unlimited classical two-way communication. Calculating these quantities is hard to compute however, motivating the search for upper bounds on these capacities. Takeoka, Guha and Wilde found the squashed entanglement of a quantum channel to be an upper bound on these capacities. In general it is hard to find the exact value of the squashed entanglement of a quantum channel, but clever, sub-optimal squashing maps still allow one to upper bound this quantity, and thus also the corresponding capacities. We follow this approach to upper bound the capacity of some specific channels, where in particular we extend the analysis of Takeoka et al. on the pure-loss channel to the general case of any Gaussian bosonic channel with equal noise in each quadrature. This bound is of practical importance, since it allows one to benchmark the implementation of quantum repeaters in quantum key distribution networks for a large class of channels.

**Tuesday, March 15, 2016 8:00AM - 11:00AM –**

**Session E45 GQI DAMOP: Hybrid Quantum Systems I** 348 - Mark Dykman, Michigan State University

**8:00AM E45.00001 Charge dynamics and spin blockade in a hybrid double quantum dot in silicon**<sup>1</sup>, ANASUA CHATTERJEE, MATIAS URDAMPILLETA, CHEUK CHI LO, JOHN MANSIR, London Centre for Nanotechnology, University College London, SYLVAIN BARRAUD, CEA-LETI, ANDREAS BETZ, M. FERNANDO GONZALEZ-ZALBA, Hitachi Cambridge Laboratory, JOHN J. L. MORTON, London Centre for Nanotechnology, University College London — Hybrid architectures combining donor atoms and quantum dots in silicon can take advantage of fast gate voltage based spin manipulations to form a hybrid singlet-triplet qubit, with access to the quantum memory offered by the nuclear spin of the donor via the hyperfine interaction. Additionally, spin buses using quantum dot chains could mediate the transfer of quantum information between long-lived donor spins. We present an approach to a novel hybrid double quantum dot by coupling a donor to an artificial atom in a CMOS-compatible nanotransistor. Using gate-based RF-reflectometry, we probe the charge stability of the system and its quantum capacitance. Through microwave spectroscopy, we find a tunnel coupling of 2.7GHz and characterize the charge dynamics, revealing a charge  $T_1$  of 100ns. We also show spin blockade at the interdot transition and investigate the spin dynamics, opening up the possibility to operate this coupled system as a singlet-triplet qubit and to coherently transfer spin information between the quantum dot and the donor electron and nucleus.

<sup>1</sup>We acknowledge support from the TOLOP project (FP7/318397), the EPSRC, ARC, and the UNEDD project, the Royal Commission for the Exhibition of 1851 and the Royal Society.

**8:12AM E45.00002 Controlling spin relaxation with a cavity**, AUDREY BIENFAIT, SPEC, CEA-Saclay, JARRYD PLA, University College of London, YUIMARU KUBO, SPEC, CEA-Saclay, XIN ZHOU, Institute of Electronics, Microelectronics, and Nanotechnology, MICHAEL STERN, University of Bar Ilan, CHEUK LO, University College of London, CHRISTOPHER WEIS, THOMAS SCHENKEL, Lawrence Berkeley National Laboratory, DENIS VION, DANIEL ESTEVE, SPEC, CEA-Saclay, JOHN MORTON, University College of London, PATRICE BERTET, SPEC, CEA-Saclay — Spontaneous emission of radiation is one of the fundamental relaxation mechanisms for a quantum system. For spins, however, it is negligible compared to non-radiative relaxation processes due to their weak coupling to the electromagnetic field. In 1946, Purcell realized [1] that spontaneous emission is strongly enhanced when the quantum system is placed in a resonant cavity - an effect now used to control the lifetime of systems with an electrical dipole [2]. Here, by coupling donor spins in silicon to a high quality factor superconducting microwave cavity of small mode volume, we reach the regime where spontaneous emission constitutes the dominant spin relaxation channel [3]. The relaxation rate is increased by three orders of magnitude when the spins are tuned to the cavity resonance, showing it can be engineered and controlled on-demand. Our results provide a novel way to initialize any spin into its ground state, with applications in magnetic resonance and quantum information processing. They also show for the first time an alteration of spin dynamics by quantum fluctuations, a step towards the coherent magnetic coupling of a spin to microwave photons. [1] E. M. Purcell, Phys. Rev. 1946, 69, 681. [2] P. Goy et al., PRL. 50, 1983. [3] A. Bienfait et al., arxiv :1508.06148

**8:24AM E45.00003 Coupling a Small Ensemble of Electrons on Helium to a Superconducting Circuit**, GE YANG, GERWIN KOOLSTRA, University of Chicago, DAVID CZAPLEWSKI, LEONIDAS OCOLA, Argonne National Laboratory Center for Nanoscale Materials, DAVID I. SCHUSTER, University of Chicago — Electrons on helium is a unique two-dimensional electron gas system formed at the interface of a quantum liquid (superfluid helium) and vacuum. If single electrons on helium can be isolated, the motional and spin states could form the building blocks for hybrid quantum computing [1,2]. Here we first review the strong coupling between a large electron ensemble and a microwave resonator [3]. Then we will describe methods to isolate small mesoscopic ensembles with less than 100 electrons in a micron-sized trap at the end of a quarter wavelength microwave cavity. Finally we will discuss the effect of helium fluctuations on the coherence of the hybrid circuit. [1] S. Lyon, Phys. Rev. A. 74, 5 (2006) [2] D.I. Schuster, et al. Phys. Rev. Lett. 105, 040503 (2010) [3] Ge Yang, et al., arXiv:1508.04847(2015)

**8:36AM E45.00004 Magnetic resonance at the quantum limit**, PATRICE BERTET, CEA Saclay — The detection and characterization of paramagnetic species by electron-spin resonance (ESR) spectroscopy has numerous applications in chemistry, biology, and materials science [1]. Most ESR spectrometers rely on the inductive detection of the small microwave signals emitted by the spins during their Larmor precession into a microwave resonator in which they are embedded. Using the tools offered by circuit Quantum Electrodynamics (QED), namely high quality factor superconducting micro-resonators and Josephson parametric amplifiers that operate at the quantum limit when cooled at 20mK [2], we report an increase of the sensitivity of inductively detected ESR by 4 orders of magnitude over the state-of-the-art, enabling the detection of 1700 Bismuth donor spins in silicon with a signal-to-noise ratio of 1 in a single echo [3]. We also demonstrate that the energy relaxation time of the spins is limited by spontaneous emission of microwave photons into the measurement line via the resonator [4], which opens the way to on-demand spin initialization via the Purcell effect. These results constitute a first step towards circuit QED experiments with magnetically coupled individual spins. [1] A. Schweiger and G. Jeschke, Principles of Pulse Electron Magnetic Resonance (Oxford University Press, 2001) [2] X. Zhou et al., Physical Review B 89, 214517 (2014). [3] A. Bienfait et al., arxiv :1507.06831 [4] A. Bienfait et al., arxiv :1508.06148

**9:12AM E45.00005 Hybrid Quantum Information Processing with Superconducting Circuits and Rydberg Atoms**, MATTHEW BECK, JOSHUA ISAACS, DONALD BOOTH, MARK SAFFMAN, ROBERT MCDERMOTT, University of Wisconsin - Madison — Hybrid approaches to quantum information processing exploit the strengths of disparate quantum technologies to realize performance that exceeds what can be reached with any single technology on its own. Here we describe steps toward realization of a hybrid superconducting circuit Rydberg atom quantum architecture that will marry a fast, high-fidelity superconducting quantum processor with a long-lived quantum memory based on trapped Rydberg atoms. The key challenge is development of a high-fidelity microwave photon Rydberg atom interface. We have designed superconducting thin-film microwave resonators that allow trapping of single Rydberg atoms at a voltage antinode, where coupling to the zero-point fields of the resonator is strongest. We discuss the dependence of resonator quality factor and achievable coupling factor on device geometry. Finally, we present preliminary results of experiments to couple Rydberg atoms and superconducting linear resonators in a custom liquid helium cryostat.

**9:24AM E45.00006 Photon-mediated interactions: a scalable tool to create and sustain entangled states of N atoms**, CAMILLE ARON, Laboratoire de Physique Thorique, cole Normale Suprieure, CNRS, Paris, France and Instituut voor Theoretische Fysica, KU Leuven, Leuven, Belgium, MANAS KULKARNI, New York City College of Technology, City University of New York, HAKAN TURECI, Princeton University — We propose and study the use of photon-mediated interactions for the generation of steady-state entanglement between N atoms that are separated by arbitrary distances. Through the judicious use of coherent drives and the placement of the atoms in a network of Cavity QED systems, a balance between their unitary and dissipative dynamics can be precisely engineered to stabilize a long-range correlated state of qubits in the steady state. We discuss the general theory behind such a scheme, and present an example of how it can be used to drive a register of N atoms to a generalized W-state, and the entanglement sustained indefinitely. The achievable steady-state fidelities for entanglement and its scaling with the number of qubits are discussed for presently existing superconducting quantum circuits. While the protocol is primarily discussed for a superconducting circuit architecture, it is ideally realized in any Cavity QED platform that permits controllable delivery of coherent electromagnetic radiation to specified locations.

**9:36AM E45.00007 Spin-cavity longitudinal coupling for two-qubit gates and measurement**, RUSKO RUSKOV, CHARLES TAHAN, Laboratory for Physical Sciences, College Park, MD 20740 — We have studied the possibility of longitudinal coupling of various encoded quantum dot spin-qubits to a microwave resonator via modulation of voltage gates. A dynamical coupling of tens of MHz can be achieved. We investigate specific procedures for entangling gates using accumulated geometrics phases and calculate possible gate times and fidelities. Implications for qubit readout and continuous quantum monitoring are also considered.

**9:48AM E45.00008 Magnetization detecting electron paramagnetic resonance spectroscopy using a dc-SQUID directly coupled to an electron spin ensemble<sup>1</sup>**, HIRAKU TOIDA, YUICHIRO MATSUZAKI, KOSUKE KAKUYANAGI, XIAOBO ZHU<sup>2</sup>, WILLIAM MUNRO, NTT Basic Research Laboratories, KAE NEMOTO, National Institute of Informatics, HIROSHI YAMAGUCHI, SHIRO SAITO, NTT Basic Research Laboratories — Electron parametric resonance (EPR) spectroscopy is one of the most widely-used tool to characterize materials containing unpaired electrons. In the case of conventional EPR spectrometers, the resonance is detected as a change of microwave transmittance of a cavity. In our method, on the other hand, magnetization of the sample induced by the resonance is detected by a direct current superconducting quantum interference device (dc-SQUID) magnetometer, which is bonded to the sample. Here, we report detection of electron spin polarization and EPR spectroscopy using a micrometer-sized dc-SQUID magnetometer. We measure temperature and in-plane magnetic field dependence of spin polarization ratio and it has good agreement to the hyperbolic tangent law. We also successfully demonstrate EPR spectroscopy by applying a continuous microwave signal to the sample with a on-chip microstrip. We estimate the sensing volume and the minimum distinguishable number of electron spins to be  $\sim 10^{-10} \text{ cm}^3$  ( $\sim 0.1 \text{ pl}$ ) and  $\sim 10^6$ , respectively. This result paves the way towards realizing highly sensitive EPR spectroscopy in nanometer-sized area.

<sup>1</sup>This work was supported by Commissioned Research of NICT and in part by MEXT KAKENHI (Grant No. 15648489 and 15H05869).

<sup>2</sup>Current address: Chinese Academy of Sciences

**10:00AM E45.00009 Coupling nanoscale spin ensembles to a SQUID embedded in superconducting circuits<sup>1</sup>**, C. EICHLER, J. R. PETTA, Department of Physics, Princeton University — Electron spin resonance is a ubiquitous phenomenon used for the characterization of paramagnetic materials and to coherently control electron spins as carriers of quantum information. The coupling strength between spins and RF magnetic fields can be increased by using microwave frequency resonators, realized either as 3D cavities or in planar geometries. Here, we study microwave resonators embedding a superconducting quantum interference device (SQUID), which couples to nearby electron spins of phosphorus donors in silicon. We compare different SQUID and resonator geometries aiming at enhanced spin sensitivity. We also study the coupled system in a sideband regime where the Zeeman energy is nonresonant with the cavity frequency, allowing for operation at lower DC magnetic fields.

<sup>1</sup> Supported by the Gordon and Betty Moore Foundation

**10:12AM E45.00010 Angular dependant micro-ESR characterization of a locally doped  $\text{Gd}^{3+}:\text{Al}_2\text{O}_3$  hybrid system for quantum applications**, I. S. WISBY, NPL, UK & Royal Holloway, UK, S.E. DE GRAAF, NPL, UK, R. GWILLIAM, ATI, University of Surrey, UK, A. ADAMYAN, Chalmers University of Technology, S. E. KUBATKIN, Chalmers University of Technology, Sweden, P. J. MEESON, Royal Holloway, UK, A. YA. TZALENCHUK, NPL, UK & Royal Holloway, UK, T. LINDSTROM, NPL, UK — Rare-earth doped crystals interfaced with superconducting quantum circuitry are an attractive platform for quantum memory and transducer applications. Here we present a detailed characterization of a locally implanted  $\text{Gd}^{3+}$  in  $\text{Al}_2\text{O}_3$  system coupled to a superconducting micro-resonator, by performing angular dependent micro-electron-spin-resonance (micro-ESR) measurements at mK temperatures. The device is fabricated using a hard  $\text{Si}_3\text{N}_4$  mask to facilitate a local ion-implantation technique for precision control of the dopant location. The technique is found not to degrade the internal quality factor of the resonators which remains above  $10^5$  (1). We find the measured angular dependence of the micro-ESR spectra to be in excellent agreement with the modelled Hamiltonian, supporting the conclusion that the dopant ions are successfully integrated into their relevant lattice sites whilst maintaining crystalline symmetries. Furthermore, we observe clear contributions from individual microwave field components of our micro-resonator, emphasising the need for controllable local implantation. 1) Wisby et al. Appl. Phys. Lett. **105**, 102601 (2014)

**10:24AM E45.00011 Strong Coupling of a Donor Spin Ensemble to a Volume Microwave Resonator**, BRENDON ROSE, ALEXEI TYRYSKIN, STEPHEN LYON, Princeton University — We achieve the strong coupling regime between an ensemble of phosphorus donor spins (5e13 total donors) in highly enriched 28-Si (50 ppm 29-Si) and a standard dielectric resonator. Spins were polarized beyond Boltzmann equilibrium to a combined electron and nuclear polarization of 120 percent using spin selective optical excitation of the no-phonon bound exciton transition. We observed a spin ensemble-resonator splitting of 580 kHz (2g) in a cavity with a Q factor of 75,000 ( $\kappa \ll \gamma \approx 120 \text{ kHz}$  where  $\kappa$  and  $\gamma$  are the external and internal resonator loss rates respectively). The spin ensemble has a long dephasing time (9  $\mu\text{s}$ ) providing a wide window for viewing the time evolution of the coupled spin ensemble-cavity system described by the Tavis-Cummings model. The free induction decay shows repeated collapses and revivals revealing a coherent and complete exchange of excitations between the superradiant state of the spin ensemble and the cavity (about 10 cycles are resolved). This exchange can be viewed as a swap of information between a long lived spin ensemble memory qubit ( $T_2 \approx 2 \text{ ms}$ ) and a cavity

**10:36AM E45.00012 Suppressing gate errors through extra ions coupled to a cavity in frequency-domain quantum computation using rare-earth-ion-doped crystal**, SATOSHI NAKAMURA, HAYATO GOTO, MAMIKO KUJIRAKA, KOUICHI ICHIMURA, Corporate RD Center, Toshiba Corporation, QUANTUM COMPUTER TEAM — The rare-earth-ion-doped crystals, such as  $\text{Pr}^{3+}:\text{Y}_2\text{SiO}_5$ , are promising materials for scalable quantum computers, because the crystals contain a large number of ions which have long coherence time. The frequency-domain quantum computation (FDQC) enables us to employ individual ions coupled to a common cavity mode as qubits by identifying with their transition frequencies. In the FDQC, operation lights with detuning interact with transitions which are not intended to operate, because ions are irradiated regardless of their positions. This crosstalk causes serious errors of the quantum gates in the FDQC. When resonance conditions between eigenenergies of the whole system and transition-frequency differences among ions are satisfied, the gate errors increase. Ions for qubits must have transitions avoiding the conditions for high-fidelity gate. However, when a large number of ions are employed as qubits, it is difficult to avoid the conditions because of many combinations of eigenenergies and transitions. We propose new implementation using extra ions to control the resonance conditions, and show the effect of the extra ions by a numerical simulation. Our implementation is useful to realize a scalable quantum computer using rare-earth-ion-doped crystal based on the FDQC.

**10:48AM E45.00013 Magneto-transport studies of a few hole GaAs double quantum dot in tilted magnetic fields.**, SERGEI STUDENIKIN, ALEX BOGAN, National Research Council of Canada, LISA TRACY, Sandia National Laboratories, LOUIS GAUDREAU, ANDY SACHRAJDA, MAREK KORKUSINSKI, National Research Council of Canada, JOHN RENO, TERRY HARGETT, Sandia National Laboratories — Compared to equivalent electron devices, single-hole spins interact weakly with lattice nuclear spins leading to extended quantum coherence times. This makes p-type Quantum Dots (QD) particularly attractive for practical quantum devices such as qubit circuits, quantum repeaters, quantum sensors etc. where long coherence time is required. Another property of holes is the possibility to tune their g-factor as a result of the strong anisotropy of the valance band. Hole g-factors can be conveniently tuned *in situ* from a large value to almost zero by tilting the magnetic field relative to the 2D hole gas surface normal. [1] In this work we explore high-bias magneto-transport properties of a p-type double quantum dot (DQD) device fabricated from a GaAs/AlGaAs heterostructures using lateral split-gate technology.[2] A charge detection technique is used to monitor number of holes and tune the p-DQD in a single hole regime around (1,1) and (2,0) occupation states where Pauli spin-blockaded transport is expected. Four states are identified in quantizing magnetic fields within the high-bias current stripe – three-fold triplet and a singlet which allows determining effective heavy hole g-factor as a function of the tilt angle from 90 to 0 degrees. [1] G. Ares et al., Phys.Rev. Lett. **110**, .046602 (2013); [2] L. A. Tracy,et al., App. Phys. Lett. **104**, 123101 (2014).

**Tuesday, March 15, 2016 8:00AM - 11:00AM –**  
**Session E46 GIMS: Advances in Scanning Probe Microscopy II: High Frequencies and Optical Techniques** 311 - Fabian Natterer, IBM Almaden Research Center

**8:00AM E46.00001 Towards microwave imaging of single two-level defects in dielectric materials**, SEBASTIAN DE GRAAF, National Physical Laboratory, Teddington, United Kingdom, ANDREY DANILOV, Chalmers University of Technology, Department of Microtechnology and Nanoscience, Gothenburg, Sweden, ALEXANDER TZALENCHUK, National Physical Laboratory, Teddington, United Kingdom, SERGEY KUBATKIN, Chalmers University of Technology, Department of Microtechnology and Nanoscience, Gothenburg, Sweden — Two-level fluctuators (TLF) are a major source of decoherence in quantum devices and significant effort is invested towards better understanding and eliminating these types of material defects. Here we propose that a near-field scanning microwave microscope (NSMM) can be used to image individual two-level defects on the nano-scale, provided that such a microscope operates in the right regime [1]. Not only would such a coherent NSMM be able to obtain nano-scale spatial distributions of defects and their locations within dielectric materials, it would also be able to determine the relative orientation of the TLF dipole with respect to the dielectric crystal, giving vital information about the nature of the TLF. We theoretically describe the operation and capabilities of a coherent NSMM and show that individual defects can be imaged in dielectric materials with low enough loss tangent, such as sapphire and silicon dioxide, relevant for solid state quantum technologies. We describe the requirements for constructing such an NSMM and report on our recent progress in setting up this technology [2]. [1] S. E. de Graaf, et al., Sci. Rep., in press (2015). [2] S. E. de Graaf, et al., Rev. Sci. Instrum. 84, 023706 (2013).

**8:12AM E46.00002 Advances in imaging and quantification of electrical properties at the nanoscale using Scanning Microwave Impedance Microscopy (sMIM)**<sup>1</sup>, STUART FRIEDMAN, FRED STANKE, YONGLIANG YANG, OSKAR AMSTER, PrimeNano, Inc — Scanning Microwave Impedance Microscopy (sMIM) is a mode for Atomic Force Microscopy (AFM) enabling imaging of unique contrast mechanisms and measurement of local permittivity and conductivity at the 10s of nm length scale. sMIM has been applied to a variety of systems including nanotubes, nanowires, 2D materials, photovoltaics and semiconductor devices. Early results were largely semi-quantitative. This talk will focus on techniques for extracting quantitative physical parameters such as permittivity, conductivity, doping concentrations and thin film properties from sMIM data. Particular attention will be paid to non-linear materials where sMIM has been used to acquire nano-scale capacitance-voltage curves. These curves can be used to identify the dopant type (n vs p) and doping level in doped semiconductors, both bulk samples and devices.

<sup>1</sup>supported in part by DOE-SBIR DE-SC0009856

**8:24AM E46.00003 Magnetic resonance force detection using a membrane resonator**, NICOLAS SCOZZARO, WILLIAM RUCHOTZKE, AMANDA BELDING, JEREMY CARDELLINO, ERICK BLOMBERG, BRENDAN MCCULLIAN, VIDYA BHALLAMUDI, DENIS PELEKHOV, P. CHRIS HAMMEL, Ohio State University - Columbus — Silicon nitride ( $\text{Si}_3\text{N}_4$ ) membranes are commercially-available, versatile structures that have a variety of applications. Although most commonly used as the support structure for transmission electron microscopy (TEM) studies, membranes are also ultrasensitive high-frequency mechanical oscillators. The sensitivity stems from the high quality factor  $Q \sim 10^6$ , which has led to applications in sensitive quantum optomechanical experiments. The high sensitivity also opens the door to ultrasensitive force detection applications. We report force detection of electron spin magnetic resonance at 300 K using a  $\text{Si}_3\text{N}_4$  membrane with a force sensitivity of 4 fN/ $\sqrt{\text{Hz}}$ , and a potential low temperature sensitivity of 25 aN/ $\sqrt{\text{Hz}}$ . Given membranes' sensitivity, robust construction, large surface area and low cost,  $\text{SiN}$  membranes can potentially serve as the central component of a compact room-temperature ESR and NMR instrument that has superior spatial resolution to conventional NMR.

**8:36AM E46.00004 Dipolar Decoupling in Magnetic Resonance Force Microscopy using Optical Control Pulses**, WILLIAM ROSE, University of Illinois at Urbana-Champaign, HOLGER HAAS, University of Waterloo, RAFFI BUDAKIAN, University of Illinois at Urbana-Champaign — We present data showing how a modified gradient ascent pulse engineering method can be used to design nuclear magnetic resonance pulses that perform a single unitary transformation over a large range of maximum Rabi field strengths ( $B_1$ ), while decoupling the secular dipolar interactions between spins. We designed dipolar-decoupling  $\pi$ -pulses that perform well over spins feeling maximum  $B_1$  fields from 131 – 274 G. By combining these  $\pi$ -pulses into a simple multiple pulse sequence, with fields produced by a silver microwire, we have increased  $T_2^*$  in a polystyrene sample attached to the tip of a silicon nanowire from 11  $\mu\text{s}$  to  $\sim 250\text{ms}$ . This dipolar decoupling could be used to improve the spatial resolution of nano-MRI experiments and to allow spectroscopy of chemical shifts in nanoscale samples.

**8:48AM E46.00005 Force-Detected Magnetic Resonance Imaging in Micron-Scale Liquids**, AIMEE SIXTA, Department of Physics, The University of Texas at Austin, Austin, TX 78712 USA, SOPHIA BOGAT, DIEGO WRIGHT, SHIRIN MOZAFFARI, DANIEL TENNANT, JEREMY PASTER, JOHN MARKERT, Department of Physics, The University of Texas at Austin — We report our efforts in the development of Nuclear Magnetic Resonance Force Microscopy (NMRFM) for the study of biological materials in liquid media at the micron scale. Our probe contains microfluidic samples sealed in thin-walled (few m) quartz tubes, with a micro-oscillator sensor nearby in vacuum to maintain its high mechanical resonance quality factor. An initial demonstration utilizes a permalloy magnet on the oscillator tip, which provides a resonant slice of thickness 0.5 m and an area of diameter 10m; these first measurements aim to demonstrate a single-shot measurement of the longitudinal relaxation time  $T_1$  in aqueous solutions of  $\text{Cu}_2\text{SO}_4$ . We also aim to implement a sawtooth 2 $\pi$  cyclic inversion of the nuclear spins, a detection scheme that effectively eliminates common measurement artifacts. At the micron scale, both spin diffusion and physical diffusion in liquids tend to blur images in conventional magnetic resonance imaging (MRI); we aim to exploit the local nature of the NMRFM probe to obtain higher resolution dynamical images, with the ultimate goal of imaging within individual biological cells.

**9:00AM E46.00006 Time-Resolved SQUID Sensor with a Nyquist Frequency up to 25 GHz**, Z. CUI, Stanford Institute for Materials and Energy Sciences, Y. H. WANG, Stanford University, P. KRATZ, Stanford Institute for Materials and Energy Sciences, A. J. ROSENBERG, Stanford University, C. A. WATSON, I. SOCHNIKOV, Stanford Institute for Materials and Energy Sciences, Y.-K.-K. FUNG, G. GIBSON, IBM Watson Research Center, J. R. KIRTLEY, Stanford Institute for Materials and Energy Sciences, M. B. KETCHEN, OcteVue, K. A. MOLER, Stanford Institute for Materials and Energy Sciences — We demonstrate a time-resolved scanning Superconducting Quantum Interference Device (SQUID) sensor with an expected maximum sampling rate of 50 GHz. The time-resolved SQUID sampler is operated by a pump-probe pulse sequence and will be particularly useful in studying high-frequency magnetic devices and the transient behavior of magnetic materials. The high sampling rate is achieved through a Josephson-interferometry technique developed at IBM[1][2]. We tested our sampler with flux signals of order 10  $m\Phi_0$  (where  $\Phi_0$  is the magnetic flux quantum), which corresponds to 25 million Bohr magnetons located 1 micron directly below the pickup loop. Operating in this regime, our sampler will have much higher sensitivity than bulk sensors like conventional SQUIDS and much larger spatial scanning range than single-spin sensors like NV centers. The SQUID sampler will thus be well-suited to characterize individual mesoscopic samples as well as bulk samples with mesoscopic features. [1]S. M. Faris, APL 36, 1005 (1980). [2]J. R. Kirtley, et al., "Advanced sensors for scanning SQUID microscopy", Superconductive Electronics Conference (ISEC 2013), invited paper F2.

**9:12AM E46.00007 Toward single atom qubits on a surface: Pump-probe spectroscopy and electrically-driven spin resonance**, WILLIAM PAUL, IBM Research - Almaden — We will discuss the characterization of spin dynamics by pump-probe spectroscopy and the use of gigahertz-frequency electric fields to drive spin resonance of a Fe atom on a MgO/Ag(001) surface. In the spirit of this session, the technical challenges in applying a precise voltage to the tip sample junction across a wide radio-frequency bandwidth will be described. The energy relaxation time,  $T_1$ , of single spins on surfaces can be measured by spin-polarized pump-probe STM (scanning tunneling microscopy) [1]. To date, the relaxation times reported for Fe-Cu dimers on Cu<sub>2</sub>N insulating films have been of the order  $\sim 100$  ns [1]. A three-order-of-magnitude enhancement of lifetime, to  $\sim 200$   $\mu$ s, was recently demonstrated for Co on a single-monolayer of MgO [2]. Here, we report on the tailoring of the  $T_1$  lifetime of single Fe atoms on single- and multi-layer MgO films grown on Ag(001). Next, we demonstrate electron spin resonance of an individual single Fe atom, driven by a gigahertz-frequency electric field applied across the tip-sample junction, and detected by a spin-polarized tunneling current. The principle parameters of the spin resonance experiment, namely the phase coherence time  $T_2$  and the Rabi rate, are characterized for Fe atoms adsorbed to the monolayer MgO film. [1] Loth et al., Science 329, 1628 (2010) [2] Rau and Baumann et al., Science 344, 988 (2014) [3] Baumann and Paul et al., Science 350, 417 (2015)

**9:48AM E46.00008 Cantilever detection of electron spin resonance in the terahertz region**, HIDEYUKI TAKAHASHI, Organization of Advanced Science and Technology, Kobe University, EIJI OHMICHII, Graduate School of Science, Kobe University, HITOSHI OHTA, Molecular Photoscience Research Center, Kobe University — Electron spin resonance (ESR) is used in a wide range of research areas. Most commercially available spectrometers operate at the X-band ( $\sim 10$  GHz). However, high-frequency ESR ( $>100$  GHz) has many advantages, such as the high spectral resolution, the ESR detection beyond the zero-field splitting etc. We report the cantilever detection of electron spin resonance in the terahertz region. This technique mechanically detects ESR as a change in magnetic torque that acts on the cantilever, while the conventional method, such as the cavity perturbation and the transmission method, directly measures the absorption of electromagnetic wave power. Backward wave oscillators (BWO) were used as THz-wave sources. Despite the small sample mass ( $m = 4$   $\mu$ g) and low power output of the BWO ( $P < 4$  mW above 1 THz), we observed ESR absorption of Co Tutton salt,  $\text{Co}(\text{NH}_4)_2(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$ , in frequencies of up to 1.1 THz. Spin sensitivity was estimated to be the order of  $10^{11}$ - $10^{12}$  spins/gauss above 1 THz. This technique will not only broaden the scope of ESR spectroscopy application but also lead to high-spectral-resolution ESR imaging. [1]H. Takahashi, E. Ohmichi and H. Ohta, Appl. Phys. Lett. **107**, 182405 (2015).

**10:00AM E46.00009 Ultrafast nano-imaging of the photoinduced phase transition dynamics in  $\text{VO}_2$** , SVEN A. DOENGES, OMAR KHATIB, BRIAN T. O'CALLAHAN, Department of Physics, Department of Chemistry, and JILA, University of Colorado, Boulder, CO 80309, JOANNA M. ATKIN, Department of Chemistry, University of North Carolina, Chapel Hill, NC 27514, JAE HYUNG PARK, DAVID H. COBDEN, Department of Physics, University of Washington, Seattle, WA 98195, MARKUS B. RASCHKE, Department of Physics, Department of Chemistry, and JILA, University of Colorado, Boulder, CO 80309 — Many quantum phase transitions in correlated matter exhibit spatial inhomogeneities with expected yet unexplored effects on the associated ultrafast dynamics. Here we demonstrate the combination of ultrafast non-degenerate pump-probe spectroscopy with scattering scanning near-field optical microscopy (s-SNOM) for ultrafast nano-imaging. In a femtosecond near-field non-degenerate near-IR (NIR) pump and mid-IR (MIR) probe experiment, we study the photoinduced insulator-to-metal (IMT) transition in nominally homogeneous  $\text{VO}_2$  micro-crystals using far-from equilibrium excitation. We observe spatial heterogeneity on 50-100 nm length scales in the fluence dependent IMT dynamics, ranging from sub-100 fs to 1 ps. With pump fluences as high as nominally 10 mJ/cm<sup>2</sup> we can reach distinct excitation and saturation regimes. These results suggest a large sensitivity of the IMT with respect to local variations in strain, doping, or defects difficult to discern microscopically.

**10:12AM E46.00010 Nanoscale dynamics of the Insulator-to-Metal transition in  $\text{VO}_2$** , AARON STERNBACH, University of California, San Diego — We have improved upon the technique of time resolved scanning near-field optical microscopy to study the development of inhomogeneous phase transitions in the time domain with 20 nanometer spatial resolution and 100 femtosecond temporal resolution. In our present work, we study Vanadium Dioxide ( $\text{VO}_2$ ), which is a canonical correlated electron system that exhibits an insulator-to-metal transition (IMT) above room temperature. We observe inhomogeneous dynamics that are related to mesoscopic strain variations. Our measurement resolves the dynamical evolution of the IMT on length scales that are short compared with the typical sizes of metallic domains in  $\text{VO}_2$ . By using Near-Infrared radiation, measured on a pulse-to-pulse basis, we are able to achieve an unprecedented Signal-to-Noise ratio. Our advances pave a pathway to study a wide range of systems with inhomogeneities properties on the nanoscale with high sensitivity, nanoscopic spatial, and ultrafast temporal resolution.

**10:24AM E46.00011 s-SNOM based IR and THz spectroscopy for nanoscale material characterization**, TOBIAS GOKUS, ANDREAS HUBER, ADRIAN CERNESCU, neaspec GmbH — Scattering-type Scanning Near-field Optical Microscopy (s-SNOM) allows to overcome the diffraction limit of conventional light microscopy enabling optical measurements at a spatial resolution of 10nm. s-SNOM employs an externally-illuminated sharp metallic AFM tip to create a nanoscale hot-spot at its apex. The optical tip-sample near-field interaction is determined by the local dielectric properties (refractive index) of the sample and detection of the elastically tip-scattered light yields nanoscale resolved near-field images simultaneous to topography. Development of a dedicated Fourier-transform detection module for analyzing light scattered from the tip which is illuminated by a broadband laser source enables IR spectroscopy of complex polymer nanostructures. Applications presented further demonstrate characterization of embedded structural phases in biominerals (bone), organic semiconductors or functional semiconductor nanostructures. Furthermore, by extending the concept of broadband-s-SNOM spectroscopy to the THz-spectral range, we demonstrate optical near-field imaging and spectroscopy at THz-frequencies (0.5-2.5 THz) by coupling the free space beam of a dedicated THz-TDS to the s-SNOM system.

**10:36AM E46.00012 Novel combination of near-field s-SNOM microscopy with peak-force tapping for nano-chemical and nano-mechanical material characterization with sub-20 nm spatial resolution**, MARTIN WAGNER, Bruker Nano Surfaces, Santa Barbara, KARINA CARNEIRO, STEFAN HABELITZ, UC San Francisco, THOMAS MUELLER, BNS, BNS TEAM, UCSF TEAM — Heterogeneity in material systems requires methods for nanoscale chemical identification. Scattering scanning near-field microscopy (s-SNOM) is chemically sensitive in the infrared fingerprint region while providing down to 10 nm spatial resolution. This technique detects material specific tip-scattering in an atomic force microscope. Here, we present the first combination of s-SNOM with peak-force tapping (PFT), a valuable AFM technique that allows precise force control between tip and sample down to 10s of pN. The latter is essential for imaging fragile samples, but allows also quantitative extraction of nano-mechanical properties, e.g. the modulus. PFT can further be complemented by KPFM or conductive AFM for nano-electrical mapping, allowing access to nanoscale optical, mechanical and electrical information in a single instrument. We will address several questions ranging from graphene plasmonics to material distributions in polymers. We highlight a biological application where dental amelogenin protein was studied via s-SNOM to learn about its self-assembly into nanoribbons. At the same time PFT allows to track crystallization to distinguish protein from apatite crystals for which amelogenin is supposed to act as a template.

**10:48AM E46.00013 Towards optically-integrated scanning tunneling microscopy studies of defects in semiconductors**, ANNE BENJAMIN, EVAN LANG, KEVIN WERNER, ENAM CHOWDHURY, JAY GUPTA, Ohio State Univ - Columbus — As electronic devices approach the nanoscale, their function is increasingly dependent on the local environment of individual defects. We are developing a combination of optical illumination and scanning tunneling microscopy techniques to study how the properties of individual defects depend on aspects of the local environment, such surface or defect proximity, applied electric fields, and illumination. Here we present studies of individual Zn and Er impurities in GaAs(110).

We use controlled motion of the STM tip during voltage sweeps to resolve previously hidden in-gap states of Zn acceptors and probe Zn further from the surface than previously accessible. We discovered two classes of Zn acceptors, one with defect states that did not shift with tip-induced band bending (TIBB), and one with states that do. Similar behavior was observed for above-gap illumination, consistent with the surface photovoltage effect (SPV). For Er on GaAs(110), we discovered three different adsorption states sharing two different sites. We found defect states near the conduction band edge, which shifted with TIBB as well as IR illumination resonant with the Er f-shell transitions.

**Tuesday, March 15, 2016 8:00AM - 11:00AM —**  
**Session E47 DCMF: Surfaces and Interfaces of Complex Oxides 312 -**

**8:00AM E47.00001 Controlling the electronic properties of  $\text{Er}_2\text{O}_3$  thin film by oxygen vacancies**, AARON WANG, ANDREW YOST, VIVEK JAIN, QILIN DAI, JINKE TANG, TEYU CHIEN, University of Wyoming — With a high dielectric constant and wide bandgap,  $\text{Er}_2\text{O}_3$  is suitable for applications in electronic and optical devices. It is known that in many oxide materials, oxygen vacancy concentration plays a decisive role in engineering the properties of the oxides. To address the oxygen vacancy concentration effects on the properties of  $\text{Er}_2\text{O}_3$ , here we present Scanning Tunneling Microscopy and Spectroscopy (STM/S) and X-Ray Diffraction (XRD) studies of the  $\text{Er}_2\text{O}_3$  thin film made by Pulsed Laser Deposition (PLD). XRD shows  $\text{Er}_2\text{O}_3$  thin film deposited at 700°C in high vacuum (HV) (sample 1) has broader peaks compared to that of the one deposited at room temperature (RT) in HV followed by 400°C annealing in air (sample 2). This indicates that, for sample 1, the loss of long range periodicity in crystal structure is mainly due to oxygen vacancies. Moreover, a relatively rough surface with 2 to 5 nm nanoclusters were observed in sample 1 by STM; while sample 2 is too resistive for STM measurements. In addition, Scanning Tunneling Spectroscopy (STS) analysis for sample 1 revealed the bandgap as well as features in the conduction band which may be related to the oxygen vacancies.

**8:12AM E47.00002 Effect of  $\text{LaInO}_3$  layer thickness on the conductance enhancement at the  $\text{LaInO}_3/\text{Ba}_{1-x}\text{La}_x\text{SnO}_3$  polar interface**, CHULKWON PARK, USEONG KIM, JUYEON SHIN, YOUNG MO KIM, YOUJUNG KIM, KOOKRIN CHAR, Seoul National University — We have recently reported on the high performance thin film transistors based on La-doped  $\text{BaSnO}_3$  (BLSO), which has high electron mobility and thermal stability, with  $\text{LaInO}_3$  (LIO) gate dielectric [1, 2]. During the course of this research we have observed  $10^4$  times enhancement of the sheet conductance of BLSO channel layer, which implies formation of 2DEG, after the interface formation with LIO. Detailed further study revealed that the La concentration in the BLSO channel layer critically affects the enhancement of sheet conductance on the LIO/BSO interface [3]. We investigated the LIO thickness dependence on the conductance of LIO/BSO interface and will discuss the origin of this phenomenon in terms of the intrinsic interface polarization in the LIO layer. This understanding is the first step towards the device application of the perovskite oxide heterostructures and may potentially lead to new interface states. [1] H. J. Kim, U. Kim *et al.*, Appl. Phys. Express **5**, 061102 (2012). [2] U. Kim *et al.*, APL Mat. **3**, 036101 (2015). [3] U. Kim *et al.*, preprint.

**8:24AM E47.00003 Optical properties of  $\text{CuFeO}_2$  and  $\text{CuFe}_{1-x}\text{Ga}_x\text{O}_2$  highly epitaxial thin films**<sup>1</sup>, A. L. CABRERA, R. A. WHEATLEY, S. ROJAS<sup>2</sup>, Instituto de Fisica, Pontificia Universidad Catolica de Chile, T. JOSHI, P. BORISOV<sup>3</sup>, D. LEDERMAN, Department of Physics and Astronomy, West Virginia University, Morgantown — Delafossite thin films of 20 and 200 nm  $\text{CuFeO}_2$  and 52 nm  $\text{CuFe}_{1-x}\text{Ga}_x\text{O}_2$  were grown by Pulsed Laser Deposition (PLD) on  $\text{Al}_2\text{O}_3$  (0001) substrates. High epitaxial quality of the films was verified by the techniques of X-Ray Diffraction and Raman spectroscopy. Optical transmission and reflection spectroscopies were performed on the films under vacuum and in  $\text{CO}_2$  controlled atmosphere, respectively. Tauc plots based on transmission data yielded direct optical band gap at 2.4 eV, 2.8eV and 3.1eV and indirect band gap at 0.9 eV and 1.3 eV for  $\text{CuFe}_{1-x}\text{Ga}_x\text{O}_2$  ( $x=0.25$ ) and the direct band gap at 1.9eV, 3.1eV and the indirect band gap at 1.1eV for the  $\text{CuFeO}_2$  films.

<sup>1</sup>Supported by FONDECYT 1130372

<sup>2</sup>CONICYT Proyecto N4386/2015

<sup>3</sup>Supported by the WV Higher Education Policy Commission (grant HEPC.dsr.12.29), by FAME, one of six centers of STARnet, a Semiconductor Research Corporation program sponsored by MARCO and DARPA (contract 2013-MA-2382) and WVU Shared Research Facilities

**8:36AM E47.00004 Comparative study of water and carbon dioxide adsorption on  $\text{CuFeO}_2$  and  $\text{CuFe}_{1-x}\text{Ga}_x\text{O}_2$  highly epitaxial thin films**<sup>1</sup>, S. ROJAS<sup>2</sup>, Instituto de Fisica, Pontificia Universidad Catolica de Chile, T. JOSHI, P. BORISOV<sup>3</sup>, D. LEDERMAN, Department of Physics and Astronomy, West Virginia University, Morgantown, A. L. CABRERA, Instituto de Fisica, Pontificia Universidad Catolica de Chile — Thermal programmed desorption (TPD) of  $\text{CO}_2$  and  $\text{H}_2\text{O}$  from a 200 nm thick  $\text{CuFeO}_2$  and 52 nm thick  $\text{CuFe}_{1-x}\text{Ga}_x\text{O}_2$  delafossite surfaces was performed in a Ultra-high vacuum (UHV) chamber. The thin films with epitaxial quality were grown by Pulsed Laser Deposition (PLD) on  $\text{Al}_2\text{O}_3$  (0001) substrates. The adsorption / desorption of  $\text{CO}_2$  and  $\text{H}_2\text{O}$  process was also monitored with X-ray Photoelectron Spectroscopy (XPS) and Auger Electron Spectroscopy (AES). Our results revealed that carbon dioxide is preferentially chemisorbed by  $\text{CuFe}_{1-x}\text{Ga}_x\text{O}_2$  over water and we observed the opposite behavior with regard to chemisorption of  $\text{CO}_2$  and  $\text{H}_2\text{O}$  over  $\text{CuFeO}_2$ . Hydroxyls and metal carbonates were formed on the surface due to the chemisorption of  $\text{H}_2\text{O}$  and  $\text{CO}_2$ . Arrhenius plots for  $\text{CO}_2$  and  $\text{H}_2\text{O}$  desorption were done and activation energy for desorption were obtained.

<sup>1</sup>supported by FONDECYT 1130372

<sup>2</sup>CONICYT Proyecto N4386/2015

<sup>3</sup>Supported by the WV Higher Education Policy Commission (grant HEPC.dsr.12.29), by FAME, one of six centers of STARnet, a Semiconductor Research Corporation program sponsored by MARCO and DARPA (contract 2013-MA-2382) and WVU Shared Research Facilities

**8:48AM E47.00005 Crystallographic orientation dependence of electronic properties at  $\text{LaAlO}_3/\text{SrTiO}_3$  interfaces**, NEIL CAMPBELL, MARK RZCHOWSKI, Department of Physics, University of Wisconsin, Madison, Wisconsin 53706, USA, SANGWOO RYU, HYUNGWOO LEE, CHANG-BEOM EOM, Department of Materials Science and Engineering, University of Wisconsin, Madison, Wisconsin 53706, USA — The two-dimensional electron liquid (2DEL) formed at the interface between perovskite oxides  $\text{LaAlO}_3$  and  $\text{SrTiO}_3$  has been found to show many interesting properties, including ones that depend on the electronic and structural properties of the interface. Most research has investigated the (001) orientation, where the crystal structure is square in the plane. Changing the crystallographic orientation can change the polarization mismatch and shift energies and occupations of the orbitals near the Fermi surface. This affects the 2DEL in many ways, particularly by changing the spatial extent and profile of the charge density. The interplay between interlayer hopping integrals and orbital energy shifts make the 2DELs in different orientations behave differently in response to gating. The interface plane defines a symmetry-breaking direction for the  $d$  orbitals and electrostatic potential, causing splitting of Ti  $d$  bands, affecting band occupation and mass near the interface. Heterostructures grown on (111)  $\text{SrTiO}_3$ , have similar Ti  $d$  orbital energies since they all have lobes crossing the interface, while in (001), the  $d_{xy}$ , and  $d_{x^2-y^2}$  orbitals do not have such lobes. We present temperature-dependent Hall and magnetotransport data probing these orientational differences.

**9:00AM E47.00006 Thickness Dependence of Electrical and Structural Properties of Tensile Strained Calcium Manganese Oxide Thin Films<sup>1</sup>**, CACIE HART, ZOEY WARECKI<sup>2</sup>, ADEEL CHAUDHRY, NATALIE FERRONE, DAVID HOUSTON, BRIDGET LAWSON, GRACE YONG, RAJESWARI KOLAGANI, Towson University — We have investigated the properties of  $\text{CaMnO}_{3-\delta}$  thin films epitaxially grown by pulsed laser deposition on lattice mismatched substrates, (100) $\text{LaAlO}_3$  and (100) $\text{SrTiO}_3$ , leading to a tensile strain of  $\sim 4\%$  and 1.5% respectively. For our films these substrates, thickness dependence of the properties is characteristically different from what has been previously observed in thin films of hole-doped manganites. We observe that the resistivity decreases significantly as the film thickness decreases. The decrease in resistivity is more pronounced in the films on (100) $\text{SrTiO}_3$  with the larger lattice mismatch, the resistivity of the thinnest films being about 3 orders of magnitude lower than the of bulk  $\text{CaMnO}_3$ . Thickness dependence of the lattice constants also show deviations from the behavior expected from strain relaxation. These results suggest a coupling between tensile strain and oxygen deficiency consistent with predictions from models based on density functional theory calculations. Our results are relevant for potential catalytic applications of  $\text{CaMnO}_{3-\delta}$  thin films.

<sup>1</sup>NSF Grant ECCS112856 and Seed Funding from the School of Emerging Technologies

<sup>2</sup>Now at University of Maryland, College Park

**9:12AM E47.00007 Role of lanthanum aluminate composition in interface formation with strontium titanate**, ABDUL RUMAIZ, National Synchrotron Light Source II, Brookhaven National Laboratory, CONAN WEILAND, National Institute of Standards and Technology, GEORGE STERBINSKY, Advanced Photon Source, Argonne National Laboratory, C. STEPHEN HELLBERG, Center for Computational Materials Science, Naval Research Laboratory, JOSEPH WOICK, National Institute of Standards and Technology, SHAOBO ZHU, DARRELL SCHLOM, Department of Materials Science and Engineering, Cornell University — While  $\text{LaAlO}_3$  (LAO) and  $\text{SrTiO}_3$  (STO) are both insulators, the interface between the two materials is conductive when the LAO is above a critical thickness and the STO is  $\text{TiO}_2$ -terminated; the origin of this conductivity is widely debated. It has also been demonstrated that the conductive interface depends on the composition of the LAO film: conductive interfaces were only found to occur for  $\text{La:Al} < 0.97$ . Hard x-ray photoelectron spectroscopy has been performed on ten unit cell thick Al-rich ( $\text{La:Al} = 0.9$ ), stoichiometric ( $\text{La:Al} = 1$ ), and La-rich ( $\text{La:Al} = 1.1$ ) LAO films deposited on STO to elucidate the role of LAO composition in the interfacial structure. A small built-in potential was observed in the Al-rich film compared to the stoichiometric and La-rich films, as determined from valence-band broadening. The stoichiometric and La-rich films were also found to have La-enrichment at the interface, while the Al-rich film did not. These results combined with first-principles calculations demonstrate the role that defects in the LAO film play in the LAO/STO interfacial structure.

**9:24AM E47.00008 Metallic interface in non- $\text{SrTiO}_3$  based titanate superlattice<sup>1</sup>**, XIAORAN LIU, Department of Physics, University of Arkansas, Fayetteville, Arkansas 72701, USA, D. CHOUDHURY, Department of Physics, Indian Institute of Technology, Kharagpur 721302, India, YANWEI CAO, M. KAREEV, S. MIDDEY, J. CHAKHALIAN, Department of Physics, University of Arkansas, Fayetteville, Arkansas 72701, USA, UNIVERSITY OF ARKANSAS TEAM, INDIAN INSTITUTE OF TECHNOLOGY TEAM — We report on the fabrication of all perovskite Mott insulator/band insulator  $\text{YTiO}_3/\text{CaTiO}_3$  superlattices by pulsed laser deposition. The combination of *in-situ* reflection high energy electron diffraction, X-ray diffraction and X-ray reflectivity confirms the high quality of the films grown in a layer-by-layer mode. Electrical transport measurements reveal that a non- $\text{SrTiO}_3$  based two-dimensional electron gas system has formed at the  $\text{YTiO}_3/\text{CaTiO}_3$  interface. These studies offer another route in the pursuit of complex oxide two-dimensional electron gas systems which allows to obtain greater insights into the exotic many-body phenomena at such interfaces.

<sup>1</sup>J.C. is supported by the Gordon and Betty Moore Foundation's EPiQS Initiative through Grant GBMF4534. S.M. is supported by the DOD-ARO under Grant No. 0402-17291. Y.C. and X.L. acknowledge the support by the Department of Energy grant DE-SC0012375.

**9:36AM E47.00009 The Effect of Polarization on Local Electronic Structure in Ferroelectric Nano-Domains in  $\text{BaTiO}_3$** , ERIE MORALES, Univ of Pennsylvania, CARLOS PEREZ, DAWN BONNELL, University of Pennsylvania, MSE TEAM — Novel ferroelectric  $\text{BaTiO}_3$  applications ranging from sensors to nanogenerators require a detailed understanding of atomic interactions at surfaces. Single crystals provide a platform that allows the exploitation of surface physical and chemical properties that can be readily transferred to other ABO<sub>3</sub> perovskites. The processes that result in the atomic and electronic structures of surfaces in tandem with polarization of domains are necessary steps towards understanding  $\text{BaTiO}_3$ . Here we treat  $\text{BaTiO}_3$  surface using sputtering-annealing cycles that yield the (6x1) reconstruction. We demonstrate that it is possible to pole a thin  $\text{BaTiO}_3$  single crystal in ultra high vacuum using scanning tunneling microscopy (STM). We determine that we can prepare  $\text{BaTiO}_3$  using *in-situ* annealing that allows us to control the size of poled region to 40nm. We pole in constant-current mode in STM by applying a bias of less than 10 V between tip and sample for 100ms. STM and scanning tunneling spectroscopy characterization allow us to map topography and local density of states, respectively. For a given unique pulse, the poled domains show a fluctuating electronic occupation of conduction bands and shifting of valence band. We will also discuss the effect of polarization on molecular adsorption.

**9:48AM E47.00010 Effect of the undoped  $\text{BaSnO}_3$  space layer on the high mobility  $\text{LaInO}_3/\text{Ba}_{1-x}\text{La}_x\text{SnO}_3$  polar interface**, JUYEON SHIN, CHULKWON PARK, YOUNG MO KIM, YOUJUNG KIM, KOOKRIN CHAR, Seoul national university — We have recently reported on the sheet conductance enhancement at the interface between two band insulators:  $\text{LaInO}_3$  (LIO) and  $\text{BaSnO}_3$  (BSO) [1, 2]. The advantages of the two-dimensional electron gas-like (2DEG) state at the LIO/ $\text{Ba}_{1-x}\text{La}_x\text{SnO}_3$  (BLSO) polar interface are its stability, the controllability of the local carrier concentration, and the high electron mobility of BLSO [3]. The origin of enhanced conductance at the interface is still under investigation, but the doping level of BSO is a critical parameter for the polar charge contribution. [2] We have investigated a new structure using an undoped BSO space layer at the LIO/BLSO interface. On one hand, this new structure will improve the mobility of the LIO/BLSO structure by reducing La impurity scattering. On the other hand, through this new structure we can answer the issues related with La diffusion at the LIO/BLSO polar interface and trace the origin of the 2DEG-like charge. This new modified structure of the LIO/BSO polar interface looks promising for higher electron mobility devices. [1] U. Kim *et al.*, APL Mat. 3, 036101 (2015). [2] U. Kim *et al.*, preprint. [3] H. J. Kim, U. Kim *et al.*, Appl. Phys. Express 5, 061102 (2012).

**10:00AM E47.00011 Electronic Structure of Epitaxial Thin Films of the Transparent Conducting Oxide La:BaSnO<sub>3</sub> Measured By In-Situ Angle-Resolved Photoemission Spectroscopy**, EDWARD LOCHOCKI, HANJONG PAIK, Cornell University, MASAKI UCHIDA, University of Tokyo, DARRELL SCHLOM, KYLE SHEN, Cornell University — Lanthanum-doped barium stannate (La:BaSnO<sub>3</sub>) is a transparent conducting oxide where single crystals have exhibited unusually high mobility and oxygen stability. Here we present in-situ angle-resolved photoemission (ARPES) measurements of La:BaSnO<sub>3</sub> epitaxial films that were co-deposited onto lattice-matched rare-earth scandate substrates by molecular-beam epitaxy (MBE). Density functional theory (DFT) calculations agree well with the observed valence bands and predict a parabolic conduction band. However, the features observed near the Fermi energy ( $E_F$ ) are non-dispersive yet localized in momentum space. This unusual appearance may be the result of quasi-localized charge carriers or out-of-plane momentum broadening. Over long measurement periods, we also observe changes to the valence band and near- $E_F$  feature that bear a strong resemblance to the beam-induced two-dimensional electron gases previously reported in SrTiO<sub>3</sub> and KTaO<sub>3</sub>. The origin of these unexpected phenomena and their relationship to the structural and transport properties of these films will be discussed.

**10:12AM E47.00012 Band gap formation in La<sub>0.7</sub>Sr<sub>0.3</sub>MnO<sub>3</sub> (LSMO) thin films measured by reflectivity/absorption and ultrafast spectroscopy**, GUERAU CABRERA, ROBBYN TRAPPEN, West Virginia University, YING-HAO CHU, National Chiao Tung University, MIKEL HOLCOMB, West Virginia University — Thin film La<sub>0.7</sub>Sr<sub>0.3</sub>MnO<sub>3</sub> (LSMO) is a prime candidate for highly spin-polarized magnetic-tunnel-junction memories. Due to its magnetic properties, it is also a good candidate for applications utilizing electrical control of magnetism when grown adjacent to a ferroelectric layer such as Pb(Zr/Ti)O<sub>3</sub> (PZT). Recently, Wu and others have seen the emergence of a band gap (about 1eV) in LSMO thin films, when grown adjacent to PZT. Currently, it is understood that LSMO is a half-metal, with a pseudo-gap due to a low density of states (DOS) near the Fermi level. The transition from pseudo-gap to band gap is not yet fully understood. It is therefore our aim to investigate the formation of this band gap through optical reflectivity/absorption and ultrafast carrier dynamics for a variety of thicknesses ranging from a few nanometers to thicker films (about 100 nm).

**10:24AM E47.00013 Interfacial stability of ultrathin film magnetite (Fe<sub>3</sub>O<sub>4</sub>) in ozone assisted MBE deposition**, HAWOONG HONG, JONGJIN KIM, Argonne National Laboratory, XINYUE FANG, University of Illinois at Urbana-Champaign, SEUNGBUM HONG, Argonne National Laboratory, TAI C. CHIANG, University of Illinois at Urbana-Champaign — Iron oxide films were grown on sapphire (0001) surfaces using nominally 100% ozone. Both of monolayer-wise deposition and continuous deposition were tried to find the structures of the films at the start of the film formation. The studies utilized x-ray scattering with synchrotron radiation from the Advanced Photon Source. Consideration of substrate and film structures predicts Fe<sub>2</sub>O<sub>3</sub>(0001) (hematite) film formation. However, in both of the deposition modes, the initial films formed as magnetite Fe<sub>3</sub>O<sub>4</sub>(111). As the film growth progresses, hematite (Fe<sub>2</sub>O<sub>3</sub>(0001)) appears. At the later stage, the magnetite disappears and the whole film turned to hematite. Real time and static x-ray diffraction results show the same result. Possibility of the oxidation limited transformation should be excluded. Other possible cause of this reverse stability will be discussed.

**10:36AM E47.00014 Effects of strain, electric field and correlations on the resistance noise in epitaxial NdNiO<sub>3</sub> films<sup>1</sup>**, G. SAMBANDAMURTHY, ALI ALSAQQA, SUJAY SINGH, State Univ of NY - Buffalo, SRIMANTA MIDDEY, MICHAEL KAREEV, JAK CHAKHALIAN, University of Arkansas - Fayetteville — Rare earth nickelates are strongly correlated materials that exhibit metal-insulator and Neel transitions as a function of temperature. The nature of the transport mechanisms in individual phases (paramagnetic metal, paramagnetic insulator and antiferromagnetic insulator) is an active area of research. We use low frequency (1 mHz < f < 10 Hz) resistance noise spectroscopy to probe the phases and the transitions between them in ultrathin epitaxial films of NdNiO<sub>3</sub> grown on substrates that introduce different strains. While the transport behavior and the transition temperatures are greatly affected by the strain, the noise behavior across the transitions is found to be similar. In the low temperature antiferromagnetic phase, an intriguing switching between two distinct ground states is observed pointing to a subtle competition in the energy landscape. The noise magnitude as a function of electric field in submicron devices will also be presented.

<sup>1</sup>This work is supported by NSF DMR 0847324

**10:48AM E47.00015 Quantitative measurements and modeling of electronic and atomic surface structure in epitaxial LaNiO<sub>3</sub> thin films by ARPES, LEED-I(V), and DFT+DMFT**, JACOB RUF, ELIZABETH NOWADNICK, Cornell University, HYOWON PARK, Columbia University, PHILIP KING, Cornell University, ANDREW MILLIS, Columbia University, DARRELL SCHLOM, KYLE SHEN, Cornell University — Careful exploration of the phase space available for artificially engineering emergent electronic properties in epitaxial thin films and superlattices of transition-metal oxides requires close feedback between materials synthesis, experimental characterization of both electronic and atomic structures, and modeling based on advanced computational methods. Here we apply this general strategy to the perovskite rare-earth nickelate LaNiO<sub>3</sub>, using molecular-beam epitaxy to synthesize thin films, performing *in situ* angle-resolved photoemission spectroscopy (ARPES) and low-energy electron diffraction (LEED) measurements, and comparing our results with the predictions of density functional theory plus dynamical mean-field theory (DFT+DMFT). Our study establishes LaNiO<sub>3</sub> as a moderately correlated metal in which the quasiparticle mass enhancement can be modeled with quantitative accuracy by DFT+DMFT. Finally, in view of efforts to produce  $e_g$  orbital polarization in nickelate heterostructures as a means of mimicking single-band cuprate-like physics, we discuss the extent to which our ARPES and LEED results suggest that such effects are intrinsically present at film surfaces due to the existence of polar distortions, as reported by coherent Bragg rod analysis of surface x-ray diffraction.

**Tuesday, March 15, 2016 8:00AM - 11:00AM –**

**Session E48 GQI: Quantum Error Correction in Superconducting Qubits** 349 - Austin Fowler, Google, Inc.

**8:00AM E48.00001 Increasing error resilience in superconducting qubits based on symmetries and parametric protocols<sup>1</sup>**, DAVID SCHUSTER<sup>2</sup>, University of Chicago — The field of superconducting quantum computing has seen remarkable advances in the past decade, and is getting closer to realizing logical qubits partially stabilized by error correction. However, achieving full scalability necessary to build a universal quantum computer remains a significant challenge which calls for new ideas to make superconducting qubits even more resilient with respect to external noise and fabrication imperfections. Past breakthroughs in this direction include circuit QED enabled measurement and long-range interactions; reliably long coherence times in transmon qubits; and additional coherence improvements by the use of 3D cavities. Here we review previous work on topological protection in superconducting circuit networks, and report on new efforts, in experiment and theory, to increase autonomous error protection of superconducting qubits by harnessing symmetry properties of circuit Hamiltonians and employing parametric processes for robust manipulation and storage of quantum information.

<sup>1</sup>This talk is based on joint work with Andrew Houck and David Schuster.

<sup>2</sup>This is joint work with Jens Koch and Andrew Houck

**8:36AM E48.00002 Engineering stabilizer measurements in circuit QED: I<sup>1</sup>** , KEVIN CHOU, JACOB BLUMOFF, M. REAGOR, C. AXLINE, R. BRIERLEY, Yale University, S. NIGG, University of Basel, P. REINHOLD, R. HEERES, C. WANG, K. SLIWA, A. NARLA, Yale University, M. HATRIDGE, University of Pittsburgh, L. JIANG, M. H. DEVORET, S. M. GIRVIN, R. J. SCHOEKOPF, Yale University — Quantum error correction based on stabilizer codes has emerged as an attractive approach towards building a practical quantum information processor. One requirement for such a device is the ability to perform hardware efficient measurements on registers of qubits. We demonstrate a new protocol to realize such multi-qubit measurements. A key feature of our approach is that it enables arbitrary stabilizer measurements to be selected in software, and requires a relatively small number of buses, ancillae, and control lines. This allows for a minimally complex sample realizing a simple dispersive hamiltonian while maintaining a high degree of decoupling between our fixed-tuned qubits. We experimentally implement these measurements in 3D circuit QED using transmon qubits coupled to a common bus resonator. In this first of two talks, we introduce our 3D cQED system and describe the protocol for measuring n-qubit parities of a three qubit register.

<sup>1</sup>We acknowledge funding from ARO

**8:48AM E48.00003 Engineering stabilizer measurements in circuit QED: II<sup>1</sup>** , JACOB BLUMOFF, KEVIN CHOU, M REAGOR, C AXLINE, R BRIERLY, Yale University, S NIGG, University of Basel, P REINHOLD, R HEERES, C WANG, K SLIWA, A NARLA, Yale University, M HATRIDGE, University of Pittsburgh, L JIANG, M H DEVORET, S M GIRVIN, R J SCHOEKOPF, Yale University — Quantum error correction based on stabilizer codes has emerged as an attractive approach towards building a practical quantum information processor. One requirement for such a device is the ability to perform hardware efficient measurements on registers of qubits. We demonstrate a new protocol to realize such multi-qubit measurements. A key feature of our approach is that it enables arbitrary stabilizer measurements to be selected in software, and requires a relatively small number of buses, ancillae, and control lines. This allows for a minimally complex sample realizing a simple dispersive hamiltonian while maintaining a high degree of decoupling between our fixed-tuned qubits. We experimentally implement these measurements in 3D circuit QED using transmon qubits coupled to a common bus resonator. In the second of two talks, we present a full characterization of the algorithm describing the outcome dependent projections via quantum process tomography.

<sup>1</sup>We acknowledge funding from ARO

**9:00AM E48.00004 Weight-4 Parity Checks on a Surface Code Sublattice with Superconducting Qubits<sup>1</sup>** , MAIKA TAKITA, ANTONIO CORCOLES, EASWAR MAGESAN, NICHOLAS BRONN, JARED HERTZBERG, JAY GAMBETTA, MATTHIAS STEFFEN, JERRY CHOW, IBM T.J. Watson Research Center — We present a superconducting qubit quantum processor design amenable to the surface code architecture. In such architecture, parity checks on the data qubits, performed by measuring their X- and Z- syndrome qubits, constitute a critical aspect. Here we show fidelities and outcomes of X- and Z-parity measurements done on a syndrome qubit in a full plaquette consisting of one syndrome qubit coupled via bus resonators to four code qubits. Parities are measured after four code qubits are prepared into sixteen initial states in each basis. Results show strong dependence on ZZ between qubits on the same bus resonators.

<sup>1</sup>This work is supported by IARPA under contract W911NF-10-1-0324

**9:12AM E48.00005 Active resonator reset in the non-linear regime of circuit QED to improve multi-round quantum parity checks<sup>1</sup>** , CORNELIS CHRISTIAAN BULTINK, M.A. ROL, X. FU, B.C.S. DIKKEN, J.C. DE STERKE, R.F.L. VERMEULEN, R.N. SCHOUTEN, A. BRUNO, K.L.M. BERTELS, L. DICARLO, QuTech, Delft University of Technology — Reliable quantum parity measurements are essential for fault-tolerant quantum computing. In quantum processors based on circuit QED, the fidelity and speed of multi-round quantum parity checks using an ancillary qubit can be compromised by photons remaining in the readout resonator post measurement, leading to ancilla dephasing and gate errors. The challenge of quickly depleting photons is biggest when maximizing the single-shot readout fidelity involves strong pulses turning the resonators non-linear. We experimentally demonstrate the numerical optimization of counter pulses for fast photon depletion in this non-analytic regime. We compare two methods, one using digital feedback and another running open loop. We assess both methods by minimizing the average number of rounds to ancilla measurement error.

<sup>1</sup>We acknowledge funding from the EU FP7 project SCALEQIT, FOM, and an ERC Synergy Grant.

**9:24AM E48.00006 Demonstration of quantum superiority in learning parity with noise with superconducting qubits<sup>1</sup>** , DIEGO RISTÈ, MARCUS DA SILVA, COLM RYAN, Raytheon BBN Technologies, ANDREW CROSS, JOHN SMOLIN, JAY GAMBETTA, JERRY CHOW, IBM T.J. Watson Research Center, BLAKE JOHNSON, Raytheon BBN Technologies — A problem in machine learning is to identify the function programmed in an unknown device, or oracle, having only access to its output. In particular, a parity function computes the parity of a subset of a bit register. We implement an oracle executing parity functions in a five-qubit superconducting processor and compare the performance of a classical and a quantum learner. The classical learner reads the output of multiple oracle calls and uses the results to infer the hidden function. In addition to querying the oracle, the quantum learner can apply coherent rotations on the output register before the readout. We show that, given a target success probability, the quantum approach outperforms the classical one in the number of queries needed. Moreover, this gap increases with readout noise and with the size of the qubit register. This result shows that quantum advantage can already emerge in current systems with a few, noisy qubits.

<sup>1</sup>We acknowledge support from IARPA under contract W911NF-10-1-0324.

**9:36AM E48.00007 A Very Small Logical Qubit** , ELIOT KAPIT, Tulane University — Superconducting qubits are among the most promising platforms for building a quantum computer. However, individual qubit coherence times are not far past the scalability threshold for quantum error correction, meaning that millions of physical devices would be required to construct a useful quantum computer. Consequently, further increases in coherence time are very desirable. In this letter, we blueprint a simple circuit consisting of two transmon qubits and two additional lossy qubits or resonators, which is passively protected against all single qubit quantum error channels through a combination of continuous driving and engineered dissipation. Photon losses are rapidly corrected through two-photon drive fields implemented with driven SQUID couplings, and dephasing from random potential fluctuations is heavily suppressed by the drive fields used to implement the multi-qubit Hamiltonian. Comparing our theoretical model to published noise estimates from recent experiments on flux and transmon qubits, we find that logical state coherence could be improved by a factor of forty or more compared to the individual qubit  $T_1$  and  $T_2$  using this technique.

**9:48AM E48.00008 Scalable in-situ qubit calibration during repetitive error detection**, J. KELLY, R. BARENDSE, A. FOWLER, J. MUTUS, Google, Santa Barbara, B. CAMPBELL, UC Santa Barbara, Y. CHEN, Google, Santa Barbara, Z. CHEN, B. CHIARO, A. DUNSWORTH, UC Santa Barbara, E. JEFFREY, E. LUCERO, A. MEGRANT, M. NEELEY, Google, Santa Barbara, C. NEILL, P.J.J. O'MALLEY, UC Santa Barbara, P. ROUSHAN, D. SANK, Google, Santa Barbara, C. QUINTANA, A. VAINSENER, J. WENNER, UC Santa Barbara, T. WHITE, Google, Santa Barbara, J.M. MARTINIS, University of California and Google, Santa Barbara — A quantum computer protects a quantum state from the environment through the careful manipulations of thousands or millions of physical qubits. However, operating such quantities of qubits at the necessary level of precision is an open challenge, as optimal control parameters can vary between qubits and drift in time. We present a method to optimize physical qubit parameters while error detection is running using a nine qubit system performing the bit-flip repetition code. We demonstrate how gate optimization can be parallelized in a large-scale qubit array and show that the presented method can be used to simultaneously compensate for independent or correlated qubit parameter drifts. Our method is  $O(1)$  scalable to systems of arbitrary size, providing a path towards controlling the large numbers of qubits needed for a fault-tolerant quantum computer.

**10:00AM E48.00009 Tracking errors of a logical qubit comprised of superpositions of cat states in a superconducting resonator**, A. PETRENKO, N. OFEK, R. HEERES, P. REINHOLD, Y. LIU, Z. LEGHTAS, B. VLASTAKIS, L. FRUNZIO, LIANG JIANG, Yale University Department of Applied Physics, M. MIRRAHIMI, INRIA Paris-Rocquencourt, M.H. DEVORET, R.J. SCHOELKOPF, Yale University Department of Applied Physics — QEC schemes involve redundantly encoding a qubit into a larger space of states that has symmetry properties that allow one to measure error syndromes. Traditional approaches involve encodings that employ large numbers of physical qubits, enhancing decay rates significantly and requiring considerable hardware overhead to realize. A hardware-efficient proposal [1,2], which we term the cat code, sheds much of this complexity by encoding a qubit in superpositions of cat states in a superconducting resonator, which has one dominant error syndrome: single photon loss. As these cat states are eigenstates of photon number parity, the loss of a photon changes the parity without corrupting the encoded information. In a superconducting cQED architecture, we demonstrate that we track these errors in real-time with repeated single shot parity measurements and map their occurrence onto applications of a unitary rotation of an arbitrary encoded state in the logical space. Our results illustrate the utility of long-lived resonators in the context of a full QEC system by highlighting the advantages of employing the cat code to suppress decoherence. [1]Leghtas et.al. PRL 111 120501 2013 [2]Mirrahipi et.al. NJP 16 045014 2014

**10:12AM E48.00010 Stabilizing the phase of superpositions of cat states in a cavity using real-time feedback**, N. OFEK<sup>1</sup>, A. PETRENKO, R. HEERES, P. REINHOLD, Y. LIU, Z. LEGHTAS, B. VLASTAKIS, L. FRUNZIO, LIANG JIANG, Yale University, Department of Applied Physics, M. MIRRAHIMI, INRIA Paris-Rocquencourt, M.H. DEVORET, R.J. SCHOELKOPF, Yale University, Department of Applied Physics — In a superconducting cQED architecture, a hardware efficient quantum error correction (QEC) scheme exists, called the cat code [1,2], which maps a qubit onto superpositions of cat states in a superconducting resonator, by mapping the occurrence of errors, or single photon jumps, onto unitary rotations of the encoded state. By tracking the parity of the encoded state, we can count the number of photon jumps and are able to apply a correcting unitary transformation. However, the situation is complicated by the fact that photon jumps do not commute with the deterministic anharmonic time evolution of a resonator state, or Kerr, inherited by the resonator from its coupling to a Josephson junction. As predicted in [1], a field in the resonator will inherit an overall phase  $\theta = KT$  in  $IQ$  space each time a photon jumps that is proportional to the Kerr  $K$  and the time  $T$  at which the jump occurs. Here I will present how we can track the errors in real time, take them into account together with the time they occur and make it possible to stabilize the qubit information. [1]Leghtas et.al. PRL 111 120501 2013 [2]Mirrahipi et.al. NJP 16 045014 2014

<sup>1</sup>Please place my talk right after the talk of Andrei Petrenko.

**10:24AM E48.00011 Encoding quantum information in a stabilized manifold of a superconducting cavity**<sup>1</sup>, S. TOUZARD, Z. LEGHTAS, S.O. MUNDHADA, C. AXLINE, M. REAGOR, K. CHOU, J. BLUMOFF, K.M. SLIWA, S. SHANKAR, L. FRUNZIO, R.J. SCHOELKOPF, Department of Applied Physics, Yale University, M. MIRRAHIMI, Department of Applied Physics, Yale University and INRIA Paris Rocquencourt, M.H. DEVORET, Department of Applied Physics, Yale University — In a superconducting Josephson circuit architecture, we activate a multi-photon process between two modes by applying microwave drives at specific frequencies. This creates a pairwise exchange of photons between a high-Q cavity and the environment. The resulting open dynamical system develops a two-dimensional quasi-energy ground state manifold. Can we encode, protect and manipulate quantum information in this manifold? We experimentally investigate the convergence and escape rates in and out of this confined subspace. Finally, using quantum Zeno dynamics, we aim to perform gates which maintain the state in the protected manifold at all times.

<sup>1</sup>Work supported by: ARO, ONR, AFOSR and YINQE

**10:36AM E48.00012 Simulation of an arbitrary quantum channel with minimal ancillary resource**, CHAO SHEN, KYUNGJOO NOH, VICTOR V. ALBERT, MICHEL H. DEVORET, ROBERT J. SCHOELKOPF, STEVEN M. GIRVIN, LIANG JIANG, Yale University — We discuss an explicit and efficient construction of quantum circuits that can simulate an arbitrary given quantum channel acting on a d-level quantum system, with the minimal quantum ancillary resource—a qubit and its QND readout. The elementary operations required are unitary evolutions and single qubit projective measurement. We further show that this technique opens up exciting new possibilities in the field of quantum control, quantum simulation, quantum error correction, and quantum state discrimination. Our proposal can be implemented on platforms such as a superconducting transmon qubit inside a microwave cavity.

**10:48AM E48.00013 Quantum Parameter Estimation in Continuous Measurement-Based Quantum Control**, LUIS CORTEZ-GONZALEZ, Universidad Autonoma de Nuevo Leon, ANDREW N. JORDAN, University of Rochester — We consider continuous measurement as a quantum tracking and control method for superconducting quantum systems. In experiments with superconducting qubits information about the quantum state of the system is extracted in the form of a noisy analog voltage signal reflected from a coupled readout resonator. Every element of the measurement sequence describes a weak measurement that provides uncertain information about the quantum state of the qubit. In this talk we describe how the information contained in the continuous readout signal is used to estimate unknown parameters of the system as well as the most probable state evolution to produce the observed measurement record. We will theoretically compare a variety of estimation techniques including Maximum Likelihood methods and Bayesian hypothesis testing among others.

**Tuesday, March 15, 2016 8:00AM - 11:00AM —**

**Session E51 DMP FIAP: Dopants and Defects in Semiconductors: Theory** Hilton Baltimore Holiday Ballroom 2 - Adam Gali, Hungarian Academy of Sciences and Budapest University of Technology and Economics

**8:00AM E51.00001 Beyond Graphene: Electronic and Mechanical Properties of Defective 2-D Materials<sup>1</sup>**, HUMBERTO TERRONES, Rensselaer Polytechnic Institute — One of the challenges in the production of 2-D materials is the synthesis of defect free systems which can achieve the desired properties for novel applications. However, the reality so far indicates that we need to deal with defective systems and understand their main features in order to perform defect engineering in such a way that we can engineer a new material. In this talk I discuss first, the introduction of defects in a hierarchic way starting from 2-D graphene to form giant Schwarzites or graphene foams, which also can exhibit further defects, thus we can have several levels of defectiveness. In this context, it will be shown that giant Schwarzites, depending on their symmetry, can exhibit Dirac-Fermion behavior and further, possess protected topological states as shown by other authors. Regarding the mechanical properties of these systems, it is possible to tune the Poisson Ratio by the addition of defects, thus shedding light to the explanation of the almost zero Poisson ratios in experimentally obtained graphene foams. Second, the idea of Haecelites, a planar sp<sup>2</sup> graphene-like structure with heptagons and pentagons, can be extended to transition metal dichalcogenides (TMDs) with square and octagonal-like defects, finding semi-metallic behaviors with Dirac-Fermions, and even topological insulating properties.

<sup>1</sup>National Science Foundation (EFRI-1433311)

**8:36AM E51.00002 Scalable, Composable Operators for Defect Analysis and Design**, ROSE WEISBURGH, PETER CHUNG, University of Maryland — Defect structures in semiconductors can profoundly affect electronic properties through electron-phonon interactions. Knowledge of the changes to phonon properties induced by defects is vital for understanding phonon effects on electronic behavior. Defects can cause the dominant phonon peaks in the spectrum to split and shift resulting in carriers that can scatter in energy levels not foreseen in the bulk. We have developed a novel mathematical and computational framework for estimating the phonon spectra in the harmonic approximation for lattices containing arbitrary defect structures. Linear operators are used to calculate defective phonon spectra directly from the spectrum of a pristine reference lattice. The primary benefit is that the full eigensolve must only be performed once for the reference defect-free crystal. The operators can be adjusted to vary the defect concentration, defective mass ratio, and/or defective potential subsequently without having to re-evaluate the eigensystem. In the talk, we will present the theory behind our methodology and initial results about the sensitivity of electro-thermal properties of semiconductors to various point defects.

**8:48AM E51.00003 First principle study of the role of oxygen non-stoichiometry in the structure and properties of amorphous InO and InGaO.<sup>1</sup>**, RABI KHANAL, JULIA MEDVEDEVA, Missouri S&T — Ab-initio molecular dynamics liquid-quench simulations of amorphous In-O and In-Ga-O are performed to investigate the structural, electronic and optical properties of these oxides. A new approach is developed to study the formation of oxygen defects in the amorphous oxides and their role in carrier generation and transport. First, the effect of oxygen non-stoichiometry on the local structure (i.e., the average Metal-Oxygen bond length and coordination) as well as on the long-range structural characteristics (i.e., the average M-M distance and the M-O-M angle) is discussed. The latter determines how the MO polyhedra are connected into a continuous network. Presence of Ga has a significant effect on the long-range structural correlations in non-stoichiometric structures. Further, the structural properties of oxygen defects as well as their effect on the electronic band structure is investigated. The results reveal charge accumulation on metal-metal bond(s) near the Fermi level suggesting the existence of two types of oxygen defect. Finally, strongly localized states near the valence band maximum originate from O<sub>2</sub> bonds and from charge imbalance associated with low coordinated oxygen atom surrounded by highly coordinated metal atoms.

<sup>1</sup>NSF grant DMR-1121262

**9:00AM E51.00004 Polarization effects in silver delafossite systems**, GIHAN PANAPITIYA, JAMES P. LEWIS, West Virginia Univ — Delafossites are a promising class of materials which has applications in catalysis and optoelectronic devices. Even though much work has been carried out on the cuprate family of delafossites, little is known about the structural and electronic properties of its silver counterpart. In this work, we present a computational study for two delafossite oxides of the form  $AgB_{1-x}Fe_xO_2$  (For B = Al, Ga). A large number of structures are studied by varying the Fe alloying percentage(x) from 0 to 5 and by choosing the impurity sites randomly. We find that the local structural changes occurring at the vicinity of Fe atoms in these two systems have opposite trends with regard to the O-O distance. The reason for this difference in the trends is identified as the polarization effects on the inter-atomic distances caused by the displacements in O atoms resulting from the incorporation of Fe in sites, previously occupied by either Al or Ga. We believe that these effects are mediated by the differences in the atomic radii of Fe, Al and Ga. Higher alloying levels coupled with nearest neighbor Fe atoms can intensify these distortions in the structure creating deformations in the O-Ag-O bonds, which are directly related to the formation of the conduction band edge in these systems.

**9:12AM E51.00005 Discriminating a deep defect from shallow acceptors in supercell calculations: gallium antisite in GaAs**, PETER SCHULTZ, Sandia National Laboratories — To make reliable first principles predictions of defect energies in semiconductors, it is crucial to discriminate between effective-mass-like defects—for which existing supercell methods fail—and deep defects—for which density functional theory calculations can yield reliable predictions of defect energy levels. The gallium antisite  $Ga_{As}$  is often associated with the 78/203 meV shallow double acceptor in Ga-rich gallium arsenide. Within a framework of level occupation patterns, analyses of structure and spin stabilization can be used within a supercell approach to distinguish localized deep defect states from shallow acceptors such as  $B_{As}$ . This systematic analysis determines that the gallium antisite is inconsistent with a shallow state, and cannot be the 78/203 shallow double acceptor. The properties of the Ga antisite in GaAs are described, predicting that the Ga antisite is a deep double acceptor and has two donor states, one of which might be accidentally shallow. — Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Company, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

**9:24AM E51.00006 *Ab Initio* Modeling of Transition-Metal Impurities in MgO<sup>1</sup>**, SERGEY V. LEVCHENKO, SEBASTIAN ALARCON VILLASECA, ALIAKSEI MAZHEIKA, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, DE — Fe- and Ni-doped MgO are promising materials for the catalytic conversion of methane and CO<sub>2</sub>. However, theoretical studies of these materials are scarce. The self-interaction error (SIE) in approximate DFT leads to an incorrect description of the electron localization and hybridization between *d* states of Ni or Fe and the oxide electronic bands. Replacing a fraction  $\alpha$  of the (semi-)local exchange by the exact exchange reduces the SIE, but  $\alpha$  remains a parameter depending on the target property. We explore the dependence of the formation energies of Ni<sub>Mg</sub> and Fe<sub>Mg</sub> substitutional defects in MgO on  $\alpha$  in the Heyd-Scuseria-Ernzerhof hybrid functional (HSE), and compare the results to CCSD(T) embedded-cluster calculations. For Ni<sub>Mg</sub> defects HSE( $\alpha$  = 0.3) reproduces CCSD(T) formation energies and CO adsorption energies on Ni<sub>Mg</sub>. However,  $\alpha$  = 0.48 is needed in the case of Fe<sub>Mg</sub>. For both Ni<sub>Mg</sub> and Fe<sub>Mg</sub>,  $\alpha$  = 0.44-0.50 satisfies best the exact DFT condition that the HOMO does not depend on occupation. Contrary to PBE and HSE06, HSE( $\alpha$   $\approx$  0.5) reproduces the experimentally observed  $O_h \rightarrow D_{4h}$  (oblate) Jahn-Teller distortion for Fe<sub>Mg</sub>.

<sup>1</sup>We thank CoE UniCat for financial support

**9:36AM E51.00007 Phase Transformations upon Doping in Tungsten Trioxide<sup>1</sup>**, WENNIE WANG, Univ of California - Santa Barbara, ANDERSON JANOTTI<sup>2</sup>, University of Delaware, CHRIS G. VAN DE WALLE, Univ of California - Santa Barbara — Tungsten trioxide (WO<sub>3</sub>) is an emerging semiconductor material, with a growing number of applications in Li-ion batteries, photocatalysis, gas sensors and electrochromic devices. As an electrochromic material, WO<sub>3</sub> turns from transparent to blue upon doping with monovalent species. Due to it having an empty A-site in the ABO<sub>3</sub> perovskite structure, high doping concentrations are possible through intercalation. Tungsten trioxide has been experimentally shown to transform from the ground-state monoclinic symmetry to cubic symmetry with increasing monovalent doping [1]. We use first-principles calculations to understand this transformation. Our calculations show that the addition of electrons to the conduction band is a primary driver of the phase transformation. We quantify the energetics and structural aspects of this transformation using density functional theory, allowing us to elucidate the mechanism. Comparison with experiment, role of the dopant species, and implications of structural changes for device applications will be discussed. [1] Q. Zhong, J. Dahn, K. Colbow. *Phys. Rev. B* **46** 2554 (1992).

<sup>1</sup>This work is supported by the DOE and NSF GRFP.

<sup>2</sup>Previously at Univ of California- Santa Barbara

**9:48AM E51.00008 Electronic structure of intrinsic defects in non-stoichiometric amorphous In-Ga-Zn-O semiconductors**, WOO HYUN HAN, KEE JOO CHANG, Korea Adv Inst of Sci & Tech — Amorphous oxide semiconductors, such as amorphous In-Ga-Zn-O (a-IGZO), have attracted much attention because of their use as a channel material in thin-film transistors (TFTs). Despite many advantages such as flexibility, transparency, and high electron mobility, a-IGZO based TFTs suffer from defects which cause the instability of threshold voltage under negative bias illumination stress (NBIS) as well as positive bias stress (PBS). Recently, we have proposed that O-vacancy and O-interstitial defects are responsible for the NBIS and PBS instabilities, respectively. In the previous studies, O-related defects were intentionally introduced in stoichiometric a-IGZO. Since the composition ratio is likely to be deviated from the ideal stoichiometry during fabrication, it is important to understand the electronic structure of non-stoichiometric a-IGZO. Here we perform density functional calculations to investigate the electronic structure of O-related defects in various a-IGZO systems with non-stoichiometric chemical compositions, which are generated through melt-and-quench molecular dynamics simulations. We consider both O-abundant and O-deficient samples and discuss the role of intrinsic defects in the device instability.

**10:00AM E51.00009 Efficient n-type doping of MoO<sub>3</sub><sup>1</sup>**, HARTWIN PEELAERS, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — MoO<sub>3</sub> is a layered material that has shown great promise as a transparent contact to organic photovoltaics and organic light-emitting diodes. It also exhibits photo- and electrochromic properties, and can be used as catalyst or sensor material. Due to its capability to reversibly accommodate Li it can be used in Li batteries. Despite these interesting properties, remarkably little is known about the properties of native defects and the possibilities of controlling the properties by intentional doping. We have used advanced hybrid functional calculations within density functional theory to investigate efficient doping strategies for this material. In particular, we explored the role of native defects in the conductivity of this material. To control the n-type conductivity and to obtain a larger amount of free carriers, intentional dopants can be used. We show that substitutional Re (on a Mo site) is a shallow donor. In contrast, substitutional doping with Mn, which also has one additional electron compared to Mo, leads to compensating behavior. Halogen impurities on the O site also act as shallow donors.

<sup>1</sup>This work was supported by NSF and DOE.

**10:12AM E51.00010 The Role of Interface Defects on Phase Selection in ZnO/MgO Core/Shell Nanowires<sup>1</sup>**, DOMINIC CRITCHLOW, Austin Peay State University, Vanderbilt University, ZHINENG LI, Stony Brook University, Vanderbilt University, XIAO SHEN, CLAIRE MARVINNEY, YEVGENIY PUZYREV, LIDA PAN, JAMES MCBRIDE, RICHARD HAGLUND, SOKRATES PANTELIDES, Vanderbilt University — ZnO nanowires, coated with MgO, have potential for optical devices. The optical properties of the ZnO/MgO core-shell structures depend on the properties of the interface. Both epitaxial interface with wurtzite MgO on ZnO and non-epitaxial interface with rocksalt MgO have been observed. Differences in MgO interface structure poses questions to what type of defects must be present to achieve these different crystal structures. Density functional theory calculations are carried out to explore the role of surface oxygen vacancies and the step edges. The results from DFT calculations show that oxygen vacancies have no effect on the crystal structure. On the other hand, the calculations show that the step edges make rocksalt MgO structure more favorable. TEM images taken on the ZnO nanowires that has rocksalt MgO coating revealed steps in the ZnO Nanowire, confirming the theoretical prediction.

<sup>1</sup>Vanderbilt Physics Research Experience for Undergraduates funded by the National Science Foundation.

**10:24AM E51.00011 Structure of self-assembled Mn atom chains on Si(001)**, RENAN VILLARREAL, MARIA LONGOBARDI, SIGRUN A. KOESTER, Department of Quantum Matter Physics, University of Geneva, Geneva, CH-1211, Switzerland, CHRISTOPHER J. KIRKHAM, Division of Precision Science and Technology and Applied Physics, Graduate School of Engineering, Osaka University, 2-1, Yamada-oka, Suita, Japan, DAVID BOWLER, London Centre for Nanotechnology and Department of Physics and Astronomy, University College London, London WC1E 6BT, United Kingdom, CHRISTOPH RENNER, Department of Quantum Matter Physics, University of Geneva, Geneva, CH-1211, Switzerland — Mn has been found to self-assemble into atomic chains running perpendicular to the surface dimer reconstruction on Si(001). They differ from other atomic chains by a striking asymmetric appearance in filled state scanning tunneling microscopy (STM) images. This has prompted complicated structural models involving up to three Mn atoms per chain unit. Combining STM, atomic force microscopy and density functional theory we find that a simple necklace-like chain of single Mn atoms reproduces all their prominent features, including their asymmetry not captured by current models. The upshot is a remarkably simpler structure for modelling the electronic and magnetic properties of Mn atom chains on Si(001).

**10:36AM E51.00012 Electronic structures in SiC/SiO<sub>2</sub> interface from first-principles calculation -Roles of peculiar electron states floating in internal space-**, YU-ICHIRO MATSUSHITA, The University of Tokyo, MAURO BOERO, The University of Strasbourg, ATSUSHI OSHIYAMA, The University of Tokyo — Silicon carbide (SiC) is a promising material for power electronic devices. We have reported that the wavefunction at the conduction-band minimum (CBM) of SiC “floats in internal space with continuum-state character” [1]. By considering the floating nature of the CBM, drastic energy-level changes of CBM observed in SiC polytypes can be explained naturally [2]. Moreover, we have clarified that floating nature of CBM varies the effective masses in SiC. In this study, we have investigated how the electronic structure of CBM is modified in SiC/SiO<sub>2</sub> interfaces, where the internal space is severely deformed, and how the floating electron state affects the material properties. We have found that we can realize 1 dimensional electron channels in the interface, and that the effective masses of CBM strongly depend on the interface structures. [1] Y. i. Matsushita, S. Furuya, and A. Oshiyama, PRL, 108, 246404 (2012). [2] Y. i. Matsushita, and A. Oshiyama, PRL 112 136403 (2014).

**10:48AM E51.00013 Ab initio study of the effect of vacancies on the thermal conductivity**, NAKIB PROTIK, Boston College, JESUS CARRETE, NATALIO MINGO, LITEN, CEA-Grenoble, NEBIL KATCHO, CIC EnergiGUNE, DAVID BROIDO, Boston College — Point defects and vacancies in particular can have a profound impact on phonon thermal transport. Examples are seen in diamond [1] and cubic boron arsenide [2, 3] where large C and As vacancy concentrations give much lower thermal conductivity than expected [2, 3]. Here, we calculate the phonon-vacancy scattering rates using an *ab initio* Green's function approach [1], which treats the scattering to all orders in contrast to standard perturbation theory approaches. The lattice thermal conductivity,  $\kappa$ , is calculated from first principles by solving the Boltzmann transport equation for phonons, with interatomic force constants determined using density functional theory. The reduction in  $\kappa$  with vacancy defect density is assessed. The phonon-vacancy scattering can show significant differences using the Green's function method compared to what would be predicted from the perturbative Born approximation, consistent with previous findings for diamond [1]. [1] N. A. Katcho J. Carrete, Wu Li and N. Mingo, Phys. Rev. B 90, 094117 (2014). [2] L. Lindsay, D. A. Broido and T. L. Reinecke, Phys. Rev. Lett. 111, 025901 (2013). [3] Bing Lv, et. al. Appl. Phys. Lett. 106, 074105 (2015).

## Tuesday, March 15, 2016 8:00AM - 10:12AM – Session E52 GERA FIAP: Physics of Batteries I Hilton Baltimore Holiday Ballroom 3 -

**8:00AM E52.00001 Diffusion and possible freezing phases of Li-ions in  $\text{LiFePO}_4$** <sup>1</sup>, YUEN YIU, Ames Laboratory, Iowa State University, RASMUS TOFT-PETERSEN, Helmholtz-Zentrum Berlin, GEORG EHLERS, Oak Ridge National Laboratory, DAVID VAKNIN, Ames Laboratory, Iowa State University — Elastic and inelastic neutron scattering studies of  $\text{LiFePO}_4$  single crystal reveal new Li-ion diffusion properties relevant to its function as Li-battery materials. In the past decade there has been broad interest in  $\text{LiFePO}_4$  and its related compounds, largely due to the applications of these materials as cathodes in Li- batteries. This is owing to these materials' high charge-discharge ability and conductivity, both of which are by virtue of the Li-ions' high mobility. In this talk, we present our findings on the temperature and directional dependence of Li-ions' diffusion in  $\text{LiFePO}_4$ .  $\text{LiFePO}_4$  adopts the olivine structure at room temperature (Space group: *Pnma*), which contains channels along principal crystalline directions that allow Li-ion motion. Elastic neutron scattering reveals lowering of symmetry from the *Pnma* structure below room temperature, which can be interpreted as the freezing of Li-ions, and can be subsequently linked to the reported decrease in Li-ion conductivity. Inelastic neutron scattering, in the 35K to 720K temperature range, shows temperature dependence, as well as anisotropy (i.e. along 0K0 versus 00L) of Li-ion diffusion.

<sup>1</sup>Ames Laboratory is supported by U.S. DOE, BES, DMSE, under contract DE-AC02-07CH11358. Spallation Neutron Source of Oak Ridge National Laboratory is sponsored by U.S. DOE, BES, SUFD.

**8:12AM E52.00002 Structural Properties and Electrochemical Performance of ZnO Nanosheets Grown Directly on Al substrate by Chemical Bath Deposition Techniques**, AHMED AL-ASADI, Department of Physics, Southern Illinois University Carbondale, Carbondale, IL 62901, United States, ROBERTO FERRERA, Department of Chemistry and Biochemistry, Southern Illinois University Carbondale, Carbondale, IL, 62901, United States, LUKE HENLEY, Department of Physics, Southern Illinois University Carbondale, Carbondale, IL 62901, United States, NESTOR LOPEZ, VICTOR CAROZO, ZHONG LIN, MAURICIO TERRONES, Department of Physics and Center for 2-Dimensional and Layered Materials, The Pennsylvania State University, University Park, PA 16802, United State, SAIKAT TALAPATRA, Department of Physics, Southern Illinois University Carbondale, Carbondale, IL 62901, United States — We will report on the synthesis & electrochemical characterization of 2-dimensional zinc oxide grown directly on Al substrate by a simple chemical bath deposition method at low temperature (below 100°C). Detail structural characterizations of the synthesized ZnO sheets will be presented and discussed. The electrochemical performances of electrochemical double layer capacitors (EDLC) on electrodes fabricated using these materials were evaluated using cyclic voltammetry, galvanostatic charge-discharge, and electrochemical impedance spectroscopy using various electrolytes. We found that high specific capacitance values (greater than 300 F/g) could be achieved using an aqueous electrolyte. The aforementioned results indicates the possibly for using 2-D ZnO architectures fabricated by this simple and cost efficient technique for future electrochemical energy storage devices.

**8:24AM E52.00003 In situ analysis of capacity fade in thin-film anodes for high performance Li-ion all-solid-state batteries**, MARINA S. LEITE, CHEN GONG, Department of Materials Science and Eng., Institute for Research in Electronics and Applied Physics, Univ. of Maryland, College Park, Maryland 20742, DMITRY RUZMETOV, Sensors and Electron Devices Directorate, US Army Research Laboratory, Adelphi, Maryland, Material Measurement Laboratory, NIST, Gaithersburg Maryland, A. ALEC TALIN, Sandia National Laboratories, Livermore, California 94550 — There is still a pressing need to understand how the solid-interfaces in Li-ion all-solid-batteries form, including their chemical composition and electrical characteristics. In order to resolve the origin of the degradation mechanism in Al anodes, we combine in situ scanning electron microscopy in ultra-high vacuum with electrochemical cycling, in addition to ex situ characterization of the morphological, chemical, and electrical changes of the Al anodes upon lithiation. An AlLi alloy capped by a stable Al-Li-O is formed on the top surface of the anode, trapping Li, which results in the capacity fade, from 48.0 to 41.5  $\mu\text{Ah}/\text{cm}^2$  in two cycles [1]. The addition of a Cu capping layer is insufficient to prevent the device degradation because of the fast Li diffusion within Al. Yet, Si present extremely stable cycling: >92% of capacity retention after 100 cycles, with average Coulombic efficiency of 98% [2]. Our in situ measurements represent a new platform for probing the real-time degradation of electrodes in all-solid-state batteries for energy storage devices. [1] M.S. Leite et al., J. Mater. Chem. A, 2, 20552 (2014). i-Cover. [2] C. Gong et al., ACS Appl. Mater. Interfaces, 2015. DOI: 10.1021/acsami.5b07058

**8:36AM E52.00004 Non-Destructive Measurement of *in-operando* Lithium Concentration in Batteries via X-Ray Compton Scattering**, HASNAIN HAFIZ, Northeastern U., K. SUZUKI, Gunma U., B. BARBIELLINI, Northeastern U., Y. ORIKASA, Kyoto U., S. KAPRZYK, Northeastern U. and AGH U. of Sc. and Tech., M. ITOU, JASRI, K. YAMAMOTO, Kyoto U., Y. J. WANG, Northeastern U. and LBNL, Y. UCHIMOTO, Kyoto U., A. BANSIL, Northeastern U., Y. SAKURAI, JASRI, H. SAKURAI, Gunma U. — Non-destructive determination of lithium distribution in a working battery is key for addressing both efficiency and safety issues. Although various techniques have been developed to map the lithium distribution in electrodes, these methods are mostly applicable to test cells. Here we propose the use of high-energy x-ray Compton scattering spectroscopy to measure the local lithium concentration in closed electrochemical cells. A combination of experimental measurements and parallel first-principles computations is used to show that the shape parameter *S* of the Compton profile is linearly proportional to lithium concentration and thus provides a viable descriptor for this important quantity. The merits and applicability of our method are demonstrated with illustrative examples of  $\text{Li}_x\text{Mn}_2\text{O}_4$  cathodes and a working commercial lithium coin battery CR2032.

**8:48AM E52.00005 In-Situ AFM Investigation of Solid Electrolyte Interphase Formation and Failure Mechanisms in Lithium-Ion Batteries.** , THOMAS MUELLER, Bruker Nano Surfaces, RAVI KUMAR, ANTON TOKRANOV, Brown University, School of Engineering, TEDDY HUANG, CHUNZENG LI, Bruker Nano Surfaces, XINGCHENG XIAO, General Motors Global RD Center, BRIAN SHELDON, Brown University, School of Engineering — The formation and evolution of the solid electrolyte interphase (SEI) is critical for lifetime and performance of lithium-ion batteries (LIBs), particularly for LIBs with high energy density materials such as silicon. Si has almost ten times theoretical specific capacity vs graphite, but its volume changes during cycling (up to 400%) put enormous strains on the SEI layer, resulting in continuous capacity loss. In this study we report in situ atomic force microscopy (AFM) investigation on the formation and failure mechanisms of SEI layer using patterned Si island structures. Due to the shear lag effect, patterned Si islands go through lateral expansion and contraction, putting the SEI layer in tension and compression during lithiation and delithiation, respectively. Experimentally, we performed the studies in a glovebox with <1 ppm O<sub>2</sub> and H<sub>2</sub>O, using PeakForce Tapping to image the extremely fragile SEI layer. We show for the first time the in operando cracking of SEI layer. To understand the mechanics of the SEI layer, the critical strain for cracking was derived from a progression of the AFM images. Our studies provide new insight into SEI formation, evolution and its mechanical response, and offer guidance to tailor passivation layers for optimal performance.

**9:00AM E52.00006 Why LiFePO<sub>4</sub> is a safe battery electrode: Coulomb repulsion induced electron-state reshuffling upon lithiation** , YUNG JUI WANG, Northeastern Univ. (NU) and ALS, LBNL, XIAOSONG LIU, ALS, LBNL, B. BARBIELLINI, HASNAIN HAFIZ, SUSMITA BASAK, NU, JUN LIU, THOMAS RICHARDSON, EETD, LBNL, GUOJIUN SHU, FANGCHENG CHOU, National Taiwan Univ., TSU-CHIEN WENG, DENNIS NORDLUND, DIMOSTHENIS SOKARAS, SLAC, B. MORITZ, T. P. DEVEREAUX, Stanford Univ. and SLAC, RUIMIN QIAO, YI-DE CHUANG, ALS, LBNL, ARUN BANSIL, NU, ZAHID HUSSAIN, WANLI YANG, ALS, LBNL — We performed systematic experimental and theoretical studies based on soft X-ray emission, absorption, and hard X-ray Raman spectroscopy of Li<sub>x</sub>FePO<sub>4</sub>. The results show a non-rigid electron-state reconfiguration of both the occupied and unoccupied Fe-3d and O-2p states during the (de)lithiation process. The critical 3d electron state configurations are consistent with the calculations based on MBJGGA+U framework, which improves the overall lineshape prediction compared with the conventionally used GGA+U method. The combined experimental and theoretical studies show that the non-rigid electron state reshuffling guarantees the stability of oxygen during the redox reaction throughout the charge and discharge process of LiFePO<sub>4</sub> electrodes, leading to the intrinsic safe performance of the electrodes. Work supported by the US DOE.

**9:12AM E52.00007 An experimental and computational investigation of structural dependence of catalytic properties of Pt-Ru nanoparticles<sup>1</sup>** , BINAY PRASAI, Central Michigan University — An approach to determining the 3D atomic structure of metallic nanoparticles (NPs) in fine detail is described and exemplified on Pt–Ru alloy NPs of importance to the development of devices for clean energy conversion such as fuel cells. NPs are characterized structurally by total scattering experiments involving high-energy synchrotron X-ray diffraction coupled to atomic pair distribution functions (PDFs) analysis. 3D structure models are built by molecular dynamics simulations and further refined against the experimental PDF data by reverse Monte Carlo simulations and analyzed in terms of structural characteristics. Structural characteristics of activated NPs and data for their catalytic activity are compared side by side and strong evidence found that electronic effects, indicated by significant changes in Pt–Pt and Ru–Ru metal bond lengths at NP surface, and practically unrecognized so far atomic ensemble effects, indicated by distinct stacking of atomic layers near NP surface and prevalence of particular configurations of Pt and Ru atoms in these layers, contribute to the observed enhancement of the catalytic activity of Pt<sub>x</sub>Ru<sub>100–x</sub> alloy NPs at  $x \sim 50$ .

<sup>1</sup>Central Michigan University, Department of Energy

**9:24AM E52.00008 Detailed characterization of lithium diffusion mechanisms in crystalline silicon using the kinetic Activation-Relaxation Technique.** , MICKAL TROCHET, OSCAR ANTONIO RESTREPO GUTIERREZ, NORMAND MOUSSEAU, Universit de Montral — Silicon displays a potential for high-capacity anode material for lithium-ion batteries as it can absorb large quantities of this metal. Yet, very little is understood about the evolution of diffusion mechanisms and migration barriers as the concentration of lithium increases. Until now, for example, simulations studies were limited by the time scale over which diffusion takes place. Here, we use the kinetic activation relaxation technique (kART[1]), an unbiased off-lattice Monte Carlo method with on-the fly catalog building, coupled with the ReaxFF forcefield to follow diffusion of Li in c–Si over timescale of seconds and more at room temperature, obtaining detailed information about the whole set of possible diffusion mechanisms as the local environment evolves. We first present a detailed characterization of Li diffusion in the presence of 1 to 3 impurities and then show the evolution of systems with a higher concentration of solute as Li aggregate. These results provide a first detailed picture of the onset of Li aggregating into this high-capacity material, as it modifies the structure through local rearrangements and long-range elastic deformations, crucial information for the development of the next generation of high-capacity anode. \pard\pard[1] M. Trochet *et al.*, “Diffusion of point defects in crystalline silicon using the kinetic activation-relaxation technique method,” *Phys. Rev. B*, vol. 91, no. 22, p. 224106, 2015.

**9:36AM E52.00009 Gold Nanoparticles-Enhanced Proton Exchange Membrane (PEM) Fuel Cell** , HONGFEI LI, CHENG PAN, Stony Brook University, PING LIU, YIMEI ZHU, RADOSLAV ADZIC, Brookhaven National Laboratory, MIRIAM RAFAILOVICH, Stony Brook University — Proton exchange membrane fuel cells have drawn great attention and been taken as a promising alternated energy source. One of the reasons hamper the wider application of PEM fuel cell is the catalytic poison effect from the impurity of the gas flow. Haruta has predicted that gold nanoparticles that are platelet shaped and have direct contact with the metal oxide substrate to be the perfect catalysts of the CO oxidation, yet the synthesis method is difficult to apply in the Fuel Cell. In our approach, thiol-functionalized gold nanoparticles were synthesized through two-phase method developed by Brust *et al.* We deposit these Au particles with stepped surface directly onto the Nafion membrane in the PEM fuel cell by Langmuir–Blodgett method, resulting in over 50% enhancement of the efficiency of the fuel cell. DFT calculations were conducted to understand the theory of this kind of enhancement. The results indicated that only when the particles were in direct surface contact with the membrane, where AuNPs attached at the end of the Nafion side chains, it could reduce the energy barrier for the CO oxidation that could happen at T<300K.

**9:48AM E52.00010 One pot electrochemical synthesis of polymer/CNT/metal nanoparticles for fuel cell applications.** , LAKSHMAN VENTRAPRAGADA, JINGYI ZHU, MEHMET KARAKAYA, RAMAKRISHNA PODILA, APPARAO RAO, Clemson University, CLEMSON NANOMATERIALS CENTER TEAM — Carbon nanotubes (CNTs) have become a key player in the design of materials for energy applications. They gained their popularity in industrial and scientific research due to their unique properties like excellent conductivity, high surface area, etc. Here we used chemical vapor deposition (CVD) to synthesize two types of CNTs namely, helically coiled CNTs and vertically aligned CNTs. These CNTs were subsequently used to make composites with conducting polymers and metal nanoparticles. One pot electrochemical synthesis was designed to electropolymerize aniline, pyrrole etc. on the surface of the electrode with simultaneous deposition of platinum and gold metal nanoparticles, and CNTs in the polymer matrix. The as synthesized composite materials were characterized with scanning electron microscope for surface morphology and spectroscopic techniques like Raman, UV-Vis for functionality. These were used to study electrocatalytic oxidation of methanol and ethanol for alkaline fuel cell applications. Electrodes fabricated from these composites not only showed good kinetics but also exhibited excellent stability. Uniqueness of this composite lies in its simple two step synthesis and it doesn't involve any surfactants unlike conventional chemical synthesis routes.

**10:00AM E52.00011 Energy storage mechanism for hybrid battery** , JUN FENG, NATASHA CHERNOVA, FREDRICK OMENYA, ALOK RASTOGI, STANLEY WHITTINGHAM, Binghamton University — Many devices require both high energy and high power density, and lithium ion batteries and super-capacitors cannot separately always meet the requirements. In this work, we study the operating mechanism of a hybrid battery, which combines the best properties of batteries and supercapacitors. We analyze the lithium ion storage mechanism using XRD, Raman, TEM and electrochemical measurements. The model system studied combines a non-intercalating carbon black anode with a  $\text{LiFePO}_4$  cathode. At 50% state of charge, XRD data for  $\text{LiFePO}_4$  cathode material shows a mixture of  $\text{LiFePO}_4$  and  $\text{FePO}_4$ , indicating battery reaction. On the other hand, the activated carbon remains structurally unchanged. We also discuss the impact of a range of activated carbon/  $\text{LiFePO}_4$  (AC/LFP) ratios. From cyclic voltammetry and charge/discharge results, the system exhibits battery-domain characteristics when the AC/ LFP ratio is below one, but showing more supercapacitor-domain traits when the ratio is higher. Besides, the systems have higher rate capacity at AC/LFP ratio around four as compared to one. This research is supported by NSF under Award Number 1318202.

**Tuesday, March 15, 2016 8:00AM - 11:00AM –**

**Session E53 FGSA: The Future of Physics: Crossing Disciplines and Collaborating** Hilton Baltimore Holiday Ballroom 4 - Krista Freeman, Carnegie Mellon University

**8:00AM E53.00001 Cross Discipline Training to Reach the Mountain Top of Your Career** , RENEE HORTON, NASA Michoud Assembly Facility — No abstract available.

**8:36AM E53.00002 Random walks along the squishy boundary of physics and engineering** , ROBERT LEHENY, Johns Hopkins University — Many of the key problems and systems of interest in soft matter physics are similarly a focus for other fields, such as chemical engineering and biomedical engineering, making the area inherently highly interdisciplinary. Although soft matter physicists and engineers share topics of interest, the reasons for their interest are of course not identical, and when brought together through collaboration, these varied perspectives can help enrich the science. In my talk, I will illustrate this point with some specific examples from projects from my research background, particularly in the area of interfacial rheology. I will also try to offer some advice on how young scientists can position themselves to contribute in an environment where cross-disciplinary interactions are increasingly important.

**9:12AM E53.00003 Collaborating Across Borders** , AMY FLATTEN, American Physical Society, Director of International Affairs — Physicists transcend national boundaries, ethnic differences, and scientific disciplines to address globally shared problems and questions. This talk will highlight how scientists have collaborated across borders – both geographic and scientific – to achieve ground-breaking discoveries through international scientific cooperation. The speaker also will address how international collaborations will be even more crucial for addressing future challenges faced by the physics community, such as building large-scale research facilities, strengthening scientific capacity in developing countries, fostering "science for diplomacy" in times of political tensions and other critical issues.

**9:48AM E53.00004 Panel Discussion –**

**Tuesday, March 15, 2016 8:00AM - 11:00AM –**

**Session E54 FIAP: Microwave and Optical Properties of Semiconductors** Hilton Baltimore Holiday Ballroom 5 - Todd Brintlinger, Naval Research Lab

**8:00AM E54.00001 Study of microwave reflection in the regime of the radiation-induced magnetoresistance oscillations in the high mobility GaAs/AlGaAs 2D electron system<sup>1</sup>** , ANNIKA KRIISA, H-C. LIU, R. L. SAMARAWEEERA, Georgia State University, Atlanta, GA 30303, M. S. HEIMBECK, Army Aviation & Missile RD & E Center, Redstone Arsenal, Huntsville, AL 35898, H. O. EVERITT, Army Aviation & Missile RD & E Center, Redstone Arsenal, Huntsville, AL 35898 and Dept. of Physics, Duke University, Durham, NC 27708, W. WEGSCHEIDER, ETH-Zurich, 8093 Zurich, Switzerland, R. G. MANI, Georgia State University, Atlanta, GA 30303 — Microwave-induced zero-resistance-states in the photo-excited GaAs/AlGaAs system evolve from the minima of microwave photo-excited quarter-cycle shifted magnetoresistance oscillations. Such magnetoresistance oscillations are known to exhibit nodes at cyclotron resonance ( $hf = \hbar\omega_c$ ) and cyclotron resonance harmonics ( $hf = n\hbar\omega_c$ ). Further, the effective mass extracted from the radiation-induced magnetoresistance oscillations is known to differ from the canonical effective mass ratio for electrons in the GaAs/AlGaAs system.[1] In an effort to reconcile this difference, we have looked for cyclotron resonance in the microwave reflection from the high mobility 2DES and attempted to correlate the observations with observed oscillatory magnetoresistance over the  $30 \leq f \leq 330$  GHz band. The results of such a study will be reported here. [1] R. G. Mani et al., Phys. Rev. Lett. 92, 146801 (2004).

<sup>1</sup>DOE-BES, Mat'l. Sci. & Eng. Div., DE-SC0001762; ARO W911NF-14-2-0076; ARO W911NF-15-1-0433

**8:12AM E54.00002 Frequency-dependence of the linear-polarization-angle phase-shift in the microwave radiation-induced magnetoresistance oscillations** , HAN-CHUN LIU, RASANGA SAMARAWEEERA, Georgia State Univ, WERNER WEGSCHEIDER, ETH-Zurich, Zurich, Switzerland , RAMESH MANI, Georgia State Univ — High-mobility GaAs/AlGaAs heterojunctions subjected to microwave photoexcitation in the perpendicular magnetic field configuration exhibit -cycle phase-shifted oscillatory magnetoresistance and zero-resistance states at low magnetic fields or high filling factors [1]. Recent studies showed that the amplitude of oscillatory magnetoresistance is polarization-angle sensitive and can be described by a fitting formula,  $R_{xx}(\theta) = A \cos 2(\theta - \theta_0)$  with diagonal resistance,  $R_{xx}$ , polarization angle  $\theta$ , and the extracted phase shift,  $\theta_0$ . Previous works have demonstrated that  $\theta_0$  is frequency-dependent by investigating some specific frequencies [2,3]. Here, we examine the continuous variation of  $\theta_0$  with frequency over the bands, 36-40 GHz and 45-49 GHz. Surprisingly, the results indicate dissimilar  $\theta_0$  variation within the two frequency bands. A comparison of  $\theta_0(f)$  with the microwave polarization reported by an in-situ polarization sensor suggests that the frequency variation of  $\theta_0$  might be caused by two different mechanisms in the two examined bands. [1] R. G. Mani et al., Nature 420, 646 (2002). [2] A. N. Ramanayaka et al., Phys. Rev. B 85, 205315 (2012). [3] Han-Chun Liu et al., J. Appl. Phys. 117, 064306 (2015)

**8:24AM E54.00003 Microwave radiation-induced magnetoresistance oscillations in the high mobility GaAs/AlGaAs system under bichromatic excitation**, BINUKA GUNAWARDANA, HAN-CHUN LIU, RASANAGA SAMARAWEEA, Georgia State Univ, WERNER WEGSCHEIDER, ETH Zurich, RAMESH MANI, Georgia State Univ — Bichromatic microwave excitation has been used in atomic physics, for example, to destabilize the populations distribution of cold atoms.[1] In semiconductor physics, bichromatic excitation of the high mobility 2D electron system is thought to provide evidence for current domains in the regime of the microwave radiation-induced zero-resistance states[2-4]. We examined radiation-induced magneto-resistance oscillations under bichromatic excitation over the  $30 < f < 100$  GHz band to obtain a better understanding of the lineshape observed in the dual excitation experiment of the high mobility GaAs/AlGaAs 2D electron system. Thus, we photo-excited the GaAs/AlGaAs Hall bar specimen at liquid helium with one microwave source at a fixed, relatively high frequency and a second microwave source at several lower frequencies corresponding to various frequency ratios. The microwave intensity due to both sources were also changed systematically to study the evolution of the oscillatory magnetoresistance lineshape. Here, we report the results of this study which aims to examine superposition- or lack thereof- in the lineshape observed in the bichromatic experiment. [1]A. Buchleitner, L. Sirko and H. Walther Europhysics Lett. 16, 35 (1991). [2] R. G. Mani et al., Nature, 420, 646 (2002) [3] M. A. Zudov et al., Phys. Rev. Lett. 96, 236804 (2004). [4] X. L. Lei and S. Y. Liu, Appl. Phys. Lett. 89, 182117 (2006).

**8:36AM E54.00004 Analysis of bell-shape negative giant-magnetoresistance in high mobility GaAs/AlGaAs 2D electron systems using multi-conduction model.**, RASANGA SAMARAWEEA, HAN-CHUN LIU, Georgia State University, WERNER WEGSCHEIDER, ETH Zurich, RAMESH MANI, Georgia State University — Recent advancements in the growth techniques of the GaAs/AlGaAs two dimensional electron system (2DES) routinely yield high quality heterostructures with enhanced physical and electrical properties, including devices with 2D electron mobilities well above  $10^7$  cm<sup>2</sup>/Vs. These improvements have opened new pathways to study interesting physical phenomena associated with the 2D electron system. Negative giant-magnetoresistance (GMR) is one such phenomenon which can be observed in the high mobility 2DES. However, the negative GMR in the GaAs/AlGaAs 2DES is still not fully understood. In this contribution, we present an experimental study of the bell-shape negative GMR in high mobility GaAs/AlGaAs devices and quantitatively analyze the results utilizing the multi-conduction model [1]. The multi-conduction model includes interesting physical characteristics such as negative diagonal conductivity, non-vanishing off-diagonal conductivity, etc. The aim of the study is to examine GMR over a wider experimental parameter space and determine whether the multi-conduction model serves to describe the experimental results. [1] R. G. Mani, A. Kriisa, and W. Wegscheider, Sci. Rep. 3, 2747 (2013).

**8:48AM E54.00005 Microwave polarization angle study of the radiation-induced magnetoresistance oscillations in the GaAs/AlGaAs 2D electron system under dc current bias**<sup>1</sup>, MUHAMMAD-ZAHIR IQBAL, HAN-CHUN LIU, Georgia State University, Atlanta, GA 30303, MARTIN S. HEIMBECK, Army Aviation & Missile RDE Center, Redstone Arsenal, Huntsville, AL 35898, HENRY O. EVERITT, Army Aviation & Missile RDE Center, Redstone Arsenal, Huntsville, AL 35898 and Dept. of Physics, Duke University, Durham, NC 27708, WERNER WEGSCHEIDER, ETH-Zurich, 8093 Zurich, Switzerland, RAMESH G. MANI, Georgia State University, Atlanta, GA 30303 — Microwave-induced magnetoresistance oscillations followed by the vanishing resistance states are a prime representation of non-equilibrium transport phenomena in two-dimensional electron systems (2DES). The effect of a dc current bias on the nonlinear response of 2DES with microwave polarization angle under magnetic field is a subject of interest. Here, we have studied the effect of various dc current bias on microwave radiation-induced magnetoresistance oscillations in a high mobility 2DES. Further, we systematically investigate the effect of the microwave polarization angle on the magneto-resistance oscillations at two different frequencies 152.78 GHz and 185.76 GHz. This study aims to better understand the effects of both dc current and microwave polarization angle in the GaAs/AlGaAs system, both of which modify the observed magneto-transport properties

<sup>1</sup>DOE-BES, Mat'l. Sci. & Eng. Div., DE-SC0001762; ARO W911NF-14-2-0076; ARO W911NF-15-1-0433

**9:00AM E54.00006 Microwave Reflection Spectroscopy of a Two-Dimensional Electron Gas**, JIE ZHANG, RUIYUAN LIU, LINGJIE DU, RUI-RUI DU, Rice University, LOREN PFEIFFER, KEN WEST, Princeton University — Cyclotron resonance (CR) is a standard method to determine the carrier effective mass in two-dimensional electron systems, typically by measuring/analyzing the absorption or transmission signal. Here we report a microwave spectrometer utilizing the reflection signal. In our experiment setup based on a top-loading helium3 cryostat and a superconducting solenoid, the microwave (up to 40GHz) is sent down via a coax cable to the sample surface, and the reflection signal is then collected by the same cable and fed upward to a directional coupler, and being detected. We demonstrate the applicability of the spectrometer by measuring the CR of high-mobility electrons or holes in GaAs/AlGaAs quantum wells. The construction of spectrometer, preliminary data, and brief discussions will be presented. The work at Rice was supported by Welch Foundation grant C-1682.

**9:12AM E54.00007 Response of Plasmonic Terahertz Detectors to Modulated Signals**, SERGEY RUDIN, GREG RUPPER, MEREDITH REED, U.S. Army Research Laboratory, MICHAEL SHUR, Rensselaer Polytechnic Institute — We present theoretical study of the response of two-dimensional gated electron gas to an amplitude modulated signals with carrier frequency in the terahertz range. Our model is based on complete hydrodynamic equations, and includes effects of viscosity, pressure gradients and thermal transport in the conduction channel of a high electron mobility semiconductor transistor. The modulation response was evaluated as a function of modulation frequency for a range of mobility values in different semiconductor materials. Maximum modulation frequency was evaluated as a function of channel mobility, with typical values in the subterahertz range of frequencies. Our analysis shows that short channel field effect transistors operating in the plasmonic regime meets the requirements for applications as terahertz detectors and modulators in high-speed wireless communication circuits.

**9:24AM E54.00008 Infrared magneto-transmission studies of the 2DEGs in (CdMn)Te and CdTe Quantum wells**<sup>1</sup>, IMTIAZ TANVEER, University at Buffalo, SUNY, MACIEJ WIATER, GRZEGORZ KARCZEWSKI, TOMASZ WÓJTOWICZ, Institute of Physics, Polish Academy of Sciences, Warsaw, Poland, B.D. MCCOMBE, University at Buffalo, SUNY — We are probing quantum hall ferromagnetism (QHF) in the 2DEG of Modulation-doped quantum wells (QWs) in the (CdMn)Te/(CdMg)Te (with 1.5% Mn) heterostructure system by THz cyclotron resonance. Samples with CdTe QWs are also studied. Both structures have the same QW width (30 nm), very similar electron densities in the wells  $\sim 3.0 \times 10^{11}$  cm<sup>-2</sup> and mobilities of 450,000 (CdTe) and 66,000 cm<sup>2</sup>/Vs ((CdMn)Te) at 1.6 K. The electron effective masses ( $m^*/m_0$ ) from cyclotron resonance measurements at 5K are  $0.110 \pm 0.001$  for CdTe and  $0.114 \pm 0.003$  for (CdMn)Te. Linear fits to the resonance positions in frequency vs. field give small non-zero intercepts which may result from small non-parabolicity or bound magneto-plasmon effects. The FWHM linewidths from Lorentzian fits of the transmission minima are  $\sim 2$  cm<sup>-1</sup>(CdTe) and  $\sim 8$  cm<sup>-1</sup>((CdMn)Te). Our present focus is on detailed studies of the CR positions and linewidths in the magnetic field region around the cusp-like behavior in the  $R_{xx}$  oscillations, which indicates the presence of the QHF state. The field position of this state is tuned via electron density in the QWs varied incrementally by a photon-dose method with an in-situ green LED.

<sup>1</sup>Work at UB was supported in part by the Office of the Provost, and work in Poland was supported in part by the National Science Centre through grant DEC-2012/06/A/ST3/00247.

**9:36AM E54.00009 Coherent coupling of magneto-excitons probed by two-dimensional Fourier transform spectroscopy<sup>1</sup>**, JAGANNATH PAUL, CUNMING LIU, University of South Florida, STEPHEN MCGILL, National High Magnetic Field Lab, Florida State University, DAVID HILTON, University of Alabama at Birmingham, DENIS KARAISKAJ, University of South Florida — We present the coherent two dimensional Fourier Transform (2DFT) spectra of magneto-excitons in undoped GaAs quantum wells at high magnetic field up to 10 Tesla. The 2DFT data reveal strong coherent coupling between resonances and line shapes which are strikingly different from the zero field spectra. 2DFT spectra measured using co-linear and co-circular polarizations at low temperatures will be discussed.

<sup>1</sup>The work at USF and UAB was supported by the National Science Foundation under grant number DMR-1409473. The work at NHMFL, Florida State University was supported by the National Science Foundation under grant numbers DMR-1157490 and DMR-1229217.

**9:48AM E54.00010 Observation of a Bound Exciton Transition in Ion-Beam Synthesized  $\beta$ -FeSi<sub>2</sub>**, A. GLEN BIRDWELL, FRANK J. CROWNE, TERRANCE P. O'REGAN, U.S. Army Research Laboratory, Adelphi, Maryland 20783, USA — Photoreflectance studies of  $\beta$ -FeSi<sub>2</sub> have revealed the presences of strong (direct) optical transitions together with several interesting lower-energy spectral features, including indirect gap excitonic transitions. In this presentation, we focus on one of these features made observable at low temperatures and located a few meV below the first direct gap. We attribute the origin of this feature to a transition that takes place on a bound exciton-ionized acceptor complex. Our observations of this transition together with results of our previous photoreflectance analysis lead us to identify it as the fundamental mechanism for the 1.5  $\mu$ m light emission in  $\beta$ -FeSi<sub>2</sub>. This result provides deeper insight into the light emission properties of  $\beta$ -FeSi<sub>2</sub>.

**10:00AM E54.00011 Langevin Bimolecular Recombination Kinetics of a Layered Exciton–Trion Gas**, FRANK CROWNE, ANTHONY BIRDWELL, Army Research Laboratory — The use of rate equations to describe various many-body kinetic processes in highly photoexcited layered semiconductors is discussed. In these systems, pairs of electrons and holes generated by photons from an external laser combine to form a multicomponent plasma whose time evolution is governed by gas dynamics and various recombination processes. At high levels of illumination this leads to a variety of secondary components in addition to neutral excitons, notably the so-called trions, which consist of exciton–electron and exciton–hole bound states. Although the recombination is modeled as bimolecular for all pairs of carrier species, the structure of the rate terms is sensitive to the dimensionality of the system due to the Langevin nature of encounters between carriers. It is demonstrated that charge neutrality does not apply to individual carrier species, e.g., electron and hole densities need not be equal in the presence of trions. In order to track the full time evolution from laser initiation to steady state, the system of rate equations is simulated numerically.

**10:12AM E54.00012 Magneto-transport properties of PbSe single crystals**, NAWREEN ANAND, University of Florida, CATALIN MARTIN, Ramapo College of NJ, Mahwah, NJ, GENDA GU, Brookhaven National Lab, Upton, NY, DAVID TANNER, University of Florida — PbSe is a low-gap semiconductor with excellent infrared photodetection properties. Here we report our high magnetic field and low temperature electrical properties measurement performed on a moderately doped PbSe single crystals with p-type bulk carrier density of around  $110^{18} \text{ cm}^{-3}$ . Longitudinal resistance ( $R_{xx}$ ) and Hall resistance ( $R_{xy}$ ) were simultaneously measured between 0 T and 18 T, and at temperatures between 0.8 K and 25 K, show quantum oscillations above 6 T. The quantum oscillation frequency is  $\sim 15 \text{ T}$ , giving an estimate for the carrier density of each L pocket in the BZ participating in these oscillations. The effective mass of the free carriers is estimated from the temperature dependence of oscillation amplitudes. Measurements as the magnetic fields is rotated reveal the magneto-transport properties of a 3D-like fermi surface. Dingle temperature and free carrier scattering rate has been estimated and compared to optical measurements. Optical measurements also show a low frequency phonon mode around  $45 \text{ cm}^{-1}$  and bandgap of around 0.2 eV along with other interband electronic transitions.

**10:24AM E54.00013 Colossal figure of merit of transparent conducting nano-ribbon networks**, JINWEI GAO, QIANG PENG, SONGRU LI, BING HAN, QIKUN RONG, XUBING LU, GUOFU ZHOU, South China Normal University, Guangzhou, China, JUN-MING LIU, Nanjing University, Nanjing, China, QIANMING WANG, South China Normal University, Guangzhou, China, ZHIFENG REN, University of Houston, Houston, USA, KRZYSZTOF KEMPA, Boston College — An inexpensive, simultaneously transparent and conducting metallic nano-ribbon network can be obtained by exploiting the self-cracking property of the egg-white film, subsequently used as a sacrificial mask for metal sputtering. The process results in a network of metallic nano-ribbons ideally suited for electroplating. Due to large inter-ribbon distance, an even 100-fold increase in the ribbon thickness has a negligible effect on the network transparency. Here we demonstrate this effect by developing a network with a colossal, by far the highest reported figure of merit of over 25000. This network can be used as an ultimate window electrode for solar cells, as well as LEDs.

**10:36AM E54.00014 Gate Tunable InSb Quantum Well Structures grown on GaSb (001)**, MIHIR PENDHARKAR, ANTHONY MCFADDEN, BORZOYEH SHOJAEI, JOON SUE LEE, CHRIS PALMSTROM, Univ of California - Santa Barbara — Study of quantum well structures with InSb channels is of special interest to the field of spintronics and quantum computing due to the strong spin orbit coupling and large g-factor of InSb. Gate control of InSb quantum wells is a necessary component in construction of an InSb based Spin-Field Effect Transistor. In this work, InSb quantum well structures have been grown on lattice mismatched GaSb substrates by Molecular Beam Epitaxy. Magneto-transport measurements at low temperatures have been used to investigate the influence of gate voltage on electron mobility and density. A conventional metal top gate, separated from the III-V structure with an Atomic Layer Deposited insulating dielectric, has been used. Use of the conducting GaSb substrate as a potential, bottom gate electrode has also been investigated. Surface morphology of as-grown films has been studied using Atomic Force Microscopy.

**10:48AM E54.00015 Reconciling Particle-Beam and Optical Stopping-Power Measurements in Silicon<sup>1</sup>**, WILLIAM KARSTENS, St. Michael's College, E. J. SHILES, Retired, DAVID Y SMITH, University of Vermont and Argonne National laboratory — A swift, charged particle passing through matter loses energy to electronic excitations via the electro-magnetic transients experienced by atoms along its path. Bethe related this process to the matter's frequency-dependent dielectric function  $\epsilon(\hbar\omega)$  through the energy-loss function,  $\text{Im}[-1/\epsilon(\hbar\omega)]$ . The matter's response may be summarized by a single parameter, the mean excitation energy, or  $I$  value, that combines the optical excitation spectrum and excitation probability. Formally,  $\ln I$  is the mean of  $\ln \hbar\omega$  weighted by the energy-loss function. This provides an independent optical check on particle energy-loss experiments. However, a persistent disagreement is found for silicon: direct particle-beam studies yield  $173.5 < I < 176 \text{ eV}$ , but a fit to the stopping-power of 36 elements suggests 165 eV. An independent determination from optical data in 1986 gave 174 eV supporting the higher values. However, recent x-ray measurements disclosed short comings in the 1986 optical data: 1. Measurements by Ershov and Lukirskii underestimated the L-edge strength, and 2. A power-law extrapolation overestimated the K-edge strength. We have updated these data and find  $I = 162 \text{ eV}$ , suggesting that silicon's recommended  $I$  value should be reconsidered. While this 5% change in  $I$  value changes the stopping power by only 1%, it is significant for precision measurements with Si detectors.

<sup>1</sup>Supported in part by the US Department of Energy, Office of Science, Office of Nuclear Physics under contract DE-AC02-06CH11357.

**Tuesday, March 15, 2016 8:00AM - 11:00AM —**  
**Session E55 DBIO: Delbruck Prize Session** Hilton Baltimore Holiday Ballroom 6 - Steven D. Schwartz, University of Arizona

**8:00AM E55.00001 Precision Measurement in Biology** , STEPHEN QUAKE, Stanford University and Howard Hughes Medical Institute — Is biology a quantitative science like physics? I will discuss the role of precision measurement in both physics and biology, and argue that in fact both fields can be tied together by the use and consequences of precision measurement. The elementary quanta of biology are twofold: the macromolecule and the cell. Cells are the fundamental unit of life, and macromolecules are the fundamental elements of the cell. I will describe how precision measurements have been used to explore the basic properties of these quanta, and more generally how the quest for higher precision almost inevitably leads to the development of new technologies, which in turn catalyze further scientific discovery. In the 21st century, there are no remaining experimental barriers to biology becoming a truly quantitative and mathematical science.

**8:36AM E55.00002 Dynamics of DNA in vitro and in vivo** , JENS-CHRISTIAN MEINERS, University of Michigan — While the structure of DNA has reached iconic status, its dynamics are equally important for its biological function. The thermal fluctuations of DNA gives rise to fundamental properties, such as its entropic elasticity, and enable many biological functions like the formation of regulatory DNA-protein complexes. More recently, evidence is emerging that active, ATP-hydrolysis driven processes also contribute to the motion of DNA in vivo. These active processes can enhance the efficiency of self-assembly processes involving DNA quite substantially. In a living cell, on the other hand, the motion of the DNA is severely constrained by numerous topological barriers, like supercoiling and protein binding, which in turn can locally enhance, but globally restrict the formation of regulatory DNA-protein complexes. In my talk I will review the dynamics of DNA and the interplay between thermal fluctuations, active processes, and topological constraints in the context of in-vitro experiments with optical tweezers, and in-vivo studies of the bacterial chromosome using fluorescence techniques, and interpret the results in the framework of statistical mechanics and polymer physics.

**9:12AM E55.00003 Dissecting human cerebral organoids and fetal neocortex using single-cell RNAseq.** , BARBARA TREUTLEIN, Max Planck Institute for Evolutionary Anthropology, Leipzig, Germany; Max Planck Institute for Molecular Cell Biology and Genetics, Dresden, Germany — Cerebral organoids – three-dimensional cultures of human cerebral tissue derived from pluripotent stem cells – have emerged as models of human cortical development. However, the extent to which in vitro organoid systems recapitulate neural progenitor cell proliferation and neuronal differentiation programs observed in vivo remains unclear. Here we use single-cell RNA sequencing (scRNA-seq) to dissect and compare cell composition and progenitor-to-neuron lineage relationships in human cerebral organoids and fetal neocortex. Covariation network analysis using the fetal neocortex data reveals known and novel interactions among genes central to neural progenitor proliferation and neuronal differentiation. In the organoid, we detect diverse progenitors and differentiated cell types of neuronal and mesenchymal lineages, and identify cells that derived from regions resembling the fetal neocortex. We find that these organoid cortical cells use gene expression programs remarkably similar to those of the fetal tissue in order to organize into cerebral cortex-like regions. Our comparison of in vivo and in vitro cortical single cell transcriptomes illuminates the genetic features underlying human cortical development that can be studied in organoid cultures.

**9:48AM E55.00004 Monitoring of organ transplants through genomic analyses of circulating cell-free DNA.** , IWIJN DE VLAMINCK, Cornell University — Solid-organ transplantation is the preferred treatment for patients with end-stage organ diseases, but complications due to infection and acute rejection undermine its long-term benefits. While clinicians strive to carefully monitor transplant patients, diagnostic options are currently limited. My colleagues and I in the lab of Stephen Quake have found that a combination of next-generation sequencing with a phenomenon called circulating cell-free DNA enables non-invasive diagnosis of both infection and rejection in transplantation. A substantial amount of small fragments of cell-free DNA circulate in blood that are the debris of dead cells. We discovered that donor specific DNA is released in circulation during injury to the transplant organ and we show that the proportion of donor DNA in plasma is predictive of acute rejection in heart and lung transplantation. We profiled viral and bacterial DNA sequences in plasma of transplant patients and discovered that the relative representation of different viruses and bacteria is informative of immunosuppression. This discovery suggested a novel biological measure of a person's immune strength, a finding that we have more recently confirmed via B-cell repertoire sequencing. Lastly, our studies highlight applications of shotgun sequencing of cell-free DNA in the broad, hypothesis free diagnosis of infection.

**10:24AM E55.00005 Accurate and High-Coverage Immune Repertoire Sequencing Reveals Characteristics of Antibody Repertoire Diversification in Young Children with Malaria** , NING JIANG, None — Accurately measuring the immune repertoire sequence composition, diversity, and abundance is important in studying repertoire response in infections, vaccinations, and cancer immunology. Using molecular identifiers (MIDs) to tag mRNA molecules is an effective method in improving the accuracy of immune repertoire sequencing (IR-seq). However, it is still difficult to use IR-seq on small amount of clinical samples to achieve a high coverage of the repertoire diversities. This is especially challenging in studying infections and vaccinations where B cell subpopulations with fewer cells, such as memory B cells or plasmablasts, are often of great interest to study somatic mutation patterns and diversity changes. Here, we describe an approach of IR-seq based on the use of MIDs in combination with a clustering method that can reveal more than 80% of the antibody diversity in a sample and can be applied to as few as 1,000 B cells. We applied this to study the antibody repertoires of young children before and during an acute malaria infection. We discovered unexpectedly high levels of somatic hypermutation (SHM) in infants and revealed characteristics of antibody repertoire development in young children that would have a profound impact on immunization in children.

**Tuesday, March 15, 2016 11:15AM - 1:39PM –**

**Session F1 DCMP GSNP: Pattern Formation** Ballroom I - Sidney Nagel, University of Chicago

**11:15AM F1.00001 Fingers, toes and tongues: the anatomy of interfacial instabilities in viscous fluids** , IRMGARD BISCHOFBERGER, Massachusetts Institute of Technology — The invasion of one fluid into another of higher viscosity is unstable and produces complex patterns in a quasi-two dimensional geometry. This viscous-fingering instability, a bedrock of our understanding of pattern formation, has been characterized by a most-unstable wavelength that sets the characteristic *width* of the fingers. We have shown that a second, previously overlooked, parameter governs the *length* of the fingers and characterizes the dominant global features of the patterns. Because interfacial tension suppresses short-wavelength fluctuations, its elimination would suggest an instability producing highly ramified singular structures. Our experimental investigations using miscible fluids show the opposite behavior – the interface becomes more stable even as the stabilizing effect of interfacial tension is removed. This is accompanied by slender structures, tongues, that form in the narrow thickness of the fluid. Among the rich variety of global patterns that emerge is a regime of blunt structures, “toes”, that exhibit the unusual features characteristic of proportionate growth. This type of pattern formation, while quite common in mammalian biology, was hitherto unknown in physical systems.

**11:51AM F1.00002 Pattern formation with proportionate growth<sup>1</sup>** , DEEPAK DHAR, Tata Institute of Fundamental Research, Mumbai — It is a common observation that as baby animals grow, different body parts grow approximately at same rate. This property, called proportionate growth is remarkable in that it is not encountered easily outside biology. The models of growth that have been studied in Physics so far, e.g diffusion -limited aggregation, surface deposition, growth of crystals from melt etc. involve only growth at the surface, with the inner structure remaining frozen. Interestingly, patterns formed in growing sandpiles provide a very wide variety of patterns that show proportionate growth. One finds patterns with different features, with sharply defined boundaries. In particular, even with very simple rules, one can produce patterns that show striking resemblance to those seen in nature. We can characterize the asymptotic pattern exactly in some special cases. I will discuss in particular the patterns grown on noisy backgrounds.

<sup>1</sup>supported by J. C. Bose fellowship from DST ( India)

**12:27PM F1.00003 Patterns in Active Nematics** , JULIA M YEOMANS, University of Oxford — Active systems, from bacterial suspensions to cellular monolayers, are continuously driven out of equilibrium by local injection of energy from their constituent elements and exhibit turbulent-like, chaotic patterns. We describe how active systems can be stabilised by tuning a physical feature of the system, friction. We demonstrate how the crossover between wet active systems, whose behaviour is dominated by hydrodynamics, and dry active matter where any flow is screened, can be achieved by using friction as a control parameter and demonstrate vortex ordering at the wet-dry crossover. We show that the self organisation of vortices into lattices is accompanied by the spatial ordering of topological defects leading to active crystal-like structures. The emergence of vortex lattices which leads to the positional ordering of topological defects may be a useful step towards the design and control of active materials.

**1:03PM F1.00004 Instabilities and pattern formation on the pore scale<sup>1</sup>** , ANNE JUEL, University of Manchester — What links a babys first breath to adhesive debonding, enhanced oil recovery, or even drop-on-demand devices? All these processes involve moving or expanding bubbles displacing fluid in a confined space, bounded by either rigid or elastic walls. In this talk, we show how spatial confinement may either induce or suppress interfacial instabilities and pattern formation in such flows. We demonstrate that a simple change in the bounding geometry can radically alter the behaviour of a fluid-displacing air finger both in rigid and elastic vessels. A rich array of propagation modes, including steady and oscillatory fingers, is uncovered when air displaces oil from axially uniform tubes that have local variations in flow resistance within their cross-sections. Moreover, we show that the experimentally observed states can all be captured by a two-dimensional depth-averaged model for bubble propagation through wide channels. Viscous fingering in Hele-Shaw cells is a classical and widely studied fluid-mechanical instability: when air is injected into the narrow, liquid-filled gap between parallel rigid plates, the axisymmetrically expanding air-liquid interface tends to be unstable to non-axisymmetric disturbances. We show how the introduction of wall elasticity (via the replacement of the upper bounding plate by an elastic membrane) can weaken or even suppress the fingering instability by allowing changes in cell confinement through the flow-induced deflection of the boundary. The presence of a deformable boundary also makes the system prone to additional solid-mechanical instabilities, and these wrinkling instabilities can in turn enhance viscous fingering.

<sup>1</sup>The financial support of EPSRC and the Leverhulme Trust is gratefully acknowledged.

**Tuesday, March 15, 2016 11:15AM - 2:15PM –**  
**Session F2 DCMP DAMOP: Topology and Localization in Floquet Systems** Ballroom II - Shivaji  
Sondhi, Princeton

**11:15AM F2.00001 Floquet States: Anomalous topological phases and steady state engineering** , GIL REFAEL, Caltech — Periodically driven quantum systems provide a novel and versatile platform for realizing topological phenomena. In my talk I'll provide a brief introduction to the Floquet path to topological behavior. Next, I will concentrate on a remarkable Floquet state that has no static analog: A 2d system which has chiral edge states, alongside fully localized bulk orbitals. This unique situation serves as the basis for a new topologically-protected non-equilibrium transport phenomenon: quantized non-adiabatic charge pumping. We identify the bulk topological invariant that characterizes this new phase, which we dub the 'anomalous Floquet Anderson Insulator'. In the second part of my talk, I will discuss recent results on stabilizing desired steady states in periodically driven fermionic semiconducting systems using bosonic and fermionic bath engineering.

**11:51AM F2.00002 When do Floquet systems fail to heat?** , ANUSHYA CHANDRAN, Perimeter Institute — Periodically driven quantum systems do not have a conserved energy. Thus, statistical mechanical lore holds that if they thermalize, it must be to infinite temperature. I will first show this holds in undriven systems that satisfy the eigenstate thermalization hypothesis. I will then present two counter-examples to infinite temperature heating. The first is the bosonic O(N) model at infinite N, in which the steady states are paramagnetic and have non-trivial correlations. The second is the Clifford circuit model, which can fail to heat depending on the choice of circuit elements. The resulting steady states can then be localized or delocalized but not ergodic. Such models shed light on the nature of interacting Floquet localization.

**12:27PM F2.00003 Floquet thermodynamics—nature of ensembles and order under periodic driving** , ACHILLEAS LAZARIDES, Max Planck Institute for the Physics of Complex Systems, Dresden — We study the long-time behaviour of many-body Floquet systems—closed quantum systems under temporally periodic driving, arguably the simplest deviation from equilibrium. We begin by showing that generically such interacting systems heat up and discuss the microscopic mechanism by which this happens. We then discuss two ways to prevent this: integrability and disorder. In the integrable case, a "periodic Gibbs ensemble" may be derived by maximising the entropy and shown to exactly describe the long-time steady state, while in the interacting disordered (many-body localised, or MBL) case, we identify the regime under which driving does not delocalise the system. We conclude by discussing the nontrivial steady-states achieved in interacting Floquet systems.

**1:03PM F2.00004 Floquet engineering with ultracold fermions: From Haldane's model of topological bands to spin-dependent lattices** , MICHAEL MESSER, ETH Zurich — Periodically driving a system of ultracold fermionic atoms in an optical lattice allows for implementing a large variety of effective Hamiltonians through Floquet engineering. Using this concept we realize the Haldane model which is a fundamental example of a Hamiltonian exhibiting topologically distinct phases of matter. By loading non-interacting degenerate fermions in a periodically modulated honeycomb lattice we can implement and characterize the topological band structure. We explore the resulting Berry-curvatures of the lowest band and map out topological phase transitions connecting distinct regimes. Such a technique may be extended to also address internal degrees of freedom. By periodically modulating a magnetic field gradient we tune the relative amplitude and sign of the tunneling for different internal states. Thereby we experimentally realize spin-dependent effective Hamiltonians where one state can be pinned to the lattice, while the other remains itinerant. For each spin state, the differing band structure can be characterized either by measuring the expansion of an atomic cloud in the lattice, or by a measurement of the effective mass through dipole oscillations. Furthermore we use the tunability of ultracold atoms to investigate the role of interactions.

**1:39PM F2.00005 Localization effects in periodically driven many-body systems<sup>1</sup>**, FRANOIS HUVE-NEERS, CEREMADE, Universit Paris Dauphine — In this talk, I will discuss the emergence of quasi, or sometimes strictly, conserved quantities in periodically driven many-body quantum systems. In the particular case of a many-body localized Hamiltonian, characterized by a full set of local integral of motions (LIOMs), I will show that the driven system itself admits a full set of strictly conserved LIOMs, if the driving frequency is high enough. Moreover, I will show that the ideas developed in the context of driven systems can be generalized to describe the emergence of pre-thermal behavior in a wide class of both closed and driven systems.

<sup>1</sup>joint work with D. Abanin, W. De Roeck, W. W. Ho

**Tuesday, March 15, 2016 11:15AM - 2:15PM —**

**Session F3 GMAG DCMP: Superconducting Spintronics** Ballroom III - Hans Nembach, National Institute of Standards and Technology

**11:15AM F3.00001 The road to superconducting spintronics<sup>1</sup>**, MATTHIAS ESCHRIG, Royal Holloway, University of London — Energy efficient computing has become a major challenge, with the increasing importance of large data centres across the world, which already today have a power consumption comparable to that of Spain, with steeply increasing trend. Superconducting computing is progressively becoming an alternative for large-scale applications, with the costs for cooling being largely outweighed by the gain in energy efficiency. The combination of superconductivity and spintronics - "superspintronics" - has the potential and flexibility to develop into such a green technology. This young field is based on the observation that new phenomena emerge at interfaces between superconducting and other, competing, phases. The past 15 years have seen a series of pivotal predictions and experimental discoveries relating to the interplay between superconductivity and ferromagnetism. The building blocks of superspintronics are equal-spin Cooper pairs, which are generated at the interface between superconducting and a ferromagnetic materials in the presence of non-collinear magnetism. Such novel, spin-polarised Cooper pairs carry spin-supercurrents in ferromagnets and thus contribute to spin-transport and spin-control. Geometric Berry phases appear during the singlet-triplet conversion process in structures with non-coplanar magnetisation, enhancing functionality of devices, and non-locality introduced by superconducting order leads to long-range effects. With the successful generation and control of equal-spin Cooper pairs the hitherto notorious incompatibility of superconductivity and ferromagnetism has been not only overcome, but turned synergistic. I will discuss these developments and their extraordinary potential. I also will present open questions posed by recent experiments and point out implications for theory.

<sup>1</sup>This work is supported by the Engineering and Physical Science Research Council (EPSRC Grant No. EP/J010618/1).

**11:51AM F3.00002 Nanoscale memory elements based on the superconductor-ferromagnet proximity effect and spin-transfer torque magnetization switching**, BURM BAEK, NIST - Boulder — Superconducting-ferromagnetic hybrid devices have potential for a practical memory technology compatible with superconducting logic circuits and may help realize energy-efficient, high-performance superconducting computers. We have developed Josephson junction devices with pseudo-spin-valve barriers <sup>1</sup>. We observed changes in Josephson critical current depending on the magnetization state of the barrier (parallel or anti-parallel) through the superconductor-ferromagnet proximity effect. This effect persists to nanoscale devices in contrast to the remanent field effect. In nanopillar devices <sup>2</sup>, the magnetization states of the pseudo-spin-valve barriers could also be switched with applied bias currents at 4 K, which is consistent with the spin-transfer torque effect in analogous room-temperature spin valve devices. These results demonstrate devices that combine major superconducting and spintronic effects for scalable read and write of memory states, respectively. Further challenges and proposals towards practical devices will also be discussed. In collaboration with: William Rippard, NIST Boulder, Matthew Pufall, NIST Boulder, Stephen Russek, NIST-Boulder, Michael Schneider, NIST Boulder, Samuel Benz, NIST Boulder, Horst Rogalla, NIST-Boulder, Paul Dresselhaus, NIST - Boulder

<sup>1</sup>B. Baek et al., Nat. Commun. 5, 3888, (2014).

<sup>2</sup>B. Baek et al., Phys. Rev. Appl. 3, 011001 (2015).

**12:27PM F3.00003 Spin-polarized superconductivity for spintronics<sup>1</sup>**, JASON ROBINSON, Cambridge University — The feasibility of superconducting spintronics depends on the spin sensitivity of ferromagnets to the spin of equal-spin triplet Cooper pairs (1). Such pairs are generated at superconductor(S) / ferromagnet(F) interfaces in which certain forms of magnetic inhomogeneity (2,3) are present. In this talk I will introduce the topic of the triplet proximity effect in S-F heterostructures and will discuss my group's recent progress, which includes: spin-selectivity of triplet Cooper pairs in F-S-F superconducting spin-valves (4) and evidence for the formation of a spin-polarized superconducting densities of state in an s-wave superconductor proximity coupled to a magnetically inhomogeneous antiferromagnet (5).

1. J Linder and JWA Robinson. *Nature Physics* 11, 307 (2015).
2. JWA Robinson, JDS Witt, MG Blamire. *Science* 329, 59 (2010).
3. C Klose *et al.*, *Phys. Rev. Lett.* 108, 127002 (2012).
4. N Banerjee, C Smiet, R Smits, A Ozaeta, F Bergeret, M Blamire, JWA Robinson, *Nature Comm.* 5, 3048 (2014).
5. A Di Bernardo, S Diesch, Y Gu, J Linder, G Divitini, C Ducati, E Scheer, MG Blamire, JWA Robinson, *Nature Comm.* 6, 8053 (2015).

<sup>1</sup>Royal Society

**1:03PM F3.00004 Quasiparticle-mediated spin Hall effect in a superconductor**, TARO WAKAMURA, Univ of Paris - Sud 11 CNRS — Superconductivity often brings novel phenomena to spintronics. According to theoretical predictions, superconductivity may enhance the spin Hall effect (SHE) due to the increase in the resistance of superconducting quasiparticles which mediate spin transport in superconductors. In this work, we show a first experimental observation of quasiparticle-mediated SHE in a superconducting NbN, which exhibits an enormous enhancement below the superconducting critical temperature ( $T_C = 10$  K). We fabricated a lateral device structure composed of Py (NiFe) and NbN wires bridged by a nonmagnetic Cu wire. A pure spin current is generated in the Cu bridge by a spin injection current ( $I$ ) between the Py and the Cu, and absorbed into the NbN wire. The absorbed spin currents are converted into charge currents via the inverse SHE, thereby generating the inverse SH voltage ( $V_{ISHE}$ ). When NbN is in the normal state at 20 K ( $>T_C$ ), inverse SH signals  $\Delta R_{ISHE}$  ( $R_{ISHE} \equiv V_{ISHE}/I$ ) are independent of  $I$ . However, at 3 K ( $<T_C$ ), as  $I$  decreases  $\Delta R_{ISHE}$  dramatically increases, and when  $I = 0.01 \mu A$ , the signal becomes more than 2000 times greater than that in the normal state. Our experimental demonstration shows a great potentiality of superconductors for spintronics and its future applications.

**1:39PM F3.00005 Cryogenic Memories based on Spin-Singlet and Spin-Triplet Ferromagnetic Josephson Junctions<sup>1</sup>**, ERIC GINGRICH, Northrop Grumman Corporation — The last several decades have seen an explosion in the use and size of computers for scientific applications. The US Department of Energy has set an ExaScale computing goal for high performance computing that is projected to be unattainable by current CMOS computing designs [1]. This has led to a renewed interest in superconducting computing as a means of beating these projections. One of the primary requirements of this thrust is the development of an efficient cryogenic memory. Estimates of power consumption of early Rapid Single Flux Quantum (RSFQ) memory designs are on the order of MW, far too steep for any real application [1]. Therefore, other memory concepts are required. S/F/S Josephson Junctions, a class of device in which two superconductors (S) are separated by one or more ferromagnetic layers (F) has shown promise as a memory element. Several different systems have been proposed utilizing either the spin-singlet or spin-triplet superconducting states [2]. This talk will discuss the concepts underpinning these devices, and the recent work done to demonstrate their feasibility. [1] - Energy-Efficient Superconducting Computing - Power Budgets and Requirements, D. Scott Holmes, Andrew L. Ripple, Marc A. Manheimer, IEEE Trans. Appl. Supercon., Vol 23, No. 3, June 2013 [2] - B. M. Niedzielski et al., "Use of Pd-Fe and Ni-Fe-Nb as soft magnetic layers in ferromagnetic Josephson junctions for nonvolatile cryogenic memory," IEEE Trans. Appl. Supercond., vol. 24, no. 4, Aug. 2014, Art. ID. 1800307.

<sup>1</sup>This research is supported in part by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA), via U.S. Army Research Office contract W911NF-14-C-0115.

**Tuesday, March 15, 2016 11:15AM - 2:15PM –**  
**Session F4 DPOLY: Polymer Architecture Effects on Structure Dynamics** Ballroom IV - Michael Rubinstein, Univ of NC - Chapel Hill

**11:15AM F4.00001 Topology Matters: Structure and dynamics of ring polymers**, DIETER RICHTER, JCNS at Forschungszentrum Jlich, 52425 Jlich Germany — In this talk I present recent experimental advances addressing the structure and dynamics of rings. I focus mainly on neutron scattering results that reveal experimental insight on a molecular scale. Structural investigations characterizing rings as compact objects in the melts are put into theoretical context. In contrast to the plateau regime common for all other high molecular weight polymer systems, the dynamic modulus of pure ring systems is characterized by a power law decay, while the viscosity displays a much weaker molecular weight dependence as a corresponding linear melt. The dynamics of ring melts is uniquely addressed by neutron spin-echo spectroscopy. The sub-diffusive center of mass motion at short times agrees well with simulation as well as theoretical concepts. In the internal dynamics the basic length scale of the ring molecule, the loop size, manifests itself clearly. The experiments reveal strong evidence for loop motions and call for further theoretical work describing them. Finally, small fractions of ring molecules in linear melts turn out to be very sensitive probes in order to scrutinize the dynamics of the host with the potential to reveal fundamental aspects of the dynamics of branched polymer systems. \pardReview Letters 131, 168302 (2014)Review Letters 115, 148302 (2015)Matter 11, DOI: 10.1039/C5SM01994J (2015)

**11:51AM F4.00002 From chromosome crumpling to the interacting randomly branched polymers**, RALF EVERAERS, Laboratoire de Physique, ENS de Lyon — The conformational statistics of ring polymers in melts or dense solutions is strongly affected by their quenched microscopic topological state. The effect is particularly strong for non-concatenated unknotted rings, which are known to crumple and segregate and which have been implicated as models for the generic behavior of interphase chromosomes. In [1] we have used a computationally efficient multi-scale approach to identify the subtle physics underlying their behavior, where we combine massive Molecular Dynamics simulations on the fiber level with Monte Carlo simulations of a wide range of lattice models for the large scale structure. This allowed us to show that ring melts can be *quantitatively* mapped to coarse-grained melts of *interacting* randomly branched primitive paths. To elucidate the behavior of interacting branched polymers, we use a combination of scaling arguments and computer simulations[2]. The simulations are carried out for different statistical ensembles: ideal randomly branching polymers, melts of interacting randomly branching polymers, and self-avoiding trees with annealed and quenched connectivities. In all cases, we perform a detailed analysis of the tree connectivities and conformations. We find that the scaling behaviour of average properties is very well described by the Flory theory of Gutin et al. [Macromolecules 26, 1293 (1993)]. A detailed study of the corresponding distribution functions allows us to propose a coherent framework of the behavior of interacting trees, including generalised Fisher-Pincus relationships and the detailed analysis of contacts statistics. [1] Ring Polymers in the Melt State: The Physics of Crumpling, Angelo Rosa and Ralf Everaers, Phys. Rev. Lett. 112, 118302 (2014)  
[2] Conformations of randomly branching polymers with volume interactions, Angelo Rosa, A.Y. Grosberg, M. Rubinstein and Ralf Everaers, in preparation.

**12:27PM F4.00003 Self-Similar Conformations and Dynamics of Non-Concatenated Entangled Ring Polymers<sup>1</sup>**, TING GE, University of North Carolina at Chapel Hill — A scaling model of self-similar conformations and dynamics of non-concatenated entangled ring polymers is developed. Topological constraints force these ring polymers into compact conformations with fractal dimension  $D=3$  that we call fractal loopy globules (FLGs). This result is based on the conjecture that the overlap parameter of loops on all length scales is equal to the Kavassalis-Noolandi number 10-20. The dynamics of entangled rings is self-similar, and proceeds as loops of increasing sizes are rearranged progressively at their respective diffusion times. The topological constraints associated with smaller rearranged loops affect the dynamics of larger loops by increasing the effective friction coefficient, but have no influence on the tubes confining larger loops. Therefore, the tube diameter defined as the average spacing between relevant topological constraints increases with time, leading to "tube dilation". Analysis of the primitive paths in molecular dynamics (MD) simulations suggests complete tube dilation with the tube diameter on the order of the time-dependent characteristic loop size. A characteristic loop at time  $t$  is defined as a ring section that has diffused a distance of its size during time  $t$ . We derive dynamic scaling exponents in terms of fractal dimensions of an entangled ring and the underlying primitive path and a parameter characterizing the extent of tube dilation. The results reproduce the predictions of different dynamic models of a single non-concatenated entangled ring. We demonstrate that traditional generalization of single-ring models to multi-ring dynamics is not self-consistent and develop a FLG model with self-consistent multi-ring dynamics and complete tube dilation. Various dynamic scaling exponents predicted by the self-consistent FLG model are consistent with recent computer simulations and experiments. We also perform MD simulations of nanoparticle (NP) diffusion in melts of non-concatenated entangled ring polymers. NPs larger than the undiluted tube diameter undergo power-law sub-diffusion in entangled rings in contrast to strong suppression in entangled linear chains. This result demonstrates that there is no long-lived confining tube in entangled ring polymers, which agrees with complete tube dilation in the self-consistent FLG model.

<sup>1</sup>This work is done in collaboration with Drs. Michael Rubinstein, Sergey Panyukov and Gary Grest and supported by NSF.

### 1:03PM F4.00004 Polymer Crystallization under Confinement , GEORGE FLOUDAS, University of Ioannina —

Recent efforts indicated that polymer crystallization under confinement can be substantially different from the bulk. This can have important technological applications for the design of polymeric nanofibers with tunable mechanical strength, processability and optical clarity. However, the question of *how, why and when* polymers crystallize under confinement is not fully answered. Important studies of polymer crystallization confined to droplets and within the spherical nanodomains of block copolymers emphasized the interplay between heterogeneous and homogeneous nucleation. Herein we report on recent studies<sup>1–5</sup> of polymer crystallization under hard confinement provided by model self-ordered AAO nanopores. Important open questions here are on the type of nucleation (homogeneous vs. heterogeneous), the size of critical nucleus, the crystal orientation and the possibility to control the overall crystallinity. Providing answers to these questions is of technological relevance for the understanding of nanocomposites containing semicrystalline polymers. [1] H. Duran, M. Steinhart, H.-J. Butt, G. Floudas, *Nano Letters* **2011**, *11*, 1671. [2] Y. Suzuki, H. Duran, M. Steinhart, H.-J. Butt, G. Floudas, *Soft Matter* **2013**, *9*, 2769. [3] Y. Suzuki, H. Duran, W. Akram, M. Steinhart, G. Floudas, H.-J. Butt, *Soft Matter* **2013**, *9*, 9189. [4] Y. Suzuki, H. Duran, M. Steinhart, H.-J. Butt, G. Floudas, *Macromolecules* **2014**, *47*, 1793. [5] Y. Suzuki, H. Duran, M. Steinhart, M. Kappl, H.-J. Butt, G. Floudas, *Nano Letters* **2015**, *15*, 1987–1992. \*In collaboration with Y. Suzuki, H. Duran, M. Steinhart, H.-J. Butt

### 1:39PM F4.00005 Rheology of Rings: Current Status and Future Challenges<sup>1</sup> , GREGORY MCKENNA,

Texas Tech Univ — Understanding the dynamics of circular or ring-like polymers has been a subject of investigation since the 1980s and is one which remains an area that is not fully understood [1–5]. Part of the reason for this is the difficulty of making synthetic rings of sufficient size to establish the nature of the entanglement dynamics, if entanglements even exist in these materials. Furthermore, there is now strong evidence that small amounts of linear impurities can impact the dynamics. Hence, one of the major challenges to our understanding of ring dynamics is to make large molecular weight rings of sufficient purity that the dynamics of the rings themselves can be determined. In the present work the current state of understanding of the dynamics of rings is outlined and current work from our group of collaborators [6] to make extremely large circular polymers using Echeverria Coli as a route to make pure rings (circular DNA) in sufficient quantity and size to determine the dynamics of these materials will be shown. First results of ring dynamics in dilute solution are presented and new results on concentrated and entangled solutions will be discussed. Remaining challenges will be elucidated. [1] J. Klein, *Macromolecules*, *19*, 105–118 (1986). [2] J. Roovers, *Macromolecules*, *18*, 1359–1361 (1985). [3] G.B. McKenna, G. Hadziioannou, P. Lutz, G. Hild, C. Strazielle, C. Straupe, P. Rempp and A.J. Kovacs, *Macromolecules*, *20*, 498–512 (1987). [4] M. Kapnistos, M. Lang, D. Vlassopoulos, W. Pyckhout-Hintzen, D. Richter, D. Cho, T. Chang and M. Rubinstein, *Nat. Matls., Nat. Mater.*, *7*, 997–1002 (2008). [5] Y. Doi, K. Matsubara, Y. Ohta, T. Nakano, D. Kawaguchi, Y. Takahashi, A. Takano and Y. Matsushita, *Macromolecules*, *48*, 3140–3147 (2015). [6] Y. Li, K.-W. Hsiao, C. A. Brockman, D. Y. Yates, R. M. Robertson-Anderson, J.A. Kornfield, M. J. San Francisco, C. M. Schroeder and G. B. McKenna, *Macromolecules*, *48*, 5997–6001 (2015).

<sup>1</sup>Partially supported by the John R. Bradford Endowment and the Paul Whitfield Horn Professorship at Texas Tech University

## Tuesday, March 15, 2016 11:15AM - 2:03PM —

Session F5 GMAG DCMP FIAP: Spin Transport in Semiconductors 301 - Pengke Li, University of Maryland, College Park

### 11:15AM F5.00001 Spin-orbit fields at semiconductor interfaces<sup>1</sup> , MARTIN GMITRA, University of Regensburg

— Solids without space inversion symmetry exhibit spin-orbit fields, which are emerging manifestations of spin-orbit coupling of the underlying atomic structure. Primary examples of spatially asymmetric systems are interfaces, which are omnipresent in electronic devices. As the device dimensions scale down, interfaces imprint their symmetries into the transport channel by proximity effects. Proximity spin-orbit fields already play important roles in anisotropic magnetoresistance of ultrathin structures such as Fe/GaAs [1], in the physics of Majorana fermions [2,3] and Andreev reflection [4] of semiconductor/superconductor junctions, in Skyrmin textures [5] in ferromagnets, or in spin-orbit torques [6]. It is thus of vital interest to gain qualitative insight and realistic quantitative description of the interfacial spin-orbit fields for various materials hybrid settings. We have proposed a methodology to extract spin-orbit fields, both their magnitudes and directions, and applied it to investigate Fe/GaAs junctions [7]. Only at low momenta the traditional description of the fields in terms of linear Rashba and Dresselhaus works. At generic momenta the fields exhibit what we call butterfly patterns, conforming to the interfacial symmetry. Remarkably, the spin-orbit fields depend rather strongly on the magnetization orientation. We will also discuss our recent results on the spin-orbit coupling in zinc-blende and wurtzite semiconductor nanostructures.

[1] T. Hupfauer *et al.*, *Nat. Nanocommun.* **6**, 7374 (2014).

[2] S. Nadj-Perge, *et al.*, *Science* **346**, 602 (2014); R. Pawlak *et al.*, arXiv:1505.06078.

[3] V. Mourik, *et al.*, *Science* **336**, 1003 (2012).

[4] P. Högl, A. Matos-Abiad, I. Zutic, and J. Fabian, *Phys. Rev. Lett.* **115**, 116601 (2015).

[5] S. Mühlbauer *et al.*, *Science* **323**, 915 (2013).

[6] K.-S. Lee *et al.*, *Phys. Rev. B* **91**, 144401 (2015).

[7] M. Gmitra, A. Matos-Abiad, C. Draxl, and J. Fabian, *Phys. Rev. Lett.* **111**, 036603 (2013).

<sup>1</sup>The work is supported by the DFG SFB 689.

### 11:51AM F5.00002 Realization of an all-electric spin transistor using quantum point contacts

, TSE-MING CHEN, POJEN CHUANG, SHENG-CHIN HO, National Cheng Kung University, LUKE SMITH, FRANCOIS SFIGAKIS, University of Cambridge, MICHAEL PEPPER, University College London, CHIN-HUNG CHEN, JU-CHUN FAN, National Cheng Kung University, JONATHAN GRIFFITHS, IAN FARRER, HARVEY BEERE, GEB JONES, DAVE RITCHIE, University of Cambridge — The spin field effect transistor envisioned by Datta and Das opens a gateway to spin information processing. Although the coherent manipulation of electron spins in semiconductors is now possible, the realization of a functional spin field effect transistor for information processing has yet to be achieved, owing to several fundamental challenges such as the low spin-injection efficiency due to resistance mismatch, spin relaxation, and the spread of spin precession angles. Alternative spin transistor designs have therefore been proposed, but these differ from the field effect transistor concept and require the use of optical or magnetic elements, which pose difficulties for the incorporation into integrated circuits. Here, we present an all-electric all-semiconductor spin field effect transistor, in which these obstacles are overcome by employing two quantum point contacts as spin injectors and detectors. Distinct engineering architectures of spin-orbit coupling are exploited for the quantum point contacts and the central semiconductor channel to achieve complete control of the electron spins—spin injection, manipulation, and detection—in a purely electrical manner. Such a device is compatible with large-scale integration and hold promise for future spintronic devices for information processing. Ref: P. Chuang *et al.*, *Nat. Nanotechnol.* *10*, 35 (2015).

### 12:03PM F5.00003 Current-induced spin polarization in InGaAs epilayers with varying doping densities , MARTA LUENGO-KOVAC, SIMON HUANG, DAVIDE DEL GAUDIO, JORDAN OCCENA, RACHEL GOLDMAN, VANESSA SIH, Univ of Michigan - Ann Arbor —

Current-induced spin polarization (CISP) is a phenomena in which an applied electric field produces a bulk spin polarization in the plane of the sample. As this is thought to arise from the spin-orbit coupling, it was originally predicted that the magnitude of CISP should be proportional to the spin-orbit (SO) splitting [1]. However, crystal axis-dependent measurements of the CISP and SO fields showed a negative differential relationship between these two quantities [2]. To develop a phenomenological understanding of the factors affecting the magnitude of CISP, we performed measurements on three In<sub>0.025</sub>Ga<sub>0.975</sub>As epilayers, Si-doped at 0.67, 9.6, and 14.1 × 10<sup>17</sup> cm<sup>-3</sup>. We will discuss the effects of the doping density and electron mobility on the magnitudes of the SO fields and CISP. [1] V. Edelstein, *Solid State Commun.* **73**, 233 (1990). [2] Norman, B. M., *et al.*, *Phys. Rev. Lett.* **112**, 056601 (2014).

**12:15PM F5.00004 Effective spin Hall properties of a mixture of materials with and without spin-orbit coupling: Tailoring the effective spin-diffusion length<sup>1</sup>**, YUE ZHANG, MEGAN PRESTGARD, ASHUTOSH TIWARI, MIKHAIL RAIKH, Univ of Utah — We study theoretically the effective spin Hall properties of a composite consisting of two materials with and without spin-orbit (SO) coupling. In particular, we assume that SO material represents a system of grains of radius,  $a$ , and density,  $n$ , in a matrix with no SO. We calculate the effective spin Hall angle,  $\theta_{eff}^{SH}$ , and the effective spin diffusion length,  $\lambda_{eff}$ , of the mixture. Our main qualitative finding is that, if the bare spin diffusion length,  $\lambda$ , is much smaller than  $a$ , then  $\lambda_{eff}$  is strongly *enhanced*, well beyond  $\lambda/(na^3)^{1/2}$ , which can be expected from purely “geometrical” consideration. The physical origin of this additional enhancement is that, with small diffusion length,  $\lambda \ll a$ , the spin current mostly flows *around the grain* without suffering much loss. We also demonstrate that the voltage, created by a spin current, is sensitive to a very weak magnetic field directed along the spin current, and even reverses sign in a certain domain of fields. The origin of this sensitivity is that the spin precession, caused by magnetic field, takes place outside the grains where SO is absent.

<sup>1</sup>Supported by NSF through MRSEC DMR-1121252.

**12:27PM F5.00005 Spin relaxation via exchange with donor impurity-bound electrons<sup>1</sup>**, IAN APPELBAUM, Univ of Maryland-College Park — In the Bir-Aronov-Pikus depolarization process affecting conduction electrons in p-type cubic semiconductors, spin relaxation is driven by exchange with short-lived valence band hole states. We have identified an analogous spin relaxation mechanism in nominally undoped silicon at low temperatures, when many electrons are bound to dilute dopant ion potentials. Inelastic scattering with externally injected conduction electrons accelerated by electric fields can excite transitions into highly spin-orbit-mixed bound excited states, driving strong spin relaxation of the conduction electrons via exchange interaction. We reveal the consequences of this spin depolarization mechanism both below and above the impact ionization threshold, where conventional charge and spin transport are restored.

<sup>1</sup>Based upon: Lan Qing, Jing Li, Ian Appelbaum, and Hanan Dery, Phys. Rev. B **91**, 241405(R) (2015). We acknowledge support from NSF, DTRA, and ONR.

**1:03PM F5.00006 Electrical spin injection and detection in Si nanowires with axial doping gradient**, KONSTANTINOS KOUNTOURIOTIS, JORGE BARREDA, TIM KEIPER, MEI ZHANG, PENG XIONG, Florida State Univ — Due to the technological importance and potential long spin coherence time in silicon, there have been significant recent efforts to realize spin injection, coherent transport, and electrical spin detection in Si nanowires (NWs). The nature of the electronic transport at the interface and its resistance are crucial factors in realizing efficient spin injection/detection between a ferromagnet (FM) and a semiconductor (SC). In this work, we examine the effects on electrical spin injection and detection by FM/SC interfaces with well-defined Schottky barriers in Si NW devices. The Si NWs are synthesized via a vapor-liquid-solid method using silane and phosphine precursor gases for the growth and doping respectively, which results in a graded phosphorus doping profile along the length of the NW. The Si NWs are dispersed on a  $p^+-Si/SiO_2/SiN_x$  substrate, and a series of CoFe electrodes are defined along a Si NW with electron beam lithography and magnetron sputtering after the removal of the native oxide by HF treatment. As a consequence of the doping gradient, the FM electrodes form Ohmic and Schottky barrier contacts of varying heights along the length of a single NW. Two-terminal local and four-terminal non-local spin-valve measurements are performed to probe spin accumulation and transport at different FM contacts, enabling a study of the dependence of the spin signals on the Schottky barrier height and interface resistance on a single device. \*Work supported by NSF grant DMR-1308613.

**1:15PM F5.00007 Room-temperature operation of Si spin MOSFET with high on/off spin signal ratio**, MASASHI SHIRAISHI, Department of Electronic Science and Engineering, Kyoto University, HAYATO KOIKE, Technology HQ, TDK Corporation, TAKAYUKI TAHARA, Department of Electronic Science and Engineering, Kyoto University, TOMOYUKI SASAKI, MAKOTO KAMENO, Technology HQ, TDK Corporation, YUICHIRO ANDO, Department of Electronic Science and Engineering, Kyoto University, KAZUHIRO TANAKA, SHINJI MIWA, YOSHISHIGE SUZUKI, Graduate School of Engineering Science, Osaka University — Si spintronics is now one of the pivotal fields in semiconductor spintronics. After the first report on successful propagation of pure spin current in Si, much effort has been paid for realization of Si spin metal-oxide-semiconductor field-effect transistor (MOSFET), since Si spin MOSFETs allow constructing reconfigurable logic circuits with ultra-low energy consumption. Our group achieved the first operation of Si spin MOSFET at room temperature by using non-degenerate n-type Si [1]. However, the remaining issue to be solved was low on/off ratio of spin signals. In this presentation, we report on our experimental demonstration of Si spin MOSFET with high on/off ratio of spin signals. The on/off ratio is greater than  $10^3$ , whereas on/off ratio in a conventional MOSFET operation is ca.  $10^5$ . More importantly, the gate voltage dependence of the spin signals and the MOSFET signals are in good agreement [2]. This achievement can pave the way to a practical application of Si spin MOSFETs. References: [1] T. Sasaki, M. Shiraishi et al., Phys. Rev. Applied 2, 034005 (2014). [2] T. Tahara, M. Shiraishi et al., Appl. Phys. Express, in press (selected as Spotlight Paper).

**1:27PM F5.00008 Electronic measurement of strain effects on spin transport in silicon<sup>1</sup>**, LAN QING, HOLLY TINKEY, IAN APPELBAUM, Center for Nanophysics and Advanced Materials and Department of Physics, University of Maryland, College Park, Maryland 20742 — Spin transport in silicon is limited by the Elliott-Yafet spin relaxation mechanism, which is driven by scattering between degenerate conduction band valleys. Mechanical strain along a valley axis partially breaks this degeneracy, and will ultimately quench intervalley spin relaxation for transitions between states on orthogonal axes. Using a custom-designed and constructed strain probe, we study the effects of uniaxial compressive strain along the  $\langle 100 \rangle$  direction on ballistic tunnel junction devices used to inject spin-polarized electrons into silicon. The effects of strain-induced valley splitting will be presented and compared to our theoretical model.

<sup>1</sup>This work is supported by the Office of Naval Research under Contract No. N000141410317, the National Science Foundation under Contract No. ECCS-1231855, the Defense Threat Reduction Agency under Contract No. HDTRA1-13-1-0013, and the Maryland NanoCenter.

**1:39PM F5.00009 Three-terminal experiments on epitaxial Si/MgO tunnel junctions**, JULIANE LAURER, MAREEN SCHAEFER, MATTHIAS KRONSEDER, MICHAELA TROTTMANN, MARKUS HAERTINGER, JOSEF ZWECK, CHRISTIAN H. BACK, DIETER WEISS, MARIUSZ CIORGA, DOMINIQUE BOUGEARD, Institut fuer Experimentelle und Angewandte Physik, Universitaet Regensburg, Germany — In the field of spin injection into semiconductors, experiments in a three-terminal (3T) Hanle geometry are widely used to determine spin life times and spin diffusion lengths. However, as charge and spin current are not separated in the 3T geometry, it is yet unclear how reliable 3T experiments are to reveal spin-related quantities of the semiconductor channel. In particular, the impact of defect states in the tunnel barrier or at its interfaces on measured 3T Hanle-like signals has intensely been discussed recently. In our contribution, we compare 3T experiments on entirely MBE-grown epitaxial Si/MgO/Fe/Au and Si/MgO/Au, i.e. ferromagnetic and nonmagnetic tunnel junctions. Both sample types show a similar Lorentzian signal comparable to those obtained by the Hanle effect of a precessing and dephasing spin ensemble. In contrast to the ferromagnetic sample, the resistance of the nonmagnetic sample increases for increasing external magnetic field. We discuss the dependence of the signal on bias, temperature and orientation of the external magnetic field, taking into account the high crystalline quality of our epitaxial tunnel junctions with atomically sharp interfaces.

**1:51PM F5.00010 Spin Transport and Precession in Epitaxial BaTiO<sub>3</sub>/Ge Heterostructures**, YICHEN JIA, CRISTINA VISANI, LIOR KORNBLUM, ERIC JIN, CHARLES AHN, FRED WALKER, Yale University — Spintronics has opened up new possibilities to leverage the spin degree of freedom in electronic devices. Spin injection from ferromagnets into semiconductors has been realized by inserting a thin tunnel barrier layer, which adjusts the conductivity mismatch. However, limited functionality in conventional tunnel barriers hinders the control and manipulation of spin. Here we report the spin injection and detection in p-type Germanium (p-Ge) through a functional BaTiO<sub>3</sub> (BTO) tunnel barrier. Epitaxial BTO thin films are grown on p-Ge by molecular beam epitaxy (MBE), followed by electron beam pattern generation (EBPG) to fabricate multi-terminal spin devices. Spin accumulation is demonstrated using the Hanle technique, where the spin signal shows a non-monotonic temperature dependence. Using this temperature dependence, we investigate the dominant spin damping pathways in each temperature regime. Furthermore, we discuss the possibility of manipulating spin transport using the BTO layer, which would allow one to integrate the unique functionalities of complex oxides with semiconductor spintronics devices.

**Tuesday, March 15, 2016 11:15AM - 2:03PM –**  
**Session F6 GMAG DMP: Iridates II** 302 - Ilija Zeljkovic, Boston College

**11:15AM F6.00001 The role of correlations in the low energy electronic structure of lightly electron doped Sr<sub>2</sub>IrO<sub>4</sub> and Sr<sub>3</sub>Ir<sub>2</sub>O<sub>7</sub>.**, ALBERTO DE LA TORRE, FLAVIO BRUNO, ZHIMING WANG, ANNA TAMAI, CHRISTOPHE BERTHOD, DIDIER JACCARD, University of Geneva, ALASKA SUBEDI, Max Planck - Hamburg, ANTOINE GEORGES, Ecole Polytechnique, CNRS, ROBIN PERRY, University College London, FELIX BAUMBERGER, University of Geneva — We characterized the emergence of exotic electronic ground states in lightly electron doped (Sr<sub>1-x</sub>La<sub>x</sub>)<sub>2</sub>IrO<sub>4</sub> and (Sr<sub>1-x</sub>La<sub>x</sub>)<sub>3</sub>Ir<sub>2</sub>O<sub>7</sub> by ARPES. In the single layer iridate, a large Fermi surface with nodal coherent spectral weight and antinodal pseudogap emerges, concomitantly with the collapse of the Mott gap, upon doping [1]. On the other hand, in Sr<sub>3</sub>Ir<sub>2</sub>O<sub>7</sub> a small non-gapped Fermi surface with coherent quasiparticles, together with a reduction of the correlated gap throughout the entire Brillouin Zone is observed when doping above the insulator to metal transition [2]. By comparing the electronic structure of these two materials, we provide evidence that the interplay between spin-orbit and electron-electron correlations ( $U$ ) in (Sr<sub>1-x</sub>La<sub>x</sub>)<sub>2</sub>IrO<sub>4</sub> and (Sr<sub>1-x</sub>La<sub>x</sub>)<sub>3</sub>Ir<sub>2</sub>O<sub>7</sub> is rather different: while in Sr<sub>2</sub>IrO<sub>4</sub> this interplay results in a pseudospin-1/2 single band Mott insulator with a phenomenology very similar to that of cuprates, in Sr<sub>3</sub>Ir<sub>2</sub>O<sub>7</sub>  $U$  enhances the bilayer splitting gap to originate a ground state resembling that of a correlated semiconductor. [1] A. de la Torre et al, PRL 115, 176402 (2015); [2] A. de la Torre et al, PRL 113, 256402 (2014)

**11:27AM F6.00002 Electrically tunable transport in antiferromagnetic Sr<sub>3</sub>Ir<sub>2</sub>O<sub>7</sub><sup>1</sup>**, HEIDI SEINIGE, CHENG WANG, The University of Texas at Austin, GANG CAO, University of Kentucky, JIANSHI-S. ZHOU, JOHN B. GOODENOUGH, MAXIM TSOI, The University of Texas at Austin — Recently we demonstrated experimentally the existence of interconnections between magnetic state and transport currents in antiferromagnetic (AFM) Mott insulator Sr<sub>2</sub>IrO<sub>4</sub>. We found a very large anisotropic magnetoresistance [1] and demonstrated a reversible resistive switching driven by high-density currents/high electric fields [2]. These results support the feasibility of AFM spintronics, where antiferromagnets are used in place of ferromagnets, however a low Néel temperature of this material (240 K) questions any practical applications. Here we present a comparative electrical transport study of its sister compound Sr<sub>2</sub>IrO<sub>4</sub> which has a higher transition temperature (285 K). Similar to the case of Sr<sub>2</sub>IrO<sub>4</sub>, we find a continuous reduction in the resistivity of Sr<sub>3</sub>Ir<sub>2</sub>O<sub>7</sub> as a function of increasing electrical bias and abrupt reversible changes above a threshold bias current. We explain these results by a reduction of activation energy associated with a field-driven lattice distortion. [1] C. Wang et al., Phys. Rev. X 4, 041034 (2014); [2] C. Wang et al, PRB 92, 115136 (2015).

<sup>1</sup>This work was supported in part by C-SPIN, one of six centers of STARnet, a Semiconductor Research Corporation program, sponsored by MARCO and DARPA, and by NSF grants DMR-1207577, DMR-1265162, and DMR-1122603.

**11:39AM F6.00003 Magnetic excitations and lattice distortions in highly-doped (Sr<sub>1-x</sub>La<sub>x</sub>)<sub>3</sub>Ir<sub>2</sub>O<sub>7</sub>**, TOM HOGAN, University of California Santa Barbara, MARY UPTON, Argonne National Laboratory, XIAOPING WANG, Oak Ridge National Laboratory, STEPHEN WILSON, University of California Santa Barbara — (Sr<sub>1-x</sub>La<sub>x</sub>)<sub>3</sub>Ir<sub>2</sub>O<sub>7</sub> has been shown to undergo a first-order phase transition from a localized antiferromagnetic insulating state to a correlated metal. We discuss the further characterization of these correlations by examining the excitation spectra of a highly-doped sample. These reveal evidence of a dispersive feature associated with an over-damped magnon mode, similar to the behavior of the undoped parent compound, as well as a higher energy excitation. The nature of the lattice distortion brought on by La-doping will also be discussed.

**11:51AM F6.00004 Nature of the magnetic correlations in photo-doped and chemically-doped spin-orbit Mott insulator Sr<sub>2</sub>IrO<sub>4</sub><sup>1</sup>**, MARK P. M. DEAN, Brookhaven National Laboratory — In the iridates, competition between spin-orbit coupling, crystal field, and electronic correlation has lead to the observation of several novel states. Particularly notable is the spin-orbit Mott insulating state in Sr<sub>2</sub>IrO<sub>4</sub> which has close analogies to the high temperature superconducting cuprates. This talk will describe the nature of the magnetic correlations in Sr<sub>2</sub>IrO<sub>4</sub> and how the magnetic correlations can be modified by two different doping schemes. I will first describe doping via photo-excitation in which we use femtosecond infrared pulses to excite carriers across the Mott gap. After excitation, we probe the resulting magnetic state as a function of time delay using the first implementation of magnetic resonant inelastic X-ray scattering at a free electron laser. We find that the non-equilibrium state 2 ps after the excitation has strongly suppressed long-range magnetic order, but hosts photo-carriers that induce strong, non-thermal magnetic correlations. The magnetism recovers its two-dimensional in-plane Néel correlations on a timescale of a few ps, while the three-dimensional long range magnetic order is restored over a far longer, fluence-dependent timescale of a few 100 ps. In the second part of the talk I will describe chemical doping via Ir-Ru substitution. In this situation, we find that with increased Ru concentration, the dispersive magnetic excitations in the parent compound become almost momentum-independent, opening a magnetic gap > 150 meV. We attribute this gap to the combined effects of disorder and Ir-Ru interactions.

<sup>1</sup>Work performed at Brookhaven National Laboratory was supported by the US Department of Energy, Division of Materials Science, under Contract No.DE-AC02-98CH10886.

**12:27PM F6.00005 Jahn-Teller effect in systems with strong on-site spin-orbit coupling**, EKATERINA PLOTNIKOVA, Leibniz Institute for Solid State and Materials Research Dresden, Germany, MARIA DAGHOFER, University of Stuttgart, Germany, JEROEN VAN DEN BRINK, Leibniz Institute for Solid State and Materials Research Dresden, Germany, KRZYSZTOF WOHLFELD, Stanford University and SLAC National Accelerator Laboratory, USA and University of Warsaw, Poland — When strong spin-orbit coupling removes orbital degeneracy, it would at the same time appear to render the Jahn-Teller mechanism ineffective. We discuss such a situation, the  $t_{2g}$  manifold of iridates, and show that, while the Jahn-Teller effect does indeed not affect the  $j = 1/2$  antiferromagnetically ordered ground state, it leads to distinctive signatures in the  $j = 3/2$  spin-orbit exciton. It allows for a hopping of the spin-orbit exciton between the nearest neighbor sites without producing defects in the  $j = 1/2$  antiferromagnet. This arises because the lattice-driven Jahn-Teller mechanism only couples to the orbital degree of freedom, but is not sensitive to the phase of the wave function that defines isospin  $j_z$ . This contrasts sharply with purely electronic propagation, which conserves isospin, and presence of Jahn-Teller coupling can explain some of the peculiar features of measured resonant inelastic x-ray scattering spectra of Sr<sub>2</sub>IrO<sub>4</sub>.

**12:39PM F6.00006 Unveiling the Origin of the Basal-plane Antiferromagnetism in the  $J_{\text{eff}}=1/2$  Mott Insulator  $\text{Ba}_2\text{IrO}_4$ : A Density Functional and Model Hamiltonian Study**, YUSHENG HOU, HONGJUN XIANG, XINGAO GONG, Fudan University, KEY LABORATORY OF COMPUTATIONAL PHYSICAL SCIENCES (MINISTRY OF EDUCATION) COLLABORATION — Based on the density functional theory and our new model Hamiltonian, we have studied the basal-plane antiferromagnetism in the novel  $J_{\text{eff}}=1/2$  Mott insulator  $\text{Ba}_2\text{IrO}_4$ . By comparing the magnetic properties of the bulk  $\text{Ba}_2\text{IrO}_4$  with those of the single-layer  $\text{Ba}_2\text{IrO}_4$ , we demonstrate unambiguously that the basal-plane antiferromagnetism is caused by the intralayer magnetic interactions rather than by the previously proposed interlayer ones. In order to reveal the origin of the basal-plane antiferromagnetism, we propose a new model Hamiltonian by adding the single ion anisotropy and pseudo-quadrupole interactions into the general bilinear pseudo-spin Hamiltonian. The obtained magnetic interaction parameters indicate that the single ion anisotropy and pseudo-quadrupole interactions are unexpectedly strong. Systematical Monte Carlo simulations demonstrate that the basal-plane antiferromagnetism is caused by the isotropic Heisenberg, bond-dependent Kitaev and pseudo-quadrupole interactions. Our results show for the first time that the single ion anisotropy and pseudo-quadrupole interaction can play significant roles in establishing the exotic magnetism in the  $J_{\text{eff}}=1/2$  Mott insulator.

**12:51PM F6.00007 Frustration in square lattice of Iridium  $J_{\text{eff}}=1/2$  moments at high pressure<sup>1</sup>**, DANIEL HASKEL, Advanced Photon Source, Argonne National Laboratory, GILBERTO FABBRI, Brookhaven National Laboratory, JONG WOO KIM, JUNG HO KIM, Advanced Photon Source, Argonne National Laboratory, BUMJOON KIM, Max Planck Institute for Solid State Research, GANG CAO, University of Kentucky, VIKTOR STRUZHNIKIN, Geophysical Laboratory, Carnegie Institution of Washington — We study the evolution of magnetic order in the weakly ferromagnetic, insulator  $\text{Sr}_2\text{IrO}_4$  under applied pressure using x-ray resonant magnetic scattering and x-ray magnetic circular dichroism techniques in the diamond anvil cell. The weak inter-layer coupling is readily tunable with pressure giving rise to a change in magnetic structure followed by coexisting and competing magnetic phases with different inter-layer coupling. Application of moderate magnetic fields stabilizes one of the magnetic phases. Higher pressures drive the system into a magnetically disordered state, possibly a quantum paramagnetic state. We discuss the results in the context of a J1-J2 model where the increasing strength of next-nearest-neighbor exchange coupling with pressure leads to frustration of in-plane interactions

<sup>1</sup>Work at Argonne is supported by the US Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC-02-06CH11357.

**1:03PM F6.00008 Effect of longer-range lattice anisotropy on the electronic structure and magnetism of spin-orbit-coupled  $5d$  transition-metal oxides**, NIKOLAY BOGDANOV<sup>1</sup>, VAMSHI KATUKURI<sup>2</sup>, JUDIT ROMHÁNYI<sup>3</sup>, Institute for Theoretical Solid State Physics, IFW Dresden, Germany, VIKTOR YUSHANKHAI, Joint Institute for Nuclear Research, Dubna, Russia, VLADISLAV KATAEV, BERNDT BÜCHNER, Institute for Solid State Research, IFW Dresden, Germany, JEROEN VAN DEN BRINK, LIVIU HOZOI, Institute for Theoretical Solid State Physics, IFW Dresden, Germany — Our detailed quantum chemistry calculations provide magnetic  $g$  factors and exchange interactions for the quasi two-dimensional iridates  $\text{Sr}_2\text{IrO}_4$  and  $\text{Ba}_2\text{IrO}_4$ . While canonical ligand-field considerations predict  $g_{||}$ -factors  $< 2$  for the positive tetragonal distortions present in  $\text{Sr}_2\text{IrO}_4$ , we find  $g_{||} > 2$ . This implies that the  $d$  levels in  $\text{Sr}_2\text{IrO}_4$  are inverted with respect to the ordering deduced from the local ligand distortions, whereas we find them in  $\text{Ba}_2\text{IrO}_4$  to be instead normally ordered. Electron spin resonance measurements confirm the level inversion in  $\text{Sr}_2\text{IrO}_4$ . This  $d$ -level switching is driven by the specific ionic charge distribution within adjacent  $\text{IrO}_2$  and  $\text{SrO}$  layers. Since polar discontinuities and the associated complications do not arise for such layers, our results highlight the tetravalent  $d$ -metal 214 oxides as ideal platforms to explore  $d$ -level reconstruction and engineering in the context of oxide heterostructures.

<sup>1</sup>Present address: Electronic structure theory, MPI-FKF, Stuttgart

<sup>2</sup>Present address: Ecole polytechnique fédérale de Lausanne

<sup>3</sup>Present address: Quantum materials, MPI-FKF, Stuttgart

**1:15PM F6.00009 Influence of isovalent doping of  $\text{Ca}^{2+}$  on the Spin orbit Mott insulator  $\text{Sr}_2\text{IrO}_4$** , XIANG CHEN, Boston Coll, STEPHEN WILSON, UCSB, WILSON GROUP TEAM — Here we investigate the influence of isoelectronic doping into the spin-orbit Mott materials  $\text{Sr}_2\text{IrO}_4$ . Specifically, we explore the influence of isovalent Ca substitution as a perturbation to the  $J_{\text{eff}}=1/2$  Mott ground state by combined transport, bulk magnetization, and scattering measurements. The evolution of the lattice geometry/structure-type as well as the electronic phase behavior will be presented as  $\text{Ca}^{2+}$  is substituted on the  $\text{Sr}^{2+}$  site.

**1:27PM F6.00010 Crystal growth and intrinsic magnetic behavior of  $\text{Sr}_2\text{IrO}_4$** , NAKHEON SUNG, H. GRETTARSSON, D. PROEPPER, J. PORRAS, M. LE TACON, A. V. BORIS, B. KEIMER, B. J. KIM, Max Planck Institute for Solid State Research — We report on the growth of stoichiometric  $\text{Sr}_2\text{IrO}_4$  single crystals, which allow us to unveil their intrinsic magnetic properties. The effect of different growth conditions has been investigated for crystals grown by the flux method. We find that the magnetic response depends very sensitively on the details of the growth conditions. We assess the defect concentration based on magnetization, X-ray diffraction, Raman scattering, and optical conductivity measurements. We find that samples with a low concentration of electronically active defects show much reduced in-gap spectral weight in the optical conductivity and a pronounced two-magnon peak in the Raman scattering spectrum. A prolonged exposure at high temperature during the growth leads to higher defect concentration likely due to creation of oxygen vacancies. We further demonstrate a systematic intergrowth of  $\text{Sr}_2\text{IrO}_4$  and  $\text{Sr}_3\text{Ir}_2\text{O}_7$  phases by varying the growth temperature. Our results thus emphasize that revealing the intrinsic magnetic properties of  $\text{Sr}_2\text{IrO}_4$  and related materials requires a scrupulous control of the crystal growth process.

**1:39PM F6.00011 Magnetic Properties comparison of 3D Kitaev candidate materials beta and gamma  $\text{Li}_2\text{IrO}_3$** , RAMON RUIZ, Univ of California - Berkeley, NICHOLAS BREZNAY COLLABORATION, ALEX FRANO COLLABORATION, TONI HELM COLLABORATION, JAMES ANALYTIS COLLABORATION — Honeycomb iridates have been the focus of substantial interest due to the strong magnetic frustration that arises from their edge-shared bonding environment, which favors a strongly anisotropic Ising-like exchange between bonds. In materials with edge-shared  $\text{IrO}_6$  octahedra, spin-anisotropy of the exchange between neighboring effective spin-1/2 states is enhanced by the interference of the two exchange paths across the planar Ir-O-Ir bond. In the honeycomb lattice, such an interaction couples different orthogonal spin components for the three nearest neighbors; no single exchange direction can be simultaneously satisfied, leading to strong frustration which can be described by the Kitaev-model. We have recently synthesized two new structures that retain the same bonding environment as the honeycomb lattice, and extend this physics to three-dimensions. In this work, we compare the magnetic properties of these two novel structures, presenting evidences that their high temperature behavior can be explained by geometric  $g$ -factor constraints while the low temperature anisotropy and degeneracy of the ground state suggest the presence of spin anisotropic exchange.

**1:51PM F6.00012 The Mott Insulating Nature of  $\text{Na}_2\text{IrO}_3$  : DFT+DMFT Study** , MINJAE KIM, CPHT, Ecole Polytechnique & College de France, BEOM HYUN KIM, RIKEN, Saitama, B. I. MIN, Pohang University of Science and Technology — We have investigated the insulating nature of  $\text{Na}_2\text{IrO}_3$ , employing both the density-functional theory (DFT) and the combination of the DFT and the dynamical mean-field theory (DFT+DMFT). We have obtained the paramagnetic (PM) insulating state even above the Neel temperature ( $T_N$ ), which reveals that  $\text{Na}_2\text{IrO}_3$  is a Mott-type insulator. The photoemission spectrum is well described by the density of states from the DFT+DMFT in this PM insulating state. However, the analysis of optical conductivity suggests that the non-local correlation effect is also important in  $\text{Na}_2\text{IrO}_3$ . We have also found sizable redistribution of both charge and spin densities upon cooling below  $T_N$  which suggests that  $\text{Na}_2\text{IrO}_3$  is not a standard Mott insulator having rigid charge density. Therefore, despite the Mott-type insulating state of  $\text{Na}_2\text{IrO}_3$ , the itineracy and the non-local correlation are important as well in describing its electronic and magnetic properties due to the extended nature of Ir 5d state.

**Tuesday, March 15, 2016 11:15AM - 1:15PM –**

**Session F7 APS SPS: Undergraduate Research/SPS V 303 - Sean Bentley, Adelphi University**

**11:15AM F7.00001 Making Physics Fun: The 2015 Science Outreach Catalyst Kit** , SHAUNA LEFEBVRE, Union College, HANNAH PELL, Lebanon Valley College — The Society of Physics Students is dedicated to performing outreach events to get the general public excited about physics. The SPS National Office established the Science Outreach Catalyst Kit program in 2001 to aid SPS chapters at colleges all around the world in their efforts to bring physics education to students of all ages. Each year SPS produces twenty-five SOCKs in conjunction with the National Institute of Standards and Technology to give to SPS chapters on a first come, first serve basis. I spent my time at the SPS offices this summer helping to develop the 2015 SOCK. We designed activities that help students from elementary to high school explore basic acoustics with everyday materials like cups, straws, string, balloons, and rubber bands. In this presentation I will discuss why we chose to include the activities we did and the process of making this years SOCK a reality.

**11:27AM F7.00002 Optimization of the Diode-Pumped Solid State Nd:YLF Amplifier Chain for the 263 nm Drive Laser at the FAST Facility<sup>1</sup>** , JULIE M. GILLIS, THEODORE A. CORCOVILOS, Dept. of Physics, Duquesne University, Pittsburgh, PA, DEAN R. EDSTROM JR., JINHAO RUAN, JAMES K. SANTUCCI, Accelerator Division, Fermi National Accelerator Laboratory, Batavia, IL — The RF photoinjector of the 50 MeV superconducting electron linear accelerator at the Fermilab Accelerator Science and Technology (FAST) Facility is driven by a phase-locked laser system. The neodymium-doped yttrium-lithium fluoride (Nd:YLF) seed laser provides short (3 ps) infrared (1053 nm) pulses to an amplifier chain before conversion to ultraviolet (263 nm) through two frequency-doubling BBO crystals. The amplification section consists of seven diode-pumped solid state (DPSS) amplifiers, which increase the pulse energy of the seed laser using optically end-pumped Nd:YLF crystals. To maximize the total gain of the amplifier chain, each stage must be properly tuned with optimized optics, alignment, and laser beam characterization. In this paper we report on one of the single-pass amplifier improvements to achieve a consistent gain of 4.83 with stabilized output pulse trains for up to 1500 seed pulses. The final ultraviolet pulses imaged onto the  $\text{Cs}_2\text{Te}$  photocathode of the RF electron gun have been doubled in energy to 10.2  $\mu\text{J}$  per pulse as a result of these alterations.

<sup>1</sup>Operated by Fermi Research Alliance, LLC under Contract No. De-AC02-07CH11359 with the United States Department of Energy

**11:39AM F7.00003 Alpha Background Rejection in Bolometer Detectors** , NICHOLAS DEPORZIO, Northeastern Univ, CUORE COLLABORATION — This study presents the modification of bolometer detectors used in particle searches to veto or otherwise reject alpha radiation background and the statistical advantages of doing so. Several techniques are presented in detail – plastic film scintillator vetoes, metallic film ionization vetoes, and Cherenkov radiation vetoes. Plastic scintillator films are cooled to bolometer temperatures and bombarded with 1.4MeV to 6.0MeV alpha particles representative of documented detector background. Quantum dot based liquid scintillator is similarly bombarded to produce a background induced scintillation light. Photomultipliers detect this scintillation light and produce a veto signal. Layered metallic films of a primary metal, dielectric, and secondary metal, such as gold-polyethylene-gold films, are cooled to milli-kelvin temperatures and biased to produce a current signal veto when incident 1.4MeV to 6.0MeV alpha particles ionize conduction paths through the film. Calibration of veto signal to background energy is presented. These findings are extrapolated to quantify the statistical impact of such modifications to bolometer searches. Effects of these techniques on experiment duration and signal-background ratio are discussed.

**11:51AM F7.00004 All-Optical Helicity Dependent Spin Switching in a Many-Spin System<sup>1</sup>** , TANNER LATTA, G. P. ZHANG, Indiana State University — All-optical helicity dependent magnetic switching (AOS) is achieved through using an ultrafast laser pulse to manipulate and switch the spin of an electron from one direction to another. This process happens in a short amount of femtoseconds after the laser pulse is introduced. All-optical helicity dependent magnetic switching (AOS) does not fall to the assistance of any external magnetic field. Linearly polarized light, as well as right and left circularly polarized light are used to manipulate the spin of the electrons. Ferrimagnetic, rather than ferromagnetic, materials are more suitable to create conditions in which AOS are viable due to the orientation of the spins within this material. In the following study we show and conclude that AOS is possible with the use of left and right circularly polarized laser pulses. All-optical helicity dependent magnetic switching has many applications in magnetic recording technology or magnetic memory devices.

<sup>1</sup>DE-FG02-06ER46304

**12:03PM F7.00005 Rapid Adiabatic Passage in a Rb gas with intense Frequency Chirped Laser Light** , BRIAN KAUFMAN, TANNER GROGAN, TRACY PALTOO, MATTHEW WRIGHT, Adelphi Univ — We will discuss our progress toward using intense frequency chirped laser light to control the excitation of atoms in a room-temperature gas cell. We illuminate  $^{87}\text{Rb}$  atoms with a 1 GHz in 8 ns frequency chirped pulse of laser light covering the  $5S_{1/2} F=1 \rightarrow 5P_{3/2}$  and explore the saturation behavior as intensity increases. We estimate that we are exciting over 90% of the atoms over 1 mm<sup>2</sup>.

**12:15PM F7.00006 Magnetic Second Harmonic Generation Imaging** , CARINA BELVIN, Department of Physics, Wellesley College, CHANGMIN LEE, Department of Physics, MIT, FERHAT KATMIS, Francis Bitter Magnet Lab and Department of Physics, MIT, PABLO JARILLO-HERRERO, Department of Physics, MIT, JAGADEESH S. MOODERA, Francis Bitter Magnet Lab and Department of Physics, MIT, NUH GEDIK, Department of Physics, MIT — Second harmonic generation is an effective probe of lattice, electronic, and magnetic symmetries of crystals where inversion symmetry is broken. In particular, magnetic second harmonic generation (MSHG) can be used to measure the magnetism induced at surfaces and interfaces of centrosymmetric materials. Imaging this MSHG signal can provide spatial information about the magnetic domains and domain boundaries that form at these interfaces. We have constructed an MSHG imaging setup using a femtosecond Ti:sapphire laser system and a highly sensitive CCD camera. Our setup can potentially be used to investigate magnetic domains and domain wall boundaries in magnetic topological insulator systems, such as  $\text{EuS}/\text{Bi}_2\text{Se}_3$  heterostructures.

**12:27PM F7.00007 High Q-factor Surface Plasmon-Polariton Resonance in a Plasmonic Perfect Absorber in the Terahertz Regime**, J ROBINSON, K BHATTARAI, S SILVA, J ZHOU, Univ of South Florida — Perfect absorption of light has become one of the exotic properties of plasmonic metamaterials which are popular due to the variety of feasible applications, particularly using them as a chemical/bio sensor. We present the plasmonic perfect absorber that exhibits strong surface plasmon-polariton (SPP) resonance. Due to the Fabry-Perot cavity effect, the SPP resonance is significantly sharpened and the Q-factor reaches 63.1. Correspondingly, the electric field of the surface wave is largely enhanced. Furthermore, we have shown numerically that the absorption peak is independent of the incident angle. The high Q-factor and enhanced surface wave are beneficial to increase the performances of the sensor and detector devices, especially in the THz regime, where such properties are hard to achieve by natural materials.

**12:39PM F7.00008 Figures and First Years: Examining first-year Calculus I student ability to incorporate figures into technical reports**, NATHAN ANTONACCI, MICHAEL ROGERS, THOMAS PFAFF, Ithaca Coll — This three-year study focused on first-year Calculus I students and their abilities to incorporate figures into technical reports. Students were handed guidelines as part of their Multidisciplinary Sustainability Education Module meant to aid them in crafting effective figures. Figure-specific questionnaires were added in the class to gain insight into the quantitative literacy skills students possessed both before starting their course and after its completion. Reviews of the figures in 78 technical reports written by 106 students showed repeated failure to refer to figures in discussion sections and use them in evidence-based arguments. Analysis of quantitative literacy skills revealed that the students could both read and interpret figures, suggesting that issues with literacy were not the main contributor to the sub-par graphs.

**12:51PM F7.00009 Simulating Entanglement Dynamics of Singlet-Triplet Qubits Coupled to a Classical Transmission Line Resonator**, MICHAEL WOLFE, JASON KESTNER, Department of Physics, UMBC — Electrons confined in lateral quantum dots are promising candidates for scalable quantum bits. Particularly, singlet-triplet qubits can entangle electrostatically and offer long coherence times due to their weak interactions with the environment. However, fast two-qubit operations are challenging. We examine the dynamics of singlet triplet qubits capacitively coupled to a classical transmission line resonator driven near resonance. We numerically simulate the dynamics of the von Neumann entanglement entropy and investigate parameters of the coupling element that optimizes the operation time for the qubit.

**1:03PM F7.00010 Simulation of weak anchoring effects on nematic liquid crystal hemispheres**, SEAN GILLEN<sup>1</sup>, DAVID A.T. SOMERS<sup>2</sup>, JEREMY N. MUNDAY<sup>3</sup>, University of Maryland, College Park — The free energy of a nematic liquid crystal droplet depends on an interplay between elastic and surface interactions. When the two contributions are of similar magnitude, there exists a transition of the nematic structure of the droplet. Because the two contributions scale differently with length scales, this transition is visible as a function of the size of the droplet. We carry out numerical simulations to explore the use of this transition in measuring surface anchoring energies. This technique could help elucidate alignment forces on liquid crystals, such as those caused by rubbed surfaces, electric fields, or even the Casimir torque.

<sup>1</sup>Electrical and Computer Engineering

<sup>2</sup>Department of Physics, Electrical and Computer Engineering

<sup>3</sup>Electrical and Computer Engineering, Institute for Research in Electronics and Applied Physics

## **Tuesday, March 15, 2016 11:15AM - 2:15PM – Session F8 DCMP DMP: Superconductivity: Novel Superconductors 304 -**

**11:15AM F8.00001 Molecular orbital polarization in Na<sub>2</sub>Ti<sub>2</sub>Sb<sub>2</sub>O: a scenario to metal-to-metal phase transition without spontaneous symmetry breaking**, HEUNG-SIK KIM, HAE-YOUNG KEE, Univ of Toronto — We suggest a scenario of partial Fermi surface (FS) gapping related to metal-to-metal phase transition without a spontaneous symmetry breaking. This theory is applied to Na<sub>2</sub>Ti<sub>2</sub>Sb<sub>2</sub>O, where the density polarization of spin-orbital entangled molecular orbitals occurs due to spin-orbit coupling. This is further enhanced by electronic correlations of Ti d-orbitals. Sharp increase of the polarization happens above a critical electronic interaction strength which then gaps out a part of FS made of d-orbitals, while the rest of FS associated with Sb p-orbitals remain almost intact. Experimental implications to test our proposal are also discussed.

**11:27AM F8.00002 Pressure dependence of the magnetic ground states in MnP<sup>1</sup>**, SACHITH DISANAYAKE, MASAAKI MATSUDA, QCMD, Oak Ridge National Laboratory, J.-G. CHENG, Chinese Academy of Sciences, China, F. YE, S. CHI, QCMD, Oak Ridge National Laboratory, J. MA, H. D. ZHOU, University of Tennessee, J.-Q. YAN, MSTD, Oak Ridge National Laboratory, S. KASAMATSU, O. SUGINO, T. KATO, K. MATSUBAYASHI, T. OKADA, Y. UWATOKO, ISSP, University of Tokyo — The newly discovered superconductor MnP shows a ferromagnetic order below  $T_C \approx 290$  K followed by a helical order below  $T_s \approx 50$  K in ambient pressure. An antiferromagnetic order is suggested in the vicinity of the pressure induced superconducting phase. We have performed single crystal neutron diffraction experiments to determine the magnetic structure under pressure. Both  $T_C$  and  $T_s$  are gradually suppressed with increasing pressure and the helical order disappears at 1.2 GPa. At intermediate pressures of 1.8 and 2.0 GPa, the ferromagnetic order first develops and is gradually suppressed below a characteristic temperature. At 4 GPa no magnetic signal was observed down to 3.5 K. Our results suggested that the new magnetic phase in the vicinity of the superconducting phase is in a short-ranged magnetic state due to frustration or in an itinerant magnetic state, where the itinerant small Mn moments are weakly interacting.

<sup>1</sup>This research at ORNLs HFIR and SNS was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

**11:39AM F8.00003 Chemical pressure effect on dynamic spin properties in CrAs<sup>1</sup>**, M. MATSUDA, M. B. STONE, Quantum Condensed Matter Division, Oak Ridge National Laboratory, J.-G. CHENG, W. WU, F. LIN, J. L. LUO, Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, J.-Q. YAN, Material Science and Technology Division, Oak Ridge National Laboratory and University of Tennessee, Knoxville, K. MATSUBAYASHI, Y. UWATOKO, Institute for Solid State Physics, University of Tokyo — CrAs is an antiferromagnetic metal, which shows a helical spin structure accompanied by an abrupt lattice expansion at  $T_N \sim 260$  K in ambient pressure. With applying pressure, the magnetic transition is suppressed and superconductivity appears with a maximum transition temperature of  $\sim 2$  K. Since Cr has the spin degree of freedom, elucidating the magnetic contribution to the superconductivity is crucial to understand the pairing mechanism. However, inelastic neutron scattering (INS) measurement under high pressure is challenging due to sample space limitation. Therefore, we studied chemical pressure effect by substituting As by P, which is found to be almost the same as the external pressure. We performed INS experiments in undoped and P-doped CrAs using powder samples. The results in the P-doped CrAs clearly indicate that the antiferromagnetic fluctuations still remain above the critical P content, where the long range magnetic order is suppressed, suggesting a coupling between the magnetism and the superconductivity.

<sup>1</sup>This research at ORNL's High Flux Isotope Reactor and Spallation Neutron Source was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

**11:51AM F8.00004 Reversal of the Upper Critical Field Anisotropy and Spin-Locked Superconductivity in K<sub>2</sub>Cr<sub>3</sub>As<sub>3</sub>**, FEDOR F. BALAKIREV, Los Alamos National Laboratory, TAI KONG, Ames Laboratory, Iowa State University, MARCELO JAIME, ROSS D. MCDONALD, CHARLES H. MIELKE, Los Alamos National Laboratory, ALEXANDER GUREVICH, Old Dominion University, PAUL C. CANFIELD, SERGEY L. BUD'KO, Ames Laboratory, Iowa State University — We report the first measurements of the anisotropic upper critical field  $H_{c2}(T)$  for K<sub>2</sub>Cr<sub>3</sub>As<sub>3</sub> single crystals up to 60 T and  $T > 0.6$  K.  $H_{c2}(T)$  was determined via resistivity and proximity detector oscillator techniques. Our results show that the upper critical field parallel to the Cr chains,  $H_{c2\parallel}$ , exhibits a paramagnetically-limited behavior, whereas no evidence of paramagnetic pair breaking was observed with field perpendicular to the Cr chains. As a result, the curves  $H_{c2\perp}(T)$  and  $H_{c2\parallel}(T)$  cross at  $T \sim 4$  K, so that the anisotropy parameter  $\gamma(T) = H_{c2\perp} / H_{c2\parallel}$  increases from  $\gamma \sim 0.35$  near  $T_c$  to  $\gamma \sim 1.7$  at 0.6 K. This behavior of  $H_{c2}(T)$  is inconsistent with triplet superconductivity but suggests a form of singlet superconductivity with the electron spins locked onto the direction of Cr chains.

**12:03PM F8.00005 Material Specific Rational Design of A<sub>1</sub>B<sub>2</sub>C<sub>3</sub>O<sub>7</sub> High-T<sub>c</sub> Superconductors without Copper [A, B, C = Cations]**, O'PAUL ISIKAKU-IRONKWE, MICHAEL J. SCHAFFER, RTS Design Technologies, San Diego CA 92101 — Soon after the discovery of YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> with  $T_c = 93$  K, a similar structured system with Ag replacing Cu was discovered with a  $T_c = 50$  K. Also, the discovery of Ba<sub>0.6</sub>K<sub>0.4</sub>BiO<sub>3</sub> with  $T_c = 30$  K indicated that Cu was not indispensable for high temperature superconductivity (HTSC). Latter, the discoveries of the Pnictide and Chalcogenide high-T<sub>c</sub> superconductors confirmed those earlier experimental indications. Using our recently developed Material Specific Characterization Dataset (MSCD) model for analysis and design of superconductors, we have computed many designs that satisfy the MSCD characteristics of YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> as a design model. Our design recognizes the valence state characteristics that make YBa<sub>2</sub>Cu<sub>3</sub>O<sub>6.8</sub> a semiconductor, while YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> is a superconductor. Here we present ten material specific rational design examples of potential A<sub>1</sub>B<sub>2</sub>C<sub>3</sub>O<sub>7</sub> HTSCs without Cu, using the YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> design model. This MSCD design model opens the possibility for search and discovery of high-T<sub>c</sub> oxide superconductor systems without copper.

**12:15PM F8.00006 Microscopic Origin of the Neutron Spin Resonance in Heavy Fermion Superconductor Ce<sub>1-x</sub>Y<sub>b</sub>xCoIn<sub>5</sub>**, YU SONG, Rice University, JOHN VAN DYKE, University of Illinois at Chicago, I. K. LUM, B. D. WHITE, University of California, San Diego, L. SHU, Fudan University, SOOYOUNG JANG, University of California, San Diego, A SCHNEIDEWIND, PETR CERMAK, Julich Center for Neutron Science, Y. QIU, NIST center for neutron scattering, M. B. MAPLE, University of California, San Diego, DIRK K. MORR, University of Illinois at Chicago, PENGCHENG DAI, Rice University — We have systematically studied the evolution of the neutron resonance mode in Ce<sub>1-x</sub>Y<sub>b</sub>xCoIn<sub>5</sub> ( $x = 0, 0.05, 0.3$ ) with neutron scattering. We uncover clear dispersive feature of the mode and show that it is quite robust to disorder due to doping. Our results suggest that the resonance in Ce<sub>1-x</sub>Y<sub>b</sub>xCoIn<sub>5</sub> is a paramagnon reminiscent of spin waves in CeRhIn<sub>5</sub>.

**12:27PM F8.00007 Consistency of measured phase boundaries of the FFLO superconducting phase for different materials and types of probes**, CHARLES AGOSTA, Clark University, NATHANAEL FORTUNE, Smith College, SCOTT HANNAHS, JU-HYUN PARK, National High Magnetic Field Laboratory, JOHN SCHLEUTER, Argonne National Laboratory, LUCY LIANG, SHUYAO GAO, Smith College, LOGAN BISHOP-VAN HORN, MAX NEWMAN, Clark University, SHUYAO GU, Smith College, LUCY LIANG — New magnetocaloric and specific heat measurements of the high field superconducting state in the organic superconductor  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu(NCS)<sub>2</sub> are compared to rf penetration depth, magnetic torque, and NMR measurements. The position of the phase lines separating the uniform superconducting state with the FFLO state and the normal state are mostly in good agreement with each other. The order of the phase transitions can only be determined from the calorimetric measurements and will be compared to theory. Results from other organic superconductors show that there is universal behavior. As an example, the distance between the lower and upper magnetic field phase line containing the FFLO state is proportional to the upper critical field. The position of the lower phase line, the Clogston Chandrasakar paramagnetic limit, will be compared to semi empirical calculations based on the specific heat for five different superconductors.

**12:39PM F8.00008 Magnetocaloric Evidence for FFLO Superconductivity in  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu(NCS)<sub>2</sub><sup>1</sup>**, NATHANAEL FORTUNE, Smith College, CHARLES AGOSTA, Clark University, SCOTT HANNAHS, JU-HYUN PARK, National High Magnetic Field Laboratory, SHUYAO GU, LUCY LIANG, Smith College, JOHN SCHLEUTER, Argonne National Laboratory — We present new magnetocaloric and calorimetric measurements of the high field superconducting state in the layered structure superconductor  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu(NCS)<sub>2</sub>. The strongly field-orientation dependent phase transition between the low field superconducting state and high field superconducting states is first order and is nearly temperature independent, occurring at the Clogston-Chandrasakar paramagnetic limit  $H_p$ . Magnetocaloric measurements  $dT/dH$  as a function of magnetic field reveal that the system becomes strongly paramagnetic at the cross over from the low field to high field state. At lower temperatures, we are able to resolve small changes at the phase boundary due to the absorption/release of latent heat when increasing/decreasing field, indicating that the high field state is higher entropy than the low field state. These results provide strong new evidence for the formation of paramagnetic spin domains within an inhomogeneous FFLO superconducting state. They also allow us to rule out alternative explanations involving the formation of spin density waves within a homogenous superconducting state.

<sup>1</sup>A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by National Science Foundation Cooperative Agreement No. DMR-1157490 and the State of Florida

**12:51PM F8.00009 Charge fluctuations and superconductivity in organic conductors: the case of  $\beta''$ -(BEDT-TTF) $_2$ SF $_5$ CH $_2$ CF $_2$ SO $_3$** , GEORGIOS KOUTROULAKIS, Univ of California - Los Angeles, H. KUHNE, Hochfeld-Magnetlabor Dresden, H.-H. WANG, Univ of California - Los Angeles, J. A. SCHLUETER, Argonne National Laboratory, J. WOSNITZA, Hochfeld-Magnetlabor Dresden, S. E. BROWN, Univ of California - Los Angeles — Superconductivity in most organic charge transfer salts is considered magnetically mediated, in part due to the proximity to antiferromagnetic ground states, as well as the preponderance of spin fluctuations in their normal state. An alternative proposal is based on mediation by charge fluctuations, close to collapsed charge-ordered insulating states. The all-organic salt  $\beta''$ -(BEDT-TTF) $_2$ SF $_5$ CH $_2$ CF $_2$ SO $_3$ , which undergoes a superconducting transition at  $T_C=4.5$ K, has been suggested as a candidate material for the realization of charge-fluctuation pairing. Here, we report on a detailed  $^{13}\text{C}$  NMR study examining the normal and superconducting states of this material, and we discuss the results in the context of the proposal for charge-fluctuation driven superconductivity.

**1:03PM F8.00010 Superconducting Properties of a Nanoparticle Assembly of the Organic Conductor (TMTSF) $_2$ ClO $_4$** , LAUREL WINTER, Los Alamos National Laboratory, National High Magnetic Field Laboratory (NHMFL), EDEN STEVEN, JAMES BROOKS, SHERMAN BENJAMIN, Florida State University, NHMFL FL, JU-HYUN PARK, NHMFL FL, DOMINIQUE DE CARO, CHRISTOPHER FAULMANN, LYDIE VALADE, KANE JACOB, IMANE CHTIOUI, CNRS, University of Toulouse, BELEN BALLESTEROS, JORDI FRAXEDAS, ICN2, CSIC Barcelona — While the study of thin-film and nanoparticle geometries on semiconductor devices, type-I elemental superconductors, and even single-molecular magnet materials have been explored, progress on thin-film and nanoparticle organic superconductors — in particular charge-transfer organic salts — has remained elusive. Recent refinements of synthesis conditions have produced nanoparticles of the Bechgaard salt (TMTSF) $_2$ ClO $_4$ . High resolution TEM studies have determined these nanoparticles are approximately 3-5 nm in size, which form nanoparticle clusters that are on average 34 nm in size<sup>1</sup>. In order to investigate the properties of these nanoparticles, randomly oriented assemblies were studied in magnetic fields up to 16 T, using a high sensitivity inductive method in a dilution refrigerator, the results of which show that the ground-state properties of the nanoparticle assembly compares favorably with the bulk-single-crystal material<sup>2</sup>. <sup>1</sup> D. de Caro *et al.*, *Eur. J. Inorg. Chem.*, **2014**, 4010 (2014). <sup>2</sup> L. E. Winter *et al.*, *Phys. Rev. B.*, **91**, 035437 (2015).

**1:15PM F8.00011 Realization of insulating state and superconductivity in Rashba semiconductor BiTeCl**, JIANJUN YING, VIKTOR STRUZHUKIN, ALEXANDER GONCHAROV, HO-KWANG MAO, Carnegie Inst of Washington, FEI CHEN, XIAN-HUI CHEN, University of Science and Technology of China, ALEXANDER GAVRILIUK, Russian Academy of Sciences, XIAO-JIA CHEN, Center for High Pressure Science and Technology Advanced Research — Measurements of the resistivity, Hall coefficient, and Raman spectroscopy are performed on a Rashba semiconductor BiTeCl single crystal at high pressures up to 50 GPa. We find that applying pressure first induces the theoretically predicted insulating state followed by a superconducting phase with the insulating normal state. Upon heavy compression, another different superconducting phase is entered with the metallic normal state. The dome-like evolution of the superconducting transition temperature with pressure is obtained with the crossover from the electron to hole carriers across the boundary of the two superconducting phases. These findings imply the possible realization of topological state of the insulating and superconducting phases in this material.

**1:27PM F8.00012 MgB $_2$  Ultrathin Films Fabricated by Hybrid Physical Chemical Vapor Deposition and Subsequent Ion Milling.**, NARENDRA ACHARYA, MATTHAEUS WOLAK, TENG TAN, Temple University, DANIEL CUNNANE, BORIS KARASIK, Jet Propulsion Laboratory, XIAOXING XI, Temple University — Hot electron bolometer (HEB) mixers are a great tool for measuring high-resolution spectroscopy at Terahertz frequencies. MgB $_2$  offers a higher critical temperature (39 K) compared to commonly used Nb and NbN and boasts a shorter intrinsic electron-phonon relaxation time, giving rise to a broader intermediate frequency (IF) bandwidth. We have fabricated high quality ultrathin MgB $_2$  films using hybrid physical-chemical vapor deposition (HPCVD) and employing ion milling to achieve thickness down to 2 nm. The thinnest achieved films show high  $T_c$  of 28 K with residual resistivity below 28  $\Omega\text{cm}$  and high critical current  $J_c$  of  $1 \times 10^6$  A/cm $^2$  at 20 K. As a result of the employed low angle ion milling process, the films remain well connected even after being thinned down since the initial thick films offer a better connectivity than as-grown thin films. The established process offers a way to realize MgB $_2$  based HEB mixers of extremely low thickness and therefore small local oscillator power requirements and increased IF bandwidth.

**1:39PM F8.00013 Epitaxial growth of MgB $_2$  films at ambient temperature**, HIROAKI SHISHIDO, TAKUYA YOSHIDA, TAKATOSHI NAKAGAMI, TAKEKAZU ISHIDA, Department of Physics and Electronics, Graduate School of Engineering, Osaka Prefecture University — We grew crystalline MgB $_2$  thin films using molecular beam epitaxy at a low substrate temperature of 110 °C under an ultrahigh vacuum of about  $10^{-6}$  Pa. MgB $_2$  thin films were deposited on the (001) surface of a 4H-SiC substrate with an epitaxial Mg buffer layer. The epitaxial growth was confirmed by X-ray diffraction measurements. MgB $_2$  thin films show a sharp superconducting transition at 27.2 K, with a relatively narrow superconducting transition width  $\Delta T_c = 0.9$  K. The growth temperature was lower than any in prior reports on superconducting MgB $_2$  thin films. The presence of the epitaxial Mg buffer layer is crucial for reducing the epitaxial temperature.

**1:51PM F8.00014 Unconventional superconductivity in half-Heusler semimetals<sup>1</sup>**, PHILIP BRYDON<sup>2</sup>, Department of Physics, University of Otago, LIMIN WANG, Center for Nanophysics and Advanced Materials, University of Maryland, MICHAEL WEINERT, DANIEL AGTERBERG, Department of Physics, University of Wisconsin, Milwaukee — We consider the superconductivity of the topological half-Heusler semimetals YPtBi and LuPtBi, where pairing occurs between  $j = 3/2$  quasiparticles. This permits Cooper pairs with quintet or septet total angular momentum, in addition to singlet and triplet states. Purely on-site interactions can generate unconventional (quintet) time-reversal symmetry-breaking states with topologically nontrivial point or line nodes. Furthermore, due to the broken inversion symmetry in these materials, the usual  $s$ -wave singlet state can mix with a  $p$ -wave septet state, also with topologically stable line-nodes.

<sup>1</sup>We acknowledge support from Microsoft Station Q, LPS-CMTC, and JQI-NSF-PFC (P.M.R.B.), J. Paglione and the U.S. Department of Energy Early Career award DE-SC-0010605 (L.W.), and the NSF via DMREF- 1335215 (D.F.A. and M.W.)

<sup>2</sup>Previously Condensed Matter Theory Center and Joint Quantum Institute, University of Maryland

**2:03PM F8.00015 Superfluid Density and Flux-Flow Resistivity Measurements of Multiple-Band Superconductor  $\beta$ -PdBi $_2$** , TATSUNORI OKADA, YOSHINORI IMAI, ATSUTAKA MAEDA, University of Tokyo —  $\beta$ -PdBi $_2$  ( $T_c^{\text{max}} = 5.4$  K) is a newcomer of the multiple-band superconductors, revealed by the specific heat and the upper critical field measurements [1], and the angle-resolved photoemission spectroscopy [2]. In addition, authors of ref. [2] observed the spin-polarized band dispersion and proposed that  $\beta$ -PdBi $_2$  is a candidate of topological superconductor. However, there is less information on superconducting properties so far. In order to clarify the superconducting gap function, we measured the temperature ( $T$ ) and magnetic field ( $B$ ) dependence of microwave complex conductivity of  $\beta$ -PdBi $_2$  single crystals. We found that the superfluid density exhibits the thermally activated  $T$  dependence, manifesting the absence of nodes in the superconducting gaps. We also found that the flux-flow resistivity increased with  $B$  with downward-convex shape. Based on some theories, we considered that such a behavior originated from the backflow of supercurrents around vortices reflecting rather small Ginzburg-Landau parameter ( $\kappa \simeq 5$ ). [1] Y. Imai *et al.*, *JPSJ* **81**, 113708 (2011). [2] M. Sakano *et al.*, arXiv:1505.07231.

<sup>1</sup>This work was supported by the JSPS KAKENHI (Grant Numbers 15K17697 and 26-9315), and the JSPS Research Fellowship for Young Scientists.

**Tuesday, March 15, 2016 11:15AM - 2:15PM –**

**Session F11 DMP: Nematicity in Fe-based Superconductors 307 - Anna Boehmer, Ames Laboratory**

**11:15AM F11.00001 Ising nematic quantum critical point in a metal: a Monte Carlo study<sup>1</sup>**

, SAMUEL LEDERER, Massachusetts Inst of Tech-MIT — The Ising nematic quantum critical point (QCP) associated with the zero temperature transition from a symmetric to a nematic *metal* is an exemplar of metallic quantum criticality. We have carried out a minus sign-free quantum Monte Carlo study of this QCP for a two dimensional lattice model with sizes up to  $24 \times 24$  sites. The system remains non-superconducting down to the lowest accessible temperatures. The results exhibit critical scaling behavior over the accessible ranges of temperature, (imaginary) time, and distance. This scaling behavior has remarkable similarities with recently measured properties of the Fe-based superconductors proximate to their putative nematic QCP.

<sup>1</sup> with Yoni Schattner, Steven A. Kivelson, and Erez Berg

**11:51AM F11.00002 NMR evidence for inhomogeneous nematic fluctuations in**

**BaFe<sub>2</sub>(As<sub>1-x</sub>P<sub>x</sub>)<sub>2</sub>**, ADAM P. DIOGUARDI, Los Alamos National Laboratory, TANAT KISSIKOV, CHING-HAN LIN, KENT R. SHIRER, MATTHEW M. LAWSON, University of California Davis, Department of Physics, HANS-JOACHIM GRAFE, IFW Dresden, Institute for Solid State Research, Dresden, Germany, JIUN-HAW CHU, IAN R. FISHER, Department of Applied Physics and Geballe Laboratory for Advanced Materials, Stanford University, & Stanford Institute of Energy and Materials Science, RAFAEL M. FERNANDES, School of Physics and Astronomy, University of Minnesota, Minneapolis, NICHOLAS J. CURRO, University of California Davis, Department of Physics — We present evidence for nuclear spin-lattice relaxation driven by glassy nematic fluctuations in isovalent P-doped BaFe<sub>2</sub>As<sub>2</sub> single crystals. Both the <sup>75</sup>As and <sup>31</sup>P sites exhibit stretched-exponential relaxation similar to the electron-doped systems. By comparing the hyperfine fields and the relaxation rates at these sites we find that the As relaxation cannot be explained solely in terms of magnetic spin fluctuations. We demonstrate that nematic fluctuations couple to the As nuclear quadrupolar moment and can explain the excess relaxation. These results suggest that glassy nematic dynamics are a universal phenomenon in the iron-based superconductors.

**12:03PM F11.00003 Measuring Nematic Susceptibilities from the Elastoresistivity Tensor<sup>1</sup>**

A. T. HRISTOV, M. C. SHAPIRO, Stanford University, PATRICK HLOBIL, Karlsruher Institut für Technologie, AKASH MAHARAJ, JIUN-HAW CHU, IAN FISHER, Stanford University — The elastoresistivity tensor  $m_{ijkl}$  relates changes in resistivity to the strain on a material. As a fourth-rank tensor, it contains considerably more information about the material than the simpler (second-rank) resistivity tensor; in particular, certain elastoresistivity coefficients can be related to thermodynamic susceptibilities and serve as a direct probe of symmetry breaking at a phase transition. The aim of this talk is twofold. First, we enumerate how symmetry both constrains the structure of the elastoresistivity tensor into an easy-to-understand form and connects tensor elements to thermodynamic susceptibilities. In the process, we generalize previous studies of elastoresistivity to include the effects of magnetic field. Second, we describe an approach to measuring quantities in the elastoresistivity tensor with a novel transverse measurement, which is immune to relative strain offsets. These techniques are then applied to BaFe<sub>2</sub>As<sub>2</sub> in a proof of principle measurement.

<sup>1</sup>This work is supported by the Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract DE-AC02-76SF00515.

**12:15PM F11.00004 Origin of the in-plane resistivity anisotropy of the iron pnictides: scattering rate or plasma frequency?<sup>1</sup>**

, MICHAEL SCHTTT, Univ of Minn - Minneapolis, JRG SCHMALIAN, Institute for Theoretical Condensed Matter Physics, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany, RAFAEL FERNANDES, Univ of Minn - Minneapolis — The prime experimental tool to probe the electronic nematic phase in the iron pnictides is the in-plane resistivity anisotropy, which can arise from an anisotropic scattering rate and/or an anisotropic plasma frequency. To shed light on its origin, we investigate the impact of spin fluctuations on the anisotropic ac conductivity of the iron pnictides. We show that two mechanisms contribute to the ac conductivity anisotropy. On the one hand, the inelastic scattering by spin fluctuations directly introduces an anisotropic scattering rate. On the other hand, the same inelastic scattering causes the renormalization of the Fermi velocity at the hot spots. Interestingly, while both mechanisms affect the ac conductivity anisotropy, only the first causes an anisotropy in the dc limit. In contrast, the second mechanism effectively renormalizes both the plasma frequency and the scattering rate. The latter effect opposes the anisotropy induced by the direct scattering of electrons, effectively reducing the observable scattering rate anisotropy. Our results agree qualitatively with recent experiments in detwinned iron pnictides and show the unavoidable entanglement between the scattering rate anisotropy and the plasma frequency anisotropy that arises from spin fluctuations.

<sup>1</sup> MS acknowledges the support from the Humboldt Foundation.

**12:27PM F11.00005 Nematic Crossover in BaFe<sub>2</sub>As<sub>2</sub> under Uniaxial Stress**

, XIAO REN<sup>1</sup>, LIAN DUAN, YUWEN HU, JIARUI LI, Peking University, Beijing 100871, China, RUI ZHANG, Rice University, Houston, Texas 77005, USA, HUIQIAN LUO, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, PENGCHENG DAI, Rice University, Houston, Texas 77005, USA, YUAN LI<sup>2</sup>, Peking University, Beijing 100871, China — The nature of the nematic order in iron-based superconductors has invoked intense research interest. A substantial portion of experimental attempts on resolving this issue required the use of single-domain samples produced under external stress. Here we use Raman scattering, a technique that can detect spontaneous point-group symmetry breaking without resorting to single-domain samples, to study BaFe<sub>2</sub>As<sub>2</sub>, the parent compound of the 122 Fe-based superconductors. We show that an applied compression along the Fe-Fe direction, which is commonly used to produce untwinned orthorhombic samples, changes the structural phase transition at temperature T<sub>s</sub> into a crossover that spans a considerable temperature range above T<sub>s</sub>. Even in crystals that are not subject to any applied force, a distribution of substantial residual stress remains, which may explain phenomena that are seemingly indicative of symmetry breaking above T<sub>s</sub>. Our results are consistent with an onset of spontaneous nematicity only below T<sub>s</sub>.

<sup>1</sup>first author

<sup>2</sup>corresponding author

**12:39PM F11.00006 Neutron scattering in detwinned  $\text{SrFe}_2\text{As}_2$  single crystals**, LI ZHANG, China Jiliang University/Rice University, YU SONG, YU LI, RUI ZHANG, WEIYI WANG, HAORAN MAN, PENGCHENG DAI, Rice University — **Abstract:** Large  $\text{SrFe}_2\text{As}_2$  single crystals (2cm) were grown with self-flux method. The basic sample characterizations were described by XRD, MPMS and PPMS. Orthorhombic  $a$  along horizontal orientation and  $b$  along vertical orientation were determined by X-ray Laue diffraction. The crystals were cut into rectangular pieces along the  $[1,1,0]$  and  $[1,-1,0]$  directions by high precision wire saw. The device for sample detwinning was made of 6061 aluminum alloy with low neutron incoherent scattering cross section. Uniaxial pressure can be applied by a spring along orthorhombic  $[0,1,0]$  direction by tuning the screw in one end. The pressure can be calculated by the known elasticity coefficient ( $k = 10.5 \text{ N/mm}$ ) and the compression of the spring ( $\Delta x$ ) [1]. Our neutron scattering experiments were carried out using the MAPS at the ISIS in England. Low Energy (such as  $E_i=80\text{meV}$ ) with different temperatures, especially around ( $T_N = T_S = 193 \text{ K}$ ) is done in the time-of-flight experiment[2]. It is interesting to find out the pressure induced spin excitation anisotropy. After careful analysis, we conclude that resistivity and spin excitation anisotropies are likely intimately connected. The results also compared with similar experiment in parent  $\text{BaFe}_2\text{As}_2$  in Murlin at the ISIS. **Keywords:** neutron scattering, detwin,  $\text{SrFe}_2\text{As}_2$ , single crystals Figure 1, Large  $\text{SrFe}_2\text{As}_2$  single crystals grown with self-flux method. References: [1] Xingye Lu *et al.*, Science 345, 657 (2014). [2] Pengcheng Dai, Rev. Mod. Phys. 87, 855(2015).

**12:51PM F11.00007 Nematic fluctuations and acoustic phonon in the Raman response of iron-based superconductors**<sup>1</sup>, M. KHODAS, University of Iowa, W.-L. ZHANG, Chinese Academy of Sci (CAS), G. BLUMBERG, Rutgers University, Piscataway, New Jersey 08854, USA, P. RICHARD, H. DING, Chinese Academy of Sci (CAS), ATHENA S. SEFAT, Oak Ridge National Laboratory — Nematicity is a generic feature in the under- and optimally-doped iron-based superconductors. Raman and shear modulus studies indicate a critical behavior of the xy symmetry susceptibility towards an extrapolated temperature  $\theta$  defining a hidden critical point tens of degrees below the structural transition  $T_S$ . It was proposed that Raman scattering is insensitive to the orthorhombic lattice deformation and a strong electron-phonon (ep) coupling could possibly lift the nematic transition from  $\theta$  to  $T_S$ , while the ep coupling strength remains unknown. Here we report a very low frequency phonon mode associated with an orthorhombic lattice deformation near  $T_S$  contributing to the xy symmetry Raman response. We propose an ep coupling model to describe the Raman response and establish the connection of Raman susceptibility and elastic shear modulus. The ep coupling strength deduced from the Raman response is insufficient to lift  $T_S$  by 60 K above  $\theta$ , suggesting that the structural phase transition at  $T_S$  and the hidden phase transition at  $\theta$  have different origins.

<sup>1</sup>This work is supported by the UI, ISF (1287/15), ICAM (NSF-IMI grant DMR-0844115), NSF (DMR-1104884), MoST (2011CBA001001) and NFSC (11274362) of China, and the U.S. DOE BES DE-SC0005463

**1:03PM F11.00008 Electronic Raman study of superconducting  $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$** <sup>1</sup>, SHANGFEI WU, GIRSH BLUMBERG, Rutgers Univ, PIERRE RICHARD, HONG DING, IOP,CAS, HAIHU WEN, Nanjing Univ — We use electronic Raman scattering to probe the superconductivity gap structure and collective modes in under-doped and optimally-doped  $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ . In the under-doped samples, we observe a sharp superconducting coherence peak at  $60 \text{ cm}^{-1}$  in the XY ( $B_{2g}$ ) geometry below  $T_c$ , which is consistent with the gap value determined by ARPES on the outer hole Fermi surface pocket <sup>2</sup>. The Raman spectrum shows a threshold at approximately  $30 \text{ cm}^{-1}$  followed by the superconducting coherence peak with a low-energy tail. We identify a peak at around  $95 \text{ cm}^{-1}$  between 13 K and 22 K in the same geometry in the orthorhombic phase below  $T_c$ , which becomes broader and weaker upon heating. A sharp and symmetric mode at  $120 \text{ cm}^{-1}$  is also observed in the optimally-doped samples in the same geometry. These collective modes have similar energy scale with the neutron spin resonance mode, the kink observed by ARPES and the bosonic mode observed by STM <sup>3</sup>, indicating that they have intimate relationship with superconductivity in the iron pnictides.

<sup>1</sup>GB and SW acknowledge support from DOE BES DE-SC0005463 and NSF DMR-1104884. PR and HD acknowledge support from MOST (2011CBA001001) and NSFC (11274362) of China. HW acknowledges support from MOST (2011CBA00102) and NSFC (11534005) of China.

<sup>2</sup>Nat. Commun. **2**, 394 (2011)

<sup>3</sup>Nature **456**, 930 (2008); PRL **102**, 047003 (2009); PRL **108**, 227002 (2012)

**1:15PM F11.00009 Numerical Study of Iron-Based Superconductors and Nematic Order**, HARRISON RUIZ, MARTIN CLAASSEN, YAO WANG, CHUNJING JIA, BRIAN MORITZ, THOMAS DEVEREAUX, SIMES, SLAC National Accelerator Laboratory/Stanford University — We perform an exact diagonalization study of the multi-orbital Hubbard model including coupling to lattice degrees of freedom. The single-particle spectral function, dynamical spin, charge, and Raman response are studied to examine a spin nematic phase due to a biquadratic exchange coupling.

**1:27PM F11.00010 The realization of nematic order in iron-pnictide superconductors**, HONG-YI CHEN, CHUNG-PIN CHOU, National Taiwan Normal University, C. S. TING, University of Houston — The interplay between the nematicity and superconductivity in iron-pnictide is studied with a proposed magnetic configuration in a microscopic model. The spin-driven order in the nematic state has been found in a small area in the electron-doped regime. In the nematic state, in the normal state, the broken degeneracy of the orbitals  $d_{xz}$  and  $d_{yz}$  causes the elliptic Fermi surface. In the state where the nematicity coexists with the superconductivity, an orthorhombic magnetic fluctuations appears and its Fourier transformation shows two uneven pairs of peaks at  $(\pm\pi, 0)$  and  $(0, \pm\pi)$ . Finally, two modulated stripe SDW perpendicularly intertwined each other and makes the charge density and the spatial distribution of the LDOS reflecting a  $d_{x^2-y^2}$ -symmetry form factor.

**1:39PM F11.00011 Spin-Driven Nematic Instability in Realistic Microscopic Models: Application to Iron-Based Superconductors**, MORTEN HOLM CHRISTENSEN, Niels Bohr Institute, University of Copenhagen and School of Physics and Astronomy, University of Minnesota, JIAN KANG, School of Physics and Astronomy, University of Minnesota, BRIAN M. ANDERSEN, Niels Bohr Institute, University of Copenhagen, RAFAEL M. FERNANDES, School of Physics and Astronomy, University of Minnesota — Electronic nematicity due to the partial melting of density waves is a prevalent phenomenon in the field of high temperature superconductivity. In contrast to usual electronic instabilities, such as magnetic and charge order, this fluctuation-driven order cannot be captured by the standard RPA method. By including fluctuations beyond RPA, we derive the orbitally-resolved nematic susceptibility of a generic multi-orbital Hubbard model, thus putting it on equal footing with other electronic susceptibilities of weakly and moderately interacting systems. Application to iron-based superconductors reveals that the  $d_{xy}$ -orbital plays a primary role in promoting a nematic transition preempting the magnetic transition. It furthermore demonstrates the importance of high-energy magnetic fluctuations in stabilizing nematic order in the absence of magnetic order. Finally, we show that the RPA ferro-orbital susceptibility shows no divergence on its own, providing strong evidence for a magnetic mechanism for nematicity.

**1:51PM F11.00012 Effect of Orbital Nematicity on Superconductivity in the Iron Pnictides and Chalcogenides**, ANDRIY NEVIDOMSKYY, Rice University, RONG YU, Renmin University of China — Orbital ordering leading to the observed nematic phase in the iron-based superconductors has been firmly established in a variety of experiments. It is therefore important to investigate the effect of the orbital order on the superconductivity. To this end, we have performed strong-coupling calculation within the slave-boson approach to the multiorbital  $t$ - $J_1$ - $J_2$  models for the iron-based superconductors. We report the phase diagram as a function of both electron/hole doping and the orbital ordering strength. We find that the amplitude of the otherwise dominant  $A_{1g}$  ( $s\pm$ ) pairing channel diminishes as the strength of orbital ordering is increased, yielding to the  $B_{1g}$  ( $d_{x^2-y^2}$ ) pairing channel. This effect is especially pronounced in the electron-doped case, with the  $d$ -wave pairing stabilized by the realistic values of the orbital splitting  $\sim 50$  meV. While the  $d$ -wave pairing has not been conclusively observed in the iron-based superconductors, the competition between the  $s$ - and  $d$ -wave pairing found in the calculations may have ramifications for FeSe,  $\text{KFe}_2\text{As}_2$  and  $\text{K}_x\text{Fe}_{2-y}\text{Se}_2$ .

**2:03PM F11.00013 Possible surface nematic order in iron pnictides<sup>1</sup>**, KOK WEE SONG, ALEXEI KOSHELEV, Argonne National Laboratory — Nematic fluctuations play important role in the physics of the iron-based superconductors. Indications for weak precursor nematic transition has been found in the compound  $\text{BaAs}_{2-x}\text{P}_x\text{Fe}_2$ [1]. However, high-resolution specific-heat measurements did not reveal any bulk transition[2]. To resolve this controversy, we consider the possibility of the surface nematic transition preceding the bulk transition. We consider the simplest model of two interacting quasi-two-dimensional electronic bands and explore the free-surface effects on the nematic order. We found that three-dimensional effects suppress the bulk nematic order and therefore this order is enhanced near the surface.

[1]Kasahara, S., et al. "Electronic nematicity above the structural and superconducting transition in  $\text{Ba}(\text{As}_{1-x}\text{P}_x\text{Fe})_2$ ." Nature 486.7403 (2012): 382-385.

[2]Luo, X., et al. "Antiferromagnetic and nematic phase transitions in  $\text{Ba}(\text{As}_{1-x}\text{P}_x\text{Fe})_2$  studied by ac microcalorimetry and SQUID magnetometry." Physical Review B 91.9 (2015): 094512.

<sup>1</sup>This work was supported by the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the US DOE, Office of Science, under Award No. DEAC0298CH1088

**Tuesday, March 15, 2016 11:15AM - 2:15PM –**

**Session F12 GPC DFD GSNP: Climate Science Frontier: Cloud and Precipitation Physics 308**

- Juan Restrepo, Oregon State Univ

**11:15AM F12.00001 Precipitation and atmospheric moisture transport responses to increased infrared opacity**, ELISABETH MOYER, University of Chicago — No abstract available.

**11:51AM F12.00002 Prototypes for the dynamics underlying precipitation and temperature extremes<sup>1</sup>**, J DAVID NEELIN, UCLA — Projecting changes in precipitation and temperature extreme events can be aided by a deeper understanding of the dynamics underlying such variations. For precipitation, this is closely connected to the interaction of fast, small-scale motions with variability of large-scale climate. Simple prototype models from the physics and applied math literature can point to analysis methods, connections among related quantities, and hypotheses for the dynamics, especially when the prototype models can be derived from climate-model equations. An overview will be provided including recent work with a number of collaborators. For distributions of precipitation-related variables, prototypes including Fokker-Planck solutions and first-passage problems for variations across an onset threshold yield insights into the form of present-day observed distributions and predictions for the form of the global warming change to evaluate in climate models. In distributions of water vapor and temperature, the widespread occurrence of non-Gaussian tails is likely explained in part by prototypes for tracer advection across a maintained gradient. The shape of these tails can have substantial implications for regional changes in probabilities of precipitation and temperature extremes with large-scale warming.

<sup>1</sup>Supported in part by the National Science Foundation

**12:27PM F12.00003 The physics of atmospheric instability, lightning, and global warming**, DAVID ROMPS, University of California, Berkeley — No abstract available.

**1:03PM F12.00004 Thermodynamic analysis of atmospheric convection**, OLIVIER PAULUIS, Courant Institute of Mathematical Sciences — No abstract available.

**1:39PM F12.00005 Aerosols, Clouds, and Precipitation as Scale Interactions in the Climate System and Controls on Climate Change**, LEO DONNER, Geophysical Fluid Dynamics Laboratory/NOAA — Clouds are major regulators of atmospheric energy flows. Their character depends on atmospheric composition, dynamics, and thermodynamic state. Clouds can assume organized structures whose scales are planetary, while processes important for determining basic properties occur on the scale of microns. The range of processes, scales, and interactions among them has precluded the development of concise theories for the role of clouds in climate, and limitations in modeling clouds in complex climate models remain among the key uncertainties in understanding and projecting climate change. The distribution function of vertical velocities (updraft speeds) in clouds is an important control on climate forcing by clouds and possibly a strong correlate with climate sensitivity. (Climate forcing refers to the change in Earth's energy balance as atmospheric composition changes, in particular, due to human activity. Climate sensitivity is defined here as the equilibrium change in globally averaged annual surface temperature as a result of doubled carbon dioxide.) Vertical velocities are central because they determine the thermodynamic environment governing phase changes of water, with both equilibrium and non-equilibrium phenomena important. The spatial and temporal spectra of relevant vertical velocities includes scales both numerically resolved by climate models and below their resolution limit. The latter implies a requirement to parameterize these smaller scale motions in models. The scale dependence of vertical velocities and emerging observational constraints on their distribution provide new opportunities for representing aerosols, clouds, and precipitation in climate models. Success in doing so could provide important breakthroughs in understanding both climate forcing and sensitivity.

**Tuesday, March 15, 2016 11:15AM - 2:15PM –**

**Session F13 DCOMP DAMOP: New Developments in the Study of Inhomogeneous Strongly Correlated Quantum Systems 309** - Mark Jarrell, Louisiana State University

**11:15AM F13.00001 New theoretical tools for quantum glasses, with and without quenched disorder**, LOUK RADEMAKER, Univ of California - Santa Barbara — Even though most solid materials are disordered or glasslike, our understanding of such non-equilibrium phases of matter is meager. Our task is thus to develop new tools to understand the nature of quantum glasses. These can be characterized into two classes: with or without quenched disorder. Interacting spin or electron models with quenched disorder are known to exhibit many-body localization (MBL). We discuss a new method based on a Hilbert-space preserving RG scheme to find the integrals of motion for an interacting system. We used this approach to numerically study MBL phases and the corresponding transition.

On the other hand, we discuss the possibility of self-generated electron glassiness in the absence of quenched disorder. Such structural quantum glasses, requiring geometric frustration and long-range interactions, are in many ways similar to the quenched disorder glasses. We will discuss the soft gap in the density of states, which is now related to short-range frozen density correlations. Using both numerical and analytic arguments we find Arrhenius-type slow relaxation and stretched exponential behavior.

**References:**

- L. Rademaker, A. Ralko, S. Fratini and V. Dobrosavljevic, Avoiding Stripe Order: Emergence of the Supercooled Electron Liquid, arXiv:1508.03065 (2015).
- L. Rademaker, M. Ortuno, Explicit Local Integrals of Motion for the Many-Body Localized State, arXiv:1507.07276 (2015).
- S. Mahmoudian, L. Rademaker, A. Ralko, S. Fratini and V. Dobrosavljevic, Glassy dynamics in geometrically frustrated Coulomb liquids without disorder, Phys. Rev. Lett. 115, 025701 (2015); arXiv:1412.4441.
- L. Rademaker, Y. Pramudya, J. Zaanen and V. Dobrosavljevic, Influence of long-range interactions on charge ordering phenomena on a square lattice, Phys. Rev. E 88, 032121 (2013); arXiv:1306.4765.

**11:51AM F13.00002 Quench and Transport Dynamics in Disordered Atomic Hubbard Lattices<sup>1</sup>**, BRIAN DEMARCO, Univ of Illinois - Urbana — I will give an overview of our experiments using ultracold atom gases trapped in optical lattices to probe transport, dynamics, and relaxation in disordered Hubbard models. By introducing disorder to naturally clean optical lattices using focused optical speckle, we realize variants of the disordered Bose- and Fermi-Hubbard models. In these systems, the distribution of Hubbard parameters is fully known, and the ratio of characteristic energy scales is completely tunable. I will discuss two measurements. In the first, we observe localization via transport measurements in the metallic regime of the Fermi-Hubbard model. We observe three phenomena consistent with many-body localization: localization at non-zero temperature, localization across a range of temperatures, and interaction-induced delocalization. These measurements show agreement with a mean-field theory in a limited parameter regime. In a separate experiment using bosonic atoms, we measure excitations following a quantum quench of disorder. Via comparison to state-of-the-art quantum Monte Carlo calculations that capture all aspects of the experiments—including all the particles—we show that the onset of excitations corresponds to the superfluid-Bose-glass transition. I will discuss how this behavior is reminiscent of the quantum Kibble-Zurek effect.

<sup>1</sup>This work is funded by the NSF and ARO.

**12:27PM F13.00003 The role of weak interactions on the mobility-edge of strongly disordered electron systems<sup>1</sup>**, CHINEDU EKUMA, Naval Research Lab, Washington D.C. — New insights into the nature of the mobility edge of a weakly correlated, disordered Anderson spectra will be presented within the typical medium dynamical cluster approximation (TMDCA). The TMDCA systematically incorporates non-local spatial correlations (beyond the single-site approximations) treating the disorder to all orders and the interacting, non-local cluster self-energy up to second order in the perturbation expansion of the interactions,  $U$ . An arbitrary small interaction is found to lead to an exponential fast crossover of the sharp mobility edge that separates the localized and extended states in the non-interacting regime below the critical disorder strength  $W_c^{U=0}$  whenever the chemical potential of the non-interacting typical density of states is below the mobility edge energy. This smearing of the mobility edge is ascribed to the inelastic scattering due to  $U$ . However, as the chemical potential,  $\mu$  approaches the smeared edge, reduction of the phase space for scattering by  $U$  causes the edge to once again become sharp. A concomitant soft-pseudogap is found at energy,  $\omega = 0$  independent of filling, which is linear rather than quadratic in  $\omega$ , due to the lack of momentum conservation. The method is demonstrated on realistic low-dimensional structures.

<sup>1</sup>This work was supported by the Office of Naval Research through the Naval Research Laboratory and NSF DMR-1237565 and the NSF EPSCoR Cooperative Agreement EPS-1003897

**1:03PM F13.00004 Precise finite-temperature properties of disordered strongly-correlated electronic systems**, EHSAN KHATAMI, San Jose State University — The interplay between disorder and electronic interactions in quantum many-body systems is not well understood. Experiments with ultracold atoms on optical lattices hold a great promise for exploring the different competing phases that arise in these systems by simulating disordered quantum lattice models in the presence of interactions. However, these experiments often rely on precise and approximate-free results from numerical calculations for various static and dynamic properties of these models in order to characterize the experimental systems. In this talk, I will present recently obtained data for the thermodynamic properties and magnetic correlations of the disordered three-dimensional Hubbard model using the determinant quantum Monte Carlo. I will also discuss new techniques within the numerical linked-cluster expansions that allow for fast and precise calculation of finite-temperature properties of disordered systems in the thermodynamic limit.

**1:39PM F13.00005 Properties of dirty bosons in disordered optical lattices**, USHNISH RAY, Princeton University — Disorder is ubiquitous in nature and its presence can lead to fascinating phenomena such as Anderson localization, Griffiths mechanisms and glassiness. These types of behavior have profound consequences on low temperature ordered phases that are difficult to study, particularly due to lack of controllable disorder. Recent advances in ultra-cold atomic systems have made it possible to make significant progress in overcoming such challenges – making direct comparisons with large scale Quantum Monte-Carlo techniques a possibility. I will talk about the disordered Bose-Hubbard model and the equilibrium properties of the domains that arise in trapped systems. I will show how they correspond to phases and explore the consequences of finite temperature and strong correlations. These aspects will be used to explain the observations of experimental measurements. In particular, I will highlight results of a recent collaborative enterprise that show excellent agreement between theory and experiment.

## Tuesday, March 15, 2016 11:15AM - 2:15PM –

Session F14 FEd: Integration of Research and Teaching Excellence: Cottrell Scholars 310 - Richard Wiener, Research Corp

**11:15AM F14.00001 From Particle Physics to Education: The Role of Tinkering**, MATS SELEN, Univ of Illinois - Urbana — The love of tinkering is perhaps the single most universal trait among scientists. From designing an experiment to building a computer application to solving a differential equation, the cycle of "observe - explain - test - revise" is at the root of the scientific creative process. Driven by the love of tinkering, we have developed a small low-cost wireless lab system with the goal of putting real scientific instrumentation in the hands of anyone with a desire to innovate and explore. I will describe how this came about and how it has changed our view of introductory physics labs at the University of Illinois.

**11:51AM F14.00002 Excellence and Diversity in Physics, and the Quest for Other Worlds**, KEIVAN STASSUN, Vanderbilt Univ — A major concern for American competitiveness today is the full engagement of US citizens in the STEM enterprise. Of particular concern is the ongoing under-representation of African Americans, Hispanic Americans, and Native Americans, who comprise 35% of the US college-age population but only 2% of physical science PhDs awarded in the US. Since 2004, with initial funding from an NSF CAREER grant and then from a Research Corp Cottrell Scholar award, the Fisk-Vanderbilt Masters-to-PhD Bridge Program has attracted 98 students, 79 of them under-represented minorities, 50% of them women, and with a PhD retention rate of 90%. Fisk has become the top producer of Black U.S. recipients of the master's degree in physics, and Vanderbilt has become the top research university to award the PhD to under-represented minorities in physics, astronomy, and materials science. Among the many "firsts" of the program are: the first member of the Sioux Nation to earn an advanced physics degree, the first Native Hawaiian woman to receive the prestigious NSF Graduate Research Fellowship, the first African American to receive NASA's top Hubble Postdoctoral Fellowship, and the first African American woman to publish an astronomy paper as first author in the prestigious journal Nature. Indeed, this latter example represents the groundbreaking discovery that the sizes and ages of stars—and therefore the sizes and ages and compositions of the planets that orbit those stars—can be measured directly and accurately via the "flicker" of the stars' light. This discovery has transformed the ability of astronomers to understand the physical nature of the exoplanets that are now being found by the thousands around distant stars.

**12:27PM F14.00003 Undergraduate research: A win-win for both students and faculty**<sup>1</sup>, TOM SOLOMON, Bucknell University — Undergraduate students benefit significantly from opportunities to do research with faculty, both at predominately undergraduate institutions (PUIs) and also at major Research I universities. If done well, these research opportunities can also benefit the faculty mentor, especially at PUIs with heavy teaching loads. In fact, the experience works best for the student if it also benefits the faculty. In this talk, I will discuss my experiences working with undergraduate research students, some of whom have been as productive as advanced graduate students. I will discuss situations where things have worked very well for everyone concerned, as well as some mistakes that I made in the past that resulted in bad research experiences. This discussion will be provided in the context of an experimental program in nonlinear dynamics, a field that is well-suited to participation by undergraduates.

<sup>1</sup>Supported by NSF Grants DMR-1361881 and PHY-1156964.

**1:03PM F14.00004 Interdisciplinary biophysics major with a comprehensive research-based capstone**, RAE ANDERSON, University of San Diego — No abstract available.

**1:39PM F14.00005 Untypical Undergraduate Research: Player Motion Analysis in Sports**, DINAH LOERKE, University of Denver — There is significant concern about the degree of attrition in STEM disciplines from the start of K-12 through to the end of higher education, and the analysis of the 'leaky pipeline' from the various institutions has identified a critical decline - which may be as high as 60 percent - between the fraction of students who identify as having an interest in a science or engineering major at the start of college/university, and the fraction of students who ultimately graduate with a STEM degree. It has been shown that this decline is even more dramatic for women and underrepresented minorities (Blickenstaff 2005, Metcalf 2010). One intervention which has been proven to be effective for retention of potential STEM students is early research experience, particularly if it facilitates the students' integration into a STEM learning community (Graham et al. 2013, Toven-Lindsey et al. 2015). In other words, to retain students in STEM majors, we would like to encourage them to 'think of themselves as scientists', and simultaneously promote supportive peer networks. The University of Denver (DU) already has a strong undergraduate research program. However, while the current program provides valuable training for many students, it likely comes too late to be effective for student retention in STEM, because it primarily serves older students who have already finished the basic coursework in their discipline; within physics, we know that the introductory physics courses already serve as gatekeeper courses that cause many gifted but 'non-typical' students to lose interest in pursuing a STEM major (Tobias 1990). To address this issue, my lab is developing a small research spinoff program in which we apply spatiotemporal motion analysis to the motion trajectories of players in sports, using video recordings of DU Pioneer hockey games. This project aims to fulfill a dual purpose: The research is framed in a way that we think is attractive and accessible for beginning students who have not yet finished the basic physics course sequence, and we hope to use it to attract untypical and retain undecided students in physics. Secondly, since mathematical techniques for trajectory analysis are independent of scale, we hope to harness the creativity and analytical intuition of undergraduates to simultaneously benefit our core biophysical research program.

**Tuesday, March 15, 2016 11:15AM - 2:15PM –**  
**Session F15 DCMP DMP: Design of 2D Materials** 314 -

**11:15AM F15.00001 Stable bound states of like charges on top of graphene in magnetic field**<sup>1</sup>, SERGEY SLIZOVSKIY, Loughborough University — We show theoretically that in the external magnetic field like charges on top of graphene monolayer may be mutually attracted to form thermodynamically stable macro-molecules. For this to happen graphene needs to be in Quantum Hall plateau state with local chemical potential being between the Landau levels. Graphene electron(s) gets localized in the middle between charges and provides overscreening of Coulomb repulsion between the charges. The size of the resulting macro-molecules is of the order of the magnetic length ( $\sim 10$  nm for magnetic field 10 T). The possible stable macro-molecules that unit charges can form on graphene in magnetic field are classified. The binding survives significant temperatures, exceeding mobility barriers for many ionically bond impurities. The influence of possible lattice-scale effects of valley-mixing are discussed. Tuning the doping of graphene or the magnetic field, the binding of impurities can be turned on and off and the macro-molecule size may be tuned. This opens the perspective to nanoscopic manipulation of ions on graphene by using magnetic field and gating.

<sup>1</sup>Acknowledge EPSRC EP/I02669X/1 and EP/H049797/1 and RSF grant 14-22-00281

**11:27AM F15.00002 Ab initio study of magnetic single layer MPX<sub>3</sub> metal-phosphorous-trichalcogenides**, BHEEMA LINGAM CHITTARI, EUYHEON HWANG, Sungkyunkwan University, JEIL JUNG, University of Seoul, ALLAN H. MACDONALD, The University of Texas at Austin — We analyze the electronic structure of two dimensional (2D) MPX<sub>3</sub> (M = V, Cr, Mn, Fe, Co, Ni, Cu, Zn, and X = S, Se, Te) transition metal thiophosphates, viewing them as single layer van der Waals materials that can exhibit magnetic order. Our ab initio calculations for MPX<sub>3</sub> single layer compounds predict both semiconducting phases with variable band gap sizes and metallic phases, and an intimate interplay between magnetic order and the presence of a gap. A systematic trend of decreasing band gaps in antiferromagnetic states is observed as the chalcogen atoms S, Se, and Te change from smaller to larger atomic number, Ferromagnetic, antiferromagnetic, and nonmagnetic phases, and lattice constant changes accompanied by distortions in crystal symmetry, occur as the metal atom is varied. The sensitive interdependence between magnetic, structural, and electronic properties suggests the important potential of this class of 2D magnetic van der Waals materials for strain and field-effect carrier tunable spintronics.

**11:39AM F15.00003 Anisotropic optical properties of few-layer transition metal dichalcogenide  $\text{ReS}_2$** , ZHENGLU LI, TING CAO, FELIPE H. DA JORNADA, MENG WU, STEVEN G. LOUIE, Physics Department, UC Berkeley and Lawrence Berkeley National Lab — We present first-principles (DFT, GW and GW-BSE) calculations of the electronic and optical properties of few-layer rhenium disulfide ( $\text{ReS}_2$ ). Monolayer  $\text{ReS}_2$  shows strong many-electron effects with a fundamental quasiparticle band gap of 2.38 eV based on  $G_0W_0$  calculation and a large exciton binding energy of 690 meV based on solving the Bethe-Salpeter equation. Highly anisotropic linear-polarized optical absorptions are revealed for few-layer and bulk  $\text{ReS}_2$ . The band gap shows a decreasing trend with the optical polarization direction near the absorption edge gradually rotating from around 67 degree in the monolayer to 85 degree in the bulk, referencing to the Re-chain. Our calculations are consistent with recent experimental data and theoretical studies, and provide a systematic understanding of the electronic and optical properties in few-layer  $\text{ReS}_2$ . This work was supported by National Science Foundation Grant No. DMR15-1508412 and the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at Lawrence Berkeley National Laboratory's NERSC facility.

**11:51AM F15.00004 Anisotropy in the optical properties of bulk and layered transition metal dichalcogenide  $\text{ReS}_2$** , SUVADIP DAS, NIHAR PRADHAN, CARLOS GARCIA, DANIEL RHODES, STEPHEN MCGILL, LUIS BALICAS, EFSTRATIOS MANOUSAKIS, National High Magnetic Field Lab. & Dept. Physics, Florida State Univ. — Unlike most transition metal dichalcogenides,  $\text{ReS}_2$  in the distorted  $1T'$  phase, is a direct gap semiconductor. We measured the temperature dependent photoluminescence in both bulk and layered  $\text{ReS}_2$  and examined the evolution of the peaks with the number of layers. We obtained strong signatures of optical anisotropy in the absorption spectroscopy and photocurrent response which makes this material a potential candidate for optoelectronic applications. Many body calculations including electron-hole interactions as implemented in the GW+BSE approach, agrees with the strong anisotropy in the optical properties of bulk and monolayer  $\text{ReS}_2$ . A shift in the excitonic peaks by about 0.8 eV introduced by solving the Bethe-Salpeter equation indicates strong contribution from excitonic bound states in this transition metal dichalcogenide.

**12:03PM F15.00005 First-principles Study of Temperature Dependence of Energy Gap in 2D Materials<sup>1</sup>**, YUNING WU, XIAOGUANG ZHANG, Department of Physics and Quantum Theory Project, University of Florida — We use a first-principles method to study the temperature dependence of energy gap in 2D semiconductors, including monolayer  $\text{MoS}_2$  and  $\text{MoSe}_2$ , etc, due to the effect of phonons on the band structure. The phonon vibrations are modeled by a set of frozen-phonon configurations, in which atomic displacements are determined by the Bose-Einstein distribution of the phonon modes. The electronic structure is calculated for each configuration, and the energy gap is extracted from configurational statistics. Calculated temperature dependence of energy gap agrees with the photoluminescence experiments [1] in terms of both the values of the band gap as well as the line shapes. [1] S. Tongay *et al.*, Nano Lett. 12, 5576, (2012)

<sup>1</sup>This work is supported by NSF grant 1508898

**12:15PM F15.00006 Ab initio studies of excitations in monolayer black phosphorus<sup>1</sup>**, TOBIAS FRANK, MARCIN KURPAS, MARTIN GMITRA, University of Regensburg, RENE DERIAN, IVAN STICH, Inst. of Physics, Slovak Academy of Sciences, JAROSLAV FABIAN, University of Regensburg — Monolayer black phosphorus, or phosphorene, represents an ideal system to study many-body electron-electron and electron-hole interactions due to its strong anisotropy driven 1d electronic nature. In particular, the size of the fundamental band gap value and excitonic binding energies remain unresolved given the different gap values of 1.6 to 2.4 eV [1] obtained by many-body GW calculations. We present our contribution to this issue studying excitations in phosphorene employing quantum monte carlo (QMC) calculations. We show the evolution of finite size effects of the fundamental and optical gap, with respect to relatively large supercell sizes in the theoretical framework of diffusion monte carlo (DMC) explicitly including electronic correlations. Our studies point to a significant influence of electron correlation on the fundamental gap as well as to a strong anisotropic nature of the excitonic state. Furthermore we address the question of a multiconfigurational ground state in monolayer black phosphorus. [1] A. N. Rudenko, Shengjun Yuan, and M. I. Katsnelson, Phys. Rev. B 92 085419 (2015)

<sup>1</sup>This work is supported by the DFG GRK 1570, SFB 689, and European Union Seventh Framework Programme under Grant Agreement No. 604391 Graphene Flagship.

**12:27PM F15.00007 Prediction of two-dimensional van der Waals ferroelectric materials**, WENJUN DING, JIANBAO ZHU, University of Science and Technology of China, YANFEI GAO, University of Tennessee, DI XIAO, Carnegie Mellon University, YI GU, Washington State University, ZHENYU ZHANG, WENGUANG ZHU, University of Science and Technology of China — Based on density functional theory calculations, we discover a class of two-dimensional van der Waals ferroelectric materials with spontaneous out-of-plane electric polarization, and the orientation of the electric polarization can be reversed by a seemingly lateral shift of a single atomic layer. We further find that the electronic structures of a bilayer of such two-dimensional ferroelectric materials can be switched to be either semiconducting or metallic, depending on their relative orientations of the electric polarization. This finding expands the family of the two-dimensional materials with ferroelectricity and offers new opportunities to tune the properties of van der Waals heterostructures for practical device applications.

**12:39PM F15.00008 Giant piezoelectricity of monolayer group IV monochalcogenides.**, RUIXIANG FEI, Department of Physics, Washington University, WENBIN LI, Research Laboratory of Electronics, Massachusetts Institute of Technology, JU LI, Department of Nuclear Science and Engineering and Department of Materials Science and Engineering, Massachusetts Institute of Technology, LI YANG, Department of Physics, Washington University — We predict enormous, anisotropic piezoelectric effects in intrinsic monolayer group IV monochalcogenides ( $\text{MX}$ ,  $\text{M}=\text{Sn}$  or  $\text{Ge}$ ,  $\text{X}=\text{Se}$  or  $\text{S}$ ), including  $\text{SnSe}$ ,  $\text{SnS}$ ,  $\text{GeSe}$ , and  $\text{GeS}$ . Using first-principle simulations based on the modern theory of polarization, we find that their piezoelectric coefficients are about one to two orders of magnitude larger than those of other 2D materials, such as  $\text{MoS}_2$  and  $\text{GaSe}$ , and bulk quartz and  $\text{AlN}$  which are widely used in industry. This enhancement is a result of the unique “puckered”  $\text{C}_{2v}$  symmetry and electronic structure of monolayer group IV monochalcogenides. Given the achieved experimental advances in the fabrication of monolayers, their flexible character, and ability to withstand enormous strain, these 2D structures with giant piezoelectric effects may be promising for a broad range of applications such as nano-sized sensors, piezotronics, and energy harvesting in portable electronic devices.

**12:51PM F15.00009 ABSTRACT WITHDRAWN —**

**1:03PM F15.00010 Structural variability and electronic properties of bulk and monolayer Si<sub>2</sub>Te<sub>3</sub>**<sup>1</sup>, COREY COMBS, University of Tennessee Knoxville Department of Materials Science and Engineering, Vanderbilt University Department of Physics and Astronomy, XIAO SHEN, Vanderbilt University Department of Physics and Astronomy, University of Memphis Department of Physics and Materials Science, YEVGENIY PUZYREV, LIDA PAN, Vanderbilt University Department of Physics and Astronomy, SOKRATES PANTELIDES, Vanderbilt University Department of Physics and Astronomy, Oak Ridge National Laboratory Materials Science and Technology Division — Silicon telluride, a layered material recently experimentally made to a few atomic layer-thick (1) has intriguing variations of optical and electronic properties, associated with the flexibility of its structure. In Si<sub>2</sub>Te<sub>3</sub>, the Te atoms form a hexagonal close packed structure, while Si atoms form Si-Si dimers and fill 2/3 of the allowed sites. There are 4 possible orientations of the Si-Si dimers, 3 in-plane directions 60 degrees to each other and one out-of-plane direction perpendicular to 2D plane. X-ray and electron diffraction data on bulk Si<sub>2</sub>Te<sub>3</sub> suggested that 1/4 of the dimers are vertical while the other 3/4 of the dimers are randomly oriented horizontally. We performed density functional calculations to show that both bulk and monolayer Si<sub>2</sub>Te<sub>3</sub> exhibit large variations in properties, resulting from reorientation of silicon dimers. These variations are up to 5 percent in lattice constant and up to 40 percent in electron band gap. Transition of Si<sub>2</sub>Te<sub>3</sub> from bulk to monolayer configuration also shows an increase in the band gap and lattice constant. We show that these properties are, in principle, controllable by temperature and strain, making Si<sub>2</sub>Te<sub>3</sub> a promising candidate as optomechanical and optoelectronic material. (1) Keuleyan, S. et al. *Nano Lett.* 2015, 15 (4), 2285-2290.

<sup>1</sup>Research funded by NSF grant: NSF EPS-1004083

**1:15PM F15.00011 Effect of functionalization on the electronic and atomic properties of layered MXenes**, KURT FREDRICKSON, Stanford University, ALEKSANDRA VOJVODIC, SLAC National Accelerator Laboratory, JENS NRSKOV, Stanford University — MXenes (M = Transition Metal, X = C or N) are a promising family of materials that have been recently manufactured from MAX phases. MXenes have already been shown as promising candidates for use in lithium ion batteries, supercapacitors, and fuel cells (1). MXenes consist of M<sub>1-x</sub>X<sub>2-x</sub>(x-1), two-dimensional sheets weakly bound by van der Waals forces. However, due to the selective removal of the A ion to manufacture MXenes, they are highly reactive, with a wide variety of possible functional groups. Previous studies have shown that the electronic properties of MXene single sheets are highly dependent on their functionalization, but so far there are few studies on the effect of functionalization of the bulk phase of MXene, which consists of many layers of MXenes bound together. In this talk, we will illustrate the effect of functionalization of bulk MXenes by H, H<sub>2</sub>, OH, and O for Mo<sub>2</sub>C and Ti<sub>2</sub>C. We will also show the effect of applied potential on the functionalization of Mo<sub>2</sub>C and Ti<sub>2</sub>C. Finally, we will compare our results with experimental measurements. (1) M. Naguib, V.D. Mochalin, M.W. Barsoum and Y. Gogotsi, *Adv. Mater.* 26, 992 (2014).

**1:27PM F15.00012 Single layer lead iodide: computational exploration of structural, electronic and optical properties, strain induced band modulation and the role of spin-orbital-coupling**, MEI ZHOU, WENHUI DUAN, Department of Physics and State Key Laboratory of Low-dimensional Quantum Physics, Tsinghua University, Beijing 100084, China, YING CHEN, Institute for Frontier Materials, Deakin University, Waurn Ponds, VIC 3216, Australia, AIJUN DU, School of Chemistry, Physics and Mechanical Engineering, Queensland University of Technology, Brisbane, QLD 4001, Australia — Graphitic like layered materials exhibit intriguing electronic structures and the search for new types of two-dimensional (2D) monolayer materials is of great interest for developing novel nano-devices. By using density functional theory method, we investigate the structure, stability, electronic and optical properties of monolayer lead iodide (PbI<sub>2</sub>). The stability of PbI<sub>2</sub> monolayer is first confirmed by phonon dispersion calculation. Compared to the calculation using generalized gradient approximation, screened hybrid functional and spin-orbit coupling effects can predicts an accurate band gap (2.63 eV). The biaxial strain can tune its band gap size in a wide range from 1 eV to 3 eV, which can be understood by the strain induced uniformly change of electric field between Pb and I atomic layer. The calculated imaginary part of the dielectric function of 2D graphene/PbI<sub>2</sub> van der Waals type hetero-structure shows significant red shift of absorption edge compared to that of a pure monolayer PbI<sub>2</sub>. Our findings highlight a new interesting 2D material with potential applications in nanoelectronics and optoelectronics.

**1:39PM F15.00013 Two-dimensional silicon and carbon monochalcogenides with the structure of phosphorene**, DARIO ROCCA, ALI ABOUD, SÉBASTIEN LEBÈGUE, Université de Lorraine and CNRS, Nancy (France), GANAPATHY VAITHEESWARAN, University of Hyderabad, Hyderabad (India) — Phosphorene has recently attracted interest for applications in transistors and photodetectors. Inspired by this material we carried out an ab initio study to predict new binary materials with a structure similar to phosphorene. Specifically, carbon or silicon atoms and chalcogen atoms (up to Te) were combined to form a phosphorene-like monolayer. The structure of these new compounds was then optimized and the dynamical stability of the structures was demonstrated by computing phonon dispersion curves. A series of materials were found to be stable: CS, CSe, CTe, SiO, SiS, SiSe, and SiTe. Electronic properties such as band gaps and effective masses were computed at the density functional theory level. By using the accurate HSE hybrid functional it was found that these materials span a broad range of bandgaps, going from the 2.1 eV of SiS to the 0.55 eV of SiTe. The effective masses were also computed; similarly to phosphorene, a strong anisotropy was found when comparing the zigzag and armchair directions. The variety of electronic properties found for these systems will contribute to broaden the technological applicability of two dimensional materials.

**1:51PM F15.00014 Electron counting and a large family of two-dimensional semiconductors**, MAOSHENG MIAO, Department of Chemistry and Biochemistry, California State University Northridge, JORGE BOTANA, Beijing Computational Science Research Center, EVA ZUREK, Department of Chemistry, University at Buffalo, JINGYAO LIU, Institute of Theoretical Chemistry, Jilin University, WEN YANG, Beijing Computational Science Research Center — Two-dimensional semiconductors (2DSC) are currently the focus of many studies, thanks to their novel and superior transport properties that may greatly influence future electronic devices. The potential applications of 2DSCs range from low-dimensional electronics, topological insulators and valleytronics all the way to novel photolysis. However, compared with the conventional semiconductors that are comprised of main group elements and cover a large range of band gaps and lattice constants, the choice of 2D materials is very limited. In this work, we propose and demonstrate a large family of 2DSCs, all adopting the same structure and consisting of only main group elements. Using advanced density functional calculations, we demonstrate the attainability of these materials, and show that they cover a large range of lattice constants, band gaps and band edge states, making them good candidate materials for heterojunctions. This family of two dimensional materials may be instrumental in the fabrication of 2DSC devices that may rival the currently employed 3D semiconductors.

**2:03PM F15.00015 Highly anisotropic Dirac fermions in square graphynes**, LIZHI ZHANG, Univ of Electronic Sci & Tech / University of Utah, ZHENGFEI WANG, University of Science and Technology of China, JIANSHENG RAO, ZIHENG LI, WULIN HUANG, ZHIMING WANG, Univ of Electronic Sci & Tech, SHIXUAN DU, HONGJUN GAO, Institute of Physics, Chinese Academy of Sciences, FENG LIU, University of Utah — Recently, there have been intense search of new 2D materials, and one especially appealing class of 2D materials is the all-carbon allotropes of Dirac materials. Here, we predict a new family of 2D carbon allotropes, square graphynes (S-graphynes) that exhibit highly anisotropic Dirac Fermions, using first-principle calculations within density functional theory. The equal-energy contour of their 3D band structure shows a crescent shape, and the Dirac crescent has varying Fermi velocities from 0.6 10<sup>5</sup> to 7.2 10<sup>5</sup> m/s along different k directions. Near the Fermi level, the Dirac crescent can be nicely expressed by an extended 2D Dirac model Hamiltonian. Furthermore, tight-binding band fitting reveals that the Dirac crescent originates from the next-nearest-neighbor interactions between C atoms. Our findings enrich the Dirac physics founded in other 2D Dirac systems, and offer a new design mechanism for creating Dirac band by tuning the interaction range. We envision that the highly anisotropic Dirac crescent may be exploited in all-carbon-based electronic devices for manipulating anisotropic electron propagation.

**Tuesday, March 15, 2016 11:15AM - 2:15PM –**

**Session F16 DMP: Exciton Dynamics in 2D Semiconductors** 315 - Xiaobo Yin, University of Colorado, Boulder

**11:15AM F16.00001 Interlayer Exciton Lifetimes in MoSe<sub>2</sub>/WSe<sub>2</sub> Heterostructures**, KYLE SEYLER, No Company Provided, PASQUAL RIVERA, University of Washington, HONGYI YU, University of Hong Kong, JOHN SCHABILEY, University of Washington, JIAQIANG YAN, DAVID MANDRUS, University of Tennessee, Oak Ridge National Lab, WANG YAO, University of Hong Kong, XIAODONG XU, University of Washington — Semiconductor heterostructures of two-dimensional (2D) transition-metal dichalcogenides (TMDs) have emerged as an exciting new platform for novel device engineering and physics. A fundamental question for the field is how the strong Coulomb interactions, electronic structure, and underlying valley physics affect the optoelectronic response. While researchers have made significant progress in understanding intralayer exciton dynamics in monolayer TMDs, there is comparatively little understanding of the interlayer excitons that form in their heterostructures. In this talk, we will report on time-resolved photoluminescence experiments of interlayer excitons in MoSe<sub>2</sub>/WSe<sub>2</sub> vertical heterostructures, which show wide tunability with gate and variability with emission energy. We will also discuss the underlying mechanisms for this behavior and show how it can be utilized to generate long-lived valley excitons.

**11:27AM F16.00002 Coupled spin-valley-dynamics in single-layer transition metal dichalcogenides**, GERD PLECHINGER, PHILIPP NAGLER, CHRISTIAN SCHÜLLER, TOBIAS KORN, Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D-93040 Regensburg, Germany — Single layers of transition metal dichalcogenides (TMDCs) like MoS<sub>2</sub> and WS<sub>2</sub> can be produced by simple mechanical exfoliation. Offering a direct bandgap at the K-points in the Brillouin zone, they represent a promising semiconductor material for flexible and transparent optoelectronic applications. Due to inversion symmetry breaking together with strong spin-orbit-interaction, the valley and spin degrees of freedom are coupled in monolayer TMDCs. Via circularly polarized optical excitation, an efficient polarization of the  $K^+$  or the  $K^-$  valley can be generated. Here, we investigate the dynamics of these coupled spin-valley polarizations in monolayer MoS<sub>2</sub> and WS<sub>2</sub> by means of photoluminescence spectroscopy and time-resolved Kerr rotation (TRKR). The results indicate a maximum achievable spin-valley-lifetime in these materials exceeding one nanosecond at low temperatures. Furthermore, we extract the dependence of the spin-valley lifetime on temperature. By varying the excitation energy, we reveal the excitonic resonances as well as the spin-polarized bandstructure around the K valleys common to monolayer TMDCs.

**11:39AM F16.00003 Measurements of ultrafast luminescence dynamics in transition metal dichalcogenide monolayers**, CEDRIC ROBERT, GANG WANG, DELPHINE LAGARDE, ANDREA BALOCCHI, THIERRY AMAND, PIERRE RENUCCI, FABIAN CADIZ, BERNHARD URBASZEK, XAVIER MARIE, CNRS/INSA Toulouse — We report time resolved photoluminescence (PL) measurements using a synchro-scan streak camera system with sub-ps time resolution, the fastest detector currently available for PL. The strong electron-hole Coulomb interaction in monolayer (ML) transition metal dichalcogenides results in excitons with high binding energies and oscillator strength. Therefore very short intrinsic radiative lifetimes can be expected. Here measurements with few ps time resolution are crucial. In our experiment we excite the ML sample with a fs laser pulse in a cryostat (T=4300 K). In the model system ML MoSe<sub>2</sub> we can separate spectrally the neutral and the charged exciton and perform detailed time-resolved PL studies on each complex. For the neutral exciton we resolve a PL emission time as short as 2ps, previous measurements were limited by the detector time-resolution. This short time depends on the experimental conditions such as temperature and applied external fields. We will discuss the different competing relaxation and recombination mechanisms, such as the intrinsic radiative recombination, the escape from the light cone through phonon scattering, the interplay between bright and dark exciton states and the possible transfer from the neutral to the charged exciton at lower energy.

**11:51AM F16.00004 Exciton Dynamics on Suspended and Substrate-supported MoS<sub>2</sub> and WS<sub>2</sub> Monolayers.**<sup>1</sup>, CHAO XU, YILING YU, YIFEI YU, ANDY BARRETTE, LINYOU CAO, KENAN GUNDOGDU, North Carolina State University, KENAN GUNDOGDU TEAM, LINYOU CAO TEAM — MoS<sub>2</sub> and WS<sub>2</sub> monolayers are promising atomic-scale platform for novel light emission devices, however, despite perfect surface passivation and strong exciton binding energy, their luminescence efficiencies are very low. Here, through the observation of exciton dynamics by ultrafast transient reflection, we revealed that the substrate can affect the exciton dynamics on MoS<sub>2</sub> and WS<sub>2</sub> monolayers, by facilitating the non-radiative recombination pathways, thus reducing the luminescence efficiency. Furthermore, strong many-body interactions such as exciton-exciton annihilation, are enhanced on suspended MoS<sub>2</sub> and WS<sub>2</sub> monolayers, whereas the defects in substrates may efficiently quench excitons thus mitigate those effects.

<sup>1</sup>North Carolina State University

**12:03PM F16.00005 Observation of excitonic Floquet states in a monolayer transition metal dichalcogenide**, EDBERT J. SIE, XI LING, MIT, YI-HSIEN LEE, NTHU Taiwan, LIANG FU, JING KONG, NUH GEDIK, MIT — Quantum systems that are driven by a time-periodic potential can form a series of new states that are called the Floquet states. In solids, the realization of Floquet states is rare and fascinating because it contains novel features that could be hybridized to create a new phase of matter. To date, such observation is limited to a recent experiment on a topological insulator (Y. H. Wang et al., Science 342, 453 (2013)). In this talk, we will show the observation of Floquet states from the excitons in a monolayer transition metal dichalcogenide that is performed using ultrafast optical spectroscopy. We will discuss the generation mechanism of these Floquet states as well as the significance of these observations.

**12:15PM F16.00006 Optical polarization and intervalley scattering in single layers of MoS<sub>2</sub> and MoSe<sub>2</sub>**<sup>1</sup>, BEREND JONKER, Naval Research Laboratory, GEORGE KIOSEOGLU, University of Crete, AUBREY HANBICKI, MARC CURRIE, ADAM FRIEDMAN, Naval Research Laboratory, NRL / U. CRETE COLLABORATION, NRL / U. CRETE COLLABORATION — We probe the valley population dynamics in MoSe<sub>2</sub> and MoS<sub>2</sub> by selectively populating the K and K' valleys with circularly polarized light while systematically varying the laser excitation energy. For both systems, the difference in the excitation energy and photoluminescence emission energy,  $dE = E_{\text{pump}} - E_{\text{PL}}$ , governs the depopulation of carriers in each valley. Adding more energy above a distinct threshold characteristic of the longitudinal acoustic (LA) phonon for each material enables inter-valley scattering and produces a sharp decrease in the observed circular polarization. LA phonons in these two systems have different energies (30 meV for MoS<sub>2</sub> and 19 meV for MoSe<sub>2</sub>), and we show that the threshold for the excess energy required to initiate the depolarization process clearly reflects the material specific phonon energy. In addition, our results show that independent of how many carriers are excited, i.e. whether you create neutral or charged excitons, the scattering process is the same. We find that the key parameter for the depolarization process is the extra kinetic energy of the exciton — depolarization is due to intervalley scattering that begins to occur when the exciton energy exceeds a threshold corresponding to twice the LA phonon energy.

<sup>1</sup>This work was supported by core programs at NRL, and by the Air Force Office of Scientific Research AOARD 14IOA018-134141.

**12:27PM F16.00007 Coherent Exciton Dynamics in Atomically Thin Semiconductors**, XIAOQIN (ELAINE) LI, Univ of Texas, Austin — The near band-edge optical response of an emerging class of semiconductors, known as the transitional metal dichalcogenides (TMDs), is dominated by tightly-bound excitons and charged excitons (i.e. trions). A fundamental property of these quasiparticles (excitons and trions) is quantum decoherence time, which reflects irreversible quantum dissipation arising from system (excitons and trions) and bath (vacuum and other quasiparticles) interactions and determines the timescale during which excitons can be coherently manipulated. Dephasing time is also equivalent to the intrinsic homogeneous linewidth of exciton resonance. In addition, excitons in TMDs are localized at the corners of the Brillouin zone and provide a convenient way to optically manipulate the valley degree of freedom, which may act as a useful information carrier analogous to electronic charge or spin. Direct measurement of valley coherence time is challenging because it corresponds to a non-radiative coherence between two degenerate states. Using ultrafast multi-dimensional optical spectroscopy, we investigate the intrinsic homogeneous linewidth of excitons, exciton valley coherence as well as coupling between excitons and trions. Our studies reveal coherent electronic dynamics on the order of  $\sim 100$  fs in monolayer TMDs. We gratefully acknowledge financial support from NSF, AFOSR, and the Welch Foundation.

**1:03PM F16.00008 Ultrafast Manipulation of the Valley Coherence in Monolayer WSe<sub>2</sub>**, ZILIANG YE, DEZHENG SUN, TONY HEINZ, Departments of Applied Physics and Photon Science, Stanford University — The valley degree of freedom in solids has been proposed as a pseudospin carrier for the future quantum electronics. Valley polarization has been created in transition metal dichalcogenide monolayers using circularly polarized light and the existence of coherence in the valley exciton pseudospin has been experimentally demonstrated<sup>1</sup>. The degeneracy of the valley degeneracy has recently been lifted both by the application of magnetic fields and dynamically by the optical Stark effect with circularly polarized light<sup>2–3</sup>. Here we demonstrate the all-optical manipulation of valley exciton coherence, i.e., of the valley exciton pseudospin, by the optical Stark effect. Using below-bandgap circularly polarized light, we rotate the valley exciton pseudospin on the femtosecond time scale. Both the direction and speed of the rotation can be optically controlled by tuning the dynamic phase of excitons in opposite valleys. In addition, by varying the time delay between the excitation and control pulses, we probe the lifetime of the intervalley coherence in monolayer WSe<sub>2</sub>.  
 1. X. Xu, W. Yao, D. Xiao, and T. F. Heinz, *Nature Physics* **10**, 343 (2014).  
 2. E. J. Sie, J. W. McIver, Y.-H. Lee, L. Fu, J. Kong, and N. Gedik, *Nature Materials* **14**, 290 (2014).  
 3. J. Kim, X. Hong, C. Jin, S. F. Shi, C. Y. S. Chang, M. H. Chiu, L. J. Li, and F. Wang, *Science* **346**, 1205 (2014).

**1:15PM F16.00009 Probing ultrafast valley dynamics in 2D semiconductors via time-resolved Kerr rotation**, JIANI HUANG, THANG HOANG, Department of Physics and Center for Metamaterials and Integrated Plasmonics, Duke University, TIAN MING, JING KONG, Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, MAIKEN MIKKELSEN, Department of Physics and Department of Electrical and Computer Engineering, Duke University — Monolayer transition metal dichalcogenides (TMDs) offer a tantalizing platform for controlling spin and valley degrees of freedom, enabling future optoelectronic devices with enhanced and novel functionalities. Here, we experimentally probe the valley dynamics in monolayer MoS<sub>2</sub> and WSe<sub>2</sub> using time-resolved Kerr rotation (TRKR) from  $T = 10$  K to 300 K. This pump-probe technique offers sub-picosecond temporal resolution, providing insight into ultrafast valley dynamics inaccessible by polarized and time-resolved photoluminescence spectroscopy. Bi-exponential decay dynamics were observed for both materials at low temperatures. Strong long-range exchange interactions between the K valleys led to a rapid exciton valley depolarization time ( $< 10$  ps), while the valley polarization of the trion and defect states decays within several tens of ps. Moreover, spatial distributions of the TRKR amplitude across monolayer flakes indicated weaker valley polarizations near the edges of MoS<sub>2</sub>, which is likely associated with the Mo- or S-zigzag terminations at the boundaries. These temporal and spatial TRKR measurements reveal insight into the complex dynamics of valley excitonic states in monolayer TMDs.

**1:27PM F16.00010 Intervalley double resonance processes in MoS<sub>2</sub>**, YUANXI WANG, Pennsylvania State University, BRUNO CARVALHO, LEANDRO MALARD, CRISTIANO FANTINI, Universidade Federal de Minas Gerais, VINCENT CRESPI, Pennsylvania State University, MARCOS PIMENTA, Universidade Federal de Minas Gerais — Intervalley scattering plays a significant role in electronic energy dissipation in semiconductors. We investigate the intervalley scattering of monolayer and few-layer MoS<sub>2</sub>, by combining density functional theory calculations and resonant Raman spectroscopy probed by up to 20 laser excitation energies. We observe that two Raman peaks within  $420\text{--}460\text{ cm}^{-1}$  are dispersive over a small range of laser energy, a clear signature of second-order processes involving intervalley scattering. Both modes involve LA and TA phonons at or near the K point. A third Raman peak at  $466\text{ cm}^{-1}$  shows a strong intensity dependence on the layer number and is assigned 2LA(M). Our results invalidate previous Raman peak assignment proposals and open up a better understanding of double resonance processes in transition metal dichalcogenides.

**1:39PM F16.00011 Interlayer Interaction Effects and Spin-Pseudospin Transfer in 2D MoSe<sub>2</sub>-WSe<sub>2</sub> Heterostructures**<sup>1</sup>, JOHN SCHABLEY, PASQUAL RIVERA, KYLE SEYLER, University of Washington, HONGYI YU, University of Hong Kong, JIAQIANG YAN, DAVID MANDRUS, Oak Ridge National Laboratory, University of Tennessee, WANG YAO, University of Hong Kong, XIAODONG XU, University of Washington — Heterostructures composed of MoSe<sub>2</sub>-WSe<sub>2</sub> monolayer semiconductors host spatially indirect interlayer excitons, which are bound states of an electron in the MoSe<sub>2</sub> layer and a hole in the WSe<sub>2</sub> layer. Interlayer excitons are observable in photoluminescence experiments as a low energy peak whose spectral position is consistent with the predicted type-II band alignment. The electron and hole which form the interlayer exciton are localized in momentum space valleys that occur at the (K and -K) corners of the Brillouin zone. To probe this interlayer valley physics, we perform two color pump-probe measurements to investigate the interactions between intralayer excitons in the heterostructure, resonantly pumping excitons in one layer and probing excitons in the other layer. We observe evidence of interlayer interaction effects in the nonlinear differential reflection spectra. Polarization dependent spectroscopy reveals evidence of interlayer spin-valley pseudospin transfer.

<sup>1</sup>We gratefully acknowledge support from the DOE, NSF, Cottrell Scholar Award, Croucher Foundation, and RGC of Hong Kong.

**1:51PM F16.00012 The role of collective motion in the ultrafast charge transfer in van der Waals heterostructures.**, HAN WANG, Rensselaer Polytechnic Institute, JUNHYEOK BANG, Spin Engineering Physics Team, Korea Basic Science Institute (KBSI), YIYANG SUN, Rensselaer Polytechnic Institute, LIANGBO LIANG, Oak Ridge National Laboratory, DAMIEN WEST, VINCENT MEUNIER, SHENGBAI ZHANG, Rensselaer Polytechnic Institute — The success of van der Waals (vdW) heterostructures made of graphene, metal dichalcogenides, and other layered materials, hinges on the understanding of charge transfer across the interface as the foundation for new device concepts and applications. In contrast to conventional heterostructures, where a strong interfacial coupling is essential to charge transfer, recent experimental findings indicate that vdW heterostructures can exhibit ultra-fast charge transfer despite the weak binding of these heterostructures. Using time-dependent density functional theory molecular dynamics, we find that the collective motion of excitons at the interface lead to plasma oscillations associated with optical excitation. Furthermore, instability of these oscillations explain the rapid charge transfer across the interface and are shown to be a general feature of vdW heterostructures provided they have a critical minimum dipole coupling. Application to the MoS<sub>2</sub>/WS<sub>2</sub> heterostructure yields good agreement with experiment, indicating near complete charge transfer within a timescale of 100 fs.

**2:03PM F16.00013 Layer- and Frequency-dependent Second-harmonic Generation from GaSe Atomic Crystals<sup>1</sup>**, YANHAO TANG, JOHN A. MCGUIRE, CHIH WEI LAI, Department of Physics and Astronomy, Michigan State University, KRISHNA C. MANDAL, Department of Electrical Engineering, University of South Carolina — GaSe is a layered semiconductor with an indirect bandgap at about 2.0 eV only ~20 meV below the direct bandgap at room temperature. Atomically thin GaSe crystals are expected to exhibit an increasing bandgap. This can be probed through the strong nonlinear optical response of GaSe. We report optical second-harmonic generation (SHG) in reflection from GaSe atomic crystals of 1 to > 100 layers on a Si substrate with a 90 nm SiO<sub>2</sub> layer. Room-temperature measurements were performed with fundamental photon energies of 0.85 to 1.4 eV as well as at 1.58 eV. By accounting for multilayer interference, the layer-dependent SHG intensity data are fit to obtain the magnitude of the second-order nonlinear optical susceptibility,  $\chi^{(2)}$ . For samples thicker than ~7 layers, we find  $|\chi^{(2)}| = 80 \pm 18$  pm/V, consistent with reported values for bulk GaSe. For samples  $\leq 6$  layers,  $|\chi^{(2)}|$  is reduced compared to that in thicker samples and shows a minimum in trilayer samples. The frequency-dependence of the SHG response suggests that this reduction of  $|\chi^{(2)}|$  in the few-layer region is due to increase of the direct bandgap.

<sup>1</sup>This work is supported by NSF grant DMR-09055944

**Tuesday, March 15, 2016 11:15AM - 2:15PM –**  
**Session F17 DMP: 2D Devices: Superconductors, Charge Density Waves, Phase Transitions**  
 316 - Vincent Meunier, Rensselaer Polytechnic Institute

**11:15AM F17.00001 hBN/graphene heterostructures for spectroscopy studies in normal and superconducting regime**, RICCARDO PISONI, Massachusetts Institute of Technology/Politecnico di Milano, JOEL I-JAN WANG, Massachusetts Institute of Technology/Harvard School of Engineering and Applied Sciences, LANDRY BRETHERAU, Massachusetts Institute of Technology, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science (NIMS), Japan, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology — Tunneling spectroscopy is a powerful tool to study the electronic properties of materials, as it has the capability of probing the electronic density of states at energies away from the Fermi level. Though local probes, such as scanning tunneling spectroscopy (STS), are widely used to elucidate the novel electronic properties of graphene, planar (2-D to 2-D) tunneling is also desirable for its capability to probe the global behavior of a 2-D electronic system. To study the intrinsic properties of the material via tunneling, one must employ a proper tunneling barrier and minimize the local doping introduced by the tunneling. Here we present a fabrication technique involving ultra thin hexagonal Boron Nitride (hBN) as both a tunneling barrier and an encapsulation overlayer to protect the 2-D Van der Waals material under study. In particular we focus on the fabrication of ultra thin hBN/graphene/hBN Van der Waals heterostructures that allows us to perform tunneling spectroscopy in graphene in normal and superconducting regime.

**11:27AM F17.00002 New Method of fabricating high-mobility graphene/LaAlO<sub>3</sub>/SrTiO<sub>3</sub> nanostructures<sup>1</sup>**, SHIVENDRA TRIPATHI, GIRIRAJ JNAWALI, LU CHEN, MENGCHENG HUANG, JEN-FENG HSU, BRIAN D'URSO, University of Pittsburgh, HYUNGWOO LEE, CHANG-BEOM EOM, University of Wisconsin-Madison, PATRICK IRVIN, JEREMY LEVY, University of Pittsburgh — Graphene and LaAlO<sub>3</sub>/SrTiO<sub>3</sub> (LAO/STO) are both two-dimensional electronic systems with a fascinating range of properties. The coupling between these two 2DEGs has the potential to produce various novel phenomena and create new functionalities. Successful integration of these two systems must overcome a number of technical challenges. Graphene-complex-oxide (GCO) heterostructures are created using Hyflon AD (2,2,4-trifluoro-5 trifluoromethoxy-1,3 dioxole) as a support layer for transferring and patterning CVD graphene on LAO/STO. This approach has advantages over more traditional methods that use Poly(Methyl Methacrylate) (PPMA) to transfer CVD graphene in that the Hyflon is easier to remove from the oxide surface after processing. To test the quality of GCO heterostructures, a graphene Hall bar structure is created. The quantum Hall regime can routinely be reached in the graphene layer, while preserving the ability of the LAO/STO to be patterned using AFM lithography. This approach opens up the possibility for the exploration of a wide range of GCO devices.

<sup>1</sup>We gratefully acknowledge the support from the following agencies and grants ONR N00014-13-1-0806 (JL,CBE)

**11:39AM F17.00003 Tunneling Spectroscopy of Andreev states in Graphene**, LANDRY BRETHERAU, Massachusetts Institute of Technology (MIT), USA, JOEL I-JAN WANG, Massachusetts Institute of Technology (MIT), USA / Harvard University (USA), RICCARDO PISONI, Massachusetts Institute of Technology (MIT), USA / Politecnico di Milano (Italy), KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science (NIMS), Japan, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology (MIT), USA — Although not intrinsically superconducting, graphene (G) can inherit electronic properties of a superconductor (S) placed in good contact with it. This proximity effect originates from the formation in the graphene of entangled electron-hole states, the Andreev states. In an S-G-S geometry, the Andreev states energies depend on the difference between the order parameter phases of the two superconductors. Such a phenomenon is usually probed by measuring the dissipationless Josephson supercurrent carried by Andreev states. Here instead, we have performed a direct tunneling spectroscopy of graphene connected to two superconducting electrodes, in a SQUID geometry that enables us to vary the phase difference. The measured energy spectra are consistent with a continuum of Andreev bound states modulating with phase with energies smaller than the superconducting gap. Interestingly, out of gap modulation is also observed and can be interpreted as Andreev scattering states. Additionally, we discuss how these phenomena evolve as a function of graphene normal DOS, which is tuned by a back-gate electrode.

**11:51AM F17.00004 Specular Interband Andreev Reflections in Graphene**, KONSTANTIN B. EFETOV, Ruhr-Universitaet Bochum, DMITRI EFETOV, Massachusetts Institute of Technology, LEI WANG, Columbia University, GIL-HO LEE, Harvard University, JIA SHUANG, ROBERT CAVA, Princeton University, TAKASHI TANIGUCHI, KENJI WATANABE, NIMS Japan, JAMES HONE, CORY DEAN, Columbia University, PHILIP KIM, Harvard University — Electrons incident from a normal metal onto a superconductor are reflected back as holes – a process called Andreev reflection. In a normal metal where the Fermi energy is much larger than a typical superconducting gap, the reflected hole retraces the path taken by the incident electron. In graphene with ultra- low disorder, however, the Fermi energy can be tuned to be smaller than the superconducting gap. In this unusual limit, the holes are expected to be reflected specularly at the superconductor-graphene interface due to the onset of interband Andreev processes, where the effective mass of the reflected holes change sign. Here we present measurements of gate modulated Andreev reflections across the low disorder van der Waals interface formed between graphene and the superconducting NbSe<sub>2</sub>. We find that the conductance across the graphene/superconductor interface exhibits a characteristic suppression when the Fermi energy is tuned to values smaller than the superconducting gap, a hallmark for the transition between intraband retro and interband specular- Andreev reflections.

**12:03PM F17.00005 Spin superconductivity and ac-Josephson effect in Graphene system under strong magnetic field**, HAIWEN LIU, International Center for Quantum Materials and School of Physics, Peking University, Beijing 100871, China, HUA JIANG, College of Physics, Optoelectronics and Energy, Soochow University, Suzhou 215006, China, QING-FENG SUN, X. C. XIE, International Center for Quantum Materials and School of Physics, Peking University, Beijing 100871, China, COLLABORATIVE INNOVATION CENTER OF QUANTUM MATTER, BEIJING, CHINA COLLABORATION — We study the spin superconductivity in Graphene system under strong magnetic field. From the microscopically Gor'kov method combined with the Aharonov-Casher effect, we derive the effective Landau-Ginzburg free energy and analyze the time evolution of order parameter, which is confirmed to be the off-diagonal long range order. Meanwhile, we compare the ground state of spin superconductivity to the canted-antiferromagnetic state, and demonstrate the equivalence between these two states. Moreover, we give out the pseudo-field flux quantization condition of spin supercurrent, and propose an experimental measurable ac-Josephson effect of spin superconductivity in this system.

**12:15PM F17.00006 Ballistic and diffusive regimes in current-phase relations of graphene SNS heterojunctions**, PHILIP KRATZ, Stanford University, FRANCOIS AMET, Duke University, CHRISTOPHER WATSON, Stanford University, KATHRYN MOLEK, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, CHUNG KE, Duke University, Durham, IVAN BORZENETS, University of Tokyo, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, RUSSELL DEACON, (CEMS), RIKEN, MICHIOHISA YAMAMOTO, University of Tokyo, YURIY BOMZE, Duke University, SEIGO TARUCHA, University of Tokyo, GLEB FINKELSTEIN, Duke University — Current-phase relations (CPRs) are an indirect measurement of the energy distribution of phase-coherent modes in Josephson junctions through the spectral supercurrent near equilibrium, probing low-energy excitations not accessible by transport. We report on planned experimental measurements of the CPRs of gated, high-mobility ( $10^5 \text{ cm}^2/\text{Vs}$ ) single-layer graphene SNS heterojunctions in ring geometries with superconducting MoRe alloy contacts, inductively read out with a scanning superconducting quantum interference device (SQUID) magnetometer. The graphene layers are encapsulated on both sides with hexagonal-BN (h-BN). We will address the CPR dependence on experimentally tunable parameters (temperature, carrier density, and channel length), and possible crossovers between the ballistic and diffusive regimes.

**12:27PM F17.00007 The role of double  $\text{TiO}_2$  layers at the interface of  $\text{FeSe}/\text{SrTiO}_3$  superconductors**, KE ZOU, Department of Applied Physics and Center for Research on Interface Structures and Phenomena (CRISP), Yale University, New Haven CT 06520, USA — The marked enhancement of the superconducting critical temperature for FeSe grown on  $\text{SrTiO}_3$  (STO) is a notable recent discovery in the field of high temperature superconductivity. A complete understanding of the mechanism for this enhancement has not been elucidated and is thought to be due to how the electronic structure is modified by the interface. We determine the surface reconstruction of  $\text{SrTiO}_3$  that is used to achieve superconducting FeSe films in experiments. In particular, we observe the existence of a double  $\text{TiO}_2$  layer and identify the symmetry of the reconstruction at the  $\text{FeSe}/\text{SrTiO}_3$  interface. The double  $\text{TiO}_2$  layer plays two important roles. First, it facilitates epitaxial growth of FeSe films. Second, *ab initio* calculations reveal that electron transfer to the FeSe is enhanced by the double layer termination more strongly than by other surface structures of  $\text{SrTiO}_3$ . The enhanced electron transfer suppresses the hole pocket near the  $\Gamma$  point, leading to a band structure characteristic of superconducting samples. The characterization of the interface structure presented here is a key step towards understanding the electronic properties of this novel superconductor.

**1:03PM F17.00008 Josephson Coupling in  $\text{Nb}/\text{SmB}_6/\text{Nb}$  Junctions<sup>1</sup>**, XIAOHANG ZHANG, SEUNGHUN LEE, CNAM, MSE, and Physics, University of Maryland, College Park, JASPER DRISKO, JOHN CUMINGS, MSE, University of Maryland, College Park, RICHARD GREENE, CNAM and Physics, University of Maryland, College Park, ICHIRO TAKEUCHI, CNAM, MSE, and Physics, University of Maryland, College Park — Josephson coupling of superconductors through a topological surface has attracted considerable attention because it may provide device applications of topological insulators with implications for Majorana fermions. However, the results of previous Josephson junction studies on topological insulators have not been fully understood due to complications arising from the conducting bulk and the non-pristine nature of the surfaces/interfaces of the topological insulator materials used. In this work,  $\text{SmB}_6$  thin films with a highly insulating bulk were adopted to minimize the influence of the bulk carriers while in-situ deposition of Nb film on  $\text{SmB}_6$  surface was used to ensure the interface quality. The bilayer structure was then patterned into  $\text{Nb}/\text{SmB}_6/\text{Nb}$  lateral junctions by e-beam lithography and ion milling. The Nb electrodes in our junctions had a typical width of  $\sim 1 \mu\text{m}$  and the gap between the two Nb electrodes was varied from 50 nm to 200 nm. A critical current up to 40  $\mu\text{A}$  has been observed in junctions with a gap around 50 nm at 2.0 K. In this talk, I will discuss the implication of our results to the desired Josephson coupling through topological surface states.

<sup>1</sup>This work was supported by NSF under grant No. DMR-1410665 and conducted at CNAM and at the Maryland NanoCenter.

**1:15PM F17.00009 Conductivity Modulation in a gated Normal-CDW-Normal configuration<sup>1</sup>**, SAUMYA BISWAS, ROGER LAKE, Univ of California - Riverside — There is considerable interest in switching by exploiting a voltage controlled phase transition, and one such phase is the charge density wave phase that occurs in a number of quasi one dimensional and two dimensional transition metal dichalcogenides. Voltage controlled switching of the charge density wave transition in  $1\text{T-TaS}_2$  has recently been demonstrated. We consider a transistor geometry with normal metal contacts and a channel of CDW material. The interaction is modeled with a negative U Hubbard term. Normal-CDW-temperature-U phase diagrams show the regime of the CDW in the ideal lattice. The wavelength of the CDW in the transistor channel is determined by both the conditions of Fermi surface nesting and also the condition of commensurability with the channel length between the two normal leads. Moving the Fermi level of the channel first results in phase boundaries within the CDW as the conditions of commensurability and Fermi surface nesting become incompatible. Moving the Fermi level from half filling by few tens of meV causes a collapsing of the CDW gap and an effective CDW-normal transition, leaving vestiges of the CDW in the channel. The transition is accompanied by one to two orders of magnitude increase in the conductivity.

<sup>1</sup>This work is supported by the National Science Foundation (NSF) Grant No. 1124733 and the Semiconductor Research Corporation (SRC) Nanoelectronic Research Initiative as a part of the Nanoelectronics for 2020 and Beyond (NEB-2020) program

**1:27PM F17.00010 Probing the Interaction of Graphene and Correlated Electron Systems by STM and Magnetotransport<sup>1</sup>**, MICHAEL ALTVATER, MARC REYNAUD, ADITYA SRIPAL, ALICE HUANG, GUOHONG LI, EVA Y. ANDREI, Rutgers University, Department of Physics and Astronomy, RUI ZHAO, JOSHUA ROBINSON, Pennsylvania State University, Materials Science and Engineering, Center for Two-Dimensional and Layered Materials — Since the discovery of 2D materials including graphene and TMDs, many have been shown to exhibit a wide variety of properties including correlated electronic phases, metal-insulator transitions, and highly tunable material properties leading to a rapid increase in research interest. Recent advances in nanostructure fabrication allow us to further study the interaction of these materials by creating heterostructures, layered devices made from low dimensional materials. In this work, we investigate the interaction of Dirac electrons in graphene with the charge density wave formed in  $1\text{T-TaS}_2$ , a van der Waals stacked TMD exhibiting a number of electronic phases including a high temperature metallic phase, several charge density wave phases, a Mott insulating phase, and superconductivity with the addition of pressure or dopants. Using STM, STS, and magnetotransport, we probe the effects of graphene on the phase transition properties of the CDW in  $\text{TaS}_2$  as well as the effect of the highly correlated substrate on the electronic spectrum in graphene. Our work will provide insight into the effects of correlated physics in heterostructures and how we might take advantage of these effects to produce novel devices and applications.

<sup>1</sup>Work supported by DOE-FG02-99ER45742, NSF DMR 1207108, NSF EFRI2-DARE 13-583

**1:39PM F17.00011 Dimensionality effect on the charge density wave and superconductivity of molecular beam epitaxy grown monolayer NbSe<sub>2</sub>**, HYEJIN RYU, YI ZHANG, ZAHID HUSSAIN, SUNG-KWAN MO, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA, Z.-X. SHEN, Geballe Laboratory for Advanced Materials, Departments of Physics and Applied Physics, Stanford University, Stanford, California 94305, USA, MIGUEL M. UGEDA, AARON J. BRADLEY, SEITA ONISHI, YI CHEN, WEI RUAN, CLAUDIA OJEDA-ARISTIZABAL, MARK T. EDMONDS, HSIN-ZON TSAI, ALEXANDER RISS, DUNGHAI LEE, ALEX ZETTL, MICHAEL F. CROMMIE, Department of Physics, University of California at Berkeley, Berkeley, California 94720, USA — Transition metal dichalcogenides are ideal compounds to investigate dimensionality effect since the weak coupling between layers enables to study single-layer material which removes interlayer interactions and introduces quantum confinement. We investigate dimensionality effect of NbSe<sub>2</sub> in which the bulk phase shows charge density wave (CDW) ( $T_{CDW} = 33$  K) and superconductivity ( $T_c = 7.2$  K). We report electronic band structure of MBE grown monolayer NbSe<sub>2</sub> measured by Angle-resolved photoemission spectroscopy compared with bulk. We find the number of bands crossing the Fermi energy reduces from three (bulk) to one (monolayer). Based on the significant suppression of superconducting  $T_c = 0.65$  K with robust CDW in monolayer NbSe<sub>2</sub>, our results imply the band remained at the Fermi level in monolayer NbSe<sub>2</sub> may play a crucial role in CDW formation and the disappeared bands are possibly in charge of superconductivity.

**1:51PM F17.00012 Reversible Semiconducting-to-Metallic Phase Transition in Chemical Vapor Deposition Grown Monolayer WSe<sub>2</sub> and Applications for Devices**, YUQIANG MA, BILU LIU, ANYI ZHANG, LIANG CHEN, MOHAMMAD FATHI, CHENFEI SHEN, AHMAD ABBAS, MINGYUAN GE, MATTHEW MECKLENBURG, CHONGWU ZHOU, Univ of Southern California, USC NANOLAB TEAM<sup>1</sup> — Two-dimensional (2D) semiconducting monolayer transition metal dichalcogenides (TMDCs) have stimulated lots of interest because they are direct bandgap materials that have reasonably good mobility values. However, contact between most metals and semiconducting TMDCs like 2H phase WSe<sub>2</sub> is highly resistive, thus degrading the performance of field effect transistors (FETs) fabricated with WSe<sub>2</sub> as active channel materials. We applied a phase engineering method to chemical vapor deposition (CVD) grown monolayer 2H-WSe<sub>2</sub> and demonstrated semiconducting-to-metallic phase transition in atomically thin WSe<sub>2</sub>. We have also shown that metallic phase WSe<sub>2</sub> can be converted back to semiconducting phase, demonstrating the reversibility of this phase transition. In addition, we fabricated FETs based on these CVD-grown WSe<sub>2</sub> flakes with phase-engineered metallic 1T-WSe<sub>2</sub> as contact regions and intact semiconducting 2H-WSe<sub>2</sub> as active channel materials. The device performance is substantially improved with metallic phase source/drain electrodes, showing on/off current ratios of  $10^7$  and mobilities up to  $66 \text{ cm}^2/\text{Vs}$  for monolayer WSe<sub>2</sub>.

<sup>1</sup>PI name: Chongwu Zhou

**2:03PM F17.00013 Metal to insulator quantum-phase transition in few-layered ReS<sub>2</sub>**<sup>1</sup>, NIHAR PRADHAN, NHMFL, Tallahassee, FL-32310, USA, AMBER MCCREARY, Dept. of Physics, Penn State University, PA 16802, USA, DANIEL RHODES, ZHENGUANG LU, DMITRY SMIRNOV, EFSTRATIOS MANOUSAKIS, NHMFL, Tallahassee, FL-32310, USA, SIMIN FENG, Dept. of Physics, Penn State University, PA 16802, USA, RAJU NAMBURU, MADAN DUBEY, U.S. Army Research Laboratory, Adelphi, MD 20783, USA, ANGELA HIGHT WALKER, NIST, Gaithersburg, MD 20899, USA, HUMBERTO TERRONES, Dept. of Physics, RPI, NY 12180, USA, MAURICIO TERRONES, Dept. of Physics, Penn State University, PA 16802, USA, VLADIMIR DOBROSAVLJEVIC, LUIS BALICAS, NHMFL, Tallahassee, FL-32310, USA — ReS<sub>2</sub> a layer-independent direct band-gap semiconductor of 1.5 eV implies a potential for its use in optoelectronic applications. Here, we present an overall evaluation of transport and anisotropic Raman of few-layered ReS<sub>2</sub> FET. ReS<sub>2</sub> exfoliated on SiO<sub>2</sub> behaves as an *n*-type semiconductor with an intrinsic carrier mobility surpassing  $\mu_i \sim 30 \text{ cm}^2/\text{Vs}$  at  $T = 300$  K which increases up to  $\sim 350 \text{ cm}^2/\text{Vs}$  at 2 K. Semiconducting behavior is observed at low electron densities *n*, but at high values of *n* the resistivity decreases by a factor  $>7$  upon cooling to 2 K and displays a metallic  $T^2$ -dependence. The electric-field induced metallic state observed in MoS<sub>2</sub> was recently claimed to result from a percolation type of transition. Instead, through a scaling analysis of the conductivity as a function of *T* and *n*, we find that the metallic state of ReS<sub>2</sub> results from a second-order metal to insulator transition driven by electronic correlations.

<sup>1</sup>Supported by U.S. Army Research Office MURI Grant No. W911NF-11-1-0362

**Tuesday, March 15, 2016 11:15AM - 2:15PM —**

**Session F18 GMAG DMP: Frustrated Magnetism: Pyrochlore and Spin Ice** 317 - Kate Ross, Colorado State University

**11:15AM F18.00001 Diffuse neutron scattering of Dy<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub> revisited**, MIKAEL TWENGSTRÖM, KTH, Sweden, MARTIN RUMINY, PSI, Switzerland, JUAN CARLOS ANDRESEN, KTH, Sweden, MAREK BARTKOWIAK, PSI, Switzerland, SEAN GIBLIN, Cardiff University, UK, STEVEN T. BRAMWELL, UCL, UK, MICHEL J. P. GINGRAS, University of Waterloo & CIFAR, Canada, TOM FENNELL, PSI, Switzerland, PATRIK HENELIUS, KTH, Sweden — Neutron scattering is a sensitive probe of correlations in condensed matter physics, and measurements of spin correlations by diffuse neutron scattering is one of the foremost methods of constraining the Hamiltonian of spin ice materials such as Dy<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>. Recent investigations of spin ices have highlighted the possibility of very slow equilibration at low temperature and/or structural defects in samples, effects which were not taken into account in the original parametrizations of the Hamiltonian. Hence, we have in this study performed a new set of diffuse magnetic neutron scattering experiments on an oxygen-annealed single crystal of the spin ice <sup>162</sup>Dy<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>. Compensation coils and an in-situ AC-susceptometer were used to control the zero magnetic field at the sample position as well as determining the thermal equilibrium of the magnetic spins respectively. In addition, we performed large-scale Monte Carlo simulations as to make a statistical fit of the dipolar spin ice model to the measured structure factor in the temperature range [0.65, 2] K, where the spin ice physics starts to develop. This will enable a most carefully controlled determination of the Hamiltonian of Dy<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>.

**11:27AM F18.00002 Radio-frequency magnetic susceptibility of spin ice crystals Dy<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub> using tunnel diode resonator**, SERAFIM TEKNOWIJOYO, KYUIL CHO, MAKARIY A. TANATAR, RUSLAN PROZOROV, Ames Laboratory and Iowa State University, ROBERT J. CAVA, JASON W. KRIZAN, Princeton University, AMES LABORATORY AND IOWA STATE UNIVERSITY TEAM, PRINCETON UNIVERSITY COLLABORATION — Spin ice compound, Dy<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>, has shown complex frequency - dependent magnetic behavior at low temperatures. While the DC measurements show conventional paramagnetic behavior, finite frequency susceptibility shows two regimes, - complex kagomé ice behavior at around 2 K and spin collective behavior above 10 K, depending on the frequency. Conventional AC susceptibility is limited to frequencies in a kHz range, but to get an insight into the possible Arrhenius activated behavior and characteristic relaxation times, higher frequencies are desired. We used self-oscillating tunnel-diode resonator (TDR) to probe magnetic susceptibility at 14.6 MHz, in the presence of a DC magnetic field and down to 50 mK. We found an unusual non-monotonic field dependence of the lower transition temperature, most likely associated with different spin configurations in a kagomé ice and an activated behavior of the upper transition, which has now shifted to 50 K range. This work was supported by the U.S. DOE BES MSED and was performed at the Ames Laboratory, Iowa State University under contract DE-AC02-07CH11358. The work at Princeton university was supported by DOE BES grant number DE-FG02-08ER46544.

**11:39AM F18.00003 Possible observation of photon excitations in the quantum spin-ice  $\text{Pr}_2\text{Zr}_2\text{O}_7$** , YOSHIFUMI TOKIWA, TAKUYA YAMASHITA, DAIKI TERAZAWA, TAKAHITO TERASHIMA, Kyoto University, KENTA KIMURA, Osaka University, MARIO HALIM, SATORU NAKATSUJI, University of Tokyo, YUJI MATSUDA, Kyoto University — It has been theoretically shown that the ground state of spin-ice system with quantum fluctuations can be quantum spin liquid, where new elementary excitations, photon, emerge [1]. In the rare-earth pyrochlore,  $\text{Pr}_2\text{Zr}_2\text{O}_7$ , which contains spin-ice correlations with significant quantum fluctuations, the absence of magnetic ordering even at very low temperature suggests formation of quantum spin liquid state [2]. In order to examine the emergence of new exotic excitations, we have performed low-temperature thermal conductivity ( $\kappa$ ) measurements of  $\text{Pr}_2\text{Zr}_2\text{O}_7$ . Interestingly, our data of  $\kappa/T$  shows a steep increase with decreasing temperature below 0.2K. Since the monopole density is negligibly small at such low temperature, the steep increase possibly indicates emergence of new elementary excitations. Anomalous magnetic-field dependence of  $\kappa/T$  observed below 0.2K further supports this possibility. [1] M. Hermele et al., Phys. Rev. B 69, 064404 (2004). [2] K. Kimura et al., Nature Commun. 4, 1934 (2013).

**11:51AM F18.00004 Thermal transport measurements of spin ice materials<sup>1</sup>**, WILLIAM TOEWS, JENNIFER REID, RAFAEL NADAS, University of Waterloo, STEFAN KYCIA, University of Guelph, TIMOTHY MUNSIE, McMaster University, HANNA DABKOWSKA, BRUCE GAULIN, McMaster University, Brockhouse Institute for Materials Research, ROBERT HILL, University of Waterloo — Extensive thermal conductivity measurements have been conducted on several rare-earth titanate materials. We report the consequences of crystalline quality and magnetic impurities on the mobility and dynamics of delocalized magnetic excitations. Detailed x-ray diffraction measurements have also been conducted on these samples to accurately characterize the sample quality. Differences between the various materials measured are also discussed.

<sup>1</sup>This research was supported by NSERC of Canada.

**12:03PM F18.00005 Atomic Structure Study of the Quantum Spin-ice Pyrochlore  $\text{Yb}_2\text{Ti}_2\text{O}_7$** , ALI MOSTAED, GEETHA BALAKRISHNAN, MARTIN LEES, RICHARD BEANLAND, Department of Physics, University of Warwick, MICROSCOPY TEAM, SUPERCONDUCTIVITY AND MAGNETISM TEAM — The quantum spin-ice candidate  $\text{Yb}_2\text{Ti}_2\text{O}_7$  (YTO) lies on the boundary between a number of competing magnetic ground states. Features in the low-temperature specific heat capacity are found to vary in sharpness and temperature depending on materials processing. It has been suggested that these changes in the magnetic ground state could be influenced by several factors, including the degree of cation stuffing, changes in oxygen occupancy and/or vacancies. In the present work, the structures of three different YTO samples, grown by the optical floating zone technique and that exhibit quite different heat capacity behaviour, have been studied by annular dark field scanning transmission microscopy (ADF-STEM). We show that the detailed intensity distribution around the visible atomic columns is sensitive to the presence of nearby atoms of low atomic number (in this case oxygen), even though they are not directly visible in the images. To the best of our knowledge, this is the first time that oxygen columns with a distance of ~30 pm have been distinguished in ADF-STEM images. Furthermore, by comparing atomic columns with different configurations of nearby oxygen atoms, we are able to distinguish between the different YTO samples. Finally, the ADF data for the crystal that exhibits no specific heat anomaly shows signs of the substitution of Yb atoms on Ti sites, supporting the view that the magnetic ground state of YTO is extremely sensitive to disorder.

**12:15PM F18.00006 Impact of Stoichiometry of  $\text{Yb}_{2+x}\text{Ti}_{2-x}\text{O}_{7-x/2}$  on its Structure and Physical Properties<sup>1</sup>**, KATHRYN ARPINO, BENJAMIN TRUMP, TYREL MCQUEEN, COLLIN BROHOLM, SEYED KOOHPAYEH, Johns Hopkins Univ — The rare-earth pyrochlores ( $R_2\text{M}_2\text{O}_7$ ) are topic of intense study in the field of magnetism as an ideal host for geometric frustration including spin-liquid and spin-ice behaviour. Specifically,  $R_2\text{Ti}_2\text{O}_7$  has proved a rich playground: compounds  $R = \text{Ho}$  and  $\text{Dy}$  are classical spin ices,  $R = \text{Tb}$  has been shown to be a spin liquid at low temperatures, and  $R = \text{Yb}$  is a candidate quantum spin ice. This system is attractive for the large anisotropic magnetic properties of rare earth ions,  $\text{Ti}^{4+}$ 's lack of magnetic moment which isolates the magnetic ordering of  $R^{3+}$ , and the comparative ease of making single crystals via the floating zone technique. This talk will present the structure and physical properties of a  $\text{Yb}_{2+x}\text{Ti}_{2-x}\text{O}_{7-x/2}$  series including both the pure and stuffed samples. The series shows a dramatic change in the low-temperature (50-200 mK) specific heat signature upon doping away from the pure compound. Understanding the magnetic and physical properties of the off-stoichiometric series sheds light both on the magnetic ordering of the ideal spin ice candidate compound as well as aids in evaluating the quality and stoichiometry of a measured sample. In this vein, proper single-crystal growth conditions in order to ensure single crystals of appropriate stoichiometry will also be discussed.

<sup>1</sup>The Institute of Quantum Matter is supported by Department of Energy (DOE), Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under award DE-FG02-08ER46544.

**12:27PM F18.00007 Magnetic monopole condensation transition out of quantum spin ice: application to  $\text{Pr}_2\text{Ir}_2\text{O}_7$  and  $\text{Yb}_2\text{Ti}_2\text{O}_7$** , GANG CHEN<sup>1</sup>, State Key Laboratory of Surface Physics, Fudan Univ; Perimeter Institute for Theoretical Physics — We study the proximate magnetic orders and the related quantum phase transition out of quantum spin ice (QSI). We apply the electromagnetic duality of the compact quantum electrodynamics to analyze the condensation of the magnetic monopoles for QSI. The monopole condensation transition represents a unconventional quantum criticality with unusual scaling laws. The magnetic monopole condensation leads to the magnetic states that belong to the 2-in 2-out spin ice manifold and generically have an enlarged magnetic unit cell. We demonstrate that the antiferromagnetic state with the ordering wavevector  $\mathbf{Q} = 2\pi(001)$  is proximate to QSI while the ferromagnetic state with the ordering wavevector  $\mathbf{Q} = (000)$  is not proximate to QSI. This implies that if there exists a direct transition from QSI to the ferromagnetic state, the transition must be strongly first order. We apply the theory to the puzzling experiments on two pyrochlore systems  $\text{Pr}_2\text{Ir}_2\text{O}_7$  and  $\text{Yb}_2\text{Ti}_2\text{O}_7$ .

<sup>1</sup>chgsgt@gmail.com

**12:39PM F18.00008 How quantum are classical spin ices?<sup>1</sup>**, MICHEL J P GINGRAS, JEFFREY G RAU, Univ of Waterloo — The pyrochlore spin ice compounds  $\text{Dy}_2\text{Ti}_2\text{O}_7$  and  $\text{Ho}_2\text{Ti}_2\text{O}_7$  are well described by classical Ising models down to low temperatures. Given the empirical success of this description, the question of the importance of quantum effects in these materials has been mostly ignored. We argue that the common wisdom that the strictly Ising moments of non-interacting  $\text{Dy}^{3+}$  and  $\text{Ho}^{3+}$  ions imply Ising interactions is too naive and that a more complex argument is needed to explain the close agreement between the classical Ising model theory and experiments. By considering a microscopic picture of the interactions in rare-earth oxides, we show that the high-rank multipolar interactions needed to induce quantum effects in these two materials are generated only very weakly by superexchange. Using this framework, we formulate an estimate of the scale of quantum effects in  $\text{Dy}_2\text{Ti}_2\text{O}_7$  and  $\text{Ho}_2\text{Ti}_2\text{O}_7$ , finding it to be well below experimentally relevant temperatures.

<sup>1</sup>Published as: PHYSICAL REVIEW B 92, 144417 (2015)

**12:51PM F18.00009 Disorder-Induced Quantum Spin Liquid in Spin Ice Pyrochlores**, LUCILE SAVARY, Massachusetts Institute of Technology, LEON BALENTS, Kavli Institute for Theoretical Physics, University of California, Santa Barbara — We discuss disorder in spin ice materials, and in particular in compounds with non-Kramers magnetic ions. We show that in the minimal relevant model, disorder succeeds in inducing a long-range entangled Coulombic quantum spin liquid phase. The phase diagram also contains an analog of the Mott glass state, envisioned in dirty boson systems with particle-hole symmetry. We discuss the relevance of our results to the material  $\text{Pr}_2\text{Zr}_2\text{O}_7$ , and how these ideas might be applied to convert a classical spin ice to a quantum one.

**1:03PM F18.00010 Low-temperature Spin-Ice State of Quantum Heisenberg Magnets on Pyrochlore Lattice**, YUAN HUANG, KUN CHEN, University of Massachusetts, Amherst; University of Science and Technology of China, YOUJIN DENG, University of Science and Technology of China; University of Massachusetts, Amherst, NIKOLAY PROKOF'EV, BORIS SVISTUNOV, University of Massachusetts, Amherst; Russian Research Center "Kurchatov Institute" — We establish that the isotropic spin-1/2 Heisenberg antiferromagnet on pyrochlore lattice enters a spin-ice state at low, but finite, temperature. Our conclusions are based on results of the bold diagrammatic Monte Carlo simulations that demonstrate good convergence of the skeleton series down to temperature  $T = J/6$ . The "smoking gun" identification of the spin-ice state is done through a remarkably accurate microscopic correspondence for static spin-spin correlation function between the quantum Heisenberg and classical Heisenberg/Ising models at all accessible temperatures. In particular, at  $T/J = 1/6$ , the momentum dependence shows a characteristic bow-tie pattern with pinch points. By numerical analytical continuation method, we also obtain the dynamic structure factor at real frequencies, showing a diffusive spinon dynamics at pinch points and spin wave continuum along the nodal lines?

**1:15PM F18.00011 Antiferromagnetic order in the pyrochlores  $\text{R}_2\text{Ge}_2\text{O}_7$  ( $\text{R} = \text{Er}, \text{Yb}$ )**, ZHILING DUN, Univ. of Tennessee, Knoxville, XIANG LI, Beijing National Laboratory for Condensed Matter Physics, RAFAEL FREITAS, EVERTON ARRIGHI, Instituto de Física, Universidade de São Paulo, Brazil, CLARINA CRUZ, Oak Ridge National Laboratory, MINSEONG LEE, EUN SANG CHOI, Florida State University and NHMFL, HUIBO CAO, Oak Ridge National Laboratory, HARLYN SILVERSTEIN, University of Manitoba, CHRIS WIEBE, Florida State University and NHMFL, University of Manitoba, University of Winnipeg, Canadian Institute for Advanced Research, JINGUANG CHEN, Beijing National Laboratory for Condensed Matter Physics, HAIDONG ZHOU, Univ. of Tennessee and NHMFL — Elastic neutron scattering, ac susceptibility, and specific heat experiments on the pyrochlores  $\text{Er}_2\text{Ge}_2\text{O}_7$  and  $\text{Yb}_2\text{Ge}_2\text{O}_7$  show that both systems are antiferromagnetically ordered in the  $\Gamma_5$  manifold. The ground state is a  $\psi_3$  phase for the Er sample and a  $\psi_2$  or  $\psi_3$  phase for the Yb sample, which suggests "Order by Disorder" (ObD) physics. Furthermore, we unify the various magnetic ground states of all known  $\text{R}_2\text{X}_2\text{O}_7$  ( $\text{R} = \text{Er}, \text{Yb}, \text{X} = \text{Sn}, \text{Ti}, \text{Ge}$ ) compounds through the enlarged XY type exchange interaction  $J_{\pm}$  under chemical pressure. The mechanism for this evolution is discussed in terms of the phase diagram proposed in the theoretical study [Wong et al., Phys. Rev. B 88, 144402, (2013)].

**1:27PM F18.00012 Theory for magnetic excitations in quantum spin ice**, SHIGEKI ONODA, Condensed Matter Theory Lab., RIKEN and Quantum Matter Theory Research Team, RIKEN Center for Emergent Matter Science, TRINANJAN DATTA, Dept. of Chemistry and Physics, Georgia Regents Univ. — Magnetic excitations in magnetic rare-earth pyrochlore oxides called quantum spin ice (QSI) systems such as  $\text{Yb}_2\text{Ti}_2\text{O}_7$ ,  $\text{Pr}_2\text{Zr}_2\text{O}_7$ , and  $\text{Tb}_2\text{Ti}_2\text{O}_7$  have attracted great interest for possible observations of the quantum dynamics of spin ice monopoles and emergent photon excitations. However, their spectral properties remain open especially for cases relevant to experimental systems. Here, we develop a theoretical framework that incorporates gauge fluctuations into a modified gauge mean-field approach, so that it reproduces key features of recent quantum Monte-Carlo results on the double broad specific heat in the simplest QSI model and can describe a continuous growth of a coherence in gauge-field correlations on cooling down to Coulomb-phase ground states. Using this new approach, we provide a theory for magnetic neutron-scattering spectra. It is found that spin-flip exchange interactions produce dispersive QSI monopole excitations which create a particle-hole continuum neutron-scattering spectrum. Gauge fluctuations give multi-particle contributions to the spectrum, which will be possibly detected in Higgs phases.

**1:39PM F18.00013 Ubiquitous Magnetic Excitations in the Ytterbium Pyrochlores**, ALANNAH HALLAS, JONATHAN GAUDET, McMaster University, NICHOLAS BUTCH, NIST Center for Neutron Research, MAKOTO TACHIBANA, National Institute for Materials Science, RAFAEL FREITAS, Universidade de São Paulo, CHRIS WIEBE, University of Winnipeg, GRAEME LUKE, BRUCE GAULIN, McMaster University — The ytterbium pyrochlores,  $\text{Yb}_2\text{B}_2\text{O}_7$  ( $\text{B} = \text{Sn}, \text{Ti}, \text{Ge}$ ) are well described in terms of  $S_{\text{eff}} = 1/2$  quantum spins with local XY anisotropy, decorating the cubic pyrochlore lattice and interacting via anisotropic exchange. While structurally only the non-magnetic B-site cation, and hence, primarily the lattice parameter, is changing across the series  $\text{Yb}_2\text{B}_2\text{O}_7$  ( $\text{B} = \text{Sn}, \text{Ti}, \text{Ge}$ ), a range of magnetic behavior is observed. The low temperature magnetism in  $\text{Yb}_2\text{Ti}_2\text{O}_7$  and  $\text{Yb}_2\text{Sn}_2\text{O}_7$  has ferromagnetic character. Conversely,  $\text{Yb}_2\text{Ge}_2\text{O}_7$  displays an antiferromagnetically ordered Neel state at low temperatures. We present a comparative analysis of the spin dynamic properties of these three systems using inelastic neutron scattering. While the static properties of the ytterbium pyrochlores are distinct from one another, we find a ubiquitous character to the spin dynamics. The inelastic scattering for each of these ytterbium pyrochlores show a gapless continuum of spin excitations, that tends to resemble over-damped ferromagnetic spin waves at low Q. Furthermore, the specific heat for each of these materials follows a common form with a broad, high-temperature anomaly followed by a sharp low-temperature anomaly. We find that the dynamic properties correlate strongly with the broad specific heat anomaly but remain unchanged across the sharp, low temperature specific heat anomaly.

**1:51PM F18.00014 Ferromagnetic correlations in  $\text{Yb}_2\text{Ti}_2\text{O}_7$  as revealed by small angle neutron scattering techniques**, CONNOR BUHARIWALLA, QIANLI MA, McMaster University, LISA DEBEER-SCHMITT, Oak Ridge National Lab, HANNA DABKOWSKA, Brockhouse Institute for Materials Research, BRUCE GAULIN, McMaster University — We report low temperature SANS measurements on frustrated  $S_{\text{eff}} = 1/2$  XY pyrochlore magnet  $\text{Yb}_2\text{Ti}_2\text{O}_7$  [1]. The ground state of this material has been proposed as a realization of a quantum spin ice; however, the low temperature phase behaviour has been complicated by sample dependencies believed to be related to weak "stuffing" [2]. Our SANS study focuses on the low Q structure of elastic "rods" of magnetic scattering which extend from  $Q=0$  along the 111 direction. Using a single crystal sample, we characterize the low Q ( $< 0.2\text{\AA}^{-1}$ ) temperature dependence of this structured diffuse scattering intensity to  $T=30\text{mK}$ , passing through the enigmatic heat capacity anomaly near  $T_c=200\text{mK}$ . The temperature dependence of this diffuse scattering near  $Q=0$  is largely consistent with that measured previously near 111 [3]. [1] K.A. Ross et al., Phys. Rev. X 1, 021002 (2011) [2] K.A. Ross et al., Phys. Rev. B 86, 174424 (2012) [3] K.A. Ross et al., Phys. Rev. B 84, 174442 (2011)

**2:03PM F18.00015 Extended spin ice**, JEFFREY G. RAU, MICHEL J. P. GINGRAS, University of Waterloo — We introduce a new classical spin liquid on the pyrochlore lattice which we call 'extended spin ice'. The ground state manifold of this model is extensive and characterized by a set of local rules that extend the conventional 2-in/2-out spin ice condition. This includes the ice states in addition to a complex set of tree structures built from 3-in/1-out, 3-out/1-in and all-in/all-out tetrahedra. Under local dynamics this model freezes heterogeneously at low temperatures into a 'spin slush', with extremely slow relaxation for some spins while other spin clusters fluctuate quickly. In addition to this dynamical heterogeneity, distinctive spherical patterns in the spin correlations serve as a further signature. Possible applications to materials as well the effects of transverse quantum exchange will be discussed.

**Tuesday, March 15, 2016 11:15AM - 2:15PM –**

**Session F19 GMAG DCMP: Kondo Physics, Heavy Fermions, and Quantum Criticality** 318 - Ivelisse Cabrera, NIST

**11:15AM F19.00001 Robust antiferromagnetism in the  $R_{1-x}\text{La}_x\text{Cu}_2\text{Ge}_2$  series: comparison of  $\text{Ce}_{1-x}\text{La}_x\text{Cu}_2\text{Ge}_2$  and  $\text{Nd}_{1-x}\text{La}_x\text{Cu}_2\text{Ge}_2$** <sup>1</sup>, SERGEY L. BUD'KO, SCOTT M. SAUNDERS, HALYNA HODOVANETS, PAUL C. CANFIELD, Ames Laboratory/Iowa State University — Recently, remarkably robust and correlated coherence and antiferromagnetism were found in the  $\text{Ce}_{1-x}\text{La}_x\text{Cu}_2\text{Ge}_2$  series [H. Hodovanets et al., *PRL* **114**, 236601 (2015)]. Whereas Ce is known to hybridize and its compounds often show a strongly correlated behavior, Nd magnetism is associated with a local moment nature. In this talk, we report new measurements on the  $\text{Ce}_{1-x}\text{La}_x\text{Cu}_2\text{Ge}_2$  series that extend the antiferromagnetic and coherence lines even further and then compare the data for  $\text{Ce}_{1-x}\text{La}_x\text{Cu}_2\text{Ge}_2$  and the data for a local moment based  $\text{Nd}_{1-x}\text{La}_x\text{Cu}_2\text{Ge}_2$  series to separate effects of Ce - hybridization from the behavior that might be common in the  $R_{1-x}\text{La}_x\text{Cu}_2\text{Ge}_2$  (R=magnetic rare earth) family.

<sup>1</sup>Supported by US DOE under the Contract No. DE-AC02-07CH11358

**11:27AM F19.00002 Possible Kondo-Lattice-Enhanced Magnetic Ordering at Anomalously High Temperature in Nd Metal under Extreme Compression**<sup>1</sup>, JAMES S. SCHILLING, JING SONG, VIKAS SONI, JINHYUK LIM, Washington University in St. Louis — Most elemental lanthanides order magnetically at temperatures  $T_o$  well below ambient, the highest being 292 K for Gd. Sufficiently high pressure is expected to destabilize the well localized magnetic  $4f$  state of the heavy lanthanides, leading to increasing influence of Kondo physics on the RKKY interaction. For pressures above 80 GPa,  $T_o$  for Dy and Tb begins to increase dramatically, extrapolating for Dy to a record-high value near 400 K at 160 GPa.<sup>2</sup> This anomalous increase may be an heretofore unrecognized feature of the Kondo lattice state; if so, one would expect  $T_o$  to pass through a maximum and fall rapidly at even higher pressures. A parallel is suggested to the ferromagnet  $\text{CeRh}_3\text{B}_2$  where  $T_o = 115$  K at ambient pressure, a temperature more than 100-times higher than anticipated from simple de Gennes scaling.<sup>3</sup> Here we discuss recent experiments on Nd where anomalous behavior in  $T_o(P)$  is found to occur at lower pressures, perhaps reflecting the fact that Nd's  $4f$  wave function is less localized.

<sup>1</sup>Work at Washington University is supported by NSF grant DMR-1104742 and CDAC through NNSA/DOE grant DE-FC52-08NA28554.

<sup>2</sup>J. Lim G. Fabbri, D. Haskel, J. S. Schilling, Phys. Rev. B **91**, 045116 & 174428 (2015).

<sup>3</sup>S. A. Shaheen, J. S. Schilling, R. N. Shelton, Phys. Rev. B **31**, 656(R) (1985).

**11:39AM F19.00003 Competition between Kondo and indirect exchange at the edges and bulk of graphene, and 2D materials.**, ANDREW ALLERDT, Northeastern University, GEORGE MARTINS, Oakland University, ADRIAN FEIGUIN, Northeastern University — We study the problem of two magnetic impurities at the surface of graphene, BN,  $\text{MoS}_2$ , phosphorene, silicene and germanene using exact numerical methods. We map the band structure of these materials onto one dimensional tight-binding chains in the same spirit as Wilson's numerical renormalization group. We use the density matrix renormalization group to solve the problem exactly, keeping all the information about the underlying lattice. Competition between Kondo and Ruderman-Kittel-Kasuya-Yosida (RKKY) interactions is non-trivial, due to strong non-perturbative effects. Depending on the presence of a pseudogap, or gap, we identify an important directionality and position dependence of the correlations. We present scenarios and regimes where impurities prefer to form their own Kondo clouds instead of an RKKY singlet state, or remain as uncoupled local moments. In the particular case of graphene, ferromagnetism is only stable at half-filling. In addition, we study the effects of spin-orbit coupling, and the presence of edge states.

**11:51AM F19.00004 Revisiting the Toulouse limit of a Kondo junction**, C.J. BOLECH, NAYANA SHAH, University of Cincinnati — Following the development of a scheme to bosonize and debosonize consistently [1,2], we present in detail the Toulouse-point analytic solution of the two-lead (nonequilibrium) Kondo junction model. The existence and location of the solvable point is not modified, but the calculational methodology and the final expressions for observable quantities change markedly as compared to the previously accepted results.

[1] See arXiv:1508.03078 and arXiv:1508.03079

[2] See also N. Shah, invited talk

**12:03PM F19.00005 Magnetic-field tuned ground states of  $\text{CeAuBi}_2$  single crystals**, H. HODOVANETS, T. METZ, H. KIM, Y. NAKAJIMA, K. WANG, J. YONG, S. R. SAHA, J. S. HIGGINS, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, College Park 20742, USA, N. BUTCH, CNAM, UMD, College Park 20742, USA/NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA, J. PAGLIONE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, College Park 20742, USA — We present detailed temperature- and field-dependent data obtained from magnetization, resistivity and heat capacity measurement performed on nearly stoichiometric  $\text{CeAuBi}_2$  single crystals. The compound orders antiferromagnetically at  $\sim 13$  K and shows large magnetic anisotropy at low temperatures with the c-direction being an easy axis. The field-dependent magnetization data at low temperatures reveal the existence of a spin-flop transition for  $\mathbf{H}||\mathbf{c}$  ( $H_c \sim 75$  kOe and  $T=1.8$  K). The zero-field resistivity and heat capacity data show features characteristic of a Ce-based intermetallic with crystal electric field splitting and possible correlated, Kondo lattice effects. The constructed  $T-H$  phase diagram, for the magnetic field applied along the easy, [001], direction shows that the magnetic field required to suppress  $T_N$  is  $\sim 75$  kOe. The possibility of realization of the field-tuned quantum critical point (QCP) in  $\text{CeAuBi}_2$  will be discussed.

**12:15PM F19.00006 Neutron scattering, magnetic, and transport properties of non-centrosymmetric  $\text{ULrSi}_3$ .**, SHANTA SAHA, I-LIN LIU, Center for Nano Physics and Advanced Materials, Department of Physics, University of Maryland, College Park, MD 20742, CRAIG BROWN, NICHOLAS BUTCH, NIST Center for Neutron Research, Gaithersburg, MD 20899, JOHNPIERRE PAGLIONE, Center for Nano Physics and Advanced Materials, Department of Physics, University of Maryland, College Park, MD 20742 — Heavy-fermion superconductivity in the non-centrosymmetric crystal structure has drawn much attention [1]. It is argued that the order parameter contains not only a spin-singlet part, but also an admixture of a spin-triplet state. The compound  $\text{ULrSi}_3$  crystallizes in the non-centrosymmetric  $\text{BaNiSn}_3$  structure which is closely related to the well-known  $\text{ThCr}_2\text{Si}_2$ -type [2]. Preliminary study on polycrystalline  $\text{ULrSi}_3$  shows antiferromagnetic order below Neel temperature  $T_N=42$  K [2]. Its lanthanide analog  $\text{CeIrSi}_3$  shows heavy-fermion superconductivity under pressure [1]. Therefore, further investigation on  $\text{ULrSi}_3$  would be meaningful. We would like to present the results of our investigation on  $\text{ULrSi}_3$  by neutron scattering, magnetic, and transport measurement on poly and single crystals grown by Czochralski method in a tetra-arc-furnace. [1] Onuki et al., J. Phys. Soc. Jpn. **77**, suppl. A 37 (2008). [2] Buffat et al., J. Mag. Mag. Mat. **62**, 53 (1986).

**12:27PM F19.00007 Single to multiparticle excitations in the itinerant helical magnet  $\text{CeRhIn}_5$** , CHRIS STOCK, Univ of Edinburgh, J. A. RODRIGUEZ-RIVERA, NIST and Univ of Maryland, K. SCHMALZL, ILL, E. E. RODRIGUEZ, Univ of Maryland, A. STUNAU, ILL, C. PETROVIC, BNL —  $\text{CeRhIn}_5$  is an itinerant magnet where the  $\text{Ce}^{3+}$  spins order in a simple helical phase. We investigate the spin excitations in this material using triple-axis neutron spectroscopy and observe sharp spin waves at low energies consistent with previous reports and a nearest neighbour exchange of  $\sim 1$  meV [1]. At higher energies, the fluctuations are heavily damped where the single-quasiparticle excitations are replaced by a momentum and energy-broadened continuum constrained by kinematics of energy and momentum conservation [2]. The delicate energy balance between localized and itinerant characters results in the breakdown of the single-quasiparticle picture in  $\text{CeRhIn}_5$ . [1] P. Das et al. Phys. Rev. Lett **113**, 246403 (2014). [2] C Stock et al. Phys. Rev. Lett. **114**, 247005 (2015). [3] T. Park et al. PNAS **105**, 6825 (2008).

**12:39PM F19.00008 Physical properties of the van der Waals bonded ferromagnet  $\text{Fe}_{3-x}\text{GeTe}_2$** , ANDREW MAY, Materials Science and Technology Division, ORNL, STUART CALDER, Quantum Condensed Matter Division, ORNL, CLAUDIA CANTONI, Materials Science and Technology Division, ORNL, HUIBO CAO, Quantum Condensed Matter Division, ORNL, MICHAEL MCGUIRE, Materials Science and Technology Division, ORNL —  $\text{Fe}_3\text{GeTe}_2$  is an itinerant ferromagnetic with a layered structure held together by van der Waals bonds. The material has been synthesized using a flux-growth technique that results in large single crystals suitable for neutron scattering, and its magnetic structure and phase diagram have been investigated. The flux-grown crystals possess a Curie temperature  $T_C \approx 150$  K, which is less than that reported for polycrystalline  $\text{Fe}_3\text{GeTe}_2$  with  $T_C \approx 230$  K. The difference is explained by intrinsic Fe-deficiency in these single crystals. This talk will summarize the physical properties of the flux grown single crystals and a series of polycrystalline samples with varying concentrations of Fe, which reveal how Fe content is correlated to structural parameters and  $T_C$ . In combination with the magnetic properties, Hall effect and thermoelectric data reveal that  $\text{Fe}_{3-x}\text{GeTe}_2$  compounds are multi-carrier type, itinerant ferromagnets. Research supported by the US DOE, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

**12:51PM F19.00009 Complex magnetic phases in non-centrosymmetric heavy fermion  $\text{CeCoGe}_3$** <sup>1</sup>, SHAN WU, Johns Hopkins University, Institute for Quantum Matter, CHRIS STOCK, University of Edinburgh, CEDOMIR PETROVIC, Brookhaven National Laboratory, J.A. RODRIGUEZ-RIVERA, NIST center for Neutron Research, COLLIN BROHOLM, Johns Hopkins University, Institute for Quantum Matter — The non-centrosymmetric nature of the tetragonal heavy fermion system  $\text{CeCoGe}_3$  has attracted much interest in the high pressure superconducting state of the material. We have explored the related ambient pressure magnetism using neutron scattering. There are three successive phase transitions at  $T_{N1} \sim 21$  K,  $T_{N2} \sim 12$  K and  $T_{N3} \sim 8$  K. The upper transition greatly enhances the susceptibility and there are meta-magnetic transitions in the lower T phases. We confirmed the previously determined AFM spin structure for  $T_{N2} < T < T_{N1}$  [1]. At lower T we find a complex commensurate structure that can be described as intertwined antiferromagnetic segments. We also report inelastic magnetic neutron scattering, which is dominated by the periodicity of the chemical cell rather than the magnetic unit cell. [1]M.Smidman, etc. *Phys. Rev. B*, **88**,134416 (2013)

<sup>1</sup>The work at IQM was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Material Sciences and Engineering, under Grant No. DEFG02-08ER46544.

**1:03PM F19.00010 Quantum criticality on ferromagnetic systems: it is not where you think it is!**, VALENTIN TAUFOR, UDHARA KALUARACHCHI, MANH CUONG NGUYEN, STELLA K KIM, XIAO LIN, EUN DEOK MUN, HYUNSOO KIM, YUJI FURUKAWA, CAI ZHUANG WANG, KAI MING HO, SERGEY L BUD'KO, PAUL C CANFIELD, Ames Laboratory / Iowa State University, Ames, IA 50011, USA, ZURAB GUGUCHIA, RUSTEM KHASANOV, Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland, PIETRO BONFA, ROBERTO DE RENZI, Dipartimento di Fisica e Scienze della Terra, Parco Area delle Scienze 7/A, I-43124 Parma, Italy — When a ferromagnetic-paramagnetic transition is tuned to 0 K by application of pressure in clean systems, the transition becomes of the first order at a tricritical point before disappearing. Instead of having a quantum critical point, i.e. a second order transition at 0 K, there is a quantum phase transition of the first order. The quantum phase transition can be from a ferromagnetic to a paramagnetic phase, or to a spatially modulated phase. We illustrate this case on a new material:  $\text{LaCrGe}_3$ . We will present the temperature-pressure-magnetic field phase diagram of  $\text{LaCrGe}_3$  and show that quantum criticality is avoided by the appearance of a modulated phase. We will also explain how quantum criticality can be re-introduced. Work at Ames Laboratory was supported by US DOE under the Contract No. DE-AC02-07CH11358. Magnetization measurements under pressure were supported by Ames Laboratory's laboratory-directed research and development (LDRD) funding.

**1:15PM F19.00011 Theory of electronic and magnetic properties of weak antiferromagnetic  $\text{TiAu}$** <sup>1</sup>, WEN FONG GOH, WARREN PICKETT, Univ of California - Davis — To date, only a few itinerant magnetic compounds have been found, viz.  $\text{ZrZn}_2$ ,  $\text{TiBe}_2$  and  $\text{Sr}_3\text{In}$ , all comprised of nonmagnetic elements.  $\text{TiAu}$ , a newly synthesized itinerant weak antiferromagnet, orders antiferromagnetically below 36 K. Neutron diffraction reveals an ordered local moment of only  $0.15 \mu_B/\text{Ti}$  at a wave vector  $Q=(0,\pi/b,0)$ . Hole doping, viz.  $\text{Ti}_{1-x}\text{Sc}_x\text{Au}$ , causes the magnetic moment to disappear at a quantum critical point  $x_{SC}=0.13$ . We present results of an extensive study of the electronic and magnetic properties of  $\text{TiAu}$ . DFT calculations reveal van Hove singularities at  $(0,0.45\pi/b,0.49\pi/c)$ , 4 meV above the Fermi level. Several types of analysis will be discussed: fixed spin moment studies and Stoner enhancement; magnetic energies; magnetism versus doping; Fermi surface nesting; corrections for spin fluctuations.

<sup>1</sup>Supported by Grant NSF DMREF DMR 1534719

**1:27PM F19.00012 Quantum Criticality in  $\text{YFe}_2\text{Al}_{10}$** , WILLIAM GANNON, Texas AM University, LIUSUO WU, Oak Ridge National Laboratory, IGOR ZALIZNYAK, Brookhaven National Laboratory, YIMING QIU, JOSE RODRIGUEZ-RIVERA, National Institute of Standards and Technology, MEIGAN ARONSON, Texas AM University — Quantum criticality has been studied in many systems, but there are few systems where observed scaling can be unified with a critical free energy  $F$ , or where the critical exponents form the basis for QC universality classes. We have identified a new layered material  $\text{YFe}_2\text{Al}_{10}$  that shows remarkably strong QC behavior, where the scaling properties of the magnetic susceptibility and specific heat are consistent with the same  $F$ . Recent neutron scattering results paint a remarkable picture of the QC fluctuations in  $\text{YFe}_2\text{Al}_{10}$ . In contrast to classical transitions, where fluctuations are relatively long ranged and inelastic scattering is observed at a magnetic zone center, in  $\text{YFe}_2\text{Al}_{10}$  the scattering is independent of wave vector in the critical plane, indicating that the fluctuations are spatially localized, while out of plane scattering indicates that the interplanar interactions are restricted to nearest neighbors. The dynamical susceptibility  $\chi'' \simeq E^{-2}$ , and is wholly temperature independent, indicating that E/T scaling is present, the signature of QC fluctuations. These results hint that the the criticality in  $\text{YFe}_2\text{Al}_{10}$  is local, which until now has only been found in a few f-electron based compounds.

**1:39PM F19.00013 Quantum criticality in single crystalline  $\text{YFe}_2\text{Al}_{10}$  determined from zero-field and longitudinal-field muon spin relaxation**<sup>1</sup>, KEVIN HUANG, CHENG TAN, JIAN ZHANG, ZHAOFENG DING, Department of Physics, Fudan University, DOUGLAS MACLAUGHLIN, Department of Physics, UC Riverside, OSCAR BERNAL, Department of Physics, CSU Los Angeles, PEI-CHUN HO, Department of Physics, CSU Fresno, LIUSUO WU, MEIGAN ARONSON, Department of Physics, Stony Brook University, LEI SHU, Department of Physics, Fudan University — Muon spin relaxation ( $\mu\text{SR}$ ) measurements were performed on single crystalline  $\text{YFe}_2\text{Al}_{10}$  down to 19 mK and in magnetic fields up to  $\sim 100$  Oe. Zero-field- $\mu\text{SR}$  measurements showed no evidence of magnetic order down to 19 mK, consistent with previous measurements. However, we also find that the depolarization rate  $\Lambda$  is temperature independent above 1 K but increases in an exponential behavior for  $T < 1$  K. Longitudinal-field  $\mu\text{SR}$  measurements also reveals a time-field scaling where  $G(t, H) = G(t/H^\gamma)$ , with  $\gamma = 0.67$ . This is further confirmed from the magnetic field dependence of  $\Lambda$ , which finds  $\Lambda(H) \propto H^{0.67}$  at 19 mK. This is further evidence that single crystalline  $\text{YFe}_2\text{Al}_{10}$  is in close proximity to a ferromagnetic quantum critical point.

<sup>1</sup>The research performed in this study was supported by the National NSF of China under Grant no. 11474060 and STCSM of China (No. 15XD1500200). Work at CSULA funded by NSF/DMR-1105380. Research at CSU-Fresno is supported by NSF DMR-1506677.

**1:51PM F19.00014 Doping-Induced Quantum Critical Point in an Itinerant Antiferromagnet TiAu**, JESSICA SANTIAGO, ETERI SVANIDZE, Rice University, TIGLET BESARA, THEO SIEGRIST, National High Magnetic Field Laboratory, Florida State University, EMILIA MOROSAN, Rice University — The recently discovered itinerant magnet TiAu is the first antiferromagnet composed of non-magnetic constituents. The spin density wave ground state develops below  $T^N \sim 36$  K, about an order of magnitude smaller than in Cr. Achieving a quantum critical point in this material would provide a better understanding of weak itinerant antiferromagnets, while giving long sought-after insights into the effects of spin fluctuations in itinerant electron systems. While the application of pressure increases the ordering temperature  $T^N$ , partial substitution of Ti provides an alternative avenue towards achieving a quantum critical point. The non-Fermi liquid behavior accompanies the quantum phase transition, as evidenced by the divergent specific heat coefficient and linear temperature dependence of the resistivity. The transition is accompanied by enhanced electron-electron correlations as well as strong spin-fluctuations, providing an experimental avenue for the verification of the self-consistent theory of spin fluctuations.

**2:03PM F19.00015 Itinerant magnetism in quantum critical  $\text{YFe}_2\text{Al}_{10}$** , WENHU XU, WEIGUO YIN, ROBERT KONIK, ALEXEI TSVELIK, Brookhaven Natl Lab, GABRIEL KOTLIAR, Rutgers University — The absence of magnetic order and the scaling laws in thermodynamical and transport properties in layered compound  $\text{YFe}_2\text{Al}_{10}$  suggest competition among different types of collective quantum states. Measurements on magnetic susceptibility have demonstrated a Curie-Weiss (CW) behavior with a reduced fluctuating Fe moment of 0.45B and  $T_{CW} \simeq -28\text{K}$ . Using first principle methods, we show that the correlation in  $\text{YFe}_2\text{Al}_{10}$  is moderate and the Fe magnetism is itinerant. Competing ground states include a paramagnetic state, an in-plane antiferromagnetic ordering (G-type) state and an in-plane collinear ordering (C-type) state. Although a bulk ferromagnetic order is not favored in total energy, both the G-type and C-type ground state prefer ferromagnetic inter-layer coupling.

**Tuesday, March 15, 2016 11:15AM - 2:15PM –**  
**Session F20 DCOMP GSCCM DMP: Materials in Extremes: High-pressure Synthesis of New Materials** 319 - Jennifer Ciezak-Jenkins, Army Research Laboratory

**11:15AM F20.00001 Extreme thermodynamic conditions: novel stoichiometries, violations of textbook chemistry, and intriguing possibilities for the synthesis of new materials.**<sup>1</sup>, ELISSAIO STAVROU, Lawrence Livermore National Laboratory — As evidenced by numerous experimental and theoretical studies, application of high pressure can dramatically modify the atomic arrangement and electronic structures of both elements and compounds. However, the great majority of research has been focused on the effect of pressure on compounds with constant stoichiometries (typically those stable under ambient conditions). Recent theoretical predictions, using advanced search algorithms, suggest that composition is another important variable in the search for stable compounds, i.e. that the more stable stoichiometry at elevated pressures is not *a priori* the same as that at ambient pressure. Indeed, thermodynamically stable compounds with novel compositions were theoretically predicted and experimentally verified even in relatively simple chemical systems including: Na-Cl, C-N, Li-H, Na-H, Cs-N, H-N, Na-He, Xe-Fe. These materials are stable due to the formation of novel chemical bonds that are absent, or even forbidden, at ambient conditions. Tuning the composition of the system thus represents another important, but poorly explored approach to the synthesis of novel materials. By varying the stoichiometry one can design novel materials with enhanced properties (e.g. high energy density, hardness, superconductivity etc.), that are metastable at ambient conditions and synthesized at thermodynamic conditions less extreme than that those required for known stoichiometries. Moreover, current outstanding questions, “anomalies” and “paradoxes” in geo- and planetary science (e.g. the Xenon paradox) could be addressed based on the stability of surprising, stoichiometries that challenge our traditional “textbook” picture. In this talk, I will briefly present recent results and highlight the need of close synergy between experimental and theoretical efforts to understand the challenging and complex field of variable stoichiometry under pressure. Finally, possible new routes for the synthesis of novel materials will be discussed.

<sup>1</sup>This work was performed under the auspices of the U. S. Department of Energy by Lawrence Livermore National Security, LLC under Contract DE-AC52-07NA27344.

**11:51AM F20.00002 Hydrogen sulfide at high pressure: change in stoichiometry**<sup>1</sup>, ALEXANDER GONCHAROV, SERGEY LOBANOV, Carnegie Inst of Washington, IVAN KRUGLOV, Moscow Institute of Physics and Technology, XIAO-MIAO ZHAO, Carnegie Inst of Washington, XIAO-JIA CHEN, Center for High Pressure Science & Technology Advanced Research (HPStar), Shanghai, China, ARTEM OGANOV, Skolkovo Institute of Science and Technology, Moscow, Russia, ZUZANA KONOPKOVA, DESY Photon Science, D-22607 Hamburg, Germany, VITALI PRAKAPENKA, Center for Advanced Radiation Sources, University of Chicago, Chicago, IL 60637, USA — Hydrogen sulfide ( $\text{H}_2\text{S}$ ) was studied by x-ray synchrotron diffraction (XRD) and Raman spectroscopy up to 144 GPa at 180-295 K. We find that  $\text{H}_2\text{S}$  compound become unstable with respect to formation of new compounds with different composition including pure S,  $\text{H}_3\text{S}$  and  $\text{HS}_2$  depending on the thermodynamic P-T path. These results are supported by our quantum-mechanical variable-composition evolutionary simulations that show the stability of the above mentioned compounds at elevated pressures. The stability of  $\text{H}_3\text{S}$  at high pressures, which we find a strong experimental and theoretical confirmation here, suggests that it is this material which is responsible for high-temperature superconducting properties reported previously.

<sup>1</sup>We thank DARPA, NSF, ISSP (Hefei, China), Government of Russian Federation, and Foreign Talents Introduction and Academic Exchange Program. Use of the Advanced Photon Source was supported by the U. S. Department of Energy Office of Science

**12:03PM F20.00003 ABSTRACT WITHDRAWN –**

**12:15PM F20.00004 A possible analog to  $\text{MgB}_2$ : Discovery of a predicted layered LiB via cold compression**<sup>1</sup>, ALEKSEY KOLMOGOROV, SAMAD HAJINAZAR, CHRIS ANGYAL, Binghamton University, VLADIMIR KUZNETZOV, University of Oxford, ANDREW JEPHCOAT, Okayama University — Stoichiometric LiB has been previously predicted [1,2] to be a new synthesizable layered material with electronic and vibrational properties desired for  $\text{MgB}_2$ -type superconductivity. However, previous experiments showed no signs of the proposed compound forming under high pressures. We report on the synthesis of the LiB via cold compression in the diamond anvil cell [3]. Remarkably, the signature powder XRD peak from the new layered compound appeared above 21 GPa and remained visible down to ambient pressure upon sample quenching. Apparent stacking disorder in LiB and a stoichiometry shift in the starting  $\text{LiB}_y$  (from  $y \approx 0.90$  down to  $y \approx 0.75$ ) made material characterization a challenge. *Ab initio* modeling allowed us to establish the pressure-dependent composition of  $\text{LiB}_y$  and predict related stable structures overlooked in previous studies. [1] A.N. Kolmogorov and S. Curtarolo, Phys. Rev. B 74, 224507 (2006) [2] A.N. Kolmogorov and S. Curtarolo, Phys. Rev. B 73, 180501(R) (2006) [3] A.N. Kolmogorov, S. Hajinazar, C. Angyal, V.L. Kuznetsov, and A.P. Jephcoat, Phys. Rev. B 92, 144110 (2015)

<sup>1</sup>Supported by NSF Grant DMR-1410514

**12:27PM F20.00005 Discovering new materials and new phenomena with evolutionary algorithms**, ARTEM OGANOV, Skolkovo Institute of Science and Technology — Thanks to powerful evolutionary algorithms, in particular the USPEX method, it is now possible to predict both the stable compounds and their crystal structures at arbitrary conditions, given just the set of chemical elements. Recent developments include major increases of efficiency and extensions to low-dimensional systems and molecular crystals (which allowed large structures to be handled easily, e.g.  $\text{Mg}(\text{BH}_4)_2$  and  $\text{H}_2\text{O}-\text{H}_2$ ) and new techniques called evolutionary metadynamics and Mendelevian search. Some of the results that I will discuss include: 1. Theoretical and experimental evidence for a new partially ionic phase of boron,  $\gamma$ -B and an insulating and optically transparent form of sodium. 2. Predicted stability of “impossible” chemical compounds that become stable under pressure – e.g.  $\text{Na}_3\text{Cl}$ ,  $\text{Na}_2\text{Cl}$ ,  $\text{Na}_3\text{Cl}_2$ ,  $\text{NaCl}_3$ ,  $\text{NaCl}_7$ ,  $\text{Mg}_3\text{O}_2$  and  $\text{MgO}_2$ . 3. Novel surface phases (e.g. boron surface reconstructions). 4. Novel dielectric polymers, and novel permanent magnets confirmed by experiment and ready for applications. 5. Prediction of new ultrahard materials and computational proof that diamond is the hardest possible material.

**1:03PM F20.00006 Structural study of superconducting sulfur hydride under high pressure**<sup>1</sup>, KATSUYA SHIMIZU, MARI EINAGA, MASAFUMI SAKATA, HARUSHIGE NAKAO, Osaka Univ, MIKHAIL EREMETS, ALEXANDER DROZDOV, IVAN TROYAN, MPI Chem, NAOHISA HIRAO, YASUO OHISHI, JASRI/SPRING-8, KYOKUGEN, GRADUATE SCHOOL OF ENGINEERING SCIENCE, OSAKA UNIVERSITY TEAM, MAX PLANCK INSTITUTE FOR CHEMISTRY TEAM, JASRI/SPRING-8 TEAM — Superconductivity exceeding 200 K was recently reported in the highly compressed hydrogen sulfide [1]. The superconductor was found to be synthesized by pressure above 90 GPa under low temperature exceeding 200 K. Here we report our high-pressure structural studies for  $\text{H}_2\text{S}$  and  $\text{D}_2\text{S}$  using a synchrotron x-ray at room temperature and low temperature [2]. The sample at 10 GPa was firstly cooled down to 200 K and compressed up to 150 GPa, then cooled down to 10 K. The resistivity and diffraction patterns were monitored at all procedures. The critical temperature and zero resistivity were confirmed. The x-ray diffraction data in both cells showed good agreement with the theoretically predicted structures [3].

<sup>1</sup>This work was supported by JSPS KAKENHI Grant Number 26000006 and the European Research Council 2010-Advanced Grant 267777

**1:15PM F20.00007 High –Pressure Synthesis and Characterization of Incompressible Titanium Pernitride**<sup>1</sup>, VENKATA BHADRAM, DUCK YOUNG KIM, TIMOTHY STROBEL, Carnegie Institution of Washington — We report the discovery of a new transition-metal pernitride,  $\text{TiN}_2$ , which was synthesized by reacting  $\text{TiN}$  with  $\text{N}_2$  at 73GPa in a laser-heated diamond anvil cell (DAC). Our *in situ* pressure dependent x-ray diffraction studies suggest that  $\text{TiN}_2$  is recoverable at ambient conditions in a crystal structure that contains single bonded nitrogen units ( $\text{N}_2$  dumbbells) embedded in the metal lattice and exhibits high bulk modulus (in the range 360-385 GPa) which is usually observed in superhard materials. We have performed *ab initio* calculations to understand the electronic properties and bonding nature in  $\text{TiN}_2$  and thereby elucidate the origin of incompressible behavior of this material which is rooted in the nearly filled anti-bonding states of the pernitride units. Although, study of transition metal pernitrides has been an active area of research for quite some time, most of the pernitrides synthesized so far are belong to noble metal group. To our knowledge, this is the first experimental report on  $\text{TiN}_2$  which is the only light metal pernitride exhibiting bonding-mechanical property relation that is usually seen in heavy metal pernitrides.

<sup>1</sup>This work was supported by Energy Frontier Research in Extreme Environments (EFree) Center, an Energy Frontier Research Center funded by the US Department of Energy, Office of Science under award No. DE-SC0001057.

**1:27PM F20.00008 Electride-like phases at extreme compression and elevated temperatures**<sup>1</sup>, STANIMIR BONEV, Lawrence Livermore National Laboratory, JONATHAN DUBOIS, Lawrence Livermore National Laboratory, Livermore, CA 94550 — The transformation of materials into electride-like structures under the application of extreme pressure has attracted a lot of interest recently. Theoretical studies have predicted the existence of low-coordinated crystal phases, where the conduction electrons are localized in the interstitial atomic regions, for a number of elements at high density. Most of these works have been limited to static lattice calculations. The pressures where such transformations are projected to occur are accessible in shock-wave experiments, but at elevated temperatures. In this talk I will discuss the temperature dependence of electride structures, both solids and liquids, as well as the requirements for their accurate simulation.

<sup>1</sup>This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344

**1:39PM F20.00009 The effects of hydrogenation and high pressure on  $\alpha$ -tetragonal boron: a first principles study**, NAOKI UEMURA, KOUN SHIRAI, ISIR, Osaka University — It is well known that boron rich crystals are superhard materials.  $\alpha$ -tetragonal ( $\alpha$ -tet) boron is one of the metastable phase in elemental boron crystals under high temperature and high pressure. This phase has a possibility of including some hydrogen atoms due to the experimental process, but it has not yet been shown crystal structures and electronic properties of hydrogenated  $\alpha$ -tet boron. Using first-principles calculations, we theoretically predicted stable structures and investigated the influences from hydrogenation of  $\alpha$ -tet boron and high pressures. According to our calculations, non-bonding states of pure  $\alpha$ -tet boron, which were mostly occupied by  $P_z$  like orbitals coming from interstitial boron atoms in  $\alpha$ -tet boron, were completely vanished by doping some hydrogen atoms and the higher the pressure was, the larger energy gaps between the valence band maximum and the conduction band minimum on  $\alpha$ -tet boron were. These results provide that the deformation potential depended on the pressure is positive, which is basically negative on semiconductors except for diamonds and is an index of the hardness under pressure on semiconductors.

**1:51PM F20.00010 Creation and formation mechanism of new carbon phases constructed by amorphous carbon.**<sup>1</sup>, MINGGUANG YAO, WEN CUI, BINGBING LIU, State Key Laboratory of Superhard Materials, Jilin University — Our recent effort is focusing on the creation of new hard/superhard carbon phases constructed by disordered carbons or amorphous carbon clusters under high pressure. We showed that the pressure-induced amorphous hard carbon clusters from collapsed fullerenes can be used as building blocks (BBs) for constructing novel carbon structures. This new strategy has been verified by compressing a series of intercalated fullerenes, pre-designed by selecting various dopants with special features. We demonstrate that the boundaries of the amorphous BBs are mediated by intercalated dopants and several new superhard materials have been prepared. We also found that the dopant-mediated BBs can be arranged in either ordered or disordered structures, both of which can be hard enough to indent the diamond anvils. The hardening mechanisms of the new phases have also been discussed. For the glassy carbon (GC) constructed by disordered fullerene-like nanosized fragments, we also found that these disordered fragments can bond and the compressed GC transformed into a transparent superhard phase. Such pressure-induced transformation has been discovered to be driven by a novel mechanism (unpublished). By understanding the mechanisms we can clarify the controversial results on glassy carbon reported recently.

<sup>1</sup>The authors would like to thank the financial support from the National Natural Science Foundation of China (No. 11474121, 51320105007).

**2:03PM F20.00011 First-principles study of MoHn (n=1, 2 and 3) crystal structures under high pressure**, XIAOLEI FENG, JURONG ZHANG, Jilin University, HANYU LIU, Carnegie Institution of Washington, HUI WANG, Jilin University — Hydrogen-rich materials have attracted attention recently, owing to their fascinating chemical bonding and potential high superconducting critical temperatures temperature. Inspired by the recent identification of polyhydrides of d metals and molybdenum hydride molecules with a high H content, we explored the crystal structures of MoHn (n = 1, 2, and 3) under high pressures using particle swarm optimization combined with first-principles electronic structure calculations. Several novel structures of MoH2 and MoH3 are predicted at high pressures. MoH is calculated to be stable at ambient pressure; at  $P > 2.3$  GPa the hexagonal phase of MoH2 becomes stable, and at 24 GPa it transforms into an orthorhombic structure, which remains stable up to 100 GPa. All three stable structures show metallic behavior under pressure. The calculated electronic properties suggest that the d-orbitals of the Mo atoms provide the dominant contribution to the density of states at the Fermi level, which is different from the density of states previously predicted for H-rich materials. The present results offer insights in understanding of chemical and physical properties in hydrogen-rich materials, especially in extreme environments.

**Tuesday, March 15, 2016 11:15AM - 2:15PM —**

**Session F21 GMAG DMP: Molecular Nanomagnets** 320 - Andrew Kent, New York University

**11:15AM F21.00001 Coherent manipulation of quantum spin states in a single molecular nano-magnet**, WOLFGANG WERNSDORFER, Institut Neel, CNRS, Grenoble — The endeavour of quantum electronics is driven by one of the most ambitious technological goals of today's scientists: the realization of an operational quantum computer (<http://quroupe.eu>). We started to address this goal by the new research field of molecular quantum spintronics. The building blocks are magnetic molecules, i.e. well-defined spin qubits. We will discuss this still largely unexplored field and present our first results: For example, using a molecular spin-transistor, we achieved the electronic read-out of the nuclear spin of an individual metal atom embedded in an SMM. We could show very long spin lifetimes ( $>10$  s). Using the hyperfine Stark effect, which transforms electric fields into local effective magnetic fields, we could not only tune the resonance frequency by several MHz, but also perform coherent quantum manipulations on a single nuclear qubit faster than a  $\mu$ s by means of electrical fields only, establishing the individual addressability of identical nuclear qubits. Using three different microwave frequencies, we could implement a simple four-level Grover algorithm. S. Thiele, F. Balestro, R. Ballou, S. Klyatskaya, M. Ruben, W. Wernsdorfer, Science 344, 1135 (2014).

**11:51AM F21.00002 Landau-Zener in a continuously measured molecular spin**, FILIPPO TROIANI, Istituto Nanoscienze, CNR (Italy), MARCO AFFRONTI, Universit di Modena e Reggio Emilia (Italy), STEPHAN THIELE, CLEMENT GODFRIN, FRANCK BALESTRO, WOLFGANG WERNSDORFER, Institut Nel, CNRS (France), SVETLANA KLYATSKAYA, MARIO RUBEN, Karlsruhe Institute of Technology (Germany) — The dynamics of a quantum system driven through an avoided level crossing represents a relevant problem in many physical contexts. Here we present a joint theoretical and experimental investigation of a single-molecule magnet (namely, a terbium double-decker complex) in a three-terminal geometry. The Tb spin is driven through an avoided level crossing by a time-dependent magnetic field, and its dynamics is monitored through a continuous measurement of the conductance. The dependence of the spin-reversal probability on the field sweeping rate presents clear deviations from the Landau-Zener formula, which applies to the case of closed systems. The comparison between direct and inverse Landau-Zener transitions points at the dominance of dephasing, with respect to inelastic incoherent processes. The spin dynamics is simulated within a master equation approach. The observed behaviors are reproduced by assuming that dephasing takes place in the basis of the time-dependent Hamiltonian eigenstates. The spin dephasing is traced back to the continuous measurement of the electron spin, and a fundamental role is played by the finite time resolution of the conductance measurement.

**12:03PM F21.00003 Magnetic hysteresis in a lanthanide molecular magnet dimer system<sup>1</sup>**, JAMES ATKINSON, REBECCA CEBULKA, ENRIQUE DEL BARCO, University of Central Florida, Physics Department, Orlando, FL, USA, OLIVIER ROUBEAU, Instituto de Ciencia de Materiales de Aragn (ICMA), CSIC and Universidad de Zaragoza, Zaragoza, Spain, VERONICA VELASCO, LEO BARRIOS, GUILLLEM AROMI, Universitat de Barcelona, Departament de Quimica Inorganica, Barcelona, Spain — Molecular magnets present a wonderful means for studying the dynamics of spin. Often synthesized as a crystal lattice of identical systems, ensemble measurements enable thorough detailing of the internal degrees of freedom. Here we present the results of characterization performed on a dimer system,  $\text{CeTm}(\text{HL})_2(\text{H}_2\text{L})\text{NO}_3\text{pyH}_2\text{O}$  (L = ligand,  $\text{C}_{45}\text{H}_{31}\text{O}_{15}\text{N}_3$ ), consisting of two lanthanide spins (Cerium and Thulium) with expected local axial anisotropies tilted with respect to each other. Microwave EPR spectroscopy at low temperature reveals hysteresis in observed absorption features, with angle dependence studies indicating the presence of several easy axis orientations. We attempt to understand this system through modelling via a spin Hamiltonian, and to determine the strength and nature of the coupling between the lanthanide centers.

<sup>1</sup>This research was funded through NSF Grant 24086159

**12:15PM F21.00004 Search for giant magnetic anisotropy in transition-metal dimers on defected hexagonal boron nitride sheet<sup>1</sup>**, JIE LI, State Key Lab. of Surface Physics, Key Lab. of Computational Physical Sciences, and Dept. of Physics, Fudan Univ., HUI WANG, Dept. of Physics and Astronomy, Univ. of California, JUN HU, College of Physics, Optoelectronics and Energy, Soochow Univ., RUQIAN WU, Dept. of Physics and Astronomy, Univ. of California — For a magnetic units at the nanometer scale, one of the most important issues is how to hold thermal fluctuation of its magnetization, i.e., how to enhance its blocking temperature ( $T_{\text{B}}^{\text{B}}\text{s}$ ) to above 300K. Through systematic density functional calculations, the structural stability and magnetic properties of many transition-metal dimers embedded in a defected hexagonal boron nitride monolayer are investigated. We find twelve cases that may have magnetic anisotropy energies (MAEs) larger than 30 meV. In particular, Ir-Ir@Dh-BN has both large MAE ( $\sim 126$  meV) and high structural stability, which makes it a promising candidate of magnetic unit in spintronics and quantum computing devices.

<sup>1</sup>Work at Fudan was supported by the Chinese National Science Foundation (11474056) and National Basic Research Program of China (2015CB921400). Work at UCI was supported by DOE-BES (Grant No. DE-FG02-05ER46237).

**12:27PM F21.00005 Molecular Magnetism in MnTe Clusters<sup>1</sup>**, JIA CHEN, Department of Applied Physics, Columbia University, ARUN NANDURI, BONNIE CHOI, Department of Chemistry, Columbia University, ANDREW MILLIS, Department of Physics, Columbia University, DAVID REICHMAN, XAVIER ROY, Department of Chemistry, Columbia University — Electron correlation in recently synthesized molecular clusters with  $\text{Mn}_4\text{Te}_4$  cores in cubane structures and ligand exteriors are studied experimentally and theoretically. We used density functional theory with on-site Coulomb interactions (DFT+U) to construct effective spin Hamiltonians and estimate the dependence of parameters on choice of ligand. The lack of inversion symmetry combined with the heavy tellurium ions leads to a significant Dzyaloshinskii-Moriya (DM) interaction. Comparison of measurements to the magnetic susceptibility calculated from the spin model is used to validate the results. We also extend this work to more complex clusters with more than one cubanes, where interesting high-spin ground state may occur. It has been measured recently,  $\text{Fe}_8\text{Te}_8$  in dicubane structure has ground state with magnetization of  $12\mu_B$ , which makes it promising candidate for single molecular magnets.

<sup>1</sup>A.J.M. acknowledges support from NSF under contract DMR-1308236. J.C. is supported by the NSF MRSEC program through Columbia in the Center for Precision Assembly of Superstratic and Superatomic Solids under Grant No.DMR-1420634.

**12:39PM F21.00006 Spin-Valve Effect at Organic-Ferromagnetic Interfaces**, NICOLAE ATODIRESEI, VASILE CACIUC, STEFAN BLÜGEL, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — The ability to reliably describe the electronic properties of carbon-based materials adsorbed on magnetic surfaces is essential to understand and assist the engineering of functionalities in hybrid organic spintronic devices. Based on the density functional theory, we performed theoretical studies [1-4] to understand how to tailor the magnetic properties of hybrid organic-ferromagnetic interfaces by adsorbing organic materials containing  $\pi$ -electrons onto several magnetic substrates. For such hybrid systems, the magnetic properties like molecular magnetic moments and their spatial orientation, spin-polarization and the magnetic exchange coupling can be specifically tuned by an appropriate choice of the organic material. \*Email: n.atodiresei@fz-juelich.de [1] N. Atodiresei et al., MRS Bulletin 39, 596 (2014). [2] J. Brede et al., Nat. Nanotech. 9, 1018 (2014). [3] K. V. Raman et al., Nature 493, 509 (2013). [4] M. Callsen et al., Phys. Rev. Lett. 111, 106805 (2013).

**12:51PM F21.00007 Magnetic dipole-dipole sensing at atomic scale using electron spin resonance STM**, T. CHOI, W. PAUL, IBM Almaden Research, S. ROLF-PISSARCZYK, Max Planck Institute, Germany, A. MACDONALD, U. of British Columbia, Canada, K. YANG, Chinese Academy of Sciences, F.D. NATTERER, EPFL, Switzerland, C.P. LUTZ, A.J. HEINRICH, IBM Almaden Research — Magnetometry having both high magnetic field sensitivity and atomic resolution has been an important goal for applications in diverse fields covering physics, material science, and biomedical science. Recent development of electron spin resonance STM (ESR-STM) promises coherent manipulation of spins and studies on magnetic interaction of artificially built nanostructures, leading toward quantum computation, simulation, and sensors. In ESR-STM experiments, we find that the ESR signal from an Fe atom underneath a STM tip splits into two different frequencies when we position an additional Fe atom nearby. We measure an ESR energy splitting that decays as  $1/r^3$  ( $r$  is the separation of the two Fe atoms), indicating that the atoms are coupled through magnetic dipole-dipole interaction. This energy and distance relation enables us to determine magnetic moments of atoms and molecules on a surface with high precision in energy. Unique and advantageous aspects of ESR-STM are the atom manipulation capabilities, which allow us to build atomically precise nanostructures and examine their interactions. For instance, we construct a dice *cinque* arrangement of five Fe atoms, and probe their interaction and energy degeneracy. We demonstrate the ESR-STM technique can be utilized for quantum magnetic sensors.

**1:03PM F21.00008 ABSTRACT WITHDRAWN —**

**1:15PM F21.00009 Spin blockade effect in single-molecule transistors<sup>1</sup>**, GUANGPU LUO, KYUNGWHA PARK, Virginia Tech, Blacksburg, Virginia — Recently single-molecule transistors consisting of individual single-molecule magnets trapped between electrodes have been experimentally realized and electron transport properties through individual single-molecule magnets have been measured. For a single-molecule magnet the  $(2S+1)$ -fold degeneracy of magnetic levels in a given spin multiplet is lifted even in the absence of external magnetic field, due to the magnetic anisotropy induced by spin-orbit coupling. This anisotropic nature of single-molecule magnets allowed one to discover interesting, unexpected transport properties. A recent theoretical study showed that an Eu-based anisotropic magnetic molecule can switch its magnetic anisotropy between magnetic easy plane and easy axis upon varying the charge state of the molecule. Motivated by this report, we investigate how this switch of magnetic anisotropy influences the electron transport through the molecule, by considering sequential electron tunneling. We calculate current-voltage characteristics by solving the master equation based on the model Hamiltonians. We explore this interesting effect in the absence and presence of external magnetic field.

<sup>1</sup>Funding from NSF DMR-1206354.

**1:27PM F21.00010 Hybrid quantum systems with YBCO coplanar resonators and spin ensembles of organic radicals**, ALBERTO GHIRRI, Istituto Nanoscienze - CNR, Centro S3, via Campi 213/a, 41125 Modena, Italy, CLAUDIO BONIZZONI, Dipartimento FIM, Università di Modena e Reggio E. and Istituto Nanoscienze - CNR, via Campi 213/a, 41125 Modena, Italy, FILIPPO TROIANI, Istituto Nanoscienze - CNR, via Campi 213/a, 41125 Modena, Italy, ANTONIO CASSINESE, CNR-SPIN and Dipartimento di Fisica, Università di Napoli Federico II, 80138 Napoli, Italy, MASSIMILIANO D'ARIENZO, LUCA BEVERINA, Department of Materials Science State University of Milano-Bicocca Via Cozzi 55 I-20125 Milano, Italy, MARCO AFFRONTI, Dipartimento FIM, Università di Modena e Reggio E. and Istituto Nanoscienze - CNR, via Campi 213/a, 41125 Modena, Italy — We have studied the coherent coupling of microwave photons in a superconducting coplanar resonator with a spin ensemble of stable open-shell organic radicals. We fabricated YBCO/sapphire coplanar resonators that show quality factors  $\simeq 3 \cdot 10^4$  at 1.8 K, that remain remarkably stable in high magnetic field applied parallel to the YBCO film [QL (7 T) = 90% QL (0 T)] [1]. Spin ensembles of (3,5-Dichloro-4-pyridyl)bis(2,4,6-trichlorophenyl)methyl organic radical (PyBTM) show sharp EPR linewidth (8 MHz) due to the effect of the exchange narrowing. The frequency of the spin transition is tuned by means of the external magnetic field. We show the achievement of the strong collective coupling with the resonant photons with coupling rates exceeding 90 MHz at 1.8 K. [1] A. Ghirri, C. Bonizzoni, D. Gerace, S. Sanna, A. Cassinese and M. Affronte, Appl. Phys. Lett. 106, 184101 (2015).

**1:39PM F21.00011 First-principles study on magnetism of Ru monolayer under an external electric field**, YUKIE KITAOKA, HIROSHI IMAMURA, AIST, Spintronics Research Center — Electric field control of magnetic properties such as magnetic moment and magnetic anisotropy has been attracted. For the  $4d$  TM films, on the other hand, it was recently reported that the ferromagnetism Pd thin-film is induced by application of an external electric field otherwise Pd thin-film shows paramagnetic [1]. However, little attention has been paid to the magnetism of other  $4d$  TMs. Here, we investigate the magnetism of the free-standing Ru monolayer and that on MgO(001) substrate under an external electric field by using first-principles FLAPW method [2]. We found that the free-standing Ru monolayer is ferromagnet with magnetic moment of  $1.50 \mu_B/\text{atom}$ . The MA energy is 3.45 meV/atom, indicating perpendicular MA, at zero electric field ( $E=0$ ) and increases up to 3.84 meV/atom by application of  $E=1$  (V/Å). The Ru monolayer on MgO(001) substrate is also ferromagnet with magnetic moment of  $0.89 \mu_B/\text{atom}$ . The MA energy is 1.49 meV/atom, indicating perpendicular MA, at  $E=0$  and decreases to 1.33 meV/atom by application of  $E=1$  (V/Å). [1] Y. Sun, J. D. Burton, E. Y. Tsymlal, PRB 81, 064413 (2010). [2] K. Nakamura, T. Ito, A. J. Freeman, L. Zhong, J. Fernandez-de-Castro, PRB, 67, 014420 (2003).

**1:51PM F21.00012 Chemically Controllable Ferromagnetic Graphene for High-Performance Spintronic Devices**, JEONGMIN HONG, UC Berkeley — The spin and charge of the electron when taken together, offer many opportunities for the creation of new information processing and storage devices applications with ultralow power consumption. Chemically controllable growth of large area nanocarbon structures has attracted considerable interests due to their superior properties. If large area nanocarbon could have by-design magnetic properties, multifunctional electronic devices could be built through modulation controlled by external factors such as 1) functionalization onto basal plane of carbon, 2) substrate effects (proximity induced ferromagnetism), and 3) external electric field. We performed soft X-ray measurement techniques using X-ray magnetic circular dichroism (XMCD) and revealed the controllable ferromagnetic properties on graphene structures. The chemically controllable nanomagnet would be an excellent building block for the applications of graphene-based high-performance spintronic devices.

**2:03PM F21.00013 Energy gap of Graphene Nanoflakes: Edge Magnetism and Self-Energy Corrections.** , ROMEO DE COSS GOMEZ, CARLOS MANUEL RAMOS CASTILLO, Departement of applied physics centro de investigacion y de estudios avanzados del instituto politecnico nacional — Previous theoretical works has predicted that graphene nanostructures with zigzag edge exhibit metallic behavior around 6-7 nm, however in such calculations the magnetic nature of zigzag edges was not considered. In this work, the influence of the edge magnetism on the size dependence of energy-gap in hexagonal graphene nanoflakes (GNFs) with zigzag borders is studied by density functional theory calculations. Thus, we found that meanwhile the calculations without spin polarization predicts that the metallic behaviour for GNFs begin at 6 nm deviating from the trend predicted for effective model of Dirac fermions, spin-polarized calculations predicts semiconducting behavior at 6 nm. This result shows clearly that the origin of metallic behaviour predicted at 6 nm in previous works is not related with the well known band-gap problem of Kohn-Sham scheme, but with neglecting spin polarization. Furthermore, to correct the band-gap problem of Kohn-Sham Scheme, we have calculated the size dependence of fundamental energy-gap using the quasiparticle formalism by adding/removing an electron to/from the system.

**Tuesday, March 15, 2016 11:15AM - 2:15PM –**  
**Session F22 DCOMP: Theory and Simulation of Excited-State Phenomena in Semiconductors and Nanostructures II** 321 - Emmanouil Kioupakis, University of Michigan

**11:15AM F22.00001 Hot Electron Dynamics at Semiconductor-Molecule Interfaces: Insights from First-Principles Dynamics Simulation** , YOSUKE KANAI, University of North Carolina at Chapel Hill — Quantum dynamics of excited electrons is fundamental to functionalities of semiconductor-molecule interfaces that are an integral part of various solar energy conversion and opto-electronic technologies. Thus, developing a predictive and quantitative understanding of the electron dynamics at the atomistic level for such complex interfaces is of great interest. In this talk, I will discuss our recent effort on addressing several challenges in understanding how atomistic features such as surface defects influence these electron dynamical processes. We tackle this problem theoretically by employing a first-principles simulation approach that synergistically combine fewest switches surface hopping, many-body perturbation theory, and first-principles molecular dynamics. New findings from the first-principles simulation will be discussed in the context of a larger effort within Solar Fuels EFRC at UNC Chapel Hill. I will also discuss how the results from atomistic theories pose a conceptual challenge when characterizing these interfacial electron processes for these complex interfaces using a simple kinetic model.

**11:51AM F22.00002 Nonadiabatic dynamics with spin-orbit couplings** , GLORIA CAPANO, 2Laboratory of ultrafast spectroscopy, Ecole Polytechnique Fédérale de Lausanne, Lausanne, 1015, Switzerland., FELIPE FRANCO DE CARVALHO, 1Centre Européen de Calcul Atomique et Moléculaire, Lausanne, 1015, Switzerland., IVANO TAVERNELLI, IBM Research Zurich, 8803 Rüschlikon, Switzerland. — In this talk I will present some recent advances in TDDFT-based nonadiabatic dynamics for molecular systems using Tully's surface hopping. In particular, I will describe a method for the efficient simulation of intersystem crossing events, which requires the on-the-fly calculation of spin-orbit coupling matrix elements along the trajectories. This approach will be applied to the study of the photophysics of metal-organic complexes in solution and of different carbon nanostructures including graphene nanoflakes and nanotubes with different wrapping topologies.

**12:03PM F22.00003 Real-time TDDFT simulations of time-resolved core-level spectroscopies in solid state systems.** , SRI CHAITANYA DAS PEMMARAJU, DAVID PRENDERGAST, Lawrence Berkeley National Laboratory, THEORY OF NANOSTRUCTURED MATERIALS FACILITY TEAM — The advent of sub-femtosecond time-resolved core-level spectroscopies based on high harmonic generated XUV pulses has enabled the study of electron dynamics on characteristic femtosecond time-scales. Unambiguous interpretation of these powerful yet complex spectroscopies however requires the development of theoretical algorithms capable of modeling light-matter interaction across a wide energy range spanning both valence and core orbitals. In this context we present a recent implementation of the velocity-gauge formalism of real-time TDDFT [1] within a linear combination of atomic orbital (LCAO) framework, which facilitates efficient numerical treatment of localized semi-core orbitals. Dynamics and spectra obtained from LCAO based simulations are compared to those from a real-space grid implementation [1]. Potential applications are also illustrated by applying the method towards interpreting recent atto-second time-resolved IR-pump XUV-probe spectroscopies investigating sub-cycle excitation dynamics in bulk silicon [2].  
[1] Yabana et al., Phys. Rev. B 85, 045134 (2012)  
[2] Schultze et al., Science, 346, 1348 (2014)

**12:15PM F22.00004 Long-range dispersion forces between molecules subject to attosecond pulses from ab initio calculations** , MICAEL OLIVEIRA, Department of Physics, University of Liege, Belgium, KSENIA KOMAROVA-VLADIMIROVA, FRANCOISE REMACLE, Department of Chemistry, University of Liege, Belgium, MATTHIEU VERTRAETE, Department of Physics, University of Liege, Belgium — The London-van der Waals dispersion forces arising from instantaneously induced dipoles in molecules are a key ingredient in a wide range of phenomena in physics, chemistry, and biology. Therefore, the ability to control and manipulate dispersion forces between atoms and molecules is of great importance. Because those dispersion interactions depend crucially on the electronic properties of the molecular systems, a simple route to achieve this would consist in manipulating their electronic states. The recent development of ultra-short optical pulses has given researchers unprecedented control over the electronic degrees of freedom. These pulses, tailored in their frequency and envelope, allow the generation of a strongly out of equilibrium population of electronic states. In this talk we show how the Hamacker constants characterizing the London-van der Waals interaction between two molecules subject to an optical pulse can be calculated using time-dependent density functional theory (TD-DFT) or standard quantum chemistry methods and present several test cases of molecules subjected to IR and UV attosecond pulses.

**12:27PM F22.00005 Nonequilibrium Green's Function approach to time-resolved photoabsorption<sup>1</sup>** , GIANLUCA STEFANUCCI, ENRICO PERFETTO, University of Rome Tor Vergata, ANNA-MAIJA UIMONEN, ROBERT VAN LEEUWEN, University of Jyväskylä — We propose a nonequilibrium Green's function (NEGF) approach to calculate the time-resolved absorption spectrum of nanoscale systems [1]. We can deal with arbitrary shape, intensity, duration and relative delay of the pump and probe fields and include ionization processes as well as hybridization effects due to surfaces. We present numerical simulations of atomic systems using different approximate self-energies and show that electron correlations are pivotal to reproduce important qualitative features. [1] E. Perfetto, A.-M. Uimonen, R. van Leeuwen and G. Stefanucci, Phys. Rev. A 92, 033419 (2015) [2] E. Perfetto, D. Sangalli, A. Marini and G. Stefanucci, Phys. Rev. B, accepted

<sup>1</sup>E.P. and G.S. acknowledge funding by MIUR FIRB Grant No. RBFR12SW0J. R.v.L. thanks the Academy of Finland for support.

**12:39PM F22.00006 AB INITIO DYNAMICS OF AN ELECTRON INTERACTING WITH A LATTICE DEFECT**, VSEVOLOD IVANOV, MARCO BERNARDI, California Institute of Technology, Pasadena, California 91125. — We study the scattering process of a charge carrier with a defect in a range of bulk and 2D materials. The scattering potential is obtained using density functional theory, the carrier is represented by a gaussian wavepacket, and the dynamics is carried out with a split-operator technique. Our parallel code can model the electron-defect scattering processes in real space and time, with an electron wavepacket of realistic size (100 - 1000 unit cells) and an accuracy typical of ab initio calculations. We apply our approach to model a carrier scattering with a vacancy in silicon and an impurity in monolayer MoS<sub>2</sub>, obtaining angular dependent scattering cross sections and resonant states.

**12:51PM F22.00007 Real-Time Time-Dependent DFT Study of Electronic Stopping in Semiconductors under Proton Irradiation**, DILLON C. YOST, KYLE G. REEVES, YOSUKE KANAI, University of North Carolina - Chapel Hill — Understanding the detailed mechanisms of how highly energetic charged particles transfer their kinetic energy to electronic excitations in materials has become an important topic in various technologies ranging from nuclear energy applications to integrated circuits for space missions. In this work, we use our new large-scale real-time time-dependent density functional theory simulation [1] to investigate details of the ion-velocity-dependent dynamics of electronic excitations in the electronic stopping process. In particular, we will discuss how point defects in semiconductor materials influence the electronic stopping process under proton irradiation, using silicon carbide (3C-SiC) as a representative material due to its great technological importance. Additionally, we will provide atomistic insights into existing analytical models that are based on the plane-wave Born approximation by examining velocity-dependence of the projectile charge from first-principles simulations. [1] “Quantum Dynamics Simulation of Electrons in Materials on High-Performance Computers” A. Schleife, E. W. Draeger, V. Anisimov, A. A. Correa, Y. Kanai, Computing in Science and Engineering, 16 (5), 54 (2014).

**1:03PM F22.00008 Semiconductors Under Ion Radiation: Ultrafast Electron-Ion Dynamics in Perfect Crystals and the Effect of Defects**, CHENG-WEI LEE, ANDRÉ SCHLEIFE, University of Illinois at Urbana-Champaign — Stability and safety issues have been challenging difficulties for materials and devices under radiation such as solar panels in outer space. On the other hand, radiation can be utilized to modify materials and increase their performance via focused-ion beam patterning at nano-scale. In order to grasp the underlying processes, further understanding of the radiation-material and radiation-defect interactions is required and inevitably involves the electron-ion dynamics that was traditionally hard to capture. By applying Ehrenfest dynamics based on time-dependent density functional theory, we have been able to perform real-time simulation of electron-ion dynamics in MgO and InP/GaP. By simulating a high-energy proton penetrating the material, the energy gain of electronic system can be interpreted as electronic stopping power and the result is compared to existing data. We also study electronic stopping in the vicinity of defects: for both oxygen vacancy in MgO and interface of InP/GaP superlattice, electronic stopping shows strong dependence on the velocity of the proton. To study the energy transfer from electronic system to lattice, simulations of about 100 femto-seconds are performed and we analyze the difference between Ehrenfest and Born-Oppenheimer molecular dynamics.

**1:15PM F22.00009 Role of non-adiabatic carrier dynamics in non-thermal phase transition of Ge-Sb-Te alloy**, JUNHYEOK BANG, Korea Basic Science Institute (KBSI), YIYANG SUN, X.-Q. LIU, Rensselaer Polytechnic Institute (RPI), F. GAO, University of Michigan, S. B. ZHANG, Rensselaer Polytechnic Institute (RPI) — Non-thermal phase transition driven by femtosecond laser irradiation has been explained by the simple static plasma annealing effect: excitation of a large fraction of valence electrons to conduction bands weakens lattices and leads to the structural phase transition in low temperature. Here, by time-dependent density functional theory and molecular dynamics study of Ge-Sb-Te alloys, we find that the energy-dependent dynamics of excited carriers is critical in determining the phase transition mechanism. For low energy carriers electron-phonon scattering becomes a dominant relaxation process, and for high energy carriers electron-electron scattering remains a dominant relaxation process. As a result, we observe significant ionic temperature increase for low energy excitation, which aids phase transition by thermal effect, and non-thermal phase transition for high energy excitation. This provides a new conceptual framework in understanding fundamental phenomenon of the phase transition.

**1:27PM F22.00010 Optimal ultrafast laser pulse-shaping to direct photo-induced phase transitions**, BIN HWANG<sup>1</sup>, JENNI PORTMAN, PHILLIP DUXBURY<sup>2</sup>, Michigan State University — Photo-induced phase transitions (PIPT) in quantum and/or complex materials are the epitome of challenging non-equilibrium many-body phenomena, that also have a wide range of potential applications. We present a computational approach to finding optimal ultrafast laser pulse shapes to control the outcome of pump-probe PIPT experiments. The Krotov approach for optimal control is combined with a Keldysh Green's function calculation to describe experimental outcomes such as photoemission, transient single particle density of states and optical responses. Results for a simple model charge density wave system will be presented.

<sup>1</sup>main author

<sup>2</sup>Advisor

US Army Research Laboratory, Aberdeen Proving Ground, MD

US Army Research Laboratory, Aberdeen Proving Ground, MD

**1:39PM F22.00011 Multiphysics modeling of non-linear laser-matter interactions for optically active semiconductors**<sup>1</sup>, BRENT KRACZEK, JAROSLAW KANP, US Army Research Laboratory — Development of photonic devices for sensors and communications devices has been significantly enhanced by computational modeling. We present a new computational method for modelling laser propagation in optically-active semiconductors within the paraxial wave approximation (PWA). Light propagation is modeled using the Streamline-upwind/Petrov-Galerkin finite element method (FEM). Material response enters through the non-linear polarization, which serves as the right-hand side of the FEM calculation. Maxwell's equations for classical light propagation within the PWA can be written solely in terms of the electric field, producing a wave equation that is a form of the advection-diffusion-reaction equations (ADREs). This allows adaptation of the computational machinery developed for solving ADREs in fluid dynamics to light-propagation modeling. The non-linear polarization is incorporated using a flexible framework to enable the use of multiple methods for carrier-carrier interactions (e.g. relaxation-time-based or Monte Carlo) to enter through the non-linear polarization, as appropriate to the material type. We demonstrate using a simple carrier-carrier model approximating the response of GaN.

<sup>1</sup>Supported by ARL Materials Enterprise

**1:51PM F22.00012 Kinetic Density Functional Theory for Plasmonic Nanostructures**, LUCAS V. BESTEIRO, Ohio University, HUI ZHANG, Rice University, ALEXANDER GOVOROV, Ohio University — We present a quantum kinetic theory of the dynamic response of typical noble metals [1]. The kinetic DFT is derived starting from the master equation of motion for the density matrix, which involves both momentum and energy relaxation processes. Therefore, the quantum system is described by two relaxation parameters, unlike the conventional time-dependent DFT incorporating only one relaxation parameter. This allows us to describe both the absorption of light and the generation of hot plasmonic electrons. The proposed theory can be employed to model and predict a variety of metal and hybrid nanostructures for applications in photocatalysis, sensors, photodetectors, metamaterials, etc. To support this, we show how the formalism can provide insights on several recent experimental results [2-4]. [1] A.O. Govorov, H. Zhang, J. Phys. Chem. C 119, 6181 (2015). [2] L. Weng, H. Zhang, A. O. Govorov, and M. Ouyang, Nature Commun. 5, 4792 (2014). [3] H. Harutyunyan, A.B.F. Martinson, D. Rosenmann, L.K. Khorashad, L.V. Besteiro, A.O. Govorov, G.P. Wiederrecht, Nature Nanotech. 10, 770 (2015). [4] W. Li, Z.J. Coppens, L.V. Besteiro, W. Wang, A.O. Govorov, J. Valentine, Nat. Commun. 6, 8379 (2015).

**2:03PM F22.00013 Electrically induced spontaneous emission in open electronic system**, RULIN WANG, Beijing Computational Science Research Center, YU ZHANG, The University of Hong Kong, CHIYUNG YAM, Beijing Computational Science Research Center, COMPUTATION ALGORITHMS DIVISION (CSRC) TEAM, THEORETICAL AND COMPUTATIONAL CHEMISTRY (HKU) COLLABORATION — A quantum mechanical approach is formulated for simulation of electroluminescence process in open electronic system. Based on nonequilibrium Greens function quantum transport equations and combining with photon-electron interaction, this method is used to describe electrically induced spontaneous emission caused by electron-hole recombination. The accuracy and reliability of simulation depends critically on correct description of the electronic band structure and the electron occupancy in the system. In this work, instead of considering electron-hole recombination in discrete states in the previous work, we take continuous states into account to simulate the spontaneous emission in open electronic system, and discover that the polarization of emitted photon is closely related to its propagation direction. Numerical studies have been performed to silicon nanowire-based P-N junction with different bias voltage.

**Tuesday, March 15, 2016 11:15AM - 2:03PM —**

**Session F23 DMP: Synthesis, Fabrication and Characterization of Nanostructures** 322 - Koray Aydin, Northwestern University

**11:15AM F23.00001 Direct Writing of Metamaterials Using Atomic Calligraphy**<sup>1</sup>, THOMAS STARK, JEREMY REEVES, LAWRENCE BARRETT, RICHARD LALLY, DAVID BISHOP, Boston University — The trend toward creating metamaterials with spectral features at shorter wavelengths demands a concomitant decrease in the minimum feature size. Many fabrication techniques have been developed to meet this challenge, all of which must address competition between resolution and throughput [1]. We fabricate metamaterials using atomic calligraphy, a technique that tackles both the throughput and resolution challenges, and present optical characterization of the metamaterials we fabricate [2]. Atomic calligraphy is a microelectromechanical systems (MEMS) based moveable stencil used to fabricate nanostructures. We increase the throughput of this technique by using many stencils in parallel and work toward further enhancing throughput by using a stage system to step the MEMS and repeat fabrication over large areas. Finally, we characterize the infrared response of the metamaterials that we fabricated. This technology can be used to fabricate metamaterials on a host of substrates, including those that are chemically incompatible with or have topological features that preclude them from use with conventional nanofabrication techniques, such as mechanical scaffolds that enable tuning of the metamaterial spectral response. [1] Imboden, M. and Bishop. D. *Physics Today*. **2014**, 67 (12), 45-50. [2] Imboden. M. et. al. *Nano Letters*. **2013**, 13 (7), 3379-3384.

<sup>1</sup>This work is funded by the DARPA A2P Program.

**11:27AM F23.00002 Graphene-like Networks in the lattice of Ag, Cu and Al metals**, LOURDES SALAMANCA-RIBA, XIAOXIAO GE, ROMAINE ISAACS, HM IFTEKAR JAIM, MANFRED WUTTIG, SERGEY RASHKEEV, MAIJA KUKLJA, LIANBING HU, University of Maryland, COVETICS TEAM TEAM — Graphene-like networks form in the lattice of metals such as silver, copper and aluminum via an electrocharging assisted process. In this process a high current of >80A is applied to the liquid metal containing particles of activated carbon. The resulting material is called M covetic (M=Al, Ag Cu). We have previously reported that this process gives rise to carbon nanostructures with sp<sup>2</sup> bonding embedded in the lattice of the metal. The carbon bonds to the metal as evidenced by Raman scattering and first principles simulation of the phonon density of states. With this process we have observed that graphene nanoribbons form along preferential crystalline directions and form 3D epitaxial structures with Al and Ag hosts. Bulk Cu covetic was used to deposit films by e-beam deposition and PLD. The PLD films contain higher C content and show higher transmittance (~90%) and resistance to oxidation than pure copper films of the same thickness. We compare the electrical and mechanical properties of covetics containing C in the 0 to 10 wt % and the transmittance of Cu covetic films compared to pure Cu films of the same thickness. Supported by ONR grant N000141410042

**11:39AM F23.00003 Patterned Fabrication of Zinc Oxide Nanowire Arrays**<sup>1</sup>, SAHAR KHAN<sup>2</sup>, THOMAS LAMSON<sup>3</sup>, HUIZHONG XU<sup>4</sup>, St. John's University — Zinc oxide nanowires possess desirable mechanical, thermodynamic, electrical, and optical properties. Although the hydrothermal growth process can be applied in tolerable growth conditions, the dimension and density of nanowires has a complex dependence on substrate pre-treatment, precursor concentrations, and growth conditions. Precise control of the geometry and density of nanowires as well as the location of nanowires would allow for the fabrication of useful nanowaveguide devices. In this work, we used electron beam lithography to pattern hole arrays in a polymer layer on gold-coated glass substrates and synthesized zinc oxide nanowires inside these holes. Arrays of nanowires with diameters ranging from 50 nm to 140 nm and various spacings were obtained. The transmission of light through these zinc oxide nanowire arrays in a silver film was also studied.

<sup>1</sup>This research was supported by the Seed Grant Program of St. Johns University and the National Science Foundation under Grant No. CBET-0953645.

<sup>2</sup>Undergraduate Student (Sophomore)

<sup>3</sup>Undergraduate Student (Senior)

<sup>4</sup>Associate Professor

**11:51AM F23.00004 Effect of Ti adhesive layer on individual gold nanodisk surface plasmon resonance**, DESALEGN TADESSE DEBU, PIJUSH GHOSH, DAVID FRENCH, STEPHEN BAUMAN, JOSEPH B. HERZOG, Univ of Arkansas-Fayetteville — We investigate localized surface plasmon resonance (SPR) of gold nanodisks of various diameter and height fabricated on extremely thin Ti adhesive layers. Dark field scattering measurements reveal significant dependence of SPR in the size nano structures and polarization of the light. Comparisons of peak resonance extracted from spectra using Gaussian fitting of different Ti adhesive layer thickness indicates significant red shifting and damping of the plasmon mode. Experimental results are supported by numerical simulation based on three dimensional finite element time domain analysis. From the simulation and experimental results we quantitatively developed optimized model equation of resonance mode of the nanodisks with respect to adhesive layer thickness and broadening effect of the line shape. Such optimized model is very helpful in guiding targeted nanofabrication such as gold nanodisk antennas or biosensors.

**12:03PM F23.00005 Aluminum Nanowire Arrays via Directed Assembly<sup>1</sup>**, NATHAN T. NESBITT, JUAN M. MERLO, AARON H. ROSE, YITZI M. CALM, LUKE A. D'IMPERIO, DAVE T. COURTNEY, STEVE SHEPARD, KRZYSZTOF KEMPA, MICHAEL J. BURNS, MICHAEL J. NAUGHTON, Boston College — Vertically-oriented metal nanowire arrays are rare. Here, freestanding, vertically-oriented, and lithographically-ordered Al nanowire arrays have been fabricated via directed assembly [1]. The fabrication technique is a variation on the preparation of anodized aluminum oxide (AAO) templates, using nanoimprint lithography (NIL) to direct the formation of pores on an Al film and produce Al nanowires. Near-field scanning optical microscope (NSOM) and conventional optical microscope data of a single nanowire lying on glass and illuminated by a laser spot show evidence of surface plasmons propagating along the nanowire. [1] N. T. Nesbitt, J. M. Merlo, A. H. Rose, Y. M. Calm, K. Kempa, M. J. Burns, M. J. Naughton, *Nano Lett.* (2015), DOI: 10.1021/acs.nanolett.5b02408

<sup>1</sup>This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. (DGE-1258923).

**12:15PM F23.00006 The total scattering atomic pair distribution function: New methodology for nanostructure analysis.**, AHMAD MASADEH, Department of Physics, The University of Jordan — The conventional x-ray diffraction (XRD) methods probe for the presence of long-range order (periodic structure) which are reflected in the Bragg peaks. Local structural deviations or disorder mainly affect the diffuse scattering intensity. In order to obtain structural information about both long-range order and local structure disorder, a technique that takes in account both Bragg and diffuse scattering need to be employed, such as the atomic pair distribution function (PDF) technique. This work introduces a PDF based methodology to quantitatively investigate nanostructure materials in general. The introduced methodology can be applied to extract quantitatively structural information about structure, crystallinity level, core/shell size, nanoparticle size, and inhomogeneous internal strain in the measured nanoparticles. This method is generally applicable to the characterization of the nano-scale solid, many of which may exhibit complex disorder and strain [1,2] (1) Ahmad. S. Masadeh, et al., *Phys. Rev. B* 76, 115413 (2007). (2) Xiaohao Yang, *Ahmad S Masadeh*, *Physical Chemistry Chemical Physics*; 15, 8480 (2013).

**12:27PM F23.00007 In-situ transmission x-ray microscopy study of photon-induced oxidation of silver nanowires**, LE YU, Department of Physics, Bryn Mawr College; School of Electronic Science and Engineering, Nanjing University, China, YUGANG SUN, Center for Nanoscale Materials, Argonne National Laboratory, YUXIN WANG, ZHONGHOU CAI, X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, PING HAN, School of Electronic Science and Engineering, Nanjing University, China, X.M. CHENG, Department of Physics, Bryn Mawr College — Oxidation of metal nanoparticles usually follows a Kirkendall process to transform solid nanoparticles to hollow metal oxide nanoshells. However the morphological trajectory of nanoparticles and the mass diffusion kinetics involved in the nanoscale Kirkendall process are complex. In this presentation we report the use of in-situ transmission x-ray microscopy (TXM) to directly image individual silver nanowires under oxidation atmosphere, which are created from radiolysis of air under illumination of the focused synchrotron x-ray beam. The in-situ results clearly show the morphological transformation from solid silver nanowires to hollow nanotubes in the course of oxidation reaction of silver. Quantitative analysis of the time-resolved TXM images provides unprecedented details on reaction kinetics and mass diffusion kinetics associated with the oxidation process. Work at Bryn Mawr College is supported by NSF grant #1207085. Use of the Advanced Photon Source and the Center for Nanoscale Materials at Argonne National Laboratory was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

**12:39PM F23.00008 Investigation of Carbon incorporation into Al 6061 alloys**, XIAOXIAO GE, LOURDES SALAMANCA RIBA, MANFRED WUTTIG, Univ of Maryland-College Park, COVETICS COLLABORATION — The incorporation of carbon nanostructures into aluminum alloys, such as Al6061 and Al7075, has the potential to further improve the mechanical, electrical and anti-corrosion properties of these alloys. We report on a novel method to incorporate up to 10.0 wt% carbon into the crystal structure of Al 6061 alloys to form a new material "Al Covetics". In this method, a DC current is applied to molten Al metal containing activated carbon particles. The current facilitates ionization of the carbon atoms and their bonding to each other, forming graphic chains and layers along preferential directions of the Al lattice. Raman mapping of the G and D peaks of graphitic carbon was used to confirm the role of the current in ensuring that the carbons remain in the metal by electro-static force and spread into the metal matrix evenly.  $sp^2$  bonding of carbon was found all over the surface in the Covetics. Carbon signals were also observed everywhere in Covetics with Energy Dispersive X-ray Spectroscopy. However, localized carbon signals were detected in samples made with activated carbon but without applying any current. The dependence of the mechanical, electrical and structural properties of Al Covetics on C content from 3 to 10 wt. % will be presented.

**12:51PM F23.00009 Electrical and Optical Characterization of Cobalt Doped Nanostructured ZnO/p-Si Heterojunctions**, AMRIT KAPHE, ECHO ADCOCK SMITH, PARAMESWAR HARI, DANIEL CRUNKLETON, TYLER JOHANNES, TODD OTANICAR, KENNETH ROBERTS, Univ of Tulsa — In this study we investigated electrical and optical properties of heterojunctions made of cobalt doped ZnO nanorods and Boron doped silicon (p-Si). ZnO nanorods were grown on a seed layer of Zn sputtered on p-Si using a chemical bath deposition technique. Cobalt percentage in the ZnO were varied from 0-20%. Scanning Electron Microscope (SEM) images indicate that the diameter of ZnO nanorods increased with higher cobalt doping. Room temperature photoluminescence shows an increase in the defect peak at 550 nm with increasing doping. Band gap was measured using UV-VIS spectroscopy. In addition, we also performed current-voltage (I-V), capacitance-voltage (C-V) measurements on ZnO/p-Si samples under both dark and illumination conditions. I-V characteristics show good rectifying behavior under dark and illumination conditions. The saturation current, diode ideality factor, carrier concentrations, built in potential, and barrier height were calculated from I-V and C-V measurements. We will discuss the implications of the band gap, I-V, and C-V measurements with variations in cobalt doping concentrations in ZnO/p-Si heterojunctions.

**1:03PM F23.00010 One-dimensional Growth of Zinc Crystals on a Liquid Surface<sup>1</sup>**, CHENXI LU, YI CHENG, QIFA PAN, XIANGMING TAO, BO YANG, GAOXIANG YE, Department of Physics, Zhejiang University, Hangzhou 310027, P. R. China, THE LAB OF FILMS ON LIQUID SUBSTRATES TEAM — The catalyst-free growth of nanocrystals on various substrates at room temperature has been a long-standing goal in the development of material science. We report the growth of one-dimensional zinc nanocrystals on silicone oil surfaces by thermal evaporation method at room temperature ( $20 \pm 2$  °C). Uniform zinc nanorods with tunable size can be obtained. The typical length and width of the nanorods are 250-500 nm and 20-40 nm, respectively. The growth mechanism can be attributed to the effect of the liquid substrate and the preferential growth direction of the crystals. This result provides a novel and simple way to fabricate the precursors (zinc crystals) for preparation of Zn-based semiconductors and other metallic crystals on liquid substrates.

<sup>1</sup>The research was funded by the National Natural Science Foundation of China (Grant No. 11374082).

**1:15PM F23.00011 Tracking and Removing Br during the Bottom-Up Synthesis of a Graphene Nanoribbon**, CHRISTOPHER BRONNER, University of California, Berkeley, JONAS BJÖRK, Linköping University, PETRA TEGEDER, Ruprecht-Karls-Universität Heidelberg — Thermally induced, two-step bottom-up synthesis from halogen-substituted molecular precursors adsorbed at metal surfaces is an intriguing concept for obtaining graphene nanoribbons with well-defined edge structure and widths on the nanometer scale. The reaction pathways of the dissociated Br atoms have so far not been in the focus of research although they may very well interfere with the on-surface synthesis. Using temperature-programmed desorption we show that Br leaves the surface as HBr in an associative desorption process during the second reaction step, the cyclodehydrogenation. Density functional theory is employed to compare this process to the competing desorption of molecular hydrogen and furthermore shows that prior to desorption, Br is submerged under the three-dimensional intermediate reaction product, polyanthrylene. Upon exposure of this intermediate co-adsorbate to an atmosphere of molecular hydrogen, Br is removed from the surface but the cyclodehydrogenation step is still feasible which demonstrates that Br does not influence the on-surface synthesis. Generally, the ability to remove Br by providing molecular hydrogen opens an effective way to exclude unfavorable influences of the halogen (e.g. side-products, steric effects) in on-surface coupling reactions.

**1:27PM F23.00012 Synthesis of metal-organic framework films by pore diffusion method.**, NAO-HIRO MURAYAMA, YUKI NISHIMURA, Tottori Univ, HIROSHI KAJIRO, Nippon Steel & Sumitomo Metal Co., SATORU KISHIDA, KENTARO KINOSHITA, Tottori Univ, TIFREC, TEDREC, TOTTORI UNIV TEAM, NIPPON STEEL & SUMITOMO METAL CO. COLLABORATION, TOTTORI INTEGRATED FRONTIER RESEARCH CENTER (TIFREC) COLLABORATION, TOTTORI UNIVERSITY ELECTRONIC DISPLAY RESEARCH CENTER (TEDREC) COLLABORATION — Metal-organic frameworks (MOFs) presents high controllability in designing the nano-scale pore, and this enable molecular storages, catalysts, gas sensors, gas separation membranes, and electronic devices for next-generation. Therefore, a simple method for film synthesis of MOFs compared with conventional methods<sup>[1]</sup> is strongly required. In this paper, we provide pore diffusion method, in which a substrate containing constituent metals of MOF is inserted in solution that includes only linker molecules of MOF. As a result, 2D growth of MOF was effectively enhanced, and the formation of flat and dense MOF films was attained. The growth time,  $t$ , dependence of film thickness,  $d$ , can be expressed by the relation of  $d = A \ln(t+1) + B$ , where A and B are constants. It means that ionized coppers diffuse through the pores of MOFs and the synthesis reaction proceeds at the MOF/solvent interface. We demonstrated the fabrication of a HKUST-1/Cu-TPA hetero structure by synthesizing a Cu-TPA film continuously after the growth of a HKUST-1 film on the CuO<sub>x</sub> substrate. [1] Denise Zacher *et al.*, *Angew. Chem. Int. Ed.* **50**, 176 (2011).

**1:39PM F23.00013 Glancing angle deposited villi-like nanostructures for enhanced chemo-resistive performances<sup>1</sup>**, HI GYU MOON, YOUNGMO JUNG, TAIKJIN LEE, SEOK LEE, Korea Institute of Science and Technology, HYUNG-HO PARK, Yonsei University, CHULKI KIM, CHONG-YUN KANG, Korea Institute of Science and Technology — Metal oxide nanostructures have attracted enormous attention for diverse applications such as solar cells, nanogenerators, nanolasers, optoelectronic devices and chemoresistive sensor. To achieve the enhanced electrical properties for these applications, one-dimensional (1D) metal oxide materials including nanowires, nanorods, nanotubes and nanobelts have been widely studied. However, the use of 1D nanomaterials as chemoresistive sensors is still in the beginning stage in how to integrate them. As an alternative, porous thin films based on 1D metal oxide nanostructures are considered as more desirable configuration due to their simplicity in synthesis, high reproducibility. In this study, we propose facile synthesis and self-assembled villi-like nanofingers (VLNF) WO<sub>3</sub> thin films with large specific surface area on the SiO<sub>2</sub>/Si substrate. Room-temperature glancing angle deposition of WO<sub>3</sub> by a simple controlling in both polar and azimuthal directions resulted in anisotropic nanostructures with large aspect ratio and porous structures with a relative surface area of 350 m<sup>2</sup>/g.

<sup>1</sup>Glancing angle deposited villi-like nanostructures for enhanced chemo-resistive performances

**1:51PM F23.00014 Replace this text with your abstract title.**, YANG LI, Ohio University Argonne National Laboratory, ANDREW DILULLO, BRANDON FISHER, Argonne National Laboratory, SAW-WAI HLA, Argonne National Laboratory & Ohio University — We investigate the interaction of graphene nanoribbon (GNR) with cobalt-porphyrin (Co-TBrPP) molecules using low temperature scanning tunneling microscopy (STM), tunneling spectroscopy, and atomic/molecular manipulation schemes. GNRs are formed by fusing 10,10'-dibromo-9,9'-bianthryl molecules on a Au(111) surface. Due to a weak binding, the Co-TBrPP molecules are mobile on GNR. The lateral manipulation scheme using the STM tip is employed to investigate the diffusion of the molecule on this surface. Guided by the edges of the GNR, the molecules diffuse in one-dimensional paths. We will also discuss the electronic properties of Co-TBrPP on GNR measured by using tunneling spectroscopy and spectroscopic mapping. We acknowledge the support of DOE SISGR grant: DE-FG02-09ER16109.

**Tuesday, March 15, 2016 11:15AM - 2:03PM –**  
**Session F24 DMP: Electronic and Optical Properties of Nanoparticle Assemblies 323 -**

**11:15AM F24.00001 Theory of light scattering at nanoparticles and optical forces between small particles**, JUAN JOSE SAENZ, Donostia International Physics Center (DIPC) — Appropriate combinations of laser beams can be used to trap and manipulate small particles with optical tweezers as well as to induce significant optical binding forces between particles. Here we review some basic concepts related to the optical forces on small (subwavelength) particles, focusing on the interplay between scattering asymmetry and momentum transfer. These forces are, in general, non-conservative (curl forces) which lead to a number of intriguing predictions regarding the dynamics of nanoparticles. Optical forces between small particles are usually strongly anisotropic depending on the interference landscape of the external fields. This is in contrast with the familiar isotropic van der Waals and, in general, Casimir-Lifshitz interactions between neutral bodies arising from random electromagnetic waves generated by equilibrium quantum and thermal fluctuations. As we will see, artificially created random fluctuating light fields can be used to induce and control dispersion forces between small colloidal particles. Interestingly, for relatively high refractive index semiconductor nanoparticles, the interactions can be tuned from attractive to strongly repulsive when the frequency of the external fluctuating field is tuned near the first magnetic Mie-resonance. Interactions induced by randomly fluctuating light fields open a path towards the control of translational invariant interactions with tuneable strength and range in colloidal systems.

**11:51AM F24.00002 Redox-driven conductance modulation of a single quantum dot in an electrolytic environment<sup>1</sup>**, GIACOMO LOVAT, University of Trieste and Columbia University, BOYEON CHOI, XAVIER ROY, LATHA VENKATARAMAN, Columbia University — Electrons confined in zero-dimensional systems exhibit shape and size-dependent electronic and optical properties of interest for many technological applications. A realization of molecular-scale quantum dots having precise shape and size is provided by the synthesis of atomically defined isostructural metal chalcogenide clusters functionalized with organic connectors, which opens the possibility of wiring up these dots without altering significantly their electronic structure. Here, we characterize the charge transport in single molecule junctions fabricated with Co<sub>6</sub>Se<sub>8</sub> clusters via the scanning tunneling microscope break junction technique. The cluster structure consists of an octahedron of Co atoms concentric with a cube of Se atoms; the electrical connection to the Au leads is provided by aurophilic thiol-terminated ligands attached at the Co sites. We demonstrate that conductance modulation in a cluster junction can be achieved by controlling the charge state of the cluster. The conductance of the oxidized species differs from that of the neutral ones, consistent with the value obtained in a control experiment with chemically oxidized clusters.

<sup>1</sup>This work was supported in part by the Columbia University NSF-MRSEC center.

**12:03PM F24.00003 First Principles Simulations of Nanoparticle Solids<sup>1</sup>**, ARIN GREENWOOD, Institute for Molecular Engineering, University of Chicago, MÁRTON VÖRÖS, Institute for Molecular Engineering, University of Chicago; Materials Science Division, Argonne National Laboratory, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago — Nanoparticle solids are gaining popularity as materials for optoelectronic devices such as solar cells [1, 2]. However, there is still much debate regarding the transport regime governing the charge carriers. To date, no comprehensive description of transport mechanisms in nanoparticle solids has been established, and there is a lack of computational studies predicting electron mobilities and transport rates at the *ab initio* level. In order to understand electron transport properties, it is an essential prerequisite to build realistic structural models of nanoparticle solids to use for prediction of electronic structure and eventually transport properties. Here we present *Ab Initio* Molecular Dynamics simulations of lead chalcogenide nanoparticles and surrounding ligands to extract relevant electronic structure properties for charge transport calculations. We tested the validity of recently observed “band-like” transport [3] by assessing the formation of bands and their dependence on nanoparticle surface structure and ligands.

[1] Crisp, Ryan et al. Scientific Reports, 2014, 5: 9945. [2] Ning, Zhijun et al. Nature Materials, 2014, 13, pp 822-828. [3] Choi, Ji-Hyuk et al. Nano Letters, 2012, 12(5), pp 2631-2638.

<sup>1</sup>Work supported by DOE-BES under DE-FG02-06ER46262

**12:15PM F24.00004 Molecularly-linked gold nanoparticle films across the insulator-to-metal transition: from hopping to strong electron correlations**, MONIQUE TIE, AL-AMIN DHIRANI, Univ of Toronto — Materials which have strong electron-electron interactions are known to display a wide variety of exotic behaviours. We have found that molecularly-linked gold nanoparticle films represent a new class of materials that exhibit correlated electronic behaviours. Most notably, (a) they undergo a percolation insulator-to-metal transition as a function of film thickness, (b) as the system transitions from an insulator to a metal, a previously unobserved zero-bias conductance peak emerges, attributed to electron correlations, and (c) Coulomb effects play an important role in the conductance on both the insulating and metallic sides near the transition. On the insulating side near the transition, we observe hopping transport with significant Coulomb charging barriers (Efros-Shklovskii variable range hopping). On the metallic side, we have found that conductance behaves as a Fermi liquid with disorder mediated electron-electron interactions. Remarkably, in this barely-metallic phase, we have found elastic scattering lengths smaller than inter-atomic Au-Au separation, violating the Ioffe-Regel limit and signalling strong electron-electron interactions. These results show that gold nanoparticle films can serve as a new test bed for studying correlated electrons and illustrate the promise

**12:27PM F24.00005 Towards the Ultimate Limit of Connectivity in Quantum Dots with High Mobility and Clean Gaps**, HUASHAN LI, DAVID ZHITOMIRSKY, SHREYA DAVE, JEFFREY GROSSMAN, Massachusetts Institute of Technology — Colloidal quantum dots (CQDs) are especially promising for commercial electronic and optoelectronic applications, yet there is a considerable lack of fundamental understanding of their electronic structure as they couple within thin films. In this work, we applied a combination of computational and experimental techniques to gain insight into the impact of connectivity in CQD assemblies. High Resolution Transmission Electron Microscopy demonstrates that a range of connectivity between dots in the film is attainable by tuning the CQD size and ligand treatment. These results were complemented by *ab-initio* simulations within the phonon-assisted charge hopping scenario. We find that both the orbital hybridization and interfacial dipole moment can change the electronic structure substantially; thus, control over the interface structure beyond stoichiometry is necessary to eliminate trap states. In addition, carrier mobility has a strong dependence on the type of connectivity (i.e., bridge vs. necking), the connectivity orientation, carrier energy, and defect states. Based on our calculations, we propose a scheme for improved carrier mobility, by necking the dots for the advantage of large electron coupling, followed by excess ligand passivation to recover the wavefunction delocalization.

**12:39PM F24.00006 Metal-Insulator Transition in nanoparticle solids: a kinetic Monte Carlo study<sup>1</sup>**, GERGELY ZIMANYI, LUMAN QU, Physics, UC Davis, Davis, CA 95616, MARTON VOROS, Materials Science Division, Argonne National Laboratory, IL — Nanoparticle (NP) solids recently emerged as a promising platform for high performance electronic/optoelectronic devices, including third generation solar cells, light emitting diodes and field effect transistors. A challenge of NP films is that their charge transport is in the unfavorable hopping/insulating regime. Recent experiments showed that it is possible to tune the NP solids through a Metal-Insulator Transition (MIT) via ligand engineering and ALD matrix infilling. However, the microscopic understanding of this transition is not yet clear. To address this challenge, we developed a Kinetic Monte Carlo transport modeling framework that builds on determining NP parameters from *ab initio*-based calculations of the energy level structures, charging energies and overlaps, and then uses these to compute the hopping mobility across a disordered NP array by the Marcus and Miller-Abrahams mechanisms. We reproduced and explained the observed non-monotonous dependence of the mobility on the NP diameter. Centrally, we extended our platform to be able to capture the MIT. We determined the MIT phase boundary on the (NP-NP overlap - Electron density) plane. We demonstrated that all mobilities fall on a universal scaling curve, allowing us to determine the critical behavior across the MIT.

<sup>1</sup>Supported by: UC Davis Office of Research RISE ANSWER grant

**12:51PM F24.00007 The effect of oxidation on charge carrier motion in PbS quantum dot thin films studied with Kelvin Probe Microscopy<sup>1</sup>**, LAN PHUONG NGUYEN HOANG, PHEONA WILLIAMS, JASON MOSCATELLO, KATHY AIDALA<sup>2</sup>, Mt Holyoke Coll, AIDALA GROUP TEAM — We developed a technique that uses scanning probe microscopy (SPM) to study the real-time injection and extraction of charge carriers in thin film devices. We investigate the effects of oxidation on thin films of Lead Sulfide (PbS) quantum dots with tetrabutyl-ammonium-iodide (TBAI) ligands in an inverted field effect transistor geometry with gold electrodes. By positioning the SPM tip at an individual location and using Kelvin Probe Force Microscopy (KPFM) to measure the potential over time, we can record how the charge carriers respond to changing the backgate voltage with grounded source and drain electrodes. We see relatively fast screening for negative backgate voltages because holes are quickly injected into the PbS film. The screening is slower for positive gate voltages, because some of these holes are trapped and therefore less mobile. We probe these trapped holes by applying different gate voltages and recording the change in potential at the surface. There are mixed reports about the effect of air exposure on thin films of PbS quantum dots, with initial exposure appearing to be beneficial to device characteristics. We study the change in current, mobility, and charge injection and extraction as measured by KPFM over hours and days of exposure to air.

<sup>1</sup>This work is supported by NSF grant DMR-0955348, and the Center for Hierarchical Manufacturing at the University of Massachusetts, Amherst (NSF CMMI-1025020).

<sup>2</sup>Research Advisor

**1:03PM F24.00008 Effects of electron-phonon interactions on the electron tunneling spectrum of PbS quantum dots**, A. ZIMMERS, H. WANG, E. LHUILLIER, Q. YU, A. MOTTAGHIZADEH, ESPCI-UPMC-CNRS Paris-France, C. ULYSSE, CNRS, Lab Photon & Nanostruct, Marcoussis, France, A. DESCAMPS-MANDINE, B. DUBERTRET, H. AUBIN, ESPCI-UPMC-CNRS Paris-France — We present a tunnel spectroscopy study of single PbS and HgSe quantum dots (QDs) as a function of temperature and gate voltage. The samples are fabricated through high-vacuum projection of the QDs on the chip circuit. For PbS, three distinct signatures of strong electron-phonon coupling are observed in the electron tunneling spectrum (ETS) of these QDs. In the shell-filling regime, the 8x degeneracy of the electronic levels is lifted by the Coulomb interactions and allows the observation of phonon subbands that result from the emission of optical phonons. At low bias, a gap is observed in the ETS that cannot be closed with the gate voltage, which is a distinguishing feature of the Franck-Condon blockade. From the data, a Huang-Rhys factor in the range 5 similar to 1.7-2.5 is obtained. Finally, in the shell-tunneling regime, the optical phonons appear in the inelastic ETS  $d(2)/dV(2)$ . For HgSe, the data show that the inter-band and intra-band gap can be clearly identified in the ETS.

**1:15PM F24.00009 Enhancement of pumped current in quantum dots.**, JUAN PABLO RAMOS, Universidad Tecnica Federico Santa Maria, Valparaíso, Chile, LUIS FOA, Universidad Nacional de Córdoba, Córdoba, Argentina, VICTOR MARCELO APEL, Universidad Catolica del Norte, Antofagasta, Chile, PEDRO ORELLANA, Universidad Tecnica Federico Santa Maria, Valparaíso, Chile — A direct current usually requires the application of a non-zero potential difference between source and drain, but on nanoscale systems (NSS) it is possible to obtain a non-zero current while the potential difference is zero. The effect is known as quantum charge pumping (QCP) and it is due to the interference provided by the existence of a time-dependent potential (TDP). QCP can be generated by a TDP in non-adiabatic limit. An example of this is a system composed by a ring with a dot embedded on it, under the application of an oscillating TDP. By the action of a magnetic field across the system, a pumped current is generated, since time reversal symmetry is broken. Decoherence is crucial, both from a scientific and technological point of view. In NSS it is expected that decoherence, among others things, decreases the QCP amplitude. In this context, we study what is the effect of a bath on the pumped current in our system. We find that for certain values of magnetic flux, the bath-system produce amplification of the pumped current. [1] J. P. Ramos *et al.* J. of appl. Phys. **115**, 124507, (2014). [2] M. Moskalets *et al.* Phys. Rev. B **64**, 201305, (2001).

**1:27PM F24.00010 Strong coupling effects in coherent electron transport in periodic quantum nanostructures**<sup>1</sup>, T. V. SHAHBAZYAN, L. S. PETROSYAN, Jackson State University — We study coherent transport in a system of periodic linear chain of quantum dots placed between two parallel quantum wires. We show that resonant-tunneling conductance between the wires exhibits Rabi splitting of the resonance peak as a function of Fermi energy in the wires. This effect is an electron transport analogue of the Rabi splitting in optical spectra of two interacting systems. The conductance peak splitting originates from anticrossing of Bloch bands in a periodic system caused by strong coupling between electron states in the quantum dot chain and quantum wires. A perpendicular magnetic field, by breaking the system left-right symmetry, gives rise to multiple Bloch band anticrossings leading to the appearance of a fine structure in the conductance lineshape.

<sup>1</sup>Supported by NSF

**1:39PM F24.00011 How many electrons make a semiconductor nanocrystal film metallic**<sup>1</sup>, KONSTANTIN REICH, TING CHEN, NICOLAAS KRAMER, HAN FU, UWE KORTSHAGEN, BORIS SHKLOVSKII, Univ of Minnesota - Twin Cities — For films of semiconductor nanocrystals to achieve their potential as novel, low-cost electronic materials, a better understanding of their doping to tune their conductivity is required. So far, it not known how many dopants will turn a nanocrystal film from semiconducting to metallic. In bulk semiconductors, the critical concentration  $n_M$  of electrons at the metal-insulator transition is described by the famous Mott criterion:  $n_M a_B^3 \simeq 0.02$ , where  $a_B$  is the effective Bohr radius. We show theoretically that in a dense NC film, where NCs touch each other by small facets, the concentration of electrons  $n_c \gg n_M$  at the metal-insulator transition satisfies the condition:  $n_c \rho^3 \simeq 0.3$ , where  $\rho$  is a radius of contact facets. In the accompanying experiments, we investigate the conduction mechanism in films of phosphorus-doped, ligand-free silicon nanocrystals. At the largest electron concentration achieved in our samples, which is half the predicted  $n_c$ , we find that the localization length of hopping electrons is close to three times the nanocrystals diameter, indicating that the film approaches the metal-insulator transition.

<sup>1</sup>This work was supported primarily by the National Science Foundation through the University of Minnesota MRSEC under Award No. DMR-1420013.

**1:51PM F24.00012 Anomalous hopping conduction in nanocrystalline/amorphous composites and amorphous semiconductor thin films**<sup>1</sup>, JAMES KAKALIOS, KENT BODURTHA<sup>2</sup>, School of Physics and Astronomy, University of Minnesota — Composite nanostructured materials consisting of nanocrystals (nc) embedded within a thin film amorphous matrix can exhibit novel optoelectronic properties. Composite films are synthesized in a dual-chamber co-deposition PECVD system capable of producing nanocrystals of material A and embedding then within a thin film matrix of material B. Electronic conduction in composite thin films of hydrogenated amorphous silicon (a-Si:H) containing nc-germanium or nc-silicon inclusions, as well as in undoped a-Si:H, does not follow an Arrhenius temperature dependence, but rather is better described by an anomalous hopping expression ( $\exp[-(T_0/T)^{3/4}]$ ), as determined from the “reduced activation energy” proposed by Zabdorskii and Shlimak. This temperature dependence has been observed in other thin film resistive materials, such as ultra-thin disordered films of Ag, Bi, Pb and Pd; carbon-black polymer composites; and weakly coupled Au and ZnO quantum dot arrays. There is presently no accepted theoretical understanding of this expression. The concept of a mobility edge, accepted for over four decades, appears to not be necessary to account for charge transport in amorphous semiconductors.

<sup>1</sup>Supported by NSF-DMR and the Minnesota Nano Center.

<sup>2</sup>Present address: Seagate, Bloomington, MN

**Tuesday, March 15, 2016 11:15AM - 2:03PM –**  
**Session F25 DCMP: Superconductivity: Mesoscopic and Nanometer Scale** 324 - Timir Datta, University of South Carolina

**11:15AM F25.00001 Magnetic Field Reentrant Superconductivity in Aluminum Nanowires\***, TERENCE BRETZ-SULLIVAN, ALLEN GOLDMAN, School of Physics and Astronomy, University of Minnesota — Reentrance to the superconducting state through the application of a magnetic field to quasi-one dimensional superconductors driven resistive by current, is counter to the expected properties of superconductors. It was not until recently that a microscopic mechanism explaining the phenomenon was proposed in which superconductivity and phase slip driven dissipation coexist in a non-equilibrium state.<sup>1</sup> Here we present additional results of magnetic field induced reentrance into the superconducting state in quasi-one-dimensional aluminum nanowires with an in-plane magnetic field both transverse to, and along the wire axis. The reentrant behavior is seen in the magnetic field dependence of the I-V characteristic and resistance vs. temperature, and in the wire's magnetoresistance at 450mK. <sup>1</sup>Y. Chen, Y.-H. Lin, S.D. Snyder, A.M. Goldman and A. Kamenev, Nature Physics **10**, 567-571 (2014). \* This work was supported by DOE Basic Energy Sciences Grant DE-FG02-02ER46004. Samples were fabricated at the Minnesota Nanofabrication Center. Parts of this work were carried out in the University of Minnesota Characterization Facility, a member of the Materials Research Facilities Network ([www.mrfn.org](http://www.mrfn.org)) funded via the NSF MRSEC program.

**11:27AM F25.00002 Andreev bound state at a strongly correlated oxide interface<sup>1</sup>**, GUANGLEI CHENG, MICHELLE TOMCZYK, Univ. of Pittsburgh, ALEXANDRE TACLA, ANDREW DALEY, Univ. of Strathclyde, SHICHENG LU, JOSH VEAZEY, MENGCHEN HUANG, PATRICK IRVIN, Univ. of Pittsburgh, SANGWOO RYU, HYUNGWOO LEE, CHANG-BEOM EOM, Univ. of Wisconsin-Madison, DAVID PEKKER, JEREMY LEVY, Univ. of Pittsburgh — Strongly correlated electrons at oxide interfaces give rise to a set of novel physics phenomena including superconductivity and magnetism. At the  $\text{LaAlO}_3/\text{SrTiO}_3$  (LAO/STO) interface, signatures of strong electron pairing persist even for conditions where superconductivity is suppressed. Meanwhile, an Andreev bound state (ABS) is a single quasiparticle excitation that mediates pair transport in confined superconductor-normal systems. Here we report a transition from pair resonant transport to ABS in sketched single electron transistors at the LAO/STO interface. This transition is consistent with a change of electron-electron interaction from attractive to repulsive, occurring at or near the Lifshitz transition. Such new electronically tunable electron-electron interaction may be useful for quantum simulation and engineering of novel quantum states in oxide materials.

<sup>1</sup>We gratefully acknowledge support from AFOSR FA9550-10-1-0524 (JL, CBE), AFOSR FA9550-12-1-0057 (JL, CBE, AD), NSF DMR-1104191 (JL), ONR N00014-15-1-2847 (JL).

**11:39AM F25.00003 Solitons in chiral p-wave superconductors and their possible link to topological phases in the non-adiabatic regime**, LEONARDO MIRANDA SANTANA, EMIL YUZHABASHYAN, Rutgers University — Solitons occur in non-linear systems where dispersion is counterbalanced by non-linearity and are ubiquitous in integrable systems. Two different types of solitons have been shown to exist in the s-wave BCS model. Normal and anomalous solitons connect unstable stationary states with zero and nonzero superconducting gaps, respectively. For the s-wave model, all the normal multi-solitons have been entirely constructed, but only the single anomalous soliton in the presence of particle-hole symmetry has been obtained. We develop a method to construct all the anomalous multi-solitons without requiring particle-hole symmetry of the initial states. Our method can be extended to the chiral p-wave BCS model, for which we also construct both normal and anomalous solitons. It is well known that the chiral p-wave BCS model describes a topological superconductor. We believe that there should exist many topological invariants encoded in its anomalous multi-solitons, extending the notion of topological phase to the non-adiabatic regime. Out of equilibrium topological superfluids are known to display richer topological phase diagrams than those in equilibrium. We believe that anomalous solitons are likely elementary objects in the characterization of these non-equilibrium topological phases.

**11:51AM F25.00004 Measuring the winding number instability in mesoscopic superconducting rings**, ANTHONY LOLLO, IVANA PETKOVIC, MICHEL DEVORET, LEONID GLAZMAN, JACK HARRIS, Yale University — In equilibrium, a flux-biased superconducting ring occupies a state that is characterized by the integer winding number of its complex order parameter. Transitions between states of differing winding number occur via phase slips of the order parameter. A number of aspects of these phase slips remain poorly understood, including the particular value of flux bias at which the transition occurs, and the particular state into which the system relaxes. We use cantilever torque magnetometry to address these questions by measuring the equilibrium supercurrent in arrays of isolated aluminum rings over a wide range of applied flux and temperature. We fit the measured supercurrent using one-dimensional stationary Ginzburg Landau theory over the entire field range  $-B_{c3} < B < B_{c3}$  and for  $T_c/2 < T < T_c$ . We show that phase slips occur at the critical flux predicted by Ginzburg Landau theory. The value of this critical flux shows the influence of the rings' finite circumference. We find that in all instances the winding number changes by unity; this may be because the dynamics of the switching events are overdamped in these rings.

**12:03PM F25.00005 Thermally activated phase slips from metastable states in mesoscopic superconducting rings**, IVANA PETKOVIC, ANTHONY LOLLO, JACK HARRIS, Yale University — In equilibrium, a flux-biased superconducting ring at low temperature can occupy any of several metastable states. The particular state that the ring occupies depends on the history of the applied flux, as different states are separated from each other by flux-dependent energy barriers. There is a critical value of the applied flux at which a given barrier goes to zero, the state becomes unstable, and the system transition into another state. In recent experiments performed on arrays of rings we showed that this transition occurs close to the critical flux predicted by Ginzburg-Landau theory. Here, we will describe experiments in which we have extended these measurements to an individual ring in order to study the thermal activation of the ring over a barrier that has been tuned close to zero. We measure the statistics of transitions as function of temperature and ramp rate.

**12:15PM F25.00006 Superconducting tunneling on thin film gold nanowires – a platform for searching Majorana fermions<sup>1</sup>**, PENG WEI, PATRICK LEE, JAGADEESH MOODERA, MIT — The metallic surface states of (111)-oriented gold thin film has been theoretically shown to be a superior candidate for Majorana fermions (MF) due to its orders of magnitude stronger spin-orbit coupling compared to semiconductor nanowires.[1] We experimentally demonstrate an ideal platform using heterostructure based nanowires for achieving this, and exploit quantum tunneling to probe the MFs forming at the end of the nanowires. By controlling the material properties of the tunnel barrier, we explore the peculiar behaviors of superconducting gold surface states in both pair tunneling (Josephson like) and quasiparticle tunneling regimes that may hint the signatures of MFs. Additionally, in the mesoscopic 1D gold nanowire superconductor, we observe a new superconducting phase with an energy gap much larger than any of the superconductors in the tunneling device, hinting possible unknown pairing mechanism. Our approach directly demonstrates a crucial step in achieving realistic fault-tolerant quantum computation devices based on non-abelian particles. [1] A. C. Potter and P. A. Lee, Phys Rev B 85, 094516 (2012)

<sup>1</sup>We acknowledge John Templeton Foundation grant-39944, NSF DMR-1207469 and ONR N00014-13-1-0301.

**12:27PM F25.00007 Spins of Andreev states in double quantum dots**, ZHAOEN SU, JUN CHEN, PENG YU, University of Pittsburgh, MOIRA HOCERVAR, Institut Neel CNRS, Grenoble, SEBASTIEN PLISSARD, CNRS, LAAS, Toulouse, France, DIANA CAR, Eindhoven University of Technology, ALEXANDRE TACLA, University of Pittsburgh, ANDREW DALEY, University of Strathclyde, DAVID PEKKER, University of Pittsburgh, ERIK BAKKERS, Eindhoven University of Technology, SERGEY FROLOV, University of Pittsburgh — Andreev (or Shiba) states in coupled double quantum dots is an open field. Here we demonstrate the realization of Andreev states in double quantum dots in an InSb nanowire coupled to two NbTiN superconductors. The magnetic field dependence of the Andreev states has been explored to resolve the spins in different double dot configurations. The experiment helps to understand the interplay between pair correlation, exchange energy and charging energy with a well-controlled system. It also opens the possibility to implement Majorana modes in Kitaev chains made of such dots.

**12:39PM F25.00008 Detection of Majorana Kramers pairs using a quantum point contact<sup>1</sup>**, JIAN LI, Princeton University, WEI PAN, Sandia National Laboratories, B. ANDREI BERNEVIG, Princeton University, ROMAN LUTCHYN, Microsoft Research Station Q — We propose a setup that integrates a quantum point contact (QPC) and a Josephson junction on a quantum spin Hall sample, experimentally realizable in InAs/GaSb quantum wells. The confinement due to both the QPC and the superconductor results in a Kramers pair of Majorana zero-energy bound states when the superconducting phases in the two arms differ by an odd multiple of  $\pi$  across the Josephson junction. We investigate the detection of these Majorana pairs with the integrated QPC, and find a robust switching from normal to Andreev scattering across the edges due to the presence of Majorana Kramers pairs. This transport signature is expected to be exhibited in measurements of differential conductance and/or current cross-correlation at low bias.

<sup>1</sup>This work was supported by ONR-N00014-14-1-0330.

**12:51PM F25.00009 Conductance through a proximitized nanowire in the Coulomb blockade regime**, BERNARD VAN HECK, Yale University, ROMAN LUTCHYN, Microsoft Station Q, LEONID GLAZMAN, Yale University — Motivated by recent experiments of the Copenhagen group on InAs nanowires with epitaxial Al [1], we investigate the two-terminal conductance of a strongly proximitized nanowire in the Coulomb blockade regime. We identify the leading electron transport processes at zero applied magnetic field  $B$  as well as at finite fields, suppressing the induced gap  $\Delta_{\text{ind}}(B)$ . In the conventional superconducting phase, the conductance is controlled by the sequential Cooper pair tunneling if  $\Delta_{\text{ind}}(B)$  exceeds the charging energy  $E_c$ , and by the elastic single-electron processes if  $\Delta_{\text{ind}}(B) < E_c$ . The latter mechanism yields smaller values of the linear conductance, and strongly asymmetric Coulomb blockade peaks, which explains the experimental finding in Ref. [1]. We also develop a quantitative theory for the differential conductance and examine its evolution across the topological transition point. [1] A. Higginbotham et al., Nature Physics (2015) doi:10.1038/nphys3461

**1:03PM F25.00010 Time-reversal asymmetry without local moments via directional scalar spin chirality**, PAVAN HOSUR, Stanford Univ — Quantum phases of matter that violate time-reversal symmetry invariably develop local spin or orbital moments in the ground state. Here, a directional scalar spin chiral order (DSSCO) phase is introduced, that disrespects time-reversal symmetry but has no static moments. It can be obtained by melting the spin moments in a magnetically ordered phase but retaining residual broken time-reversal symmetry. Orbital moments are then precluded by the spatial symmetries of the spin rotation symmetric state. Interestingly, polar Kerr effect in the 3D DSSCO has the same symmetries as those observed experimentally in the pseudogap phase of several underdoped cuprates. Finally, it is shown that the DSSCO provides a phenomenological route for reconciling the results of Kerr effect and nuclear magnetic resonance experiments in the cuprates, with charge ordering tendencies — observed in X-ray diffraction studies — playing a crucial role. The so-called "memory effect" in the cuprates can be incorporated into this picture as well.

**1:15PM F25.00011 Reentrant phase coherence in a quasi-one-dimensional superconductor<sup>1</sup>**, DIANE ANSERMET, ALEXANDER P. PETROVIC, SHIKUN HE, Nanyang Technological University, DMITRI CHERNYSHOV, European Synchrotron Radiation Facility, MORITZ HOESCH, Diamond Light Source, DIALA SALLOUM, Lebanese University, PATRICK GOUGEON, MICHEL POTEL, University of Rennes 1, LILIA BOERI, Graz University of Technology, OLE K. ANDERSEN, Max Planck Institute for Solid State Research, CHRISTOS PANAGOPOULOS, Nanyang Technological University — Short coherence lengths characteristic of low-dimensional superconductors are related to high critical fields or temperatures. Fatally, such materials are often sensitive to disorder and suffer from phase fluctuations in the order parameter which diverge with temperature  $T$ , magnetic field  $H$  or current  $I$ . To solve synthesis and fluctuation problems, we propose to build superconductors from inhomogeneous composites of nanofilaments. Single crystals of quasi-one-dimensional  $\text{Na}_{2-\delta}\text{Mo}_6\text{Se}_6$  featuring Na vacancy disorder ( $\delta \sim 0.2$ ) behave as percolative networks of superconducting nanowires. Long range order is established via transverse coupling between individual filaments, yet phase coherence is unstable to fluctuations and localization in the zero- $(T, H, I)$  limit. A region of reentrant phase coherence develops upon raising  $(T, H, I)$  and is attributed to an enhancement of the transverse coupling due to electron delocalization. The observed reentrance in the electronic transport coincides with a peak in the Josephson energy  $E_J$  at non-zero  $(T, H, I)$ .  $\text{Na}_{2-\delta}\text{Mo}_6\text{Se}_6$  is a blueprint for a new generation of low dimensional superconductors with resilience to phase fluctuations at high  $(T, H, I)$ .

<sup>1</sup>This work was supported by the National Research Foundation, Singapore, through Grant NRF-CRP4-2008-04.

**1:27PM F25.00012 Probing Andreev and Majorana States with Voltage Pulses<sup>1</sup>**, JOSEPH WESTON, XAVIER WAIN TAL, CEA, INAC-SPSMS, F-38000 Grenoble, France — We study the effect of time-resolved voltage pulses applied to normal-insulator-superconductor junctions. With the aid of cutting-edge numerical techniques, we see that applying an alternating train of voltage pulses allows us to manipulate the (Andreev) quasi-bound states that form between the insulator and superconductor. When the superconductor is rendered topologically nontrivial, the presence of a Majorana state gives a zero-bias peak (ZBP) in the conductivity of the junction<sup>2</sup>. We show that by applying different amplitudes/frequencies of voltage pulses we can eliminate or recreate the ZBP and hence probe its Majorana character<sup>3</sup>. The persistence of this effect in the presence of finite temperature and moderate disorder is promising for the validation of recent experimental results concerning detection of Majoranas in nanowire-superconductor junctions<sup>4</sup>.

<sup>1</sup>This work was supported by the ERC grant MESOQMC from the European Union

<sup>2</sup>C. Beenakker, Annu. Rev. Condens. Matter Phys., Vol. 4: 113 -136

<sup>3</sup>J. Weston et al., Phys. Rev. B **92**, 020513(R)

<sup>4</sup>V. Mourik et al., Science **336**, 1003

**1:39PM F25.00013 Large variance of  $T_c$  at large length scales in granular mesoscopic Nb islands**, RITA GARRIDO MENACHO, MALCOLM DURKIN, University of Illinois at Urbana-Champaign, SARANG GOPALAKRISHNAN, Harvard University, JIAN-MIN ZUO, NADYA MASON, University of Illinois at Urbana-Champaign — Superconductivity in granular mesoscopic islands, in which the average grain size is smaller than the superconducting coherence length, remains largely unstudied. We performed transport measurements of single Nb islands to study the relation between the critical temperature ( $T_c$ ) and the island diameter. We found that  $T_c$  is largely suppressed at scales much larger than the coherence length of Nb. This can be explained by considering a proximity effect between the grains in the island in which the largest grains define the onset of superconductivity. Following this logic, the grain distribution is proportional to the island area and large  $T_c$  fluctuations are expected as the diameter of the island decreases. We perform a  $T_c$  variance study of large sets of islands at various diameters, and demonstrate an exponential decay relation reaching bulk Nb properties as the island diameter increases.

**1:51PM F25.00014 Quantum interference in a Cooper pair splitter device**, SZABOLCS CSONKA, G. FULOP, Department of Physics, Budapest University of Technology and Economics, F. DOMINGUEZ, A. LÉVY YEYATI, Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, S. D'HOLLOSZY, A. BAUMGARTNER, P. MAKK, C. SCHONENBERGER, Department of Physics, University of Basel, V. A. GUZENKO, Laboratory for Micro- and Nanotechnology, Paul Scherrer Institute, M. H. MADSEN, J. NYGARD, Nano-Science Center, Niels Bohr Institute, University of Copenhagen — Cooper pair splitting (CPS) is a process in which the electrons of naturally occurring spin singlet pairs in a superconductor are spatially separated using two quantum dots. In the present work we investigate the evolution of the conductance correlations in an InAs nanowire based CPS device in the presence of an external magnetic field. In our experiments the gate dependence of the signal that depends on both quantum dots continuously evolves from a slightly asymmetric Lorentzian to a strongly asymmetric Fano-type resonance with increasing B field. Our experiments can be understood in a simple 3 site model, which shows that the nonlocal CPS leads to symmetric line shapes, while the local transport processes can exhibit an asymmetric shape due to quantum interference. These findings demonstrate that the electrons from a Cooper pair splitter can propagate coherently after their emission from the superconductor and how a magnetic field can be used to optimize the performance of a CPS device. In addition CPS devices were developed where the nanowire segments between the two dots were removed, nonlocal measurement on such CPS devices will also be presented.

**Tuesday, March 15, 2016 11:15AM - 2:15PM —**

**Session F26 DCMP DMP: Weyl Semimetal - Theory** 325 - Catalin Martin, Ramapo College of New Jersey

**11:15AM F26.00001 Raman spectroscopy of exfoliated few-layered n-type  $\text{Bi}_2\text{Te}_3$**  , FENGJIAO LIU, MEHMET KARAKAYA, POOJA PUNEET, Clemson Nanomaterials Center, Department of Physics and Astronomy, Clemson University, Clemson, SC USA 29634, RAMAKRISHNA PODILA, Laboratory of Nano-biophysics and COMSET, Clemson Nanomaterials Center, Dept. of Physics & Astronomy, Clemson University, Clemson, SC USA 29634, SRIPARNA BHATTACHARYA, Clemson Nanomaterials Center, Department of Physics and Astronomy, Clemson University, Clemson, SC USA 29634, APPARAO M. RAO, Clemson Nanomaterials Center, Laboratory of Nano-biophysics and COMSET, Dept. of Physics and Astronomy, Clemson University, Clemson, SC USA 29634, CLEMSON NANOMATERIALS CENTER, DEPT. OF PHYSICS & ASTRONOMY, CLEMSON UNIVERSITY, CLEMSON, SC 29634 COLLABORATION, LABORATORY OF NANO-BIOPHYSICS AND COMSET, CLEMSON UNIVERSITY, CLEMSON, SC USA 29634 COLLABORATION — A novel chemical-exfoliation spark-plasma-sintering (CE-SPS) process was applied to enhance the thermoelectric figure of merit and compatibility factor of few-layered n-type  $\text{Bi}_2\text{Te}_3$ . New vibrational modes were observed in the micro-Raman spectra of the few-layered  $\text{Bi}_2\text{Te}_3$  samples, which are absent in the bulk. Here we focus on the emergence of the new intermediate and high-frequency Raman modes and their dependence on the layer thickness. A detailed Raman study probing the origin of these exfoliation induced defect modes will be presented.

**11:27AM F26.00002 Disorder and metal-insulator transitions in Weyl semimetals** , HUA JIANG, College of Physics, Optoelectronics and Energy, Soochow University, Suzhou 215006, China, CHUI-ZHEN CHEN, International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China, JUNTAO SONG, Department of Physics, Hebei Normal University, Hebei 050024, China, QING-FENG SUN, International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China, ZIJIANG WANG, Department of Physics, Boston College, Chestnut Hill, Massachusetts 02167, USA, X. C. XIE, International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China — The Weyl semimetal (WSM) is a newly proposed quantum state of matter. It has Weyl nodes in bulk excitations and Fermi arcs surface states. We study the effects of disorder and localization in WSMs and find three novel phase transitions. (I) Two Weyl nodes near the Brillouin zone boundary can be annihilated pairwise by disorder scattering, resulting in the opening of a topologically nontrivial gap and a transition from a WSM to a three-dimensional (3D) quantum anomalous Hall state. (II) When the two Weyl nodes are well separated in momentum space, the emergent bulk extended states can give rise to a direct transition from a WSM to a 3D diffusive anomalous Hall metal. (III) Two Weyl nodes can emerge near the zone center when an insulating gap closes with increasing disorder, enabling a direct transition from a normal band insulator to a WSM. We determine the phase diagram by numerically computing the localization length and the Hall conductivity, and propose that the novel phase transitions can be realized on a photonic lattice.

**11:39AM F26.00003 Critical exponents at the unconventional disorder-driven transition in a Weyl semimetal** , SERGEY SYZРАНOV, Univ of Colorado - Boulder, PAVEL OSTROVSKY, Max Planck Institute for Solid State Research, Stuttgart, Germany; L. D. Landau Institute for Theoretical Physics RAS, Moscow, Russia, VICTOR GURARIE, LEO RADZIHOVSKY, Univ of Colorado - Boulder — Disordered non-interacting systems in sufficiently high dimensions have been predicted to display a non-Anderson disorder-driven transition that manifests itself in the critical behaviour of the density of states and other physical observables. Recently the critical properties of this transition have been extensively studied for the specific case of Weyl semimetals by means of numerical and renormalisation-group approaches. Despite this, the values of the critical exponents at such a transition in a Weyl semimetal are currently under debate. We present an independent calculation of the critical exponents using a two-loop renormalisation-group approach for Dirac fermions in  $2 + \varepsilon$  dimensions and resolve controversies currently existing in the literature.

**11:51AM F26.00004 Elastic Gauge Fields in Weyl Semimetals<sup>1</sup>** , ALBERTO CORTIJO, YAGO FERREIROS, KARL LANDSTEINER, MARIA ANGELES HERNANDEZ VOZMEDIANO, Consejo Superior de Investigaciones Científicas — We show that, as it happens in graphene, elastic deformations couple to the electronic degrees of freedom as pseudo gauge fields in Weyl semimetals. We derive the form of the elastic gauge fields in a tight-binding model hosting Weyl nodes and see that this vector electron-phonon coupling is chiral, providing an example of axial gauge fields in three dimensions. As an example of the new response functions that arise associated to these elastic gauge fields, we derive a non-zero phonon Hall viscosity for the neutral system at zero temperature. The axial nature of the fields provides a test of the chiral anomaly in high energy with three axial vector couplings.

<sup>1</sup> European Union structural funds and the Comunidad de Madrid MAD2D-CM Program (S2013/MIT-3007)

**12:03PM F26.00005 Quantum oscillations in Weyl semimetals** , JAN BORCHMANN, TAMI PEREG-BARNEA, McGill University — In this work we present recent progress on quantum oscillations of a Weyl semimetal in a slab geometry. Based on semiclassical arguments, it has been conjectured that the Fermi arcs present on the surface of the slab can lead to quantum oscillations with a characteristic dependence on the applied magnetic field as well as the thickness of the slab, which differ from the quantum oscillations in the bulk. To further investigate this we present results from a calculation via a Floquet formalism as well as a lattice quantum treatment of the problem. We present results on the oscillation frequency as well as the phase offset.

**12:15PM F26.00006 Characterization of the Weyl semimetal via the “Fermi arc” of Wannier-Stark ladder** , KUN WOO KIM, WOO-RAM LEE, Korea institute for advanced study, YONG BAEK KIM, University of Toronto, KWON PARK, Korea institute for advanced study — Weyl semimetals have been characterized unequivocally by the Fermi-arc spectrum of the surface states in photoemission experiments. While successful, such a method reveals the topological nature of the Weyl phase in the bulk indirectly via the surface spectrum. In this talk, we propose an alternative method to characterize the Weyl phase via the bulk spectrum of the Wannier-Stark ladder (WSL) emerging under an electric field. Specifically, we show that, for weak-to-moderate strengths of electric field, the WSL exhibits its own “Fermi arc” precisely corresponding to the surface spectrum counterpart, which can be used to characterize the Weyl phase directly in the bulk spectrum.

**12:27PM F26.00007 Phase diagrams of disordered Weyl semimetals** , HASSAN SHAPOURIAN, TAYLOR L. HUGHES, Univ of Illinois - Urbana — Weyl semimetals are gapless quasi-topological materials with a set of isolated nodal points forming their Fermi surface. They manifest their quasi-topological character in a series of topological electromagnetic responses including the anomalous Hall effect. Here we study the effect of disorder on Weyl semimetals while monitoring both their nodal/semi-metallic and topological properties through computations of the localization length and the Hall conductivity. We present detailed phase diagrams of three different lattice tight-binding models and we find that weak disorder preserves the nodal points up to the diffusive limit, but does affect the Hall conductivity. We show that the trend of the Hall conductivity is consistent with an effective picture in which disorder causes the Weyl nodes move within the Brillouin zone along a specific direction that depends deterministically on the properties of the model and the neighboring phases to the Weyl semimetal phase.

**12:39PM F26.00008 Dynamical axion string, screw dislocation in Weyl semimetals and Axion insulators** , YI-ZHI YOU, University of California, Santa Barbara, GIL YOUNG CHO, Korea Advanced Institute of Science and Technology, TAYLOR HUGHES, University of Illinois Urbana- Champaign — We study the interplay between the geometry and axion string resulting from a chiral symmetry breaking in 3D. The chiral symmetry is spontaneously broken by charge density wave (CDW) order parameter nesting two Weyl points, which turns it into an axion insulator. The phase fluctuation of the CDW order parameter acts as a dynamical axion field coupled to electromagnetic field via  $\theta F \wedge F$  term. When the axion insulator is coupled with the background geometry with torsional defects, i.e. screw dislocations, there is a novel interplay between the dislocation and the dynamical axion string. First, we show that the screw dislocation traps an axial charge. This then implies that if an axion string braids with a parallel screw dislocation, there is Berry phase accumulated during the braiding procedure. In addition, the cubic coupling between the axial current and the torsion bilinear shows the Berry phase accumulated by the three-loop braiding procedure, where we braid one dislocation loop around the other dislocation loop where the both are linked by an axion string loop. We also observe a chiral magnetic effect induced by a screw dislocation in the absence of chemical potential imbalance between Weyl points.

**12:51PM F26.00009 Non-Fermi liquid phase and non-Gaussian itinerant quantum criticality of Weyl semimetals<sup>1</sup>**, PALLAB GOSWAMI, University of Maryland, College Park — A Weyl semimetal is a gapless topological phase in three dimensions, for which the touching points between two nondegenerate bands act as monopoles and antimonopoles of Abelian Berry curvature, with monopole strength  $m$ . Such a gapless phase can support  $m$  Fermi arcs as the protected, zero energy surface states. We consider the stability of a generalized Weyl semimetal with  $m > 1$  in the presence of interaction and disorder by employing a renormalization group analysis, which is controlled by the parameter  $\epsilon = (1 - \frac{1}{m})$ . For any  $m > 1$ , we show how the long range Coulomb interaction gives rise to an infra-red stable, non-Fermi liquid phase without any sharp quasiparticle pole. In the presence of sufficiently strong short range interactions, the non-Fermi liquid can transform into a translational symmetry breaking, axionic insulator. We demonstrate that the associated itinerant quantum critical point possesses non-Gaussian scaling properties. We establish the stability of the emergent non-Fermi liquid phase and the itinerant quantum critical point against weak disorder. Finally, we discuss the scaling properties of physical quantities, the fate of the Fermi arcs, and the experimental relevance of our results for some candidate materials.

<sup>1</sup>NSF

**1:03PM F26.00010 Detecting monopole charge via quantum interference transport**, XIN DAI, Tsinghua Univ, HAIZHOU LU, South University of Science and Technology China, HONG YAO, Tsinghua Univ — Topological Weyl and double-Weyl semimetals host different monopole charges in momentum space. How to detect the signature of the monopole charges in quantum transport remains a challenging topic. Here, we reveal the connection between the parity of monopole charge in topological semimetals and the quantum-interference correction to the conductivity. We demonstrate that the parity of monopole charge determines the sign of quantum-interference correction, with odd and even parity yielding the weak anti-localization and weak localization effect, respectively. This is attributed to the Berry phase difference between time-reversed trajectories circulating the great circle of the Fermi sphere that encloses the monopole charges. From standard Feynman diagram calculations, we further show that the weak-field magnetoconductivity is proportional to  $\pm\sqrt{B}$  for double-Weyl semimetals and Weyl semimetals, respectively, which could be verified experimentally.

**1:15PM F26.00011 Chirality-dependent Hall Effect in Weyl Semimetals<sup>1</sup>**, SHENGYUAN YANG, Singapore University of Technology and Design, HUI PAN, Beihang University, FAN ZHANG, University of Texas at Dallas — We generalize a semiclassical theory and use the argument of angular momentum conservation to examine the ballistic transport in lightly-doped Weyl semimetals, taking into account various phase-space Berry curvatures. We predict universal transverse shifts of the wave-packet center in transmission and reflection, perpendicular to the direction in which the Fermi energy or velocities change adiabatically. The anomalous shifts are opposite for electrons with different chirality, and can be made imbalanced by breaking inversion symmetry. We discuss how to utilize local gates, strain effects, and circularly polarized lights to generate and probe such a chirality-dependent Hall effect.

<sup>1</sup>Journal Ref: Phys. Rev. Lett. 115, 156603 (2015).

**1:27PM F26.00012 Full quantum theory of the chiral anomaly transport in a Weyl semimetal<sup>1</sup>**, WOO-RAM LEE, KWON PARK, Korea Inst for Advanced Study, KIAS TEAM — In relativistic field theory, the chiral anomaly means a violation of the number conservation of chiral fermions. In condensed matter physics, the chiral anomaly can be manifested in a Weyl semimetal as a negative magnetoresistance in the presence of parallel electric and magnetic fields. In this work, we use the Keldysh-Floquet Greens function formalism to develop a full quantum theory of the chiral anomaly transport, which can be valid in a broad range of both electric and magnetic field strengths.

<sup>1</sup>The authors thank KIAS Center for Advanced Computation (CAC) for providing computing resources.

**1:39PM F26.00013 Effect of disorder in three dimensional layered Chern insulator**, SHANG LIU, School of Physics, Peking University, Beijing, 100871, China, TOMI OHTSUKI, Department of Physics, Sophia University, Chiyoda-ku, Tokyo, 102-8554, Japan, RYUICHI SHINDOU, International Center for Quantum Materials, Beijing, 100871, China — Critical nature of quantum phase transition between topological phase and non-topological phase is one of the most fundamental research issues in the studies of topological phases, where a bulk delocalized state is universally observed between distinct phases as a holographic requirement from the stable surface states. In this work, we studied the effects of disorder in a three dimensional layered Chern insulator, which, in the clean limit, is either a Chern insulator or Weyl semimetal (WSM) depending on the strength of an inter-layer coupling. By calculating the localization length with the transfer matrix method and density of states with the kernel polynomial expansion, we found two distinct types of metallic phases between the Anderson insulator and Chern insulator phases; one is a diffusive metallic (DM) phase and the other is a renormalized WSM phase. We showed that the longitudinal conductivity at the zero energy state remains finite not only in the DM phase but also in the renormalized WSM phase, while goes to zero at the semimetal-metal quantum phase transition point. Based on the Einstein relation combined with the self-consistent Born analysis, we also argue the conductivity scaling near the quantum transition point.

**1:51PM F26.00014 The appearance of a switch in orbital texture and the resulting absence of complete spin polarization in a Rashba semiconductor<sup>1</sup>**, QIHANG LIU, XIUWEN ZHANG, ALEX ZUNGER, University of Colorado, Boulder — We consider spin-orbit coupling (SOC) induced spin splitting and spin polarization in nonmagnetic bulk materials lacking inversion symmetry, in which a pair of side-by-side bands that cross at some wavevector  $K$  is formed. We find that (i) even though in the semi-classical single-electron model the two bands manifest complete spin polarization, we find via density functional theory and  $k \cdot p$  modeling that SOC-induced spin splitting in real materials does not necessarily manifest complete spin polarization. (ii) Away from band crossing point  $K$  and looking at the same wavevector, the spin polarization in different branches does not compensate each other. When considering the full pair of spin-split bands this leads to a net spin texture. We explain this unexpected phenomenon and find that the key factor here is the complex interplay between spin and orbital textures entangled by SOC. (iii) In surprising analogy to the surface states of topological insulators (such as  $\text{Bi}_2\text{Se}_3$ ), a bulk Rashba compound (such as  $\text{BiTeI}$ ) also exhibits a switch of in-plane orbital character between radial and tangential orbital at the critical band crossing point  $K$ . These observations provide a different thinking on the fundamental concept of SOC-induced spin polarization, and opens a new route for manipulating spin degree of freedom by the atomic-orbital feature.

<sup>1</sup>This work was supported by National Science Foundation (Grant DMR-13-34170).

**2:03PM F26.00015 Quantum Mechanics of Palladium Nanostructures**, AJIT HIRA, JAMES MCKEOUGH, BRIDGET ORTIZ, JUAN DIAZ, Northern New Mexico College — We continue our interest in the chemisorption of different atomic and molecular species on small clusters of metallic elements, by examining the interactions of  $\text{H}$ ,  $\text{H}_2$ ,  $\text{Li}$  and  $\text{O}$  adsorbates with  $\text{Pd}_n$  clusters ( $n = 2$  thru 20). The study of clusters can reveal the effects of substrate geometry on the behavior of adsorbates. Transition-metal clusters are especially suited for the study of quantum size effects and for formation of metallic states, and are ideal candidates for catalytic processes. Hybrid ab initio methods of quantum chemistry (particularly the DFT-B3LYP model) are used to derive optimal geometries for the clusters of interest. We compare calculated binding energies, bond-lengths, ionization potentials, electron affinities and HOMO-LUMO gaps for the clusters. Of particular interest are the comparisons of binding strengths at the three important types of sites: edge (E), hollow (H), on-top (T), threefold sites and fourfold sites. Effects of crystal symmetries corresponding to the bulk structures are investigated. The capacity of Pd clusters to adsorb H atoms will be compared to Ni clusters. Admixture with Pt atoms will also be considered.

**Tuesday, March 15, 2016 11:15AM - 2:15PM –**

**Session F27 DMP: Carbon Nanotube & Related Materials: Optical & Other Properties 326 -**

Shu-Jen Han, IBM T. J. Watson Research Center

**11:15AM F27.00001 Terahertz Science and Technology of Macroscopically Aligned Carbon Nanotube Films**, JUNICHIRO KONO, Rice Univ — One of the outstanding challenges in nanotechnology is how to assemble individual nano-objects into macroscopic architectures while preserving their extraordinary properties. For example, the one-dimensional character of electrons in individual carbon nanotubes leads to extremely anisotropic transport, optical, and magnetic phenomena, but their macroscopic manifestations have been limited. Here, we describe methods for preparing macroscopic films, sheets, and fibers of highly aligned carbon nanotubes and their applications to basic and applied terahertz studies. Sufficiently thick films act as ideal terahertz polarizers, and appropriately doped films operate as polarization-sensitive, flexible, powerless, and ultra-broadband detectors. Together with recently developed chirality enrichment methods, these developments will ultimately allow us to study dynamic conductivities of interacting one-dimensional electrons in macroscopic single crystals of single-chirality single-wall carbon nanotubes.

**11:51AM F27.00002 Photocurrent generation efficiency of a carbon nanotube pn junction**, DANIEL MCCULLEY, LEE ASPITARTE, ETHAN MINOT, Oregon State University — Carrier multiplication effects can enhance the quantum efficiency of photovoltaic devices. For example, quantum dot solar cells have demonstrated photon-to-electron conversion efficiencies greater than 100% when photon energies exceed twice the band gap. Carbon nanotube photodiodes exhibit carrier multiplication effects (Gabor et al, Science 2009), but the quantum efficiency of such photodiodes has not previously been characterized. We have reproduced the carrier multiplication phenomena in individual CNT pn junctions and investigated the conditions under which it occurs. We will present early results quantifying the internal quantum efficiency of the process.

**12:03PM F27.00003 Excitonic Contribution to Near-Field Enhancements of a Carbon Nanotube Antenna<sup>1</sup>**, BENJAMIN SOFKA, SLAVA V ROTKIN, Lehigh University — Complexes containing rare earth ions (REI) and single-walled carbon nanotubes (SWNT) show promise to be utilized for the optical sensing of biomolecules. We theoretically study the near-field electromagnetic effects in such a system using a propagating polariton model for the SWNT antenna. To be in resonance with the REI transitions that are in the NIR/optical range, excitonic transitions in the SWNT must be included in the model. We calculate measurable field enhancements in the vicinity of the SWNT antenna that lead to an increase of the REI photoluminescence.

<sup>1</sup>NSF ECCS-1509786

**12:15PM F27.00004 Electroluminescence from individual air-suspended carbon nanotubes within split-gate structures<sup>1</sup>**, N. HIGASHIDE, T. UDA, M. YOSHIDA, A. ISHII, Y. K. KATO, The University of Tokyo — Electrically induced light emission from chirality-identified single-walled carbon nanotubes are investigated by utilizing split-gate field-effect devices fabricated on silicon-on-insulator substrates. We begin by etching trenches through the top silicon layer into the buried oxide, and the silicon layer is thermally oxidized for use as local gates [1]. We partially remove the oxide and form gate electrodes, then contacts for nanotubes are deposited on both sides of the trench. Catalyst particles are placed on the contacts, and nanotubes are grown over the trench by chemical vapor deposition. We use photoluminescence microscopy to locate the nanotubes and perform excitation spectroscopy to identify their chirality. Gate-induced photoluminescence quenching is used to confirm carrier doping [2], and electroluminescence intensity is investigated as a function of the split-gate and bias voltages.

[1] M. Jiang, Y. Kumamoto, A. Ishii, M. Yoshida, T. Shimada, Y. K. Kato, Nature Commun. 6, 6335 (2015).

[2] S. Yasukochi, T. Murai, S. Moritsubo, T. Shimada, S. Chiashi, S. Maruyama, Y. K. Kato, Phys. Rev. B 84, 121409(R) (2011).

<sup>1</sup>Work supported by JSPS (KAKENHI 24340066, 26610080), MEXT (Photon Frontier Network Program, Nanotechnology Platform), Canon Foundation, and Asahi Glass Foundation.

**12:27PM F27.00005 Theory of quadruple plasmon in doped carbon nanotubes**, KEN-ICHI SASAKI, NTT Basic Research Laboratories, SHUICHI MURAKAMI, Tokyo Institute of Technology — A single-wall carbon nanotube possesses two different types of plasmons specified by wavenumbers in the azimuthal and axial directions. In this presentation we show that the azimuthal plasmons consist of underdamped oscillations forming electric dipoles inside a nanotube and overdamped oscillations forming magnetic dipoles. These, originating from the surface plasmons of graphene, are of prime importance in the optical properties of doped "metallic" tubes, such as depolarization effect and relaxation of photo-excited carriers. The axial plasmons also consist of underdamped and overdamped oscillations which are inherent in the cylindrical waveguide-structures of nanotubes and relevant to optics and transport. We discuss the exact configurations of the electromagnetic fields in connection with Aharonov-Bohm effect and point out a possibility of the generation of transient energy band gaps in metallic nanotubes.

**12:39PM F27.00006 Electrical Activation of Dark Excitonic States in Carbon Nanotubes<sup>1</sup>**, TAKUSHI UDA, MASAHIRO YOSHIDA, AKIHIRO ISHII, YUICHIRO K. KATO, The University of Tokyo — Electrical activation of optical transitions to parity-forbidden dark excitonic states in individual carbon nanotubes is reported. We examine electric field effects on various excitonic states by simultaneously measuring both photocurrent and photoluminescence. As the applied field increases, we observe an emergence of new absorption peaks in the excitation spectra. From the diameter dependence of the energy separation between the new peaks and the ground state of  $E_{11}$  excitons, we attribute the peaks to the dark excited states which became optically active due to the applied field. A simple field-induced exciton dissociation model is introduced to explain the photocurrent threshold fields, and the edge of the  $E_{11}$  continuum states have been identified using this model.

<sup>1</sup>Work supported by JSPS (KAKENHI 24340066, 26610080), MEXT (Photon Frontier Network Program, Nanotechnology Platform), Canon Foundation, and Asahi Glass Foundation.

**12:51PM F27.00007 Multi-Excitonic Emission from Solitary Dopant States of Carbon Nanotubes.** , H. HTOON, Center for Integrated Nanotechnologies, Los Alamos National Laboratory, X. MA, N. F. HARTMANN, L. ADAMSKA, K. A. VELIZHANIN, S. TRETIK, J. K. S. BALDWIN, S. K. DOORN, Los Alamos National Laboratory — Oxygen doping of single wall carbon nanotubes (SWCNTs) has been rapidly emerging as an effective mean for introduction of new functionalities. Recently, through demonstration of fluctuation free, room temperature single photon generation<sup>1</sup>, we established these states as a new type of solid-state two level atom with potentials in quantum information technologies. This study further showed that while some doped tubes were characterized with a near complete photon antibunching, significant numbers of doped tubes exhibit some degree of photon bunching indicating that they emit more than one photon in one excitation cycle. Here in this work, by separating slow and fast photons in the time domain, we show for the first time that the multiple photon emissions originated from higher order multi-exciton states of solitary dopants. We also show that such multi-exciton states can allow emission of photon pairs with efficiency as high as 20-30% of single exciton emission. With this work, we bring out multi-excitonic processes of the solitary dopant states as a new area to be explored for potential applications in lasing, entangled photon generation and carrier multiplication. <sup>1</sup> X. Ma et al., Nature Nanotech. **10**, 671 (2015)

**1:03PM F27.00008 Gate-voltage induced trions in suspended carbon nanotubes<sup>1</sup>** , MASAHIRO YOSHIDA, ALEXANDER POPERT, YUICHIRO K. KATO, The University of Tokyo — We observe trion emission from suspended carbon nanotubes where carriers are introduced electrostatically using field-effect transistor structures [1]. The trion peak emerges below the  $E_{11}$  emission energy at gate voltages that coincide with the onset of bright exciton quenching. By investigating nanotubes with various chiralities, we verify that the energy separation between the bright exciton peak and the trion peak becomes smaller for larger diameter tubes. Trion binding energies that are significantly larger compared to surfactant-wrapped carbon nanotubes are obtained, and the difference is attributed to the reduced dielectric screening in suspended tubes.

[1] M. Yoshida, A. Popert, and Y. K. Kato, arXiv:1510.08996.

<sup>1</sup>Work supported by JSPS (KAKENHI 24340066), the Canon Foundation, the Sasakawa Scientific Research Grant, and MEXT (Photon Frontier Network Program, Nanotechnology Platform). M.Y. is supported by ALPS.

**1:15PM F27.00009 New Feature Observed in the Raman Resonance Excitation Profiles of (6,5)-Enriched, Selectively Bundled SWCNTs** , A. R. HIGHT WALKER, J. R. SIMPSON, National Institute of Standards and Technology, O. ROSLYAK, Fordham University, E. HAROZ, H. TELG, J. G. DUQUE, J. J. CROCHET, A. PIRYATINSKI, S. K. DOORN, Los Alamos National Lab — Understanding the photophysics of exciton behavior in single wall carbon nanotube (SWCNT) bundles remains important for opto-electronic device applications. We report resonance Raman spectroscopy (RRS) measurements on (6,5)-enriched SWCNTs, dispersed in aqueous solutions and separated using density gradient ultracentrifugation into fractions of increasing bundling. Near-IR to UV absorption spectroscopy shows a redshift and broadening of the main excitonic transitions with increasing bundling. A continuously tunable dye laser coupled to a triple-grating spectrometer affords measurement of Raman resonance excitation profiles (REPs) over a range of wavelengths covering the (6,5)- $E_{22}$  range (505 to 585) nm. REPs of both the radial breathing mode (RBM) and G-band reveal a redshifting and broadening of the (6,5)  $E_{22}$  transition energy with increasing bundling. Additionally, we observe an unexpected peak in the REP of bundled SWCNTs, which is shifted lower in energy than the main  $E_{22}$  and is anomalously narrow. We compare these observations to a theoretical model that examines the origin of this peak in relation to bundle polarization-enhanced exciton response.

**1:27PM F27.00010 Simulations of resonant Raman response in bundles of semiconductor carbon nanotubes.** , OLEKSIY ROSLYAK, <sup>1</sup>Physics and Engineering Physics Department, Fordham University, Bronx, NY 10458, ANDREI PIRYATINSKI, STEPHEN DOORN, ERIK HAROZ, HAGEN TELG, JUAN DUQUE, JARED CROCHET, Los Alamos Natl Lab, J. R. SIMPSON, A. R. HIGHT WALKER, Engineering Physics Division, NIST, Gaithersburg, MD 20886, LANL COLLABORATION, FORDHAM COLLABORATION, NIST COLLABORATION — This work is motivated by an experimental study of resonant Raman spectroscopy under  $E_{22}$  excitation, which shows a new, sharp feature associated with bundling in (6,5) semiconductor carbon nanotubes. In order to provide an insight into the experimental data, we model Raman excitation spectra using our modified discrete dipole approximation (DDA) method. The calculations account for the exciton states polarized along and across the nanotube axis that are characterized by a small energy splitting. Strong polarization of the nanotubes forming the bundle results in the exciton state mixing whose spectroscopic signatures such as peaks positions, line widths, and depolarization ratio are calculated and compared to the experiment. Furthermore, the effects of the energy and structural disorder, as well as structural defects within the bundle are also examined and compared with the experimental data.

**1:39PM F27.00011 Improvement of polypyrrole nanowire devices by plasmonic space charge generation: high photocurrent and wide spectral response by Ag nanoparticle decoration<sup>1</sup>** , SEUNG-HOON LEE, Department of Physics, Pukyong National University, SEUNG WOO LEE, School of Chemical Engineering, Yeungnam University, JAW-WON JANG<sup>2</sup>, Department of Physics, Pukyong National University — In this study, improvement of the opto-electronic properties of non-single crystallized nanowire devices with space charges generated by localized surface plasmon resonance (LSPR) is demonstrated. The photocurrent and spectral response of single polypyrrole (PPy) nanowire (NW) devices are increased by electrostatically attached Ag nanoparticles (Ag NPs). The photocurrent density is remarkably improved, up to 25.3 times, by the Ag NP decoration onto the PPy NW (PPy<sub>AgNPs</sub> NW) under blue light illumination. In addition, the PPy<sub>AgNPs</sub> NW shows a photocurrent decay time twice that of PPy NW, as well as an improved spectral response of the photocurrent. The improved photocurrent efficiency, decay time, and spectral response resulted from the space charges generated by the LSPR of Ag NPs. Furthermore, the increasing exponent ( $m$ ) of the photocurrent ( $J_{PC} \sim V_m$ ) and finite-differential time domain (FDTD) simulation straightforwardly indicate relatively large plasmonic space charge generation.

<sup>1</sup>Supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (no. 2013K1A3A1A32035429 and 2015R1A1A1A05027681)

<sup>2</sup>Corresponding Author

**1:51PM F27.00012 Optical Properties of waste derived carbon dots** , PRASHANT SARSWAT, MICHAEL FREE, University of Utah — Carbon dots (CDs) have been extensively examined recently, mainly due to their luminescence and excitation wavelength dependent emission behavior. These dots can be derived from a variety of carbonaceous sources. Some of the possible sources are carbonaceous waste materials. Although it is possible to synthesize CDs using waste and their applications in light source, few steps such as to purification of starting material and removal of other impurities during solvothermal processing can enhance the performance of CDs and associated devices. Our primary results suggest that carbonaceous waste in liquid form is easy to process. In contrast the solid carbonaceous wastes are relatively difficult to process, but their availability is higher. In this regard, a detailed study has been performed to formulate the appropriate processing parameters for best performing CDs.

**2:03PM F27.00013 C<sub>8</sub>-structured carbon quantum dots: Synthesis, blue and green double luminescence, and origins of surface defects**, CHEN XIFANG, ZHANG WENXIA, Department of Physics, Southeast University, Nanjing 211189, PR China, WANG QIANJIN, National Laboratory of Solid State Microstructures and Department of Materials Science and Engineering, Nanjing University, Nanjing 210093, PR China, FAN JIYANG, Department of Physics, Southeast University, Nanjing 211189, PR China — Carbon quantum dots (CQDs) have attracted great attention in the past few years due to their low cytotoxicity, exploited various synthesis methods, unexampled abundance of raw materials on earth, and robust near-infrared to near-UV luminescence. Carbon nanoparticles have applications in biological labeling, delivery of drugs and biological molecules into cells, and light emitting diodes and lasing. CQDs generally exist as nanodiamonds or graphite quantum dots according to previous research reports. In this study, we report the first synthesis of the third-allotrope CQDs through carbonization of sucrose and study their luminescence properties. These CQDs have a body-centered cubic structure and each lattice point is composed of eight atoms which form a sub-cube (so called C<sub>8</sub> crystal structure). High-resolution transmission electron microscopy and X-ray diffraction confirm the C<sub>8</sub> structure of the synthesized carbon nanocrystallites with an average size of 2 nm. The C<sub>8</sub> CQDs exhibit double-band luminescence with two peaks centered at around 432 and 520 nm. The study based on the photoluminescence, UV-Vis absorption, Fourier-transform infrared, and X-ray photoelectron spectroscopies reveals that the green emission originates from the C=O related surface defect.

**Tuesday, March 15, 2016 11:15AM - 2:15PM —**

**Session F28 DMP: Topological Insulator Thin Films** 327 - Matthew Brahlek, Pennsylvania State University

**11:15AM F28.00001 Interfacing Topological Insulators with Ferromagnetism<sup>1</sup>**, ANTHONY RICHARDELLA, Department of Physics, The Pennsylvania State University — In topological insulators, the surface states arise from strong spin-orbit coupling while the degeneracy of the Dirac point is protected by time reversal symmetry. Introducing magnetism in proximity to the surface states breaks this symmetry, destroying the non-trivial Berry phase at the Dirac point and leads to a hedgehog spin texture near the newly opened magnetic gap.<sup>2</sup> This symmetry broken phase leads to a host of unusual physics, such as the quantum anomalous Hall (QAH) effect. In this talk, we discuss the growth by molecular beam epitaxy and characterization of such magnetically interfaced and magnetically doped topological insulators. Such materials often suffer from structural defects and interfacial layers, as well as from degradation during device fabrication.<sup>3</sup> In particular, it is shown that Cr doped (Bi<sub>1-x</sub>Sb<sub>x</sub>)<sub>2</sub>Te<sub>3</sub> can exhibit perfect Hall quantization at low temperatures despite these defects. However, the magnetic ordering of this material was found to be quite unusual, displaying a super-paramagnetic like character, perhaps reflecting this disorder.<sup>4</sup> Such observations highlight the surprising behavior of such broken symmetry phases in topological materials. This work was performed in collaboration with A. Kandala, M. Liu, W. Wang, N.P. Ong, C.-X. Liu, and N. Samarth, in addition to the authors of the references cited.

<sup>1</sup>This work was supported by funding from ARO/MURI, DARPA and ONR.

<sup>2</sup>S.-Y. Xu, M. Neupane, C. Liu, D. Zhang, A. Richardella, L. A. Wray, ... M. Zahid Hasan. Nature Physics, 8, 616 (2012)

<sup>3</sup>A. Richardella, A. Kandala, J. S. Lee, N. Samarth. APL Materials, 3(8), 083303 (2015)

<sup>4</sup>E. O. Lachman, A. F. Young, A. Richardella, J. Cuppens, H. R. Naren, Y. Anahory, ... E. Zeldov. Science Advances 1, e1500740 (2015)

**11:51AM F28.00002 Structure and transport of topological insulators on epitaxial graphene<sup>1</sup>**, JAMES KALLY, Dept. of Physics, Penn State Univ., DANIELLE REIFSNEYDER HICKEY, Dept. of Chemical Engineering and Materials Science, Univ. of Minnesota, YU-CHUAN LIN, Dept. of Materials Science and Engineering, Penn State Univ., ANTHONY RICHARDELLA, JOON SUE LEE, Dept. of Physics, Penn State Univ., JOSHUA ROBINSON, Dept. of Materials Science and Engineering, Penn. State Univ., K. ANDRE MKHOYAN, Dept. of Chemical Engineering and Materials Science, Univ. of Minnesota, NITIN SAMARTH, Dept. of Physics, Penn State Univ. — Recent advancements in spintronics have shown that a class of materials, topological insulators (TI), can be used as a spin-current generator or detector. Topological insulators have protected surface states with the electrons spin locked to its momentum. To access these surface states, (Bi, Sb)<sub>2</sub>Te<sub>3</sub> can be grown by molecular beam epitaxy to have the Fermi energy near the Dirac point so that transport occurs only through the spin-dependent surface states. Graphene is another 2D material of great interest for spintronics because of its very long spin diffusion length. This is an ideal material to act as a spin channel in devices. The van der Waals nature of the growth exhibited by 2D materials such as (Bi, Sb)<sub>2</sub>Te<sub>3</sub> and graphene allows heterostructures to be formed despite the large lattice mismatch. We explore the structure and transport of (Bi, Sb)<sub>2</sub>Te<sub>3</sub> grown on epitaxial graphene on 6H-SiC substrates for spintronic applications.

<sup>1</sup>This work was supported in part by C-SPIN and LEAST, two of the six centers of STARnet, a Semiconductor Research Corporation program, sponsored by MARCO and DARPA.

**12:03PM F28.00003 Band Bending Inversion in Bi<sub>2</sub>Se<sub>3</sub> Nanostructures**, LOUIS VEYRAT, IFW-Dresden, Institute for Solid State Research, FABRICE IACOVELLA, Laboratoire National des Champs Magnétiques Intenses (LNCMI-EMFL), JOSEPH DUFOULEUR, CHRISTIAN NOWKA, HANNES FUNKE, IFW-Dresden, Institute for Solid State Research, MING YANG, WALTER ESCOFFIER, MICHEL GOIRAN, Laboratoire National des Champs Magnétiques Intenses (LNCMI-EMFL), BARBARA EICHLER, OLIVER G. SCHMIDT, BERND BCHNER, SILKE HAMPEL, ROMAIN GIRAUD, IFW-Dresden, Institute for Solid State Research — Shubnikov-de-Haas oscillations were studied under high magnetic field in Bi<sub>2</sub>Se<sub>3</sub> nanostructures grown by Chemical Vapor Transport, for different bulk carrier densities ranging from  $3 \times 10^{19} \text{ cm}^{-3}$  to  $6 \times 10^{17} \text{ cm}^{-3}$ . The contribution of topological surface states to electrical transport can be identified and separated from bulk carriers and massive two-dimensional electron gas. Band bending is investigated, and a crossover from upward to downward band bending is found at low bulk density, as a result of a competition between bulk and interface doping. These results highlight the need to control electrical doping both in the bulk and at interfaces in order to study only topological surface states[1]. [1] : Veyrat et al., Nano Lett., Article ASAP, DOI: 10.1021/acs.nanolett.5b03124

**12:15PM F28.00004 High-mobility surface states and conductance fluctuations in Bismuth Telluro-Sulfide topological insulator devices**, TANUJ TRIVEDI, SUSHANT SONDE, HEMA C. P. MOVVA, SANJAY K. BANERJEE, Microelectronics Research Center, The University of Texas at Austin — Since the experimental discovery of three-dimensional topological insulators (TI), (Bi,Sb)<sub>2</sub>(Se,Te)<sub>3</sub> binary compounds are the principal material systems to explore TI physics. However, transport experiments studying surface-states are complicated by parallel bulk conductivity contribution, which is expected to improve for ternary and quaternary chalcogenide compounds of Bi and Sb. A promising alternative is the Sulfur-based tetradymite with an ideal formula of Bi<sub>2</sub>Te<sub>2</sub>S, which has received little attention. We present van der Waals epitaxial growth and magnetotransport in Bismuth Telluro-Sulfide (BTS) crystalline nanosheets. Gating-enhanced Weak-antilocalization (WAL) and Universal Conductance Fluctuations (UCF) are observed in BTS devices. Empirical modeling of the data shows the existence of two-dimensional surface transport. A three-channel Hall conductivity model is proposed, which is utilized in conjunction with an extended-WAL analysis, showing the presence of a high-mobility surface component and indication for separation of transport channels in BTS devices. Our growth and comprehensive transport experiments demonstrate BTS as a promising candidate TI material.

**12:27PM F28.00005 In Situ Thin Film Growth and Characterization of Topological Dirac Semimetal  $\text{Na}_3\text{Bi}$** <sup>1</sup>, JACK HELLERSTEDT, MARK EDMONDS, CHANG LIU, Monash Centre for Atomically Thin Materials, NAVNEETH RAMAKRISHNAN, NUS Singapore, SHAFFIQUE ADAM, Yale-NUS College, MICHAEL FUHRER, Monash Centre for Atomically Thin Materials — The alkali pnictide  $\text{Na}_3\text{Bi}$  is a three-dimensional Dirac semimetal possessing Dirac-like dispersions in  $k_x$ ,  $k_y$  and  $k_z$ , that has attracted recent interest as a condensed matter system for realizing the chiral anomaly [1]. The high reactivity of sodium makes conventional synthesis and characterization extremely difficult: we circumvent this issue by combining thin film growth with low temperature STM and magnetotransport in one comprehensive UHV system. We have successfully grown  $\text{Na}_3\text{Bi}$  on  $\alpha\text{-Al}_2\text{O}_3$  (0001) substrates, achieving low temperature mobilities in excess of  $3,500 \text{ cm}^2/\text{Vs}$  and carrier densities as low as  $5 \times 10^{12} \text{ cm}^{-2}$ . Perpendicular magnetoresistance up to 1T shows quadratic behavior with weak anti-localization at low field. Quantitative analysis of this data suggests that our samples are in a charge inhomogeneous regime reminiscent of charge puddling in graphene [2]. [1] Xiong et. al Science (2015) doi:10.1126/science.aac6089 [2] Ramakrishnan et. al arXiv:1501.03815 (2015)

<sup>1</sup>JH, MTE and MSF are supported by MSFs ARC Laureate Fellowship (FL120100038)

**12:39PM F28.00006 Epitaxial  $\text{Cd}_3\text{As}_2$  Thin Films Synthesized by Molecular Beam Epitaxy**, TIMO SCHUMANN, MANIK GOYAL, SUSANNE STEMMER, Univ of California - Santa Barbara —  $\text{Cd}_3\text{As}_2$  is a three-dimensional (3D) Dirac semimetal, i.e. it possesses Dirac cones in a 3D bulk state where the band dispersion relation is linear near the Fermi energy.  $\text{Cd}_3\text{As}_2$  has raised considerable interest due to its high electron mobilities in bulk crystals and for novel quantum phenomena, such as chiral anomalies. However, few studies have been performed using thin films of  $\text{Cd}_3\text{As}_2$ . In this presentation, we report on the synthesis of  $\text{Cd}_3\text{As}_2$  thin films by molecular beam epitaxy (MBE). Single phase, epitaxial films were grown on undoped GaSb(111)B substrates with the (112) facet of  $\text{Cd}_3\text{As}_2$  parallel to the GaSb(111) surface. We report on the structural quality and orientation variants in the films. Electrical transport properties indicate electron mobilities exceeding  $6000 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ . We discuss the impact of the MBE growth parameters and substrate preparation on the structural and electrical properties of the films.

**12:51PM F28.00007 Asymmetric topological interfaces and charge transfer in epitaxial  $\text{Bi}_2\text{Se}_3$ /II-VI superlattices**, ZHIYI CHEN, The Graduate Center - CUNY, The City College of New York - CUNY, LUKASF ZHAO, INNA KORZHOVSKA, THOR GARCIA, MARIA TAMARGO, LIA KRUSIN-ELBAUM, The City College of New York - CUNY, KYUNGWHA PARK, Virginia Tech. — Access to charge transport through Dirac surface states in topological insulators (TIs) can be challenging due to their intermixing with the bulk or with non-topological subsurface two-dimensional electron gas (2DEG) quantum well states. Formed by bending of bulk electronic bands near the surface, 2DEG states arise via charge transfer to the topological surfaces, so the choice of layers abutting these surfaces is critical. Here we report molecular beam epitaxial growth of  $\text{Bi}_2\text{Se}_3/\text{Zn}_x\text{Cd}_{1-x}\text{Se}$  superlattices that support only one topological surface channel per TI layer. The topological nature of conducting channels is evidenced by  $\pi$ -Berry phase and by the two-dimensional weak antilocalization. Both density functional theory calculations and transport measurements suggest that a single topological Dirac cone per TI layer arises from the asymmetry between the Se-terminated and Zn-terminated interfaces of  $\text{Zn}_x\text{Cd}_{1-x}\text{Se}$  with  $\text{Bi}_2\text{Se}_3$ . Our findings suggest that topological transport could be controlled by adjusting charge transfer from non-topological spacers in hybrid structures. \*Supported by NSF-DMR-1420634, NSF-DMR-1312483, DOD-W911NF-13-1-0159, NSF DMR-1206354 and computer resources from SDSC under DMR060009N and VT ARC

**1:03PM F28.00008 Study of the circular photo-galvanic effect in electrically gated  $(\text{Bi,Sb})_2\text{Te}_3$  thin films**, YU PAN, TIMOTHY PILLSBURY, ANTHONY RICHARDELLA, THOMAS FLANAGAN, NITIN SAMARTH, The Pennsylvania State University — Illumination with circularly polarized light is known to produce a helicity dependent photocurrent in topological insulators such as  $\text{Bi}_2\text{Se}_3$  [Nature Nanotech. 7, 96 (2012)]. Symmetry considerations suggest that this circular photo-galvanic effect (CPGE) arises purely from the surface. However, whether or not the CPGE is directly related to optical excitations from the helical surface states is still under debate. To clarify the origin of the CPGE, we first compare the helicity dependent photocurrent in intrinsic  $(\text{Bi,Sb})_2\text{Te}_3$  to Cr doped  $(\text{Bi,Sb})_2\text{Te}_3$  thin films in which the Dirac surface states are perturbed by magnetic coupling. Secondly, we discuss the tunable CPGE in electrically gated  $(\text{Bi,Sb})_2\text{Te}_3$  thin films excited by optical excitations at different wavelengths. The dependence on the chemical potential and the photon energy of the excitation unveils the origin of the CPGE. Funded by ONR.

**1:15PM F28.00009 Low Temperature Quantum Transport Properties of  $\text{Bi}_2\text{Se}_3$  Topological Insulator Thin Films**<sup>1</sup>, DAVID LEDERMAN<sup>2</sup>, SERCAN BABAKIRAY, PAVEL BORISOV, AMIT KC, YURI GLINKA, West Virginia University —  $\text{Bi}_2\text{Se}_3$  thin films with nominal thickness values of 12, 16, 20 and 25 quintuple layers (QLs) were grown by molecular beam epitaxy (MBE) on  $\text{Al}_2\text{O}_3$  substrates. The magnetoconductance (MC) was analyzed using the two-dimensional Altshuler-Aronov (AA) and Hikami-Larkin-Nagaoka (HLN) mechanisms. Using a simple model where the channels for the bulk and surface states are independent from each other, and assuming that all channels undergo WAL, it was possible to determine the phase coherence length ( $L_\phi$ ) of the carriers of the surface and bulk contributions independently from the MC with the field perpendicular to the surface. The value of  $L_\phi$  for the surface states was independent of thickness, as expected, while  $L_\phi$  for the bulk channel was strongly dependent on film thickness. WAL was also measured with the field applied parallel to the surface, and from the MC data in this configuration, it was possible to obtain values for  $L_\phi$  that were similar to the perpendicular configuration for all samples except for the thinnest sample (12 QL), which may be a result of interactions between the metallic surface states on opposite sides of the film. We will discuss these results in view of other results from the literature.

<sup>1</sup>This work was supported at WVU by a Research Challenge Grant from the West Virginia Higher Education Policy Commission and by the WVU Shared Research Facilities.

<sup>2</sup>Physics Department, University of California, Santa Cruz

**1:27PM F28.00010 High quality topological insulator thin films grown by molecular beam epitaxy using  $\text{MoS}_2$  monolayer as buffer layer**, K. H. CHEN, H. Y. LIN, C. Y. WANG, S. R. YANG, J. KWO, Dept. of Physics, Natl Tsing Hua Univ., Hsinchu 30013, Taiwan, C. K. CHENG, M. HONG, Graduate Institute of Applied Physics and Dept. of Physics, National Taiwan Univ., Taipei 10617, Taiwan, X. Q. ZHANG, Y. H. LEE, Dept. of Material Science and Engineering, Natl Tsing Hua Univ., Hsinchu 30013, Taiwan — Topological insulators (TIs), a new state of quantum matter, display a rich variety of physical phenomena. High quality TI films of  $\text{Bi}_2\text{Se}_3$  and  $\text{Bi}_2\text{Te}_3$  have been obtained by van der Waals epitaxy on various substrates. To further reduce the high defect density level common in these films, we have extended the investigation to utilize 2D layered materials of hexagonal symmetry as substrates, such as large area CVD-grown  $\text{MoS}_2$  monolayer. Streaky RHEED patterns were observed during growth. Normal scans of x-ray diffraction indicated that the c-axis of films grown on both  $\text{Al}_2\text{O}_3$ (0001) and  $\text{MoS}_2/\text{Al}_2\text{O}_3$ (0001) were fully strain relaxed with a FWHM varying from 0.01 to 0.03, suggesting a very high degree of crystallinity. Using AFM, we found that size of triangular shaped domains were substantially bigger ( $\sim 1.5\mu\text{m}$ ) than those without  $\text{MoS}_2$  ( $\sim 0.6\mu\text{m}$ ). Furthermore, reduction by  $\sim 16\%$  in carrier concentration and a mobility as high as  $5700 \text{ cm}^2/\text{Vs}$  were observed in our 50nm film with  $\text{MoS}_2$ . Other thickness dependent transport properties such as WAL are underway, along with ARPES study of the electronic structures.

**1:39PM F28.00011 Visualizing virgin magnetic domains of V-doped  $\text{Sb}_2\text{Te}_3$  thin films<sup>1</sup>**, WENBO WANG, Department of Physics and Astronomy, Rutgers University, Piscataway, NJ, 08854 USA, CUI-ZU CHANG, JAGADEESH S. MOODERA, Francis Bitter Magnet Lab, Massachusetts Institute of Technology, Cambridge, MA 02139, USA., WEIDA WU, Department of Physics and Astronomy, Rutgers University, Piscataway, NJ, 08854 USA — Quantum anomalous Hall effect (QAHE) was experimentally realized in a ferromagnetic topological insulator Cr-doped  $(\text{Bi,Sb})_2\text{Te}_3$  thin film for the first time[1]. Recently, a more robust QAHE has been observed in V-doped  $(\text{Bi,Sb})_2\text{Te}_3$  thin film, which has a much larger coercive field and higher Curie temperature at the same doping level[2]. However, a mysterious self-magnetization phenomenon was observed in the V-doped  $\text{Sb}_2\text{Te}_3$ , where net magnetization spontaneously develops after zero field cooling. In this talk, we utilize cryogenic magnetic force microscopy (MFM) technique to study the domain states of V doped  $\text{Sb}_2\text{Te}_3$  film under various cooling fields. A zero net magnetization state with equally distributed up and down domains was observed after zero-field cooling. In addition, a small external magnetic field ( $\sim 5$  Oe) is able to significantly polarize the magnetization of the film. Our MFM results are qualitatively consistent with in-situ magnetoresistance measurements. [1] C.-Z. Chang et al., Science 340, 167 (2013). [2] C.-Z. Chang et al., Nature Materials 14, 473477(2015).

<sup>1</sup>This work is supported by DOE BES under award DE-SC0008147.

**1:51PM F28.00012 Controlling the 2DEG states evolution at a metal/ $\text{Bi}_2\text{X}_3$  ( $\text{X}=\text{Se,Te}$ ) interface**, HAN-JIN NOH, JINWON JEONG, EN-JIN CHO, Department of Physics, Chonnam National University, JOONBUM PARK, JUN SUNG KIM, Department of Physics, Pohang University of Science and Technology, ILYOU KIM, BYEONG-GYU PARK, Pohang Accelerator Laboratory, Pohang University of Science and Technology, HYEONG-DO KIM, Department of Physics and Astronomy, Institute for Basic Science — We have demonstrated that the evolution of the two-dimensional electron gas (2DEG) system at an interface of metal and the model topological insulator (TI)  $\text{Bi}_2\text{X}_3$  ( $\text{X}=\text{Se, Te}$ ) can be controlled by choosing an appropriate kind of metal elements and by applying a low temperature evaporation procedure. In particular, we find that only topological surface states (TSSs) can exist at a  $\text{Mn}/\text{Bi}_2\text{X}_3$  interface, which would be useful for implementing a TI-based device with surface current channels only. The existence of the TSSs alone at the interface was confirmed by angle-resolved photoemission spectroscopy (ARPES). Based on the ARPES and core-level x-ray photoemission spectroscopy measurements, we propose a cation intercalation model to explain our findings.

**2:03PM F28.00013 Characterization of high-quality  $\text{Bi}_2\text{Se}_3$  films grown using a selenium cracker source<sup>1</sup>**, THERESA GINLEY, STEPHANIE LAW, University of Delaware — Topological insulators, including  $\text{Bi}_2\text{Se}_3$ , are becoming increasingly prevalent in research due to their unique electronic properties. These materials exhibit an insulating bulk but conducting surfaces with electron spin-momentum locking. Using Molecular Beam Epitaxy (MBE) it is possible to grow high-quality thin films of  $\text{Bi}_2\text{Se}_3$ . Yet these films have not lived up to their potential, in part due to significant bulk conductivity arising from material defects like selenium vacancies. Current MBE growth methods for  $\text{Bi}_2\text{Se}_3$  use standard selenium sources that evaporate large selenium molecules which must then be cracked into smaller molecules to be incorporated into the film. This process is inefficient and requires very high fluxes of selenium for good quality growths. However, using a selenium cracking source results in the evaporation of monomers and dimers, facilitating incorporation into the film. We will present electrical, structural, and optical measurements demonstrating that the use of a cracker source allows films to be grown using much lower selenium:bismuth flux ratios with good mobility and low carrier density.

<sup>1</sup>T. G. and S. L. gratefully acknowledge funding from the University of Delaware Research Foundation grant 15A00862

**Tuesday, March 15, 2016 11:15AM - 2:15PM –**

**Session F29 DCMP DMP: Novel Topological Phases: Theory** 328 - Bitan Roy, University of Maryland

**11:15AM F29.00001 Chiral topological superconductor and half-integer conductance plateau from quantum anomalous hall plateau transition**, QUAN ZHOU, Stanford Univ, JING WANG, BIAO LIAN, SHOUCHENG ZHANG, Stanford University, ZHANG'S GROUP TEAM — We propose to realize a two-dimensional chiral topological superconducting (TSC) state from the quantum anomalous hall plateau transition in a magnetic topological insulator thin LM through the proximity ECT to a conventional s-wave superconductor. This state has a full pairing gap in the bulk and a single chiral majorana mode at the edge. The optimal condition for realizing such chiral tsc is to have inequivalent superconducting pairing amplitudes on top and bottom surfaces of the doped magnetic topological insulator. We further propose several transport experiments to detect the chiral TSC. One unique signature is that the conductance will be quantized into a half-integer plateau at the coercive eld in this hybrid system. In particular, with the point contact formed by a superconducting junction, the conductance oscillates between  $E_2=2H$  AND  $E_2=H$  with the frequency determined by the voltage across the junction. we close by discussing the feasibility of these experimental proposals.

**11:27AM F29.00002 Bona fide interaction-driven topological phase transition in correlated SPT states**, ZI YANG MENG, Institute of Physics, Chinese Academy of Sciences, YUAN-YAO HE, HAN-QING WU, Department of Physics, Renmin University of China, Beijing 100872, China, YI-ZHUANG YOU, CENKE XU, Department of Physics, University of California, Santa Barbara, California 93106, USA, ZHONG-YI LU, Department of Physics, Renmin University of China, Beijing 100872, China — It is expected the interplay between non-trivial band topology and strong electron correlation will lead to very rich physics. Thus a controlled study of the competition between topology and correlation is of great interest. Here, employing large-scale quantum Monte Carlo simulations, we provide a concrete example of the Kane-Mele-Hubbard model on an AA stacking bilayer honeycomb lattice with inter-layer antiferromagnetic interaction. Our simulation identified several different phases: a quantum spin-Hall insulator (QSH), a xy-plane antiferromagnetic Mott insulator (xy-AFM) and an inter-layer dimer-singlet insulator (dimer-singlet). Most importantly, a bona fide topological phase transition between the QSH and the dimer-singlet insulators, purely driven by the inter-layer antiferromagnetic interaction is found. At the transition, the spin and charge gap of the system close while the single-particle excitations remain gapped, which means that this transition has no mean field analogue and it can be viewed as a transition between bosonic SPT states. At one special point, this transition is described by a  $(2+1)\text{d}$   $\text{O}(4)$  nonlinear sigma model with exact  $\text{SO}(4)$  symmetry, and a topological term at  $\theta=\pi$ . Relevance of this work towards more general interacting SPT states is discussed.

**11:39AM F29.00003 Topological Phases on Non-orientable Surfaces: Twisting by Parity Symmetry**, PAK ON CHAN, ICMT at University of Illinois Urbana-Champaign, CHI YAN TEO, Physics at the University Of Virginia, SHINSEI RYU, ICMT at University of Illinois Urbana-Champaign — We discuss  $(2+1)\text{D}$  topological phases on non-orientable spatial surfaces, such as Möbius strip, real projective plane and Klein bottle, etc., which are obtained by twisting the parent topological phases by their underlying parity symmetries through introducing parity defects. We construct the ground states on arbitrary non-orientable closed manifolds and calculate the ground state degeneracy. Such degeneracy is shown to be robust against continuous deformation of the underlying manifold. We also study the action of the mapping class group on the multiplet of ground states on the Klein bottle. The physical properties of the topological states on non-orientable surfaces are deeply related to the parity symmetric anyons which do not have a notion of orientation in their statistics. For example, the number of ground states on the projective plane equals the root of the number of distinguishable parity symmetric anyons, while the ground state degeneracy on the Klein bottle equals the total number of parity symmetric anyons; In deforming the Klein bottle, the Dehn twist encodes the topological spins whereas the Y-homeomorphism tells the particle-hole relation of the parity symmetric anyons.

**11:51AM F29.00004 Analysis of the Kane-Mele-Kondo lattice at finite temperatures.**<sup>1</sup>, TSUNEYA YOSHIDA, Condensed Matter Theory Laboratory, RIKEN, ROBERT PETERS, Computational Condensed Matter Physics Laboratory, RIKEN, NORIO KAWAKAMI, Department of Physics, Kyoto University — Recently, correlation effects on topological insulators are extensively studied because the interplay of topological properties and electron correlations is expected to induce exotic phenomena. A promising candidate for a topological insulator in heavy-fermion systems is  $\mathrm{SmB}_{6}$  where the Kondo effects play an essential role. In this article, we study the Kane-Mele-Kondo lattice at finite temperatures. By using the dynamical mean-field theory, we obtain a temperature vs. interaction phase diagram (a Doniach phase diagram). Furthermore, we have observed an intriguing crossover behavior induced by the interplay of electron correlations and topologically nontrivial properties. In the bulk system, the spin-Hall conductivity which is proportional to the spin Chern number is zero at low temperatures while the conductivity rapidly increases with increasing temperature. Correspondingly, gapless modes are restored by temperature effects at the edge sites, which are destroyed by the Kondo effect at low temperature.

<sup>1</sup>This work is partly supported by KAKENHI (No. 25400366, and 15H05855). The numerical calculations were performed at the ISSP in the University of Tokyo and on the SR16000 at YITP in Kyoto University.

**12:03PM F29.00005 Bulk Topological Proximity Effect**, TIMOTHY HSIEH, HIROAKI ISHIZUKA, LEON BALENTS, Kavli Institute for Theoretical Physics, TAYLOR HUGHES, University of Illinois at Urbana-Champaign — Existing proximity effects stem from systems with a local order parameter, such as a local magnetic moment or a local superconducting pairing amplitude. Here, we demonstrate that despite lacking a local order parameter, topological phases also may give rise to a proximity effect of a distinctively inverted nature. We focus on a general construction in which a topological phase is extensively coupled to a second system, and we argue that in many cases, the inverse topological order will be induced on the second system. To support our arguments, we rigorously establish this “bulk topological proximity effect” for all gapped free fermion topological phases and representative integrable models of interacting topological phases. We present a terrace construction which illustrates the phenomenological consequences of this proximity effect. Finally, we discuss generalizations beyond our framework, including how intrinsic topological order may also exhibit this effect.

**12:15PM F29.00006 Electrically tunable spin polarization of chiral edge modes in a quantum anomalous Hall insulator**, RUI-XING ZHANG, HSIU-CHUAN HSU, CHAO-XING LIU, Department of Physics, The Pennsylvania State University — In the quantum anomalous Hall effect, chiral edge modes are expected to conduct spin polarized current without dissipation and thus hold great promise for future electronics and spintronics with low energy consumption. However, spin polarization of chiral edge modes has never been established in experiments. In this work, we theoretically study spin polarization of chiral edge modes in the quantum anomalous Hall effect, based on both the effective model and more realistic tight-binding model constructed from the first principles calculations. We find that spin polarization can be manipulated by tuning either a local gate voltage or the Fermi energy. We also propose to extract spin information of chiral edge modes by contacting the quantum anomalous Hall insulator to a ferromagnetic (FM) lead. The establishment of spin polarization of chiral edge modes, as well as the manipulation and detection in a fully electrical manner, will pave the way to the applications of the quantum anomalous Hall effect in spintronics.

**12:27PM F29.00007 Topological invariants in interacting topological insulators: Success and Breakdown**, YUAN-YAO HE, HAN-QING WU, Department of Physics, Renmin University of China, Beijing 100872, China, ZI YANG MENG, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, ZHONG-YI LU, Department of Physics, Renmin University of China, Beijing 100872, China — The content of this talk is twofold. In the first part, we provide a paradigm of efficient numerical evaluation scheme for topological invariants via zero-frequency single-particle Green's function in quantum Monte Carlo (QMC) simulations. Especially, we introduce a periodization process to overcome the ubiquitous finite-size effect and make use of symmetry properties of the underlying systems to reduce the computational effort. This scheme is tested to be successful on models of interacting topological insulators, where there is single-particle gap closing at the transition. In the second part, we apply the above scheme to wider classes of interacting topological insulators, in which the breakdown of constructing topological invariant via single-particle Green's functions is presented. These systems host novel interaction-driven topological phase transitions without symmetry breaking, and hence fermionic degree of freedom is not involved at the critical point, instead, collective bosonic mode become critical.

**12:39PM F29.00008 Of Bulk and Boundaries: Generalized Transfer Matrices for Tight-Binding Models**<sup>1</sup>, VATSAL DWIVEDI, VICTOR CHUA, Univ of Illinois - Urbana — We construct a generalized transfer matrix corresponding to noninteracting tight-binding lattice models, which can subsequently be used to compute the bulk bands as well as the edge states. Crucially, our formalism works even in cases where the hopping matrix is non-invertible. Following Hatsugai [PRL 71, 3697 (1993)], we explicitly construct the energy Riemann surfaces associated with the band structure for a specific class of systems which includes systems like Chern insulator, Dirac semimetal and graphene. The edge states can then be interpreted as non-contractible loops, with the winding number equal to the bulk Chern number. For these systems, the transfer matrix is symplectic, and hence we also describe the windings associated with the edge states on  $Sp(2, R)$  and interpret the corresponding winding number as a Maslov index. This work is discussed in arXiv preprint arXiv:1510.04279.

<sup>1</sup>National Science Foundation Grant NSF DMR 13-06011 and Gordon and Betty Moore Foundation's EPiQS Initiative Grant GBMF4305

**12:51PM F29.00009 Topological Edge States with Zero Hall Conductivity in a Dimerized Hofstadter Model**, ALEXANDER LAU, CARMINE ORTIX, JEROEN VAN DEN BRINK, Institute for Theoretical Solid State Physics, IFW Dresden — The Hofstadter model is one of the most celebrated models for the study of topological properties of matter and allows the study of the quantum Hall effect in a lattice system. Indeed, the Hofstadter Hamiltonian harbors the topological chiral edge states that are responsible for the quantized Hall conductivity. Here, we show that a lattice dimerization in the Hofstadter model opens an energy gap at half-filling. What is more, we demonstrate that even if the ensuing insulator has a Chern number equal to zero, concomitantly a doublet of edge states appear that are pinned to specific momenta. We show that the presence of these states can be understood from the topological properties of lower dimensional cuts of the system, using a mapping of the Hofstadter Hamiltonian to a collection of one-dimensional Aubry-André-Harper (AAH) models. A sub-set of AAH chains in this collection preserve inversion symmetry. This guarantees the presence of topologically protected doublets of end modes to which the edge states are pinned. To explicitly prove the robustness of the emerging edge states, we define and calculate the topological invariant that protects them, which turns out to be an integer invariant for inversion-symmetric AAH models.

**1:03PM F29.00010 Field theory of symmetry protected valence bond solid states in (2+1) dimensions**, AKIHIRO TANAKA, National Institute for Materials Science, Jpn, SHINTARO TAKAYOSHI, Department of Quantum Matter Physics, University of Geneva — With the scope of identifying possible symmetry-protected topological (SPT) states, we revisit the effective field theory description of 2d antiferromagnets in terms of nonlinear sigma models with topological Berry phase terms. We focus on ground states that can be characterized as spatially-uniform valence-bond-solid states residing on a square lattice, which implies that the spin quantum number  $S$  be an even integer. A path integral representation of wave functionals allows us to study the topological properties of the ground state in terms of a field theory defined in a space whose dimensionality is reduced by one, which leads us to an interesting incarnation of the well-known Haldane-gap argument for 1d antiferromagnets. From this, we conclude that the ground state can be an SPT state when  $S = 2 \times \text{odd integer}$ , while for  $S = 2 \times \text{even integer}$  it is topologically trivial. We also discuss how our method generalizes to 1d and 3d antiferromagnets.

**1:15PM F29.00011 First-Order Character and Observable Signatures of Topological Quantum Phase Transitions**, GIORGIO SANGIOVANNI, University of Wuerzburg, Germany, ADRIANO AMARICCI, SISSA Trieste, Italy, JAN CARL BUDICH, University of Innsbruck, Austria, MASSIMO CAPONE, SISSA Trieste, Italy, BJOERN TRAUZETTEL, University of Wuerzburg, Germany — Topological quantum phase transitions are characterized by changes in global topological invariants. These invariants classify many-body systems beyond the conventional paradigm of local order parameters describing spontaneous symmetry breaking. For noninteracting electrons, it is well understood that such transitions are continuous and always accompanied by a gap closing in the energy spectrum, given that the symmetries protecting the topological phase are maintained. Here, we demonstrate that a sufficiently strong electron-electron interaction can fundamentally change the situation: we discover a topological quantum phase transition of first-order character in the genuine thermodynamic sense that occurs without a gap closing. Our theoretical study reveals the existence of a quantum critical endpoint associated with an orbital instability on the transition line between a 2D topological insulator and a trivial band insulator. Remarkably, this phenomenon entails unambiguous signatures related to the orbital occupations that can be detected experimentally. Part of the results presented in this talk have been published in Phys. Rev. Lett. 114, 185701 (2015)

**1:27PM F29.00012 Construction of non-Abelian topological insulators using non-Abelian bosonization**, PO-HAO HUANG, Boston University, JYONG-HAO CHEN, Paul Scherrer Institute, PEDRO GOMES, Universidade de Sao Paulo, TITUS NEUPERT, Princeton University, CHRISTOPHER MUDRY, Paul Scherrer Institute, CLAUDIO CHAMON, Boston University — A way to construct 2D topological insulators and superconductors is to couple an array of wires. The advantage of this construction is that one can use bosonization. Many 2D integer and fractional topological quantum states have been proposed using Abelian bosonization. In this talk we show how to use non-Abelian bosonization to construct non-Abelian topological insulators and superconductors in 2D. With the help of conformal field theory, we construct topological states whose edge states are described by coset theories of the Wess-Zumino-Witten model. In this construction, all the interactions we use to gap the bulk are physical, i.e. tunneling of electrons and current-current interactions.

**1:39PM F29.00013 Constructing parent Hamiltonians for  $SU(N)$  AKLT states - a diagrammatic method**, ABHISHEK ROY, THOMAS QUELLA, Institute of Theoretical Physics, University of Cologne — Over the last decade, there has been increasing experimental interest in alkaline cold atom systems which exhibit  $SU(N)$  symmetry. Theoretical work has shown that a one-dimensional  $SU(N)$  chain can have  $N - 1$  symmetric protected states distinguished by fractionalized boundary spins. We introduce a new method for constructing  $SU(N)$  invariant Hamiltonians for Haldane phases in one dimension. Working at the AKLT point where the ground state is known exactly, we show a universal form of the Hamiltonian for any appropriate choice of physical and boundary spins. We apply our method to the case where the physical spin is in the adjoint representation and obtain a general expression for the Hamiltonian as well the Transfer Matrix for any  $N$ . Finally we comment on the relevance of our results to the generalized Haldane conjecture.

**1:51PM F29.00014 Topological Nonsymmorphic Crystalline Superconductors**, QING-ZE WANG, CHAO-XING LIU, The Pennsylvania State University — Topological superconductors possess a nodeless superconducting gap in the bulk and gapless zero energy modes, known as "Majorana zero modes", at the boundary of a finite system. In this work, we introduce a new class of topological superconductors, which are protected by nonsymmorphic crystalline symmetry and thus dubbed "topological nonsymmorphic crystalline superconductors". We construct an explicit Bogoliubov-de Gennes type of model for this superconducting phase in the D class and show how Majorana zero modes in this model are protected by glide symmetry. Furthermore, we generalize the classification of topological nonsymmorphic crystalline superconductors to the classes with time reversal symmetry, including the DIII and BDI classes, in two dimensions. Our theory provides a guidance to search for new topological superconducting materials with nonsymmorphic crystal structures.

**2:03PM F29.00015 Equivalence of topological insulators and superconductors**, GERARDO ORTIZ, Indiana Univ - Bloomington, EMILIO COBANERA, Dartmouth College — Systems of free fermions are classified by symmetry, space dimensionality, and topological properties described by K-homology. We show that by taking a many-body/Fock space viewpoint it becomes possible to establish equivalences of topological insulators and superconductors in terms of duality transformations [1]. These mappings connect topologically inequivalent systems of fermions, jumping across entries in existent classification tables, because of the phenomenon of symmetry transmutation by which a symmetry and its dual partner have identical algebraic properties but very different physical interpretations and electromagnetic response. Since our analysis extends to interacting fermion systems we also briefly discuss some such applications. To illustrate main concepts we will present dual superconducting partners of paradigmatic models, such as the Haldane Chern insulator as well as a quantum spin Hall effect graphene model. [1] Phys. Rev. B 92, 155125 (2015).

**Tuesday, March 15, 2016 11:15AM - 2:15PM –**

**Session F30 DMP: Orbital and Electronic Transitions in Oxide Heterostructures** 329 - Hyowon Park, University of Illinois, Chicago

**11:15AM F30.00001 Orbital reconstruction through interlayer cation charge imbalance: insights from wave-function-based quantum chemistry calculations**, LIVIU HOZOI, IFW Dresden, Germany — A promising route to engineering the electronic properties of quantum materials and devices rests on the idea of orbital reconstruction in multilayered oxide heterostructures. In this context, we identify and discuss in detail one simple, appealing mechanism for tailoring the sequence of d-electron energy levels: interplanar cation charge imbalance (ICCI) along successive metal-oxygen layers [1,2]. Through interplay with distortions of the ligand cages, it provides a knob for tuning the order of electronic levels in even intrinsically stacked oxides. We analyze in this regard electron spin resonance data for the 214 Sr-iridate oxide compound [1]. While canonical ligand-field theory predicts z-axis g factors smaller than 2 for positive tetragonal distortions as present in Sr214, the experiment indicates values larger than 2. This implies that the iridium d levels are inverted with respect to their normal ordering. State-of-the-art quantum chemistry calculations confirm the level switching in Sr214, whereas we find them to be instead normally ordered in the sister compound Ba214. Given the nonpolar character of the metal-oxygen layers, our findings highlight the tetravalent transition-metal 214 oxides as ideal platforms to explore d-orbital engineering in the context of oxide electronics. The crucial role of internal anisotropic fields related to the environment beyond nearest-neighbor ligands is further highlighted by ab initio quantum chemistry calculations on 3D pyrochlore osmates and iridates [3,4]. [References: [1] N. Bogdanov et al., Nature Commun. 6, 7306 (2015); [2] V. Katukuri et al., Inorg. Chem. 53, 4833 (2014); [3] L. Hozoi et al., Phys. Rev. B 89, 115111 (2014); [4] N. Bogdanov et al., Phys. Rev. Lett. 110, 127206 (2013).]

**11:51AM F30.00002 Enhancement of conductivity in ultrathin films of  $\text{LaNiO}_3$** , JENNIFER FOWLIE, MARTA GIBERT, SARA CATALANO, JEAN-MARC TRISCONE, University of Geneva — In order to achieve tailor-made properties in oxide heterostructures it is essential to first fully understand the physics of these materials and their behavior when pushing the 2-D limit. That is the principle goal of this work.  $\text{LaNiO}_3$  (LNO), a metal in bulk, has previously been found to be insulating in ultrathin form and this behavior was attributed to the onset of weak, and then strong, localization. A key feature of ultrathin films is that a significant portion of the sample is under the influence of the two "boundaries", these are the interfaces with the substrate and with the vacuum respectively. The effects of both of these boundaries have been studied previously by changing substrate material and with the addition of an encapsulating layer. In this work we show that, for LNO grown on  $\text{LaAlO}_3$  (001) substrates, there is an enhancement of conductivity that occurs on the verge of the ultrathin regime (less than 10 unit cells) and we hypothesize that this stems from a structural distortion imposed at the substrate-film interface.

**12:03PM F30.00003 Metal-insulator transition and emergence of spontaneous polarization in  $(\text{La}_{1-x}\text{Sr}_x\text{MnO}_3)_m/(\text{LaNiO}_3)_n$  superlattices constructed from metallic building blocks<sup>1</sup>**, SAURABH GHOSH, Vanderbilt University, Oak Ridge National Laboratory, USA, ROHAN MISHRA, Washington University in St. Louis, USA, JASON HOFFMAN, ANAND BHATTACHARYA, Argonne National Laboratory, USA, ALBINA Y. BORISEVICH, Oak Ridge National Laboratory, USA, SOKRATES T. PANTELIDES, Vanderbilt University, USA —  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$  and  $\text{LaNiO}_3$  are metallic oxides. However, short-period superlattices of the form  $(\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3)_m/(\text{LaNiO}_3)_n$  show insulating behavior depending on  $m$  and  $n$ . In particular, the insulating property is robust when  $m = n = 2$  (SL 2/2). Here, using first-principles density functional theory (DFT) and DFT+U (static  $d-d$  Coulomb interaction), we explain the experimental observation and discuss a general mechanism that underlies such metal-insulator transition for different  $m$  and  $n$ . The general mechanism is based on the finding that disproportionation on Ni sites is the key. Further, we predict that insulating SL 2/2 is ferroelectric with large spontaneous polarization. The ferroelectric distortion persists in the cases where the superlattices are metallic, which leads to the possibility of designing a new family of 'polar metals'. Finally, we discuss the origin of such polar distortion and its coupling with the magnetic properties (by considering spin-phonon coupling) of the material.

<sup>1</sup>This work is supported by DOE Grant number DE-FG02-09ER46554 and DOE BES DMSE

**12:15PM F30.00004 Polarity and the Metal-Insulator Transition in ultrathin  $\text{LaNiO}_3$  on  $\text{SrTiO}_3$** , J.W. FREELAND, I.C. TUNG, Advanced Photon Source, Argonne National Laboratory, G. LUO, University of Wisconsin, Madison, H. ZHOU, Advanced Photon Source, Argonne National Laboratory, J.H. LEE, Korea Atomic Energy Research Institute, S.H. CHANG, Materials Science Division, Argonne National Laboratory, D. MORGAN, University of Wisconsin, Madison, M.J. BEDZYK, Northwestern University, D.D. FONG, Materials Science Division, Argonne National Laboratory — Dimensionality and strain control of nickelates has been shown as a route for control of interesting electronic and magnetic phases. However, little is known about the evolution of atomic structure in these layered architectures and the interplay with these states. Here we present, a detailed study of lattice structures measured real time during the layer-by-layer growth of  $\text{LaNiO}_3$  on  $\text{SrTiO}_3$ . Using hard X-rays coupled with oxide MBE, we have tracked the lattice structure evolution as a function of depth across the regime where transport shows a clear metal to insulator transition. At the same time X-ray absorption shows the films are closer to  $\text{LaNiO}_{2.5}$  when thin and evolve to  $\text{LaNiO}_3$  by 10 unit cells thickness. Analysis of the structure during growth displays a very complex evolution throughout the film of the lattice parameter and displacement of the B-site from the unit cell center, which theory connects with pathways of compensating the polar mismatch at the surface and interface. Work at the APS, Argonne is supported by the U.S. Department of Energy, Office of Science, and Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

**12:27PM F30.00005 Tailoring the electronic transitions of  $\text{NdNiO}_3$  films through  $(111)_{\text{pc}}$ -oriented interfaces**, SARA CATALANO, University of Geneva, MARTA GIBERT, University of Geneva Switzerland, VALENTINA BISOGNI, SLS PSI Villigen Switzerland, FEIZHOU HE, RONNIE SUTARTO, CLS Saskatoon Canada, MICHEL VIRET, CEA CNRS Saclay France, PAVLO ZUBKO, JEN-NIFER FOWLIE, University of Geneva Switzerland, GEORGE A. SAWATZKY, UBC Vancouver Canada, THORSTEN SCHMITT, SLS PSI Villigen Switzerland, JEAN-MARC TRISCONI, University of Geneva Switzerland — Bulk  $\text{NdNiO}_3$  displays a 1<sup>st</sup> order metal to insulator transition (MIT) that occurs simultaneously with a paramagnetic to antiferromagnetic Néel transition. For  $\text{NdNiO}_3$  epitaxial thin films grown along the  $(001)_{\text{pc}}$  axis, the MIT can be tuned between 0 and 200K through a variety of parameters, such as epitaxial strain or electrostatic carrier doping. Here, we extend the control of the electronic transitions of  $\text{NdNiO}_3$  thin films over an unprecedented temperature range by selecting  $(111)_{\text{pc}}$ -oriented substrates as a template for the growth. We show that  $(111)_{\text{pc}}$   $\text{NdNiO}_3/\text{NdGaO}_3$  heterostructures exhibit a MIT above room temperature, at  $T=335\text{K}$ , and a Néel transition at  $T=230\text{K}$ . By comparing the behavior of  $\text{NdNiO}_3$  layers grown on substrates with different symmetries and lattice parameters, we conclude that the particularly large tuning of the critical temperatures of the system is produced by the specific lattice matching conditions imposed along the  $(111)_{\text{pc}}$  axis of orthorhombic substrates.

**12:39PM F30.00006 Electronic and magnetic structure of ultra-thin film of  $\text{EuNiO}_3$** , SRIMANTA MIDDEY, D. MEYERS, M KAREEV, Department of Physics, University of Arkansas, Fayetteville, AR 72701 USA, J. LIU, Department of Physics and Astronomy, The University of Tennessee, Knoxville, TN 37996, USA, J. W. KIM, Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, USA, P. SHAFER, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA, P. J. RYAN, Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, USA, J. CHAKHALIAN, Department of Physics, University of Arkansas, Fayetteville, AR 72701 USA — In order to uncover the effect of reduced dimensionality on electronic and magnetic structure of rare earth nickelates series, we have investigate ultra thin film of  $\text{EuNiO}_3$  (ENO) using hard and soft resonant x-ray scattering. Despite of such small thickness, it exhibits checker board type charge ordering, and E antiferromagnetic transition highlighting bulk-like electronic and magnetic structure can be retained for highly distorted member of  $\text{RENiO}_3$  family. The presence of charge ordering at room temperature also provides opportunity for their use in novel electric field controlled devices.

**12:51PM F30.00007 Modeling Correlation Effects in Nickelates with Slave Particles<sup>1</sup>**, ALEXANDRU BOGDAN GEORGESCU, Department of Physics and Center for Research on Interface Structures and Phenomena, Yale University, SOHRAB ISMAIL-BEIGI, Department of Applied Physics, Physics, Mechanical Engineering and Center for Research on Interface Structures and Phenomena, Yale University — Nickelate interfaces display interesting electronic properties including orbital ordering similar to that of cuprate superconductors and thickness dependent metal-insulator transitions. One-particle band theory calculations do not include dynamic localized correlation effects on the nickel sites and thus often incorrectly predict metallic systems or incorrect ARPES spectra. Building on two previous<sup>1,2</sup> successful slave-particle treatments of local correlations, we present a generalized slave-particle method that includes prior models and allows us to produce new intermediate models<sup>3</sup>. The computational efficiency of these slave-boson methods means that one can readily study correlation effects in complex heterostructures. We show some predictions of these methods for the electronic structure of bulk and thin film nickelates.

1. Florens and Georges, PRB (2002); Lau and Millis, PRL (2013).
2. deMedici, Georges and Biermann, PRB (2005); deMedici, Giovannetti and Capone, PRL (2014).
3. Georgescu and Ismail-Beigi, arXiv:1506.03515, in press at PRB (2015)

<sup>1</sup>Work supported by NSF Grant MRSEC DMR-1119826

**1:03PM F30.00008 Testing for Quantum Criticality in the  $(\text{Nd,L a})\text{NiO}_3$  phase space by Inelastic Tunneling Electron Spectroscopy (IETS)**, ANDREW KLEVITCH, University of Alabama, ANKIT DISA, FRED WALKER, Center for Research on Interface Structures and Phenomena and Department of Applied Physics, Yale University, GINA ADAM, Department of Electrical and Computer Engineering, University of California at Santa Barbara, JAMES ALLEN, Department of Physics, University of California, CHARLES AHN, Center for Research on Interface Structures and Phenomena and Department of Applied Physics, Yale University, ADAM HAUSER, University of Alabama — Continuous (2<sup>nd</sup> order)  $T=0\text{K}$  Mott transitions are highly sought after because they are predicted to produce interesting quantum critical phenomena at higher temperatures such as quantum spin liquid states and marginal Fermi behavior. The rare earth nickelate system has generated significant interest for understanding charge and spin ordering phenomena in correlated materials and for potential application in novel switching devices. We will present Inelastic Electron Tunneling Spectroscopy (IETS) measurements from a series of films across the  $(\text{Nd,L a})\text{NiO}_3$  compositional system, yielding the single particle density of states at and across the quantum phase transition. Previous work has shown that pure  $\text{NdNiO}_3$  thin films have a characteristic bandgap, and pure  $\text{LaNiO}_3$  films have a characteristic pseudo-gap, satisfying a major requirement for a quantum critical transition point. Accordingly, our films undergo a metal-to-insulator transition upon cooling for high Nd content, while remaining metallic at all temperatures for high La content.

**1:15PM F30.00009 Suppression of charge and spin order in confined NdNiO<sub>3</sub> layers**, ANKIT DISA, DIVINE KUMAR, ANDREI MALASHEVICH, SOHRAB ISMAIL-BEIGI, FRED WALKER, CHARLES AHN, Yale University — Atomic-layer synthesis allows one to study and control the complex phase behavior correlated systems by controllably modifying dimensionality and interfacial constraints. To this end, the rare-earth nickelates (*R*NiO<sub>3</sub>) embody a remarkable model system, as exhibited by the bulk metal-insulator and paramagnetic-antiferromagnetic ordering transitions, which are sensitive to structural and electronic conditions. We present evidence from transport, x-ray absorption, and resonant x-ray scattering measurements of NdNiO<sub>3</sub>/NdAlO<sub>3</sub> superlattices of a suppression of charge and spin order induced by interfacial confinement. We find that the spectroscopic signatures of charge localization and antiferromagnetic ordering remain for NdNiO<sub>3</sub> layers thicker than a single unit cell. The disappearance of ground state order in single NdNiO<sub>3</sub> layers is attributed to enhanced *e<sub>g</sub>* orbital polarization from the interaction with the NdAlO<sub>3</sub> confining layers. We also observe a crossover region of thickness with no metal-insulator transition but distinct charge and spin ordering temperatures. These findings shed light on the interplay between competing ground states in nickelates and help guide efforts to controlling long-range order in such systems.

**1:27PM F30.00010 Effect of strain on ferroelectric field effect in strongly correlated oxide Sm<sub>0.5</sub>Nd<sub>0.5</sub>NiO<sub>3</sub>**<sup>1</sup>, LE ZHANG, XUEGANG CHEN, H. JEFFREY GARDNER, Dept. of Physics and Astronomy, University of Nebraska Lincoln, MARK A. KOTEN, JEFFREY E. SHIELD, Dept. of Mechanical Engineering, University of Nebraska Lincoln, XIA HONG, Dept. of Physics and Astronomy, University of Nebraska Lincoln — We report the effect of epitaxial strain on the magnitude and retention of the ferroelectric field effect in a prototype FerroFET based on a charge transfer-type Mott insulator, Sm<sub>0.5</sub>Nd<sub>0.5</sub>NiO<sub>3</sub> (SNNO). It has been shown that epitaxial strain can change the transition temperature *T<sub>MI</sub>* in SNNO by more than 100 K, and modify the metal-insulator transition (MIT) characteristic between first-order and second-order. We have fabricated epitaxial PbZr<sub>0.3</sub>Ti<sub>0.7</sub>O<sub>3</sub> (PZT)/3.8–4.3 nm SNNO heterostructures on (001) LaAlO<sub>3</sub> (LAO) and SrTiO<sub>3</sub> (STO) substrates. The magnitude of the field effect modulation can differ by more than one order of magnitude in these two systems, which has been attributed to strain modified MIT characteristic in SNNO. In both systems, we also observe a pronounced relaxation of off state resistance *R<sub>OFF</sub>*, showing a thermally activated behavior with corresponding activation energy of 22 meV (28 meV) for devices on LAO (STO). The time dynamics and thermal response of the retention behavior suggest that strain-induced oxygen vacancies play a critical role in the ferroelectric field effect instability.

<sup>1</sup>L. Zhang et al., Appl. Phys. Lett. 107, 152906 (2015)

**1:39PM F30.00011 Current-voltage profile of a strongly correlated materials heterostructure using non-equilibrium dynamical mean field theory**, KHADIJEH NAJAFI, JAMES FREERICKS, Georgetown university — We investigate the nonlinear electronic transport across a multilayered heterostructure which consists of Mott insulator layers connected to ballistic metal leads on both sides. To create current flow, we turn on an electric field in the leads for a finite period of time and then turn it off and let the system reach the steady state by adding an electric field over the correlated region. We use nonequilibrium dynamical mean-field theory to obtain the current-voltage relation. To do so, we current bias the device, and adjust the voltage profile to ensure current conservation and charge conservation throughout. The calculation ultimately works directly in the steady-state limit.

**1:51PM F30.00012 Photoinducing the hidden M2 phase in VO<sub>2</sub>**<sup>1</sup>, D.A. WALKO, Argonne National Laboratory, R.K. SMITH<sup>2</sup>, Bowling Green State University, HAIDAN WEN, A.D. DICHARA, Argonne National Laboratory, JAEWOO JEONG, MAHENS H. SAMANT, IBM Almaden Research Center, STUART S.P. PARKIN, IBM Almaden Research Center and Max Planck Institute for Microstructure Physics — We used time-resolved x-ray diffraction to study photoinduced structural phase transitions in a 170-nm-thick VO<sub>2</sub> film grown on sapphire (1,0,-1,0). Heating the unstrained film from room temperature induces the well-known phase transition from the monoclinic (M1) phase directly to the high-temperature tetragonal rutile (R) phase. In contrast, upon ultrafast optical excitation, the phase transition depends strongly on the laser intensity. At low fluences, the film is partially transformed into the monoclinic M2 phase, a phase which generally is observed only in doped or strained materials. Above a threshold at higher fluences, a small portion of the film is transformed into the M2 phase, decaying on a time scale of a few nanoseconds, while the majority of the film is transformed into the R phase which can persist for tens of nanoseconds. We further discuss the effects of laser wavelength on the efficiency of producing the M2 phase.

<sup>1</sup>Work at the Advanced Photon Source supported by DOE Contract No. DE-AC02-06CH11357.

<sup>2</sup>Present address: The Ohio State University

**2:03PM F30.00013 Quantum capacitance in thin film vanadium dioxide metal insulator transition**<sup>1</sup>, ZHE WU, TALBOT KNIGHTON, VINICIO TARQUINI, Department of Physics and Astronomy, Wayne State University, DAVID TORRES, TONGYU WANG, NELSON SEPULVEDA, Electrical and Computer Engineering Department, Michigan State University, JIAN HUANG, Department of Physics and Astronomy, Wayne State University — We present capacitance measurements of the electronic density of states performed in high quality vanadium dioxide (VO<sub>2</sub>) thin films on sapphire (Al<sub>2</sub>O<sub>3</sub>) substrate. These films show the expected metal insulator transition near 60 °C with resistivity changing by 3 orders of magnitude with a hysteresis of 10 °C. To make a capacitive probe, a gate is suspended above the film surface using a flip-chip method with microfabricated supports. The geometric capacitance per-area reached is 40 pF/mm<sup>2</sup>. Such a large capacitance can be significantly modified by electron interaction and band charging/discharging which appear as an extra term known as the quantum capacitance (*C<sub>q</sub>*). An AC signal applied to the gate allows measurement of the changing density of states (DOS) across the MIT. The DOS abruptly increases as the sample is heated through the transition point. Conversely the low temperature drop of *dμ/dn* is consistent with an energy gap opening in the insulating phase. These parameters shed light on the transition mechanism.

<sup>1</sup>NSF DMR-1105183, NSF ECCS 1306311.

**Tuesday, March 15, 2016 11:15AM - 2:15PM –**  
**Session F31 DCMP: Superconductivity: Spectroscopy of Cuprates 331 -**

**11:15AM F31.00001 Ultrafast Gap Dynamics in Bi<sub>2</sub>Sr<sub>2</sub>CaCu<sub>2</sub>O<sub>8+δ</sub> Studied by High Resolution trARPES**, STEPHEN PARHAM, HAOXIANG LI, JUSTIN WAUGH, XIAOQING ZHOU, THOMAS NUMMY, JUSTIN GRIFFITH, University of Colorado Boulder, Z. XU, J. SCHNEELOCH, R.D. ZHONG, GENDA GU, Brookhaven National Lab, DANIEL DESSAU, University of Colorado Boulder, DESSAU GROUP TEAM, GU GROUP TEAM — We perform time and angle resolved photoemission spectroscopy on optimally doped Bi<sub>2</sub>Sr<sub>2</sub>CaCu<sub>2</sub>O<sub>8+δ</sub> (BSCCO-2212) using higher energy resolution than previously reported. This technique allows us to observe quasiparticle and gap dynamics directly in the time domain. We find that the quasiparticle decays have a rich momentum and energy dependence, with the general trend of faster decays closer to the antinode and faster decays inside the superconducting gap scale. We can understand this entire landscape by modeling the electrons as following a non-equilibrium, “pseudo”-temperature that controls all electrons in the zone. Using this model, which has zero free parameters, we find excellent agreement with the data.

**11:27AM F31.00002 A Tight Binding Approach to Understanding the Orbital Character of Pb-BSSCO and its Effects on Photoemission Matrix Elements<sup>1</sup>**, THOMAS NUMMY, University of Colorado Boulder, YUE CAO, Brookhaven National Lab, JUSTIN WAUGH, STEPHEN PARHAM, HAOXIANG LI, XIAOQING ZHOU, University of Colorado Boulder, SUNG-KWAN MO, Lawrence Berkeley National Lab, A. MAGREZ, H. BERGER, EPFL Lausanne, DANIEL DESSAU, University of Colorado Boulder — We measure the near Fermi energy electronic structure of Pb-BSSCO using Angle Resolved Photoemission Spectroscopy (ARPES) for various light polarization, incident at a glancing angle. A strong dependence of the photocurrent for a given crystal momentum on the polarization of light is observed. A minimal model tight binding calculation in a basis of local atomic orbitals is then utilized to determine the orbital composition of the single particle wavefunction as a function of crystal momentum in a single CuO<sub>2</sub> plane. Building off of these results, we simulate the relative ARPES photocurrent throughout crystal momentum space in the dipole approximation and compare to our experimental data. These comparisons confirm the presence of changing wavefunction orbital composition throughout the Brillouin zone in Pb-BSSCO.

<sup>1</sup>Acknowledgement: NSF GRFP

**11:39AM F31.00003 Phonon modes in cuprates possibly related to the 10 meV ARPES kink<sup>1</sup>**, ADRIAN MERRITT, University of Colorado - Boulder, SEUNG-RYONG PARK, Incheon National University, JOHN-PAUL CASTELLAN, Karlsruhe Institute of Technology, GENDA GU, Brookhaven National Laboratory, DMITRY REZNIK, University of Colorado - Boulder — One of the possible mechanisms of high T<sub>c</sub> superconductivity is Cooper pairing with the help of bosons responsible for kinks in electronic dispersion observed by angle-resolved photoemission (ARPES). Up to now most effort has been devoted to the kinks near 70 meV. More recent ARPES experiments revealed an additional energy scale near 10 meV. Since no magnetic excitations peaked at these energies have been identified, the likeliest candidates appear to be phonons. We recently performed measurements of low-energy phonons in a large single crystal sample of optimally-doped 2212 BSSCO. We measured all phonons below 15 meV. There are many branches, in particular an optic branch disperses from 7 meV from the zone center with an anticrossing with an acoustic branch near h=0.2. In addition, there is evidence for a very low energy branch dispersing through 3-4 meV. I will present these results as well as similar data on LSCO and YBCO. A comparison with recent ultrafast optics experiment detecting lattice modes around 10 meV will also be made.

<sup>1</sup>This work was supported by the DOE Basic Energy Sciences Neutron Scattering Program.

**11:51AM F31.00004 Power Law Liquid – A Unified Form of Low-Energy Nodal Electronic Interactions in Hole Doped Cuprate Superconductors**, DANIEL DESSAU, TED REBER, XIAOQING ZHOU, NICK PLUMB, STEPHEN PARHAM, JUSTIN WAUGH, YUE CAO, ZHE SUN, HAOXIANG LI, QIANG WANG, Univ of Colorado - Boulder, J.S. WEN, Z.J. XU, GENDA GU, Brookhaven National Labs, Y. YOSHIDA, HIROSHI EIASHI, AIST, Tsukuba, Japan, GERALD ARNOLD, Univ of Colorado - Boulder, UNIVERSITY OF COLORADO, BOULDER TEAM, BROOKHAVEN NATIONAL LABS TEAM, AIST, TSUKUBA, JAPAN TEAM — Based upon detailed ARPES measurements of Bi<sub>2</sub>Sr<sub>2</sub>CaCu<sub>2</sub>O<sub>8+δ</sub> over a wide range of doping levels, we present a new unifying phenomenology for the non-Fermi liquid normal-state interactions (scattering rates) in the nodal direction. This new phenomenology has a continuously varying power law exponent (hence named a Power Law Liquid or PLL), which with doping varies smoothly from a quadratic Fermi Liquid to a linear Marginal Fermi Liquid and beyond. Using the extracted PLL parameters we can calculate the optics and resistivity over a wide range of doping and normal-state temperature values, with the results closely matching the experimental curves. This agreement includes the presence of the T\* “pseudogap” temperature scale observed in the resistivity curves including the apparent quantum critical point.

**12:03PM F31.00005 ARPES Study of Triple Layer Nickelate R<sub>4</sub>Ni<sub>3</sub>O<sub>10</sub> (R=Pr, La)**, HAOXIANG LI, XIAOQING ZHOU, THOMAS NUMMY, Department of Physics, University of Colorado at Boulder, Boulder, CO 80309, USA, JUNJIE ZHANG, Material Science Division, Argonne National Lab, Argonne, IL 60439, USA, VICTOR PARDO, Departamento de Fisica Aplicada, Universidade de Santiago de Compostela, E-15782 Campus Sur s/n, Santiago de Compostela, Spain, WARREN E. PICKETT, Department of Physics, University of California, Davis, CA, 95616, USA, JOHN F. MITCHELL, Material Science Division, Argonne National Lab, Argonne, IL 60439, USA, DANIEL S. DESSAU, Department of Physics, University of Colorado at Boulder, Boulder, CO 80309, USA — Layered nickelates present a similar crystal and electronic structure to the high-T<sub>c</sub> cuprates. They are potential candidates to host superconductivity, and have demonstrated intriguing anomalies in resistivity, magnetic susceptibility, and specific heat [1-3]. Here we present an ARPES study of the triple layer nickelate R<sub>4</sub>Ni<sub>3</sub>O<sub>10</sub> (R=Pr, La) and compare it with density functional calculations. A large hole pocket centered at the zone corners similar to the cuprates is observed, with additional zone folding due to the structural/magnetic cell doubling. An additional band-like feature is found near the Fermi surface at the gamma point, and shows a different symmetry than that of the hole pocket. These details of the fermiology and their relevance to the properties of these materials will be discussed. [1] Z. Zhang et al. J. Solid State Chem. 117, 236 (1995). [2] M. D. Carvalho et al. J. Appl. Phys. 88, 544 (2000). [3] M. Zinkevich et al. J. Alloys Compd. 438, 92 (2007).

**12:15PM F31.00006 ABSTRACT WITHDRAWN —**

**12:27PM F31.00007 Photodoping of Effects in Underdoped Bi<sub>2</sub>Sr<sub>2</sub>CaCu<sub>2</sub>O<sub>8+x</sub> Revealed by Time and Angle Resolved Photoemission Spectroscopy<sup>1</sup>**, JONATHAN RAMEAU, Brookhaven Natl Lab, S. FREUTEL, I. AVIGO, M. LIGGES, L. RETTIG<sup>2</sup>, P. ZHOU, University of Duisburg-Essen, J. SCHNEELOCH, R. ZHONG, Z. XU, GENDA GU, PETER JOHNSON, Brookhaven Natl Lab, UWE BOVENSIEPEN, University of Duisburg-Essen — While in the last several years great strides have been made in the use of ultrafast optical excitation to induce non-equilibrium effects in the superconducting state of cuprate high T<sub>c</sub> superconductors, less attention has been paid to what such pump-probe experiments might reveal about the equilibrium properties of these materials, particularly in their normal states. Recently we have investigated the non-equilibrium properties of the normal state of optimally doped Bi<sub>2</sub>Sr<sub>2</sub>CaCu<sub>2</sub>O<sub>8+x</sub> (T<sub>c</sub> = 91 K) using time and angle resolved photoelectron spectroscopy (tr-ARPES). This effort revealed a pump-induced modification of the nodal mass renormalization at 70 meV as well as a longer-lived photodoping effect. Building on this work, we will present further findings related to the photodoping effect as it is manifested in the normal state of underdoped (T<sub>c</sub> = 50 K) Bi<sub>2</sub>Sr<sub>2</sub>CaCu<sub>2</sub>O<sub>8+x</sub>.

<sup>1</sup>Center for Emergent Superconductivity, a DOE EFRC

<sup>2</sup>Current Affiliation at Paul Scherrer Institute

**12:39PM F31.00008 The self-energies and bosonic spectrum of high T<sub>c</sub> cuprate from laser-based ARPES.**, JIN MO BOK, JONG JU BAE, HAN-YONG CHOI, Sungkyunkwan Univ, LI YU, X. J. ZHOU, Institute of Physics, Chinese Academy of Science, CHANDRA M. VARMA, University of California, Riverside — While phonon mediated conventional superconductors are revealed by comparing tunneling and neutron scattering experiment, high T<sub>c</sub> cuprate which has d-wave symmetry is still in debate. Laser-based AREPS can provide both momentum and energy dependence of spectral function that enables self-energy extraction using one particle Greens function. It is well known that anisotropy of electronic structure and d-wave superconducting gap on ARPES experiments. We analyzed high resolution APRES data of under and overdoped Bi2212 and extracted both normal and pairing self-energy. Here we report the extracted normal and pairing self-energy in superconducting state. Also we obtained bosonic spectrum from both self-energies by performing maximum entropy method. Implications of these results for understanding the superconductivity mechanism will be discussed.

**12:51PM F31.00009 Photoinduced Chemical Potential Shifts in Bi2212**, TRISTAN MILLER, CHRISTOPHER SMALLWOOD, WENTAO ZHANG, Lawrence Berkeley National Laboratory and UC Berkeley, HIROSHI EISAKI, Electronics and Photonics Research Institute, National Institute of Advanced Industrial Science and Technology, JOSEPH ORENSTEIN, ALESSANDRA LANZARA, Lawrence Berkeley National Laboratory and UC Berkeley — In superconducting materials, the chemical potential is particularly important because it is the energy of the superconducting condensate. The chemical potential may be perturbed by laser pulses, giving us new insight into the equilibrium properties of cuprate superconductors. Here, we report on studies of the photoinduced change of chemical potential in Bi2212 using time- and angle-resolved photoemission spectroscopy. We make an important distinction between the chemical potential relative to the vacuum energy, and relative to the valence band energy. The observations can be explained with considerations of the density of states. Measurements on different dopings of Bi2212 also provide new clues to the pseudogap phase.

**1:03PM F31.00010 Quasi-particles ultrafastly releasing kink bosons to form Fermi arcs in a cuprate superconductor**, Y. ISHIDA, T. SAITOH, ISSP, U. Tokyo, Japan, T. MOCHIKU, T. NAKANE, K. HIRATA, NIMS, Japan, S. SHIN, ISSP, U. Tokyo, Japan — In a conventional framework, superconductivity is lost at a critical temperature ( $T_c$ ) because, at higher temperatures, gluing bosons can no longer bind two electrons into a Cooper pair. In high  $T_c$  cuprates, it is still unknown how superconductivity vanishes at  $T_c$ . Recent angle-resolved photoemission (ARPES) studies revealed a remnant feature of the  $d$ -wave superconducting gap in the so-called Fermi arc occurring at  $T > T_c$ . The loss of superconductivity is thereby attributed to the filling of the near-nodal gap due to spectral broadenings as opposed to the closure of the gap at  $T_c$  [Reber *et al.*, PRB2013; Kondo *et al.*, Nature Phys. 2015]. The next step would be to elucidate the underlying mechanism of the spectral broadenings that cause the unconventional loss of superconductivity. We provide evidence that the so-called  $\sim 70$ -meV kink bosons that dress the quasi-particle excitations are playing the key role. We performed time-resolved ARPES on Bi2212 and monitored the responses of the superconducting gap and dressed quasi-particles to a light pulse. We observe an ultrafast loss of superconducting gap near the  $d$ -wave node, or light-induced Fermi arcs, which is accompanied by spectral broadenings and weight redistributions occurring within the kink binding energy. We discuss that the spectral broadening that induce the Fermi arc is due to the undressing of quasi-particles from the kink bosons. The loss mechanism is beyond the conventional framework, and can accept the unconventional phenomena such as the signatures of Cooper pairs remaining at  $T > T_c$ .

**1:15PM F31.00011 Superconducting Gap and Pseudogap in Heavily Underdoped Bi2212**, CHENG HU, LIN ZHAO, SHAOLONG HE, GUODONG LIU, LI YU, CHUANGTIAN CHEN, ZUYAN XU, GENDA GU, XINGJIANG ZHOU, Chinese Academy of Sci (CAS) — The relationship between the pseudogap and superconducting gap in high temperature cuprate superconductors remains an outstanding issue. In this talk, we will present laser-based angle-resolved photoemission spectroscopy results on underdoped Bi2Sr2(Ca,Dy)Cu2O8 high temperature superconductor. The latest generation of ARPES system equipped with the narrow-bandwidth VUV laser and the time-of-flight (TOF) electron energy analyzer is utilized here, which enables us to have super-high energy resolution, high momentum resolution, and simultaneous coverage of two-dimensional momentum space. From detailed temperature dependence near the nodal and antinodal regions, we will discuss the relationship between the pseudogap and superconducting gap in the underdoped cuprate superconductors.

**1:27PM F31.00012 Interplay of low-energy bosonic collective modes with incipient charge order in Bi-2212 characterized by momentum-resolved electron energy loss spectroscopy<sup>1</sup>**, SEAN VIG, ANSHUL KOGAR, Univ of Illinois - Urbana, VIVEK MISHRA, Argonne National Laboratory, MELINDA RAK, ALI HUSAIN, Univ of Illinois - Urbana, GENDA GU, Brookhaven National Laboratory, MIKE NORMAN, Argonne National Laboratory, PETER ABBAMONTE, Univ of Illinois - Urbana — Classifying the collective electronic dynamics of materials is critical to addressing the high temperature superconductivity problem and understanding related collective phenomena. Most current probes are unable to measure the full energy and momentum dependence of the dynamic charge susceptibility in these strongly correlated materials at the meV energy scale relevant to superconductivity. We use our momentum-resolved electron energy loss spectroscopy (M-EELS) technique to perform this measurement, characterizing both the static charge density and the bosonic electronic excitations in the cuprate superconductor Bi2Sr2CaCu2O8+ $\delta$  (Bi-2212). I present our measurement of a low temperature diffuse charge ordered state at optimal doping which modulates the observed dispersionless low energy collective excitations. Performing a one-loop correction to the bare electron dispersion, we show these modes reproduce the self-energy anomaly, or “kink”, as measured by ARPES. I discuss the nature of the charge dynamics that we measured with our technique and its relation to the superconducting state.

<sup>1</sup>This work was supported as part of the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science

**1:39PM F31.00013 Resonant inelastic x-ray scattering as a band structure probe of high-temperature superconductors<sup>1</sup>**, MARTON KANASZ-NAGY, Harvard University, YIFEI SHI, ISRAEL KLICH, University of Virginia, EUGENE DEMLER, Harvard University — I will analyze recent resonant inelastic x-ray scattering (RIXS) experimental data on YBa2Cu3O6+x [Minola *et al.*, Phys. Rev. Lett. 114, 217003 (2015)] within quasi-particle theory. This measurement has been performed with the incoming photon energy detuned at several values from the resonance maximum, and, surprisingly, the data shows much weaker dependence on detuning than expected from recent measurements on a different cuprate superconductor, Bi2Sr2CuO6+x [Guarise *et al.*, Nat. Commun. 5, 5760 (2014)]. I will demonstrate, that this discrepancy, originally attributed to collective magnetic excitations, can be understood in terms of the differences between the band structures of these materials. We found good agreement between theory and experiment over a large range of dopings [M. Kanasz-Nagy *et al.*, arXiv:1508.06639]. Moreover, I will demonstrate that the RIXS signal depends sensitively on excitations at energies well above the Fermi surface, that are inaccessible to traditionally used band structure probes, such as angle-resolved photoemission spectroscopy. This makes RIXS a powerful probe of band structure, not suffering from surface preparation problems and small sample sizes, making it potentially applicable to a wide range of materials.

<sup>1</sup>The work of M. K.-N. was supported by the Harvard-MIT CUA, NSF Grant No. DMR-1308435, AFOSR Quantum Simulation MURI, the ARO-MURI on Atomtronics, and ARO MURI Quism program.

**1:51PM F31.00014 Doping dependent charge correlation in electron-doped cuprates.**, EDUARDO DA SILVA NETO, F. BOSCHINI, M. ZONNO, G. A. SAWATZKY, A. DAMASCELLI, Univ of British Columbia, M. MINOLA, M. BLUSCHKE, M. LE TACON, B. KEIMER, Max Planck Institute for Solid State Research, B. WU, Y. LI, G. YU, M. GREVEN, University of Minnesota, J. HIGGINS, Y. JIANG, R. L. GREENE, University of Maryland, R. SUTARTO, F. HE, Canadian Light Source, E. SCHIERLE, E. WESCHKE, Helmholtz-Zentrum Berlin — We use resonant x-ray scattering to measure the charge order in electron-doped high- $T_c$  superconductors and its relationship to antiferromagnetism and superconductivity. First, we establish the presence of charge order in a second family of electron-doped cuprates, LCCO thin films, with similar characteristics to previous observations in NCCO [1]. Second, doping and temperature dependent measurements of NCCO single crystals show that charge order is present in the  $x = 0.059$  to  $0.166$  doping range, and its doping-dependent wavevector is consistent with the separation between the hot spots on the Fermi surface. For NCCO samples near optimal doping ( $x = 0.14$ ) the charge order remains constant through the superconducting transition temperature and we find that magnetic fields up to  $6$  T have a negligible effect on its intensity. The implications of our data to the connections of charge order to antiferromagnetism and superconductivity will be discussed. [1] E. H. da Silva Neto, *et al.* Science 347, 282 (2015).

**2:03PM F31.00015 Resonant Soft X-ray Scattering studies of charge orders in high-temperature cuprates with Transition Edge Sensors<sup>1</sup>**, YIZHI FANG, Univ of Illinois - Urbana; Argonne National Laboratory, PETER ABBAMONTE, Univ of Illinois - Urbana, FANNY RODOLAKIS, JESSICA MCCHESENEY, Argonne National Laboratory, HIDEYUKI TATSUNO, National Institute of Standards and Technology; Lund University, YOUNG IL JOE, JOE FOWLER, KELSEY MORGAN, WILLIAM DORIESE, DANIEL SWETZ, JOEL ULLOM, National Institute of Standards and Technology — Resonant Soft X-ray studies of high  $T_c$  cuprates have implied a complex yet unresolved relationship between charge orders, antiferromagnetism and superconductivity. Unfortunately, at resonance the inelastic fluorescence background makes it hard to distinguish weak charge orders. To eliminate this issue, we have developed an energy-resolving detector comprised of 240-pixels superconducting Transition-Edge Sensor microcalorimeters. These superconducting sensors obtain exquisite resolution by exploiting the superconducting-to-normal transition to transduce photon energy to temperature and by operating at cryogenic temperatures ( $\sim 100$  mK) where thermal noise is minimal. Initial commissioning was accomplished at Advanced Photon Source Sector 29 in August 2015 and have demonstrated 1.0 eV resolution below 1 keV with efficiency (solid angle  $\times$  quantum efficiency)  $\sim 50$  times than that of grating spectrometers. An experiment to study charge orders in LBCO, LESCO and YBCO as a function of doping will take place in November 2015.

<sup>1</sup>This work was supported by the U.S. Department of Energy under Grant No. DE-FG02-06ER46285.

## Tuesday, March 15, 2016 11:15AM - 2:15PM – Session F33 DPOLY: The Physics of Confined Structural Fluids II 336 - Erik Watkins, UC - Davis

**11:15AM F33.00001 Coherent X-ray Scattering from Liquid-Air Interfaces<sup>1</sup>**, OLEG SHPYRKO, University of California, San Diego — Advances in synchrotron x-ray scattering techniques allow studies of structure and dynamics of liquid surfaces with unprecedented resolution. I will review x-ray scattering measurements of thermally excited capillary fluctuations in liquids, thin polymer liquid films and polymer surfaces in confined geometry. X-ray Diffuse scattering profile due to Debye-Waller like roughening of the surface allows to probe the distribution of capillary fluctuations over a wide range of length scales, while using X-ray Photon Correlation Spectroscopy (XPCS) one is able to directly couple to nanoscale dynamics of these surface fluctuations, over a wide range of temporal and spacial scales. I will also discuss recent XPCS measurements of lateral diffusion dynamics in Langmuir monolayers assembled at the liquid-air interface.

<sup>1</sup>This research was supported by NSF CAREER grant 0956131

**11:51AM F33.00002 A particle-in-mesh method for Brownian Dynamics simulation of many-particle systems with hydrodynamics interactions in a confined geometry**, XUJUN ZHAO, Argonne National Laboratory, JUAN HERNANDEZ-ORTIZ, Univ. Nacional de Colombia, DMITRY KARPEYEV, Argonne National Laboratory, JUAN DE PABLO, University of Chicago, BARRY SMITH, Argonne National Laboratory — In this work, we present an efficient parallel particle-in-mesh method for Brownian Dynamics simulations of many-particle systems confined in micro- and nano-fluidic devices. A general geometry Ewald-like method (GGEM) combined with finite element method is used to account for the hydrodynamic interaction. A fast parallel Krylov-type iterative solver with hybrid preconditioning techniques is developed for solving the large sparse systems of equations arising from finite element discretization of the Stokes equations. In addition, the current computer code is developed based on PETSc, a scalable library of numerical algorithms developed at Argonne, SLEPc - Scalable Library for Eigenvalue Problem Computations, and libMesh, a finite element library for numerical solution of PDEs built on top of PETSc, which allows for direct simulation of large scale systems with arbitrary confined geometries. This scheme is applied to Brownian dynamics simulations of flowing confined polymer solutions and colloidal dispersions in micro-fluid channels. The effects of hydrodynamics interactions and geometric confinement on the migration phenomena are illustrated.

**12:03PM F33.00003 Structural and dynamical properties of water on chemically modified surfaces: The role of the instantaneous surface<sup>1</sup>**, SELEMON BEKELE, MESFIN TSIGE, The University of Akron, Department of Polymer Science, Akron, Ohio — Surfaces of polymers such as atactic polystyrene (aPS) represent very good model systems for amorphous material surfaces. Such polymer surfaces are usually modified either chemically or physically for a wide range of applications that include friction, lubrication and adhesion. It is thus quite important to understand the structural and dynamical properties of liquids that come in contact with them to achieve the desired functional properties. Using molecular dynamics (MD) simulations, we investigate the structural and dynamical properties of water molecules in a slab of water in contact with atactic polystyrene surfaces of varying polarity. We find that the density of water molecules and the number distribution of hydrogen bonds as a function of distance relative to an instantaneous surface exhibit a structure indicative of a layering of water molecules near the water/PS interface. For the dynamics, we use time correlation functions of hydrogen bonds and the incoherent structure function for the water molecules. Our results indicate that the polarity of the surface dramatically affects the dynamics of the interfacial water molecules with the dynamics slowing down with increasing polarity.

<sup>1</sup>This work was supported by NSF Grant DMR1410290

**12:15PM F33.00004 Ion transport and dehydration in sub-nanoscale pores<sup>1</sup>**, SUBIN SAHU, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, Gaithersburg, MD 20899, MASSIMILIANO DI VENTRA, Department of Physics, University of California, San Diego, CA 9500, MICHAEL ZWOLAK, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, Gaithersburg, MD — Ions in solution develop tightly bound layers of water – hydration layers – which stabilize disassociation and enable ionic currents to flow. Sub-nanometer pores in a membrane enable ions to pass provided that they shed their hydration shell. This process has an associated large energy penalty that is predicted to give rise to "quantized" steps in the ionic conductance.<sup>2,3</sup> Using all-atom molecular dynamics simulation, we demonstrate that the ionic current begins to show nonlinear behavior as the radius of the pore is reduced to the sub-nanometer scale. This nonlinear behavior is seen as a sharp rise in the pore resistance and excess noise in the current. Our work sheds light on basic mechanism of ion transport through sub-nanoscale pores.

<sup>1</sup>S. Sahu acknowledges support by UMD/CNST Cooperative Research Agreement, Award 70NANB10H193 through University of Maryland

<sup>2</sup> Zwolak, M., Lagerqvist, J. & Di Ventra, M. Quantized ionic conductance in nanopores. *Phys. Rev. Lett.* **103**, 128102 (2009).

<sup>3</sup> Zwolak, M., Wilson, J. & Di Ventra, M. Dehydration and ionic conductance quantization in nanopores. *J. Phys.: Condens. Matter* **22**, 454126 (2010).

**12:27PM F33.00005 Coordinated Water Under Confinement Eases Sliding Friction**, ADRIAN DE-FANTE, NISHAD DHOPOTKAR, ALI DHINOJWALA, Univ of Akron — Water is essential to a number of interfacial phenomena such as the lubrication of knee joints, protein folding, mass transport, and adsorption processes. We have used a biaxial friction cell to quantify underwater friction between a hydrophobic elastomeric lens and a hydrophobic self-assembled monolayer in the presence of surfactant solutions. To gain an understanding of the role of water in these processes we have coupled this measurement with surface sensitive sum frequency generation to directly probe the molecular constitution of the confined contact interface. We observe that role of confined coordinated water between two hydrophobic substrates covered with surfactants is the key to obtaining a low coefficient of friction.

**12:39PM F33.00006 Understanding dynamic changes in live cell adhesion with neutron reflectometry**, ANN JUNGHANS, Los Alamos National Laboratory — Understanding the structure and functionality of biological systems on a nanometer-resolution and short temporal scales is important for solving complex biological problems, developing innovative treatment, and advancing the design of highly functionalized biomimetic materials. For example, adhesion of cells to an underlying substrate plays a crucial role in physiology and disease development, and has been investigated with great interest for several decades. In the talk, we would like to highlight recent advances in utilizing neutron scattering to study bio-related structures in dynamic conditions (*e.g.* under the shear flow) including *in-situ* investigations of the interfacial properties of living cells. The strength of neutron reflectometry is its non-perturbative nature, the ability to probe buried interfaces with nanometer resolution and its sensitivity to light elements like hydrogen and carbon. That allows us to study details of cell - substrate interfaces that are not accessible with any other standard techniques. We studied the adhesion of human brain tumor cells (U251) to quartz substrates and their responses to the external mechanical forces. Such cells are isolated within the central nervous system which makes them difficult to reach with conventional therapies and therefore making them highly invasive. Our results reveal changes in the thickness and composition of the adhesion layer (a layer between the cell lipid membrane and the quartz substrate), largely composed of hyaluronic acid and associated proteoglycans, when the cells were subjected to shear stress. Further studies will allow us to determine more conditions triggering changes in the composition of the bio-material in the adhesion layer. This, in turn, can help to identify changes that correlate with tumor invasiveness, which can have significant medical impact for the development of targeted anti-invasive therapies.

**1:15PM F33.00007 Adsorption of CO<sub>2</sub> in hydrated MCM-41 Studied by SANS**, BO WANG, GARFIELD T. WARREN, MATTHEW BRYAN, PAUL E. SOKOL, Indiana University, INDIANA UNIVERSITY TEAM — Adsorption of CO<sub>2</sub> in hydrated MCM-41 was studied as a function of CO<sub>2</sub> pressure by Small-Angle Neutron Scattering (SANS). Measurements were carried out on hydrophobic Si-MCM-41 and hydrophilic Al-MCM-41 with pore sizes of 4nm with no aqueous layer as well as monolayers and bilayers of water pre-adsorbed on the surface. SANS was measured as CO<sub>2</sub> was introduced into the pores, which has the ability to probe the microscopic arrangement of water and CO<sub>2</sub> confined within the pores. We will present the results of analysis indicating whether water or CO<sub>2</sub> is more strongly attracted to the surface in these different samples. This study was prepared by Indiana University under award 70NANB10H255 from the National Institute of Standards and Technology, U.S. Department of Commerce.

**1:27PM F33.00008 Probing the Hydrodynamic Boundary Condition from Surface Perturbations in Thin Liquid Films**, OLIVER BAEUMCHEN, Max Planck Institute for Dynamics and Self-Organization (MPIDS), Goettingen, Germany, PAUL FOWLER, Department of Physics and Astronomy, McMaster University, Hamilton, Canada, THOMAS SALEZ, MICHAEL BENZAQUEN, ESPCI Paris-Tech, PSL Research University, Paris, France, MARK ILTON, Department of Physics and Astronomy, McMaster University, Hamilton, Canada, JOSHUA MCGRAW, Departement de Physique, Ecole Normale Supérieure, PSL Research University, Paris, France, ELIE RAPHAEL, ESPCI ParisTech, PSL Research University, Paris, France, KARI DALNOKI-VERESS, Department of Physics and Astronomy, McMaster University, Hamilton, Canada — For flows on the micro- and nanoscale, the hydrodynamic boundary condition of a liquid at a solid surface plays an enormous role. In recent years much has been learned about this slip boundary condition from flows that are driven by capillary forces, *e.g.* dewetting thin liquid films featuring a three-phase contact line [1]. Recently, we have shown that the amplification of surface perturbations in thin liquid films allows for a quantification of slippage in the absence of a contact line [2]. We also show that the opposite approach, *i.e.* the capillary levelling of initially perturbed free surfaces [3], is sensitive to the slip boundary condition at the solid/liquid interface. Thin film models comprising slip enable a quantification of the slip length of viscous liquids of various molecular properties. [1] O. Bäümchen et al., Phys. Rev. Lett. 113, 014501 (2014). [2] S. Haefner et al., Nature Comm. 6, 7409 (2015). [3] J.D. McGraw et al., Phys. Rev. Lett. 109, 128303 (2012).

**1:39PM F33.00009 Dynamic arrest of colloids in quenched-disordered nanofiber networks**, ANH PHAN, Department of Physics, University of Illinois at Urbana-Champaign, KENNETH SCHWEIZER, Department of Materials Science and Engineering, University of Illinois — The effect of quenched-disordered high aspect ratio nanorod networks on the kinetic arrest of relatively dilute colloid or nanoparticle suspensions is theoretically studied using equilibrium replica integral equation and dynamical activated hopping theories. The adsorbing templates act as an external field which can destroy macrophase separation and induce variable colloidal microstructures. When the colloid-template attraction is weak, a large-mesh network only weakly perturbs dynamical arrest in pores driven by colloid aggregation. Reducing the mesh size increases constraints and enhances colloid localization. For strong interfacial attraction templates, colloids can be kinetically arrested in large-mesh networks even when they are purely repulsive hard spheres due to dynamic blocking effects. However, the localization length is significantly larger, more akin to a glass-like, not gel-like, form of arrest. Decreasing the template mesh results in colloid localization at smaller interfacial attraction strengths. An overall kinetic arrest map is constructed based on the interplay of inter-colloid attraction, colloid-template attraction, and template mesh size. The effect of colloid localization on the composite dynamic elastic shear modulus can be estimated.

**1:51PM F33.00010 Effect of confinement on ionic liquid molecules in porous polymeric network**, PRASAD RAUT, Department of Polymer Engineering, The University of Akron, SHICHEN YUAN, DR. TOSHIKAZU MIYOSHI, Department of Polymer Science, The University of Akron, DR. SADHAN JANA, Department of Polymer Engineering, The University of Akron — Ionic liquids (ILs) have attractive physicochemical properties but their room temperature liquid state necessitates pairing of IL with other solid, porous materials for fabrication of devices. Such materials are called ionogels. Loading of bulky IL molecules in the pores can dramatically affect the physical properties as function of the pore surface chemistry, pore size, and IL polarity. In this study porous syndiotactic polystyrene (sPS) network was made via thermos-reversible gelation. 1-Butyl-1-methylpyrrolidinium bis(trifluoromethanesulfonyl)imide (PYR14TFSI) is incorporated into the pores of sPS. DSC study and the temperature dependence of <sup>13</sup>C-CPMAS NMR show that on confinement; the melting point of PYR14TFSI contained in the ionogel increased in comparison to the bulk PYR14TFSI. At room temperature, WAXD study of the ionogels showed diffraction pattern for PYR14TFSI in nanopores, correspondingly <sup>1</sup>H NOESY experiments show strong non-bonded cation-cation correlation in ionogels. The results for the bulk IL does not show non-bonded correlation at room temperature, this increment of local order in ionogel might be the results of crystallization of IL molecules in confined geometry.

**2:03PM F33.00011 Spacetime of Fluid and Gas**, DAYONG CAO, AEEA — The spacetime coordinates do not measure the spacetime. It measures a structure of the object. The structure is massenergy center and spacetime around. It is build up by massenergy and spacetime together. The density of massenergy of solid is bigger than the one of the fluid or gas; contrariwise, the density of spacetime of the fluid or gas is bigger than the one of the solid. Because the density of spacetime is inversely proportional to the density of massenergy. The Einstein's equation has the other formula for the structure of the center of spacetime. The spacetime is wave, and the spacetime effect of the fluid and gas are about buoyancy, pressure, resistance, and temperature will be taken into Einstein's equation. It should explain of the low density asteroid-1950 DA and a rock hull of 67P/Churyumov-Gerasimenko. <http://meetings.aps.org/link/BAPS.2015.APR.T1.24> <http://meetings.aps.org/link/BAPS.2015.APR.H14.8>

**Tuesday, March 15, 2016 11:15AM - 1:51PM —**

Session F34 GSOFD DBIO GSNP/DFD: Active Matter IV 337 - Cristina Marchetti, Syracuse University

**11:15AM F34.00001 Self-Pumping Active Gel.** , KUN-TA WU, JEAN BERNARD HISHAMUNDA, SETH FRADEN, ZVONIMIR DOGIC, Department of Physics, Brandeis University — Isotropic active gels are the network which is consist of cross-linked building blocks and the structure of which changes randomly and isotropically with time. Dogic et. al. show that pairs of anti-parallel microtubules form extensile bundles, which merge, extend, and buckle. In an unconfined system, the dynamics of these bundles causes spontaneous turbulent-like flow driven by motion of microscopic molecular motors. We found that confining these active gels in a millimeter sized toroids causes a transition into a new dynamical state characterized by circulation currents persisting for hours until ATP is depleted. We show how toroid dimensions impact the properties of self-organized circular currents, how directions of circulation can be designed by engineering ratchet-shaped boundaries, and how circulations of connected toroids can be either synchronized or antisynchronized. Furthermore, we demonstrate that the flow rate in the circulation is independent of curvature and length of flow path. The flow rate persists for centimeters without decay, disregarding conventional pipe flow resistance. Such findings pave the path to self-pumping pipe transport and performing physical work with biological system.

**11:27AM F34.00002 Synchronization of oscillations in hybrid gel-piezoelectric active materials.** , VICTOR V. YASHIN, Department of Chemical Engineering, University of Pittsburgh, STEVEN P. LEVITAN, Department of Electrical and Computer Engineering, University of Pittsburgh, ANNA C. BALAZS, Department of Chemical Engineering, University of Pittsburgh — We model the hybrid gel-piezoelectric active material that could perform oscillator based unconventional computing tasks (materials that compute). The material is assumed to have a cellular structure, where each cell contains a polymer gel, which undergoes cyclic swelling and deswelling due to the oscillatory Belousov-Zhabotinsky (BZ) reaction, and is coupled to a piezoelectric (PZ) film. Upon electrical connection, oscillations in the BZ-PZ units get synchronized, and the mode of synchronization is shown to depend on the number of units in the system, type of circuit connection, etc. Introduction of capacitors into the circuits allows us to further manipulate the synchronization modes, i.e., the distinctive patterns in phase of oscillations. The results indicate the BZ-PZ systems could be used for spatio-temporal pattern recognition.

**11:39AM F34.00003 Photo-programming Semicrystalline Shape Actuators<sup>1</sup>** , YUAN MENG, JASON YANG, MITCHELL ANTHAMATTEN, Univ of Rochester, ANTHAMATTEN LAB TEAM — A semi-crystalline double network is formed that contains two types of molecular junctions: covalent junctions and reversible molecular linkages. The reversible junctions have the ability to rearrange/reshuffle upon irradiation, and, therefore give rise to a competitive double network architecture that actuates upon crystallization without an applied external load. Poly(caprolactone) networks containing reconfigurable allyl-sulfide linkages are melted, strained to various elongations (hundreds of percent), and irradiated. The network connectivity is reconfigured through a series of light-induced AFCT events, causing a unique built-in stress to be introduced. After irradiation and unloading, the resulting double networks assume a mechanical state-of-ease, and polymer strands adopt biased configurations; when cooled, they crystallize along a preferred direction leading to fully reversible shape actuation. Sample networks can be programmed in multi-steps under constant strain or constant stress, leading to different dynamics and equilibrium states-of-ease. Stress free actuation of 18 percent was achieved.

<sup>1</sup>Pump Primer Award from Univ. of Rochester

**11:51AM F34.00004 Designing Self-powered Nanomotors and Pumps** , AYUSMAN SEN, Pennsylvania State University — Self-powered nano and microscale moving systems are currently the subject of intense interest due in part to their potential applications in nanomachinery, nanoscale assembly, robotics, fluidics, and chemical/biochemical sensing. We will demonstrate that one can build autonomous nanomotors over a wide range of length-scales “from scratch” that mimic biological motors by using catalytic reactions to create forces based on chemical gradients. These motors are autonomous in that they do not require external electric, magnetic, or optical fields as energy sources. Instead, the input energy is supplied locally and chemically. These “bots” can be directed by information in the form of chemical and light gradients. Furthermore, we have developed systems in which chemical secretions from the translating nano/micromotors initiate long-range, collective interactions among themselves. This behavior is reminiscent of quorum sensing organisms that swarm in response to a minimum threshold concentration of a signaling chemical. In addition, an object that moves by generating a continuous surface force in a fluid can, in principle, be used to pump the fluid by the same catalytic mechanism. Thus, by immobilizing the nano/micromotors, we have developed nano/microfluidic pumps that transduce energy catalytically. These non-mechanical pumps provide precise control over flow rate without the aid of an external power source and are capable of turning on in response to specific analytes in solution.

**12:27PM F34.00005 Emergent Ultra-Long-Range Interactions Between Active Particles in Hybrid Active-Inactive Systems** , JOSHUA STEIMEL, JUAN ARAGONES, HELEN HU, MIT, NASER QURESHI, UNAM, ALFREDO ALEXANDER-KATZ, MIT — Particle-particle interactions determine the state of a system. Control over the range and magnitude of such interactions has been an active area of research for decades due to the fundamental challenges it poses in science and technology. Effective interactions between active particles have gathered much attention as they can lead to out-of-equilibrium cooperative states such as flocking. Inspired by nature, where active living cells coexist with lifeless, immobile objects and structures, here we study the effective interactions that appear in systems composed of active and passive mixtures of colloids. Our system is a two dimensional colloidal monolayer composed primarily of passive (inactive) colloids and a very small fraction of active (sinning) ferromagnetic colloids. We find an emergent ultra-long-range attractive interaction between active particles induced by the activity of the spinning particles and mediated by the elasticity of the passive medium. Interestingly, the appearance of such interaction depends on the spinning protocol and has a minimum actuation time scale below which no attraction is observed. Overall, these results clearly show that in the presence of elastic components, active particles can interact across very long distances without any chemical modification of the environment. Such a mechanism might potentially be important for some biological systems and can be harnessed for newer developments in synthetic active soft materials.

**12:39PM F34.00006 Noise and diffusion in vibrated self-propelled particles** , LEE WALSH, University of Massachusetts Amherst, SARAH SCHLOSSBERG, University of California San Diego, APARNA BASKARAN, Brandeis University, NARAYANAN MENON, University of Massachusetts Amherst — Active-matter systems are often modeled in the lab by studying the two-dimensional dynamics of granular particles driven by vibration in the third dimension. If the vibrational noise is rectified by the shape of the particle, the resulting motion of the particle shows directed motion superimposed on diffusion. We use particles designed for polar motion along a body axis as well as others that break isotropy in various ways. The long-term motion is typically theoretically modeled by a Langevin equation that encodes a self-propulsion velocity along the body axis as well as uncorrelated rotational and translational noise, all of which are treated as independent parameters. For a dilute system of granular tiles confined to a horizontal plane and vertically vibrated, we measure the long-time single-particle dynamics as well as the short-time distributions of translational and rotational motion. From these we characterize the different correlation functions that determine the noise and test the assumptions of the conventional Langevin dynamics used for self-propelled particles.

**12:51PM F34.00007 Glassy dynamics of self-propelled particles** , ELIJAH FLENNER, Colorado State University, LUDOVIC BERTHIER, CNRS and Universite Montpellier, GRZEGORZ SZAMEL, Colorado State University — We examine the glassy dynamics of a system of self-propelled, interacting particles. The self-propulsion is described as an internal driving force that evolves according to the Ornstein-Uhlenbeck process. It can be characterized by an effective temperature and a persistence time for the self-propelled motion. For a fixed effective temperature, as the persistence time approaches zero the particles dynamics becomes equivalent to overdamped Brownian (thermal) dynamics. Our goal is to investigate how the average structure and dynamics evolves with increasing persistence time, which corresponds to increasing departure from the Brownian limit. To this end we simulate a system whose glassy dynamics has been extensively studied in Brownian dynamics simulations, the Kob-Andersen binary mixture. We examine how the effective mode-coupling transition, the fragility and heterogeneous dynamics change with increasing persistence time.

**1:03PM F34.00008 Emergent motion patterns of delay-coupled swarms<sup>1</sup>**, KLEMENTYNA SZWAYKOWSKA, U.S. Naval Research Laboratory, Code 6792, Plasma Physics Division, LUIS MIER-Y-TERAN-ROMERO, Department of Epidemiology, Johns Hopkins University Bloomberg School of Public Health, IRA SCHWARTZ, U.S. Naval Research Laboratory, Code 6792, Plasma Physics Division — Emergent pattern-forming behaviours of aggregates of interacting autonomous agents are a topic of great interest in complex systems research, with applications including biology, environmental monitoring, and defence. We model, and experimentally verify, pattern formation in a swarm of delay-coupled agents, using a simple but general model of agent interactions. Using mean-field dynamics, we perform a thorough analytical study of the bifurcation structure as a function of network connectivity and delay to describe the emergence of pattern formation. We show that swarm motion patterns observed for a homogeneous swarm with all-to-all communication are robust to decreasing network connectivity and to heterogeneity in the parameters governing individual agent behaviours. We perform systematic numerical studies to show where the mean-field theory deviates from simulation and experiment.

<sup>1</sup>This research is funded by the Office of Naval Research (ONR) (Contract No. N0001412WX20083 and NRL Base Funding Contract No. N0001414WX00023). KS holds a NRC Research Associateship Award. LMR is a post-doctoral fellow at JHU, supported by NIH.

**1:15PM F34.00009 Trapping and sorting active granular rods**, SRIRAM RAMASWAMY<sup>1</sup>, TIFR Centre for Interdisciplinary Sciences, 21 Brundavan Colony, Narsingi, Hyderabad 500 075, NITIN KUMAR, James Franck Institute, University of Chicago, Chicago IL 60637, HARSH SONI, School of Engineering, Brown University, Providence RI 02912, RAHUL GUPTA, TIFR Centre for Interdisciplinary Sciences, 21 Brundavan Colony, Narsingi, Hyderabad 500 075, AJAY SOOD, Department of Physics, Indian Institute of Science, Bangalore 560 012 — We report experiments and simulations on collective trapping in a horizontal monolayer of tapered granular rods rendered motile by mechanical vibration. A macroscopic fraction of the particles are trapped by a V-shaped obstacle if its opening angle is less than a threshold value of about 120 degrees, consistent with active Brownian simulations [PRL 108, 268307 (2012)]. the transition between trapped and untrapped states becomes sharper with increasing system size in our numerical studies. We offer a theoretical understanding of this nonequilibrium phase transition based on collective noise suppression and an analysis of fluxes. We show also that the trap can serve to separate particles based on their motility and rotational diffusivity.

<sup>1</sup>on leave from Dept of Physics, Indian Institute of Science

**1:27PM F34.00010 Pattern Formation in Driven Systems<sup>1</sup>**, KATHERINE KLYMKO, Univ of California - Berkeley — Model colloidal particles of two types, driven in opposite directions, will in two dimensions segregate into lanes, a phenomenon studied extensively by Lowen and co-workers [Dzubiella et al. Phys. Rev. E 65, 021402 (2002)]. We have simulated mixtures of oppositely-driven particles using three numerical protocols. We find that laning results from enhanced diffusion, in the direction perpendicular to the drive, of particles surrounded by particles of the opposite type, consistent with the observation of Vissers et al. [Soft Matter 7, 6, 2352 (2011)]. By comparing protocols we find that enhanced diffusion follows from a simple geometrical constraint: oppositely-driven particles must, in the time taken to encounter each other in the direction of the drive, diffuse in the perpendicular direction by about one particle diameter. This constraint implies that the effective lateral diffusion constant grows linearly with drive speed and as the square root of the packing fraction, a prediction supported by our numerics. By invoking an analogy between hard particles with environment-dependent mobilities and mutually attractive particles we argue that there exists an equilibrium system whose pattern-forming properties are similar to those of the driven system.

<sup>1</sup>Katherine Klymko acknowledges support from the NSF Graduate Research Fellowship.

**1:39PM F34.00011 How many dissenters does it take to disorder a flock?<sup>1</sup>**, DAVID YLLANES, M. CRISTINA MARCHETTI, Syracuse University — Minimal models of active particles have had much success in the study of flocking behavior. Typically one considers a system of self-propelled particles with noisy aligning interactions. By varying the density of the system or the intensity of the noise one can switch between a disordered phase where the particles move randomly and independently and a flocking state where the velocities of the particles are aligned. In this work we consider what happens if a fraction  $p$  of the particles does not experience the aligning interaction. This is an interesting problem from a statistical mechanics point of view, with applications to collective behavior of living systems, where not all the members of a community (a flock of birds, a herd of sheep, etc.) behave in the same way. By carrying out extensive molecular dynamics simulations we show that even a very small fraction of such "individualistic" particles can have a dramatic effect on the whole system and, indeed, that the flocking can be destroyed for a very low value of  $p$ .

<sup>1</sup>We acknowledge support from NSF-DMR-305184 and the Syracuse Soft Matter Program

## Tuesday, March 15, 2016 11:15AM - 2:15PM – Session F35 DBIO GSNP: Population and Evolutionary Dynamics II 338 - Uwe Tauber, Virginia Tech

**11:15AM F35.00001 The effect of extrinsic noise on the dynamics of simple gene network motifs**, MICHAEL ASSAF, Hebrew University of Jerusalem — Cellular processes do not follow deterministic rules; even in identical environments genetically identical cells can make random choices leading to different phenotypes. This randomness originates from fluctuations present in the biomolecular interaction networks. Most previous work has been focused on the intrinsic noise of these networks. Yet, especially for high-copy-number biomolecules, extrinsic or environmental noise has been experimentally shown to dominate the variation. Here we develop an analytical formalism that allows for calculation of the combined effect of intrinsic and extrinsic noise on gene expression motifs. We introduce a new and generic method for modeling bounded extrinsic noise as an auxiliary species in the master equation. We focus our study on motifs that can be viewed as the building blocks of genetic switches: a non-regulated gene, a self-inhibiting gene, and a self-promoting gene. The role of the extrinsic noise properties (magnitude, correlation time, and distribution) on the statistics of interest are systematically investigated, and the effect of fluctuations in different reaction rates is compared. Due to its analytical nature, our formalism can be used to quantify the effect of extrinsic noise on the dynamics of biochemical networks and can also be used to improve the interpretation of data from single-cell gene expression experiments.

**11:51AM F35.00002 Backward evolution from gene network dynamics**, MERZU BELETE, University of Houston and Laufer Center for Physical and Quantitative Biology, Stony Brook University, Stony Brook, New York, United States of America, DANIEL CHARLEBOIS, GÁBOR BALÁZSI, Laufer Center for Physical and Quantitative Biology, Stony Brook University, Stony Brook, New York, United States of America — Gene expression is often controlled by regulator genes that form gene regulatory network cascades. How mutation in the genes comprising regulatory cascades influences cell populations dynamics has not been adequately investigated. In this study, we developed a model to study how a mutation in a regulator gene that reaches the effector gene with a time delay affects short-term and long-term population growth. We find a paradoxical outcome of evolution, where a mutation in a regulator gene leads to an interaction between gene regulatory network dynamics and population dynamics, causing in certain cases a permanent decrease in population fitness.

**12:03PM F35.00003 Collective evolution of cyanobacteria and cyanophages mediated by horizontal gene transfer**, HONG-YAN SHIH, Department of Physics and Woese Institute for Genomic Biology, University of Illinois at Urbana-Champaign, TIM ROGERS, Department of Mathematical Sciences, University of Bath, NIGEL GOLDENFELD, Department of Physics and Woese Institute for Genomic Biology, University of Illinois at Urbana-Champaign — We describe a model for how antagonistic predator-prey coevolution can lead to mutualistic adaptation to an environment, as a result of horizontal gene transfer. Our model is a simple description of ecosystems such as marine cyanobacteria and their predator cyanophages, which carry photosynthesis genes. These genes evolve more rapidly in the virosphere than the bacterial pan-genome, and thus the bacterial population could potentially benefit from phage predation. By modeling both the barrier to predation and horizontal gene transfer, we study this balance between individual sacrifice and collective benefits. The outcome is an emergent mutualistic coevolution of improved photosynthesis capability, benefiting both bacteria and phage. This form of multi-level selection can contribute to niche stratification in the cyanobacteria-phage ecosystem. This work is supported in part by a cooperative agreement with NASA, grant NNA13AA91A/A0018.

**12:15PM F35.00004 Environmental quality modulates the cooperative and competitive nature of a microbial cross-feeding mutualism**, TIM HOEK, CSnD Master Program, University Utrecht, Utrecht, The Netherlands, KEVIN AXELROD, Biophysics PhD Program, Harvard University, Cambridge, MA, EUGENE YURTSEV, JEFF GORE, Physics of Living Systems, Department of Physics, Massachusetts Institute of Technology, Cambridge, MA — Mutualisms are essential for ecosystem function and stability. However, in some environments the competitive aspects of an interaction may dominate the mutualistic aspects. Although these transitions could have far-reaching implications, it has been difficult to study the causes and consequences of this mutualistic-competitive transition in experimentally tractable systems. Here we experimentally study a microbial cross-feeding mutualism in which each yeast strain supplies an essential amino acid for its partner strain. We find that, depending upon the amino acid concentration, this pair of strains can exhibit any of: obligatory mutualism, facultative mutualism, competition, parasitism, competitive exclusion, or failed mutualism leading to extinction of the population. A simple model capturing the essential features of this interaction predicts that environmental quality specifies the outcome and provides a “phase diagram” of net interactions in this mutualism. In addition, the model accurately predicts that changes in the dynamics of the mutualism in deteriorating environments can predict that population collapse is imminent. Our results provide a general framework for how mutualisms may transition between qualitatively different regimes of interaction.

**12:27PM F35.00005 Predicting evolutionary dynamics**, GABOR BALAZSI, Laufer Center for Physical and Quantitative Biology, Stony Brook University — We developed an ordinary differential equation-based model to predict the evolutionary dynamics of yeast cells carrying a synthetic gene circuit. The predicted aspects included the speed at which the ancestral genotype disappears from the population; as well as the types of mutant alleles that establish in each environmental condition. We validated these predictions by experimental evolution. The agreement between our predictions and experimental findings suggests that cellular and population fitness landscapes can be useful to predict short-term evolution.

**12:39PM F35.00006 Complex dynamics of selection and cellular memory in adaptation to a changing environment<sup>1</sup>**, EDO KUSSELL, WEI-HSIANG LIN, New York University — We study a synthetic evolutionary system in bacteria in which an antibiotic resistance gene is controlled by a stochastic on/off switching promoter. At the population level, this system displays all the basic ingredients for evolutionary selection, including diversity, fitness differences, and heritability. At the single cell level, physiological processes can modulate the ability of selection to act. We expose the stochastic switching strains to pulses of antibiotics of different durations in periodically changing environments using microfluidics. Small populations are tracked over a large number of periods at single cell resolution, allowing the visualization and quantification of selective sweeps and counter-sweeps at the population level, as well as detailed single cell analysis. A simple model is introduced to predict long-term population growth rates from single cell measurements, and reveals unexpected aspects of population dynamics, including cellular memory that acts on a fast timescale to modulate growth rates.

<sup>1</sup>This work is supported by NIH grant no. R01-GM097356.

**12:51PM F35.00007 Exploiting temporal gradients of antibiotic concentration against the emergence of resistance**, MARIANNE BAUER, Ludwig-Maximilians-Universitt Munich, VUDTIWAT NGAMPRUETIKORN<sup>1</sup>, Okinawa Institute of Science and Technology, ERWIN FREY, Ludwig-Maximilians-Universitt Munich, GREG STEPHENS, Vrije Universiteit Amsterdam and Okinawa Institute of Science and Technology — A very simple model for antibiotic resistance - involving one normal and one more resistant species interacting indirectly through a carrying capacity - shows that the temporal variation of the antibiotic can affect the effect of the antibiotic. For a single antibiotic pulse, we find that for different minimal inhibitory concentrations of the two species an optimal pulse shape may exist, which increases the likelihood of bacterial extinction. For a long series of pulses, efficiency does not vary monotonically with the length of the gap between two individual pulses, but instead, the gap length can be optimised by exploiting the competition between the two species. Finally, a series of pulses is not always more efficient than a single pulse. Shorter pulses may be more efficient in an initial time window without risking population level resistance. We elucidate this behaviour with a phase diagram, and discuss the meaning of this work for current experiments.

<sup>1</sup>(equally contributing author)

**1:03PM F35.00008 Emergence of elevated levels of multiple infections in spatial host-virus dynamics**, BRADFORD TAYLOR, Georgia Inst of Tech, CATHERINE PENINGTON, Queensland Univ of Tech, JOSHUA WEITZ, Georgia Inst of Tech — Bacteria are subject to infection and potentially to multiple simultaneous infections by viruses. Multiply infected hosts have altered life-history traits (e.g., viral burst size) and evolutionary rates (e.g., viral recombination). Yet our understanding of multiple infections of microbes is limited to lab settings where the ratio of inoculant viruses to hosts is controlled. In contrast, rates of multiple infection in natural environments are unknown. Here, we develop an individual based model to quantify rates of multiple infections by a single viral type. We explore different dispersal regimes by varying the viral adsorption rate. High dispersal regimes lead to spatial dynamics and rates of multiple infection equivalent to predictions from mean field models. Local clustering of bacterial hosts occurs for low dispersal. Comparing to mean field, the clustering leads to increased rates of multiple infection and fatter tails in the distribution of the number of internal viruses. The emergence of increased colocalization of viruses with infected hosts leads to these deviations. We show these deviations result from the wave-like spread of viruses when invading clusters of bacteria. Our work represents a key step in understanding the population-level effects of multiple infections.

### 1:15PM F35.00009 Focusing antibody responses against distraction and loss in diversity<sup>1</sup>

SHENSHEN WANG<sup>2</sup>, MEHRAN KARDAR, ARUP CHAKRABORTY, Massachusetts Institute of Technology — Pathogens are complex and evolving fast. They have developed full ranges of disguises to divert immune responses and often manage to escape recognition and thereby outpace natural immunity. A prominent example is the scarce and staggered development of broadly neutralizing antibodies against highly mutable viruses. It remains unclear under what evolutionary conditions these exceptional antibodies could emerge and dominate the response. To address this challenge, we construct an individual-based stochastic model of the Darwinian evolution of antibody-producing immune cells. We consider complexity of viral epitopes, vary seeding diversity of the immune cell population, and allow a time varying population size and extinction – new aspects essential for designing a realistic vaccine. We show that various temporal statistics of antigenic environments would select distinct evolutionary paths that lead to predominantly non-neutralizing, strain-specific or broadly neutralizing antibody responses. We suggest strategies to focus antibody responses on the targeted vulnerability of the virus and confer selective advantage to cross-reactive lineages. This implies a new step toward an effective vaccine against rapidly mutating complex pathogens.

<sup>1</sup>This work is supported by NIH.

<sup>2</sup>Current affiliation: Department of Physics, University of California Los Angeles

### 1:27PM F35.00010 Modeling the interactions between pathogenic bacteria, bacteriophage and immune response

, CHUNG YIN (JOEY) LEUNG, JOSHUA S. WEITZ, School of Biology and School of Physics, Georgia Institute of Technology — The prevalence of antibiotic-resistant strains of pathogenic bacteria has led to renewed interest in the use of bacteriophage (phage), or virus that infects bacteria, as a therapeutic agent against bacterial infections [1]. However, little is known about the theoretical mechanism by which phage therapy may work. In particular, interactions between the bacteria, the phage and the host immune response crucially influences the outcome of the therapy. Few models of phage therapy have incorporated all these three components, and existing models [2] suffer from unrealistic assumptions such as unbounded growth of the immune response. We propose a model of phage therapy with an emphasis on nonlinear feedback arising from interactions with bacteria and the immune response. Our model shows a synergistic effect between the phage and the immune response which underlies a possible mechanism for phage to catalyze the elimination of bacteria even when neither the immune response nor phage could do so alone. We study the significance of this effect for different parameters of infection and immune response, and discuss its implications for phage therapy. References: [1] C. Potera, Environ. Health Perspect. 121, A48 (2013). [2] B. R. Levin and J. J. Bull, Nature Rev. Microbiol. 2, 166 (2004).

### 1:39PM F35.00011 Modeling HIV Cure<sup>1</sup>

, ALAN PERELSON, Los Alamos National Laboratory, JESSICA CONWAY, Pennsylvania State University, YOUFANG CAO, Los Alamos National Laboratory — A large effort is being made to find a means to cure HIV infection. I will present a dynamical model of post-treatment control (PTC) or functional cure of HIV-infection. Some patients treated with suppressive antiviral therapy have been taken off of therapy and then spontaneously control HIV infection such that the amount of virus in the circulation is maintained undetectable by clinical assays for years. The model explains PTC occurring in some patients by having a parameter regime in which the model exhibits bistability, with both a low and high steady state viral load being stable. The model makes a number of predictions about how to attain the low PTC steady state. Bistability in this model depends upon the immune response becoming exhausted when over stimulated. I will also present a generalization of the model in which immunotherapy can be used to reverse immune exhaustion and compare model predictions with experiments in SIV infected macaques given immunotherapy and then taken off of antiretroviral therapy. Lastly, if time permits, I will discuss one of the hurdles to true HIV eradication, latently infected cells, and present clinical trial data and a new model addressing pharmacological means of flushing out the latent reservoir.

<sup>1</sup>Supported by NIH Grants AI028433 and OD011095

### 1:51PM F35.00012 The kinetics and location of intra-host HIV evolution to evade cellular immunity are predictable

, JOHN BARTON, Massachusetts Inst of Tech-MIT, NILU GOONETILLEKE, University of North Carolina, THOMAS BUTLER, Massachusetts Inst of Tech-MIT, BRUCE WALKER, Ragon Institute of MGH, MIT & Harvard, ANDREW MCMICHAEL, University of Oxford, ARUP CHAKRABORTY, Massachusetts Inst of Tech-MIT — Human immunodeficiency virus (HIV) evolves within infected persons to escape targeting and clearance by the host immune system, thereby preventing effective immune control of infection. Knowledge of the timing and pathways of escape that result in loss of control of the virus could aid in the design of effective strategies to overcome the challenge of viral diversification and immune escape. We combined methods from statistical physics and evolutionary dynamics to predict the course of *in vivo* viral sequence evolution in response to T cell-mediated immune pressure in a cohort of 17 persons with acute HIV infection. Our predictions agree well with both the location of documented escape mutations and the clinically observed time to escape. We also find that that the mutational pathways to escape depend on the viral sequence background due to epistatic interactions. The ability to predict escape pathways, and the duration over which control is maintained by specific immune responses prior to escape, could be exploited for the rational design of immunotherapeutic strategies that may enable long-term control of HIV infection.

### 2:03PM F35.00013 Outbreak and Extinction Dynamics in a Stochastic Ebola Model

, GARRETT NIEDDU, Montclair State University, SIMONE BIANCO, IBM Almaden Research Center, LORA BILLINGS, Montclair State University and National Science Foundation, ERIC FORGOSTON, Montclair State University, JAMES KAUFMAN, IBM Almaden Research Center — A zoonotic disease is a disease that can be passed between animals and humans. In many cases zoonotic diseases can persist in the animal population even if there are no infections in the human population. In this case we call the infected animal population the reservoir for the disease. Ebola virus disease (EVD) and SARS are both notable examples of such diseases. There is little work devoted to understanding stochastic disease extinction and reintroduction in the presence of a reservoir. Here we build a stochastic model for EVD and explicitly consider the presence of an animal reservoir. Using a master equation approach and a WKB ansatz, we determine the associated Hamiltonian of the system. Hamilton's equations are then used to numerically compute the 12-dimensional optimal path to extinction, which is then used to estimate mean extinction times. We also numerically investigate the behavior of the model for dynamic population size. Our results provide an improved understanding of outbreak and extinction dynamics in diseases like EVD.

**Tuesday, March 15, 2016 11:15AM - 1:15PM –**

**Session F36 GSOF BIO DPOLY: Physics of Bioinspired Materials II** 339 - Sung Hoong Kang, Johns Hopkins University

**11:15AM F36.00001 The Effect of Water Molecules on Mechanical Properties of Bamboo Microfibrils<sup>1</sup>** , NIMA RAHBAR, Worcester Polytechnic Institute — Bamboo fibers have higher strength-to-weight ratios than steel and concrete. The unique properties of bamboo fibers come from their natural composite structures that comprise mainly cellulose nanofibrils in a matrix of intertwined hemicellulose and lignin called lignin-carbohydrate complex (LCC). Here, we have utilized atomistic simulations to investigate the mechanical properties and mechanisms of interactions between these materials, in the presence of water molecules. Our results suggest that hemicellulose exhibits better mechanical properties and lignin shows greater tendency to adhere to cellulose nanofibrils. Consequently, the role of hemicellulose found to be enhancing the mechanical properties and lignin found to be providing the strength of bamboo fibers. The abundance of Hbonds in hemicellulose chains is responsible for improving the mechanical behavior of LCC. The strong van der Waals forces between lignin molecules and cellulose nanofibrils is responsible for higher adhesion energy between LCC/cellulose nanofibrils. We also found out that the amorphous regions of cellulose nanofibrils is the weakest interface in bamboo Microfibrils. In presence of water, the elastic modulus of lignin increases at low water content (less than 10

<sup>1</sup>NSF CAREER grant no. 1261284

**11:27AM F36.00002 Water-Floating Giant Nanosheets from Helical Peptide Pentamers.<sup>1</sup>** , JAE-HUN LEE, KI TAE NAM, Seoul Natl Univ — One of the important challenges in the development of protein-mimetic materials is to understand the sequence specific assembly behavior and the dynamic folding change. Conventional strategies to construct two dimensional nanostructures from the peptides have been limited to beta-sheet forming sequences in use of basic building blocks because of their natural tendency to form sheet like aggregations. Here we identified a new peptide sequence, YFCFY that can form dimers by the disulfide bridge, fold into helix and assemble into macroscopic flat sheet at the air/water interface. Because of large driving force for two dimensional assembly and high elastic modulus of the resulting sheet, the peptide assembly induces the flattening of initially round water droplet. Additionally, we found that stabilization of helix by the dimerization is a key determinant for maintaining macroscopic flatness over a few tens centimeter even with a uniform thickness below 10 nm. Furthermore, the capability to transfer 2D film from water droplet to other substrates allows for the multiple stacking of 2D peptide nanostructure, suggesting possible applications in the biomimetic catalysts, biosensor and 2D related electronic devices.

<sup>1</sup>This work was supported by Samsung Research Funding Center of Samsung Electronics under Project Number SRFC-MA1401-01

**11:39AM F36.00003 DNA-linked NanoParticle Lattices with Diamond Symmetry: Stability and Shape** , HAMED EMAMY, Wesleyan University, Physics Department, ALEXEI TKACHENKO, OLEG GANG, Brookhaven National Laboratory, Center for Functional Nanomaterials, FRANCIS STARR, Wesleyan University, Physics Department — The linking of nanoparticles (NP) by DNA has been proven to be an effective means to create NP lattices with specific order. Lattices with diamond symmetry are predicted to offer novel photonic properties, but self-assembly of such lattices has proven to be challenging due to the low packing fraction, sensitivity to bond orientation, and local heterogeneity. Recently, we reported an approach to create diamond NP lattices based on the association between anisotropic particles with well-defined tetravalent DNA binding topology and isotropically functionalized NP. Here, we use molecular dynamics simulations to evaluate the Gibbs free energy of these lattices, and thereby determine the stability of these lattices as a function of NP size. The lattice free energy has a minimum for NP size near 50 nm, and rapid increases for larger NP, destabilizing the lattice. We also predict the equilibrium shape for the cubic diamond crystallite using the Wulff construction method. Specifically, we predict the equilibrium shape using the surface energy for different crystallographic planes. We evaluate surface energy directly from molecular dynamics simulation, which we correlate with theoretical estimates from the expected number of broken DNA bonds along a facet.

**11:51AM F36.00004 Multifunctional Memprocessor Device with DNA-Guided Nickel Ions Chain<sup>1</sup>** , CHIA-CHING CHANG, Department of Biological Science and Technology, National Chiao Tung University, WEN-BIN JIAN, YU-CHANG CHEN, Department of Electrophysics, National Chiao Tung University, YUN-LIANG SOO, Department of Physics, National Tsing Hua University, CHIUN-JYE YUAN, Department of Biological Science and Technology, National Chiao Tung University, MASSIMILIANO DI VENTRA, Department of Physics, University of California, San Diego — Molecular metal ion wires are highly desirable for their potential applications in the field of molecular electronics. However, synthesis of a scaffold-free and long metal chain is exceptional challenging. DNA is a self-assembly wire that chelates metal ions with its base-pairs. By using DNA as template, an 830-nm equivalent conducting nickel ion chain was fabricated. This nickel ion chain device demonstrates the functionality of memristor (memory resistor), memcapacitor (memory capacitor), and redox-induced hysteresis effects. The memory state operation is attributed to the dynamic response of nickel-ion states caused by redox reaction. The redox state of Ni ions is controllable by external bias, making it a multi-state memory component for a possible memcomputer, namely a computer that uses memory to store and process information simultaneously [1]. Ref: [1] M. Di Ventra and Y.V. Pershin, Nature Physics, 9, 200 (2013).

<sup>1</sup>Research is supported by MOST 104-2627-M-009-007 Taiwan and is partially supported by CMRR.

**12:03PM F36.00005 Elastic Properties of Lysozyme Confined in Nanoporous Polymer Films** , HAOYU WANG, PINAR AKCORA, Stevens Inst of Tech — Retaining the conformational structure and bioactivity of immobilized proteins is important for biosensor designs and drug delivery systems. It is known that confined media provide a protective environment to the encapsulated proteins and prevent diffusion of the denaturant. In this study, different types of proteins (streptavidin, lysozyme and fibrinogen) were chemically attached into the nanopores of poly(methyl methacrylate) thin films. Heterogeneous flat surfaces with varying cylinder pore sizes (10-50 nm) were used to confine proteins of different sizes and shapes. Stiffness of protein functionalized nanopores was measured in nanoindentation experiments. Our results showed that streptavidin behaved more stiffly when pore dimension changed from micron to nanosize. Further, it was found that lysozyme confined within nanopores showed higher specific bioactivity than proteins on flat surfaces. These results on surface elasticity and protein activity may help in understanding protein interactions with surfaces of different topologies and chemistry.

**12:15PM F36.00006 Bioinspired Non-iridescent Structural Color from Polymer Blend Thin Films** , ASRITHA NALLAPANENI, MATTHEW SHAWKEY, ALAMGIR KARIM, Univ of Akron — Colors exhibited in biological species are either due to natural pigments, sub-micron structural variation or both. Structural colors thus exhibited can be iridescent (ID) or non-iridescent (NID) in nature. NID colors originate due to interference and coherent scattering of light with quasi-ordered micro- and nano- structures. Specifically, in Eastern Bluebird (*Sialia sialis*) these nanostructures develop as a result of phase separation of  $\beta$ -keratin from cytoplasm present in cells. We replicate these structures *via* spinodal blend phase separation of PS-PMMA thin films. Colors of films vary from ultraviolet to blue. Scattering of UV-visible light from selectively leached phase separated blends are studied in terms of varying domain spacing (200nm to 2 $\mu$ m) of film. We control these parameters by tuning annealing time and temperature. Angle-resolved spectroscopy studies suggest that the films are weakly iridescent and scattering from phase-separated films is more diffused when compared to well-mixed films. This study offers solutions to several color-based application in paints and coatings industry.

**12:27PM F36.00007 Colloidal-based additive manufacturing of bio-inspired composites**, ANDRE R STUDART, ETH Zurich — Composite materials in nature exhibit heterogeneous architectures that are tuned to fulfill the functional demands of the surrounding environment. Examples range from the cellulose-based organic structure of plants to highly mineralized collagen-based skeletal parts like bone and teeth. Because they are often utilized to combine opposing properties such as strength and low-density or stiffness and wear resistance, the heterogeneous architecture of natural materials can potentially address several of the technical limitations of artificial homogeneous composites. However, current man-made manufacturing technologies do not allow for the level of composition and fiber orientation control found in natural heterogeneous systems. In this talk, I will present two additive manufacturing technologies recently developed in our group to build composites with exquisite architectures only rivaled by structures made by living organisms in nature. Since the proposed techniques utilize colloidal suspensions as feedstock, understanding the physics underlying the stability, assembly and rheology of the printing inks is key to predict and control the architecture of manufactured parts. Our results will show that additive manufacturing routes offer a new exciting pathway for the fabrication of biologically-inspired composite materials with unprecedented architectures and functionalities.

**1:03PM F36.00008 Mesh Size Control of Friction**, ANGELA PITENIS, JUAN MANUEL URUENA, KYLE D. SCHULZE, ANDREW C. COOPER, THOMAS E. ANGELINI, W. GREGORY SAWYER, Univ of Florida - Gainesville — Soft, permeable sliding interfaces in aqueous environments are ubiquitous in nature but their ability to maintain high lubricity in a poor lubricant (water) has not been well understood. Hydrogels are excellent materials for fundamental soft matter and biotribology studies due to their high water content. While mesh size controls the material and transport properties of a hydrogel, its effects on friction were only recently explored. Polyacrylamide hydrogels slid in a Gemini (self-mated) interface produced low friction under low speeds, low pressures, macroscopic contact areas, and room temperature aqueous environments. The friction coefficients at these interfaces are lowest at low speeds and are speed-independent. This behavior is due to thermal fluctuations at the interface separating the surfaces, with water shearing in this region being the main source of dissipation. We found that mesh size had an inverse correlation with friction. We further investigated a transition from this behavior at higher speeds, and found that the transition speed correlated with the mesh size and relaxation time of the polymer network. Very soft and correspondingly large mesh size Gemini hydrogels show superlubricity under specific conditions with friction being less than 0.005.

## Tuesday, March 15, 2016 11:15AM - 2:15PM –

**Session F37 GSOF: Clustering and Gelation with Competing Interactions I** 340 - Emanuela Del Gado, Georgetown University

**11:15AM F37.00001 Inverse design of voids: clusters of nothing**, BETH LINDQUIST, RYAN JADRIC, THOMAS TRUSKETT, University of Texas at Austin — Much work has been done to find and characterize potentials (both pair and many-body) that result in interesting fluid architectures, particularly with respect to clustered fluids. In this work, we inverse design a pair potential possessing competitive attractions and repulsions that forms voids/clusters of empty space. We show that these voids are relatively spherical and reasonably monodisperse in size. We study the behavior of this potential with respect to modulating system density and temperature and we find that, like clusters of particles, these voids are capable of self-assembling into columns, lamellar sheets, as well as a bicontinuous structure. Moreover, we find that this potential can form both clusters and voids, depending on the state point, demonstrating a correspondence between the competitive interactions that are suitable to form these two structural motifs.

**11:27AM F37.00002 Inverse Design of Equilibrium Cluster Fluids**, RYAN JADRIC, JONATHAN BOLLINGER, BETH LINDQUIST, THOMAS TRUSKETT, University of Texas at Austin — Equilibrium cluster fluids have garnered much recent attention, but the types of interparticle forces that can lead to self-assembly of such entities have not been systematically explored. As a step towards addressing this, we leverage powerful inverse design tools to fabricate a fluid of monodisperse, spherical, liquid-droplet-like clusters of a desired size and good center of mass mobility. The inverse designed pair potential possesses a broad attractive well and narrow repulsive barrier at larger separations a qualitatively different form as compared to the so-called SALR potential [short-range attractive (SA) and long-range repulsive (LR)] often associated with equilibrium cluster formation in colloids. Such differences suggest alternative mechanisms for cluster formation leading to structured fluids with qualitatively different static and dynamic properties. Lastly, we explore the representability of our inverse designed potentials through simple parametrized forms.

**11:39AM F37.00003 Decoding the pair correlations and properties of equilibrium microscopic cluster phases**, JONATHAN BOLLINGER, RYAN JADRIC, THOMAS TRUSKETT, University of Texas at Austin — Due to competing interactions acting between particles, dispersed colloidal suspensions can reversibly transition to phases comprising aggregate clusters. Cluster phases have been reported for both model colloidal particles and complex monomers (e.g., proteins); however, many questions remain regarding how to detect and characterize cluster phases given only pair structural correlations (the information most accessible across diverse systems) and how to relate clustering susceptibility and behavior to underlying monomer-monomer interactions. Using molecular simulations and liquid-state theory across a wide survey of conditions, we decode the widely-observed intermediate range order pre-peak in the structure factor by: (1) validating a physically-intuitive rule for detecting clustering based on the pre-peak thermal correlation length; and (2) relating pre-peak position to cluster size and bulk monomer density. We further demonstrate how clustering transitions and resultant properties relate to monomer interactions along coordinates tunable in experiments. These trends are suitable for comparing against clustering systems that can be directly visualized (via, e.g., confocal microscopy), which should aid in assessing the realism of commonly-adopted monomer interaction potentials.

**11:51AM F37.00004 Multiscale modeling of the thixotropic behavior of aggregating soft colloidal particle suspensions<sup>1</sup>**, PAUL MWASAME, NORMAN WAGNER, ANTONY BERIS, University of Delaware — A multiscale model is presented that incorporates microscopic information at the soft, aggregating, colloidal particle level to a macroscopic description of a thixotropic suspension with a yield stress. This is accomplished by incorporating the relevant physics describing aggregation and breakage at the particle level into a population balance microscopic framework. A moment approach is followed to allow for model coarsening and its incorporation into a macroscopic description. Furthermore, to describe the aggregate dynamics under flow, it is necessary to include an additional description of the aggregate deformation. The yielding behavior of gel networks observed in thixotropic suspensions is modeled by adapting micromechanical models of emulsions and pastes to describe aggregate deformation under flow. A key outcome of this work is the recognition of the important role of competition between orthokinetic and perikinetic aggregation on polydispersity and dynamical behavior. Comparison to rheological experiments on a model thixotropic suspension will also be presented to validate the model developed.

<sup>1</sup>NSF CBET 312146

**12:03PM F37.00005 Elasto-hydrodynamic network analysis of colloidal gels**, JAMES SWAN, ZSIGMOND VARGA, Massachusetts Inst of Tech-MIT — Colloidal gels formed at low particle volume fractions result from a competition between two rate processes: aggregation of colloids and compaction of pre-gel aggregates. Recent work has shown that the former process is highly sensitive to the nature of the hydrodynamic interactions between suspended colloids. This same sensitivity to hydrodynamic flows within the gel leads to pronounced differences in the spectrum of relaxation times and response to deformation of the gel. This talk explores those differences and their consequences through computational simulations and the framework of elasto-hydrodynamic network analysis. We demonstrate a significant impact of hydrodynamic interactions between gelled colloids on macroscopic gel dynamics and rheology as well as the effect of hydrodynamic screening in gelled materials.

**12:15PM F37.00006 Shape mismatch in self assembly leads to fiber-like aggregates<sup>1</sup>**, MARTIN LENZ, CNRS - Orsay, EFRIM EFRATI, Weizmann Institute of Science, THOMAS A. WITTEN, University of Chicago — Aggregating proteins tend to form fibers, often for the worse - think of Alzheimer's disease. Could this propensity to form fibers be a generic physical property of irregular aggregating objects, rather than something specific to protein chemistry? We investigate the aggregation of simple ill-fitting, deformable objects and find that geometrical frustration can lead to self-assembly into slender aggregates.

<sup>1</sup>ML acknowledges support from Universit Paris-Sud and CNRS, the University of Chicago FACCTS program, Marie Curie Integration Grant PCIG12-GA-2012-334053 and Investissements d'Avenir LabEx PALM (ANR-10-LABX-0039-PALM).

**12:27PM F37.00007 Gelation And Mechanical Response of Patchy Rods.<sup>1</sup>**, NAVID KAZEM, Carnegie Mellon Univ, CARMEL MAJIDI, Carnegie Mellon University, CRAIG MALONEY, Northeastern University — We perform Brownian Dynamics simulations to study the gelation of suspensions of attractive, rod-like particles. We show that details of the particle-particle interactions can dramatically affect the dynamics of gelation and the structure and mechanics of the networks that form. If the attraction between the rods is perfectly smooth along their length, they will collapse into compact bundles. If the attraction is sufficiently corrugated or patchy, over time, a rigid space spanning network forms. We study the structure and mechanical properties of the networks that form as a function of the fraction of the surface that is allowed to bind. Surprisingly, the structural and mechanical properties are non-monotonic in the surface coverage. At low coverage, there are not a sufficient number of cross-linking sites to form networks. At high coverage, rods bundle and form disconnected clusters. At intermediate coverage, robust networks form. The elastic modulus and yield stress are both non-monotonic in the surface coverage. The stiffest and strongest networks show an essentially homogeneous deformation under strain with rods re-orienting along the extensional axis. Weaker, clumpy networks at high surface coverage exhibit relatively little re-orienting with strong non-affine deformation. These results suggest design strategies for tailoring surface interactions between rods to yield rigid networks with optimal properties.

<sup>1</sup>National Science Foundation and the Air Force Office of Scientific Research

**12:39PM F37.00008 Protein gelation kinetics near the overlap concentration**, PASHA TABATABAI, Georgetown University, BENJAMIN PARTLOW, DAVID KAPLAN, Tufts University, DANIEL BLAIR, Georgetown University — Proteins can be crosslinked to form gel networks either as a tool to study biological problems or as a method for creating novel materials. The bulk mechanical properties of protein gels in steady state are a manifestation of the gel structure, but the polymerization kinetics are often disregarded. Using the gelation of an aqueous denatured silk protein solution as a model polymer system, we probe the gelation kinetics (modulus vs. time) and find two regimes that depend on whether the initial protein concentration ( $c$ ) is near or below the overlap concentration ( $c^*$ ). We find that systems with  $c/c^* \sim 1$  exhibit immediate and single-mode modulus growth until the completion of polymerization that can be scaled onto a characteristic polymerization curve. However, systems with  $c/c^* < 1$  display delayed modulus development followed by two-stage modulus growth that can be normalized onto a separate distinctive polymerization curve. These two regimes are probed by changing both the initial concentration and the overlap concentration separately, emphasizing the importance of the overlap concentration on the assembly of polymeric/complex fluids.

**12:51PM F37.00009 Coupled diffusion processes and 2D affinities of adhesion molecules at synthetic membrane junctions**, CHRISTOPHER PEEL, University of Oxford, KAUSHIK CHOUDHURI, University of Michigan Medical School, EVA M. SCHMID, MATTHEW H. BAKALAR, HYOUNG SOOK ANN, DANIEL A. FLETCHER, University of California, Berkeley, CELINE JOURNOT, ANDREW TURBERFIELD, MARK WALLACE, MICHAEL DUSTIN, University of Oxford — A more complete understanding of the physically intrinsic mechanisms underlying protein mobility at cellular interfaces will provide additional insights into processes driving adhesion and organization in signalling junctions such as the immunological synapse. We observed diffusional slowing of structurally diverse binding proteins at synthetic interfaces formed by giant unilamellar vesicles (GUVs) on supported lipid bilayers (SLBs) that shows size dependence not accounted for by existing models. To model the effects of size and intermembrane spacing on interfacial reaction-diffusion processes, we describe a multistate diffusion model incorporating entropic effects of constrained binding. This can be merged with hydrodynamic theories of receptor-ligand diffusion and coupling to thermal membrane roughness. A novel synthetic membrane adhesion assay based on reversible and irreversible DNA-mediated interactions between GUVs and SLBs is used to precisely vary length, affinity, and flexibility, and also provides a platform to examine these effects on the dynamics of processes such as size-based segregation of binding and non-binding species.

**1:03PM F37.00010 Enhanced gel formation in binary mixtures of nanocolloids with tunable short-range attraction**, R. LEHENY, Johns Hopkins University, H. GUO, NIST, M. BERTRAND, University of Ottawa, T. SHENDRUK, University of Oxford, S. RAMAKRISHNAN, Florida State University, J. HARDEN, University of Ottawa — We report a combined experimental, theoretical, and simulation study of the phase behavior and microstructural dynamics of concentrated binary mixtures of spherical nanocolloids with a size ratio near two and with a tunable, intrinsic short-range attraction. In the absence of the attraction, the suspensions behave as well mixed, hard-sphere liquids. For sufficiently strong attraction, the suspensions undergo a gel transition. Rheometry measurements show that the fluid-gel boundary of the mixtures does not follow an ideal mixing law, but rather the gel state is stable at weaker interparticle attraction in the mixtures than in the corresponding monodisperse suspensions. X-ray photon correlation spectroscopy measurements reveal that, in contrast with depletion-driven gelation at larger size ratio, gel formation in the mixtures coincides with dynamic arrest of the smaller colloids while the larger colloids remain mobile. Molecular dynamics simulations indicate the arrest results from microphase separation that is caused by a subtle interplay of entropic and enthalpic effects and that drives the smaller particles to form dense regions.

**1:15PM F37.00011 Gelation of calcium-silicate-hydrate in cement**, KATERINA IOANNIDOU, MSE2, joint MIT-CNRS lab, MIT, Cambridge, MA 02139, US, MATEJ KANDUC, Department of Physics, Free University Berlin, D-14195 Berlin, Germany, LUNNA LI, DAAN FRENKEL, Department of Chemistry, University of Cambridge, Cambridge, UK, JURE DOBNIKAR, IRCSM, Beijing University of Chemical Technology, Beijing, P. R. China, ROLAND PELLENG, MSE2, joint MIT-CNRS lab, MIT, Cambridge, MA 02139, US, EMANUELA DEL GADO, Department of Physics and Institute for Soft Matter Synthesis and Metrology, Georgetown University, Washington, DC 20057, US — The calcium-silicate-hydrate (C-S-H) gel forms and densifies via precipitation and aggregation of nano-scale hydrates within a couple of hours during cement hydration and it is the main responsible for cement strength. We have investigated equilibrium and arrested states representative of the effective interactions between the nano-scale C-S-H at different stages of the hydration. The inter-hydrate interactions are due to ion correlation forces arising from strong surface charge heterogeneities and change from repulsive to strongly attractive during the early stages of cement hydration, according to the ionic concentration. We analyze the cluster size distributions, the morphology, the local packing and the free energy of aggregates and crystalline phases, using molecular dynamics and Monte Carlo simulations. We compare the results of equilibrium calculations with non-equilibrium simulations that capture the main features of the hydration kinetics. The emerging picture is that the evolving effective interactions provide a thermodynamic driving for the growth of the gel and for its continuous densification that is crucial to cement strength.

**1:27PM F37.00012 Effects on gelation transition by tuning the interaction of solvent-solute molecules in a bridging system<sup>1</sup>**, GUANGCUI YUAN, NIST - Natl Inst of Stds & Tech, JUNHUA LUO, CHARLES C. HAN, Institute of Chemistry CAS, YUN LIU, University of Delaware — A mixed suspension of large hard spheres and small soft microgels with well-defined bridging interaction is used to construct a new short-range attractive system. Soft poly (N-isopropylacrylamide) microgels ( $R = 80$  nm) are absorbable to the surface of hard polystyrene spheres ( $R = 960$  nm) in aqueous solution. For a constant volume fraction of hard spheres ( $\Phi_{MS}$ ), gradually increasing amount of microgels ( $\Phi_{MG}$ ) leads to a liquid-gel-liquid transitions through bridging and steric stabilized mechanisms. Rheological measurements were performed on suspensions with  $\Phi_{MS}$  ranging up to 0.35 to carefully identify the transition boundaries between liquid-like and solid-like behaviors triggered by  $\Phi_{MG}$ . Meanwhile, neutron scattering technique with Baxter's sticky hard-sphere potential fit was used to investigate the effective interparticle potential at and around the gelation boundaries. By exhibiting a set of experimental results from this explicit model system and comparing with the theoretical data, we try to clarify a debate issue about the relative position of the gel line and the liquid-gas coexistence line in the potential  $U - \Phi$  plane.

<sup>1</sup>This work is supported by the Chinese National Science Foundation (Project 21474121).

**1:39PM F37.00013 Gelation of anisotropic silica colloids with thermoreversible short-range interactions**, RYAN MURPHY, NORMAN WAGNER, University of Delaware — Colloidal suspensions containing anisotropic particles are widely used in particle-based technologies including pharmaceuticals, consumer products, and coatings. The rheological properties of colloidal suspensions are known to be affected by particle shape; however, the combined influence of particle shape and attraction strength is not quantitatively understood for dynamic arrest transitions such as gelation. A model system of anisotropic silica colloids with thermoreversible, short-range attractions was developed to quantify the effect of particle shape and attractions on the gelation behavior. This tunable model system aims to map a fundamental state diagram for anisotropic particle suspensions as a function of particle shape, volume fraction, and interaction strength. Macroscopic rheological properties of thermoreversible gels were explored to determine the influence of particle shape on the gel transition. Neutron and x-ray scattering methods further probed the underlying fluid and gel microstructure at various temperatures, volume fractions, and aspect ratios. Linking these fundamental macroscopic and microscopic measurements will provide practical insight into particle technologies and manufacturing processes containing anisotropic colloidal suspensions.

**1:51PM F37.00014 Colloidal interactions: bridging the gap from atomistic-scale descriptions to the mesoscale Primitive Model and introducing the Explicit Solvent Primitive Model approach**, ROLAND PELLENQ, CNRS/MIT, jMSE<sub>2</sub>, MIT, 77 Massachusetts Avenue, Cambridge, US, BENOIT CARRIER, MATTHIEU VANDAMME, Laboratoire Navier (ENPC/IFSTTAR/CNRS), Marne-la-Vallée, France, HENRI VAN DAMME, CNRS/MIT, jMSE<sub>2</sub>, MIT, 77 Massachusetts Avenue, Cambridge, US, CNRS/MIT, jMSE<sub>2</sub> TEAM, LABORATOIRE NAVIER TEAM — We investigated the interactions responsible for the cohesion of colloidal materials such as clays, cement... The swelling/cohesive properties of these (lamellar) materials depend both on the nature of the (interlayer) cations and on the surface charge of the layers. The overall goal of this work is determining the right level of modelling complexity required to capture the cohesive behaviour of charged materials immersed in an electrolyte. In addition to the analytical mean-field DLVO theory, we used various numerical modelling approaches of increasing complexity from the so-called Primitive Model to full-atomistic description. In particular, we introduced the Explicit Solvent Primitive Model (ESPM), in which ions are modelled as charged hard spheres and solvent molecules as soft spheres with embedded point dipoles. We showed that taking explicitly into account the solvent in such a Primitive Model description, significantly impacts the cohesion. Ionic correlation interactions are always present between charged objects immersed in an electrolyte and always play an important role, even in the case of system carrying a low surface charge balanced by monovalent counter-ions.

**2:03PM F37.00015 Coupling of gelation and glass transition in a biphasic colloidal mixture—from gel-to-defective gel-to-glass<sup>1</sup>**, HE CHENG, DI JIA, CHARLES HAN, Chinese Academy of Sci (CAS) — The state transition from gel to glass is studied in a biphasic mixture of polystyrene core/poly (N-isopropylacrylamide) shell (CS) microgels and sulfonated polystyrene (PSS) particles. At 35 °C, the interaction between CS is due to short-range Van der Waals attraction while that between PSS is from long-range electrostatic repulsion. During variation of the relative ratio of the two species at a fixed apparent total volume fraction, the mixture exhibits a gel-to-defective gel-to-glass transition. When small amounts of PSS are introduced into the CS gel network, some of them are kinetically trapped, causing a change in its fractal structure, and act as defects to weaken the macroscopic gel strength. An increase of PSS content in the mixture promotes the switch from gel to defective gel, *e.g.*, the typical two-step yielding gel merges into one-step yielding. This phenomenon is an indication that inter-cluster bond breakage coincides with intra-cluster bond fracture. As the relative volume fraction of PSS exceeds a critical threshold, the gel network can no longer be formed; hence, the mixture exhibits characteristics of glass. A state diagram of the biphasic mixture is constructed, and the landscape of the different transitions will be described in future studies

<sup>1</sup>The financial support from the National Basic Research Program of China (973 Program, 2012CB821500) is gratefully acknowledged.

**Tuesday, March 15, 2016 11:15AM - 1:15PM —**

**Session F38 DPOLY: Padden Award Symposium 341 - Wesley Burghardt, Northwestern University**

**11:15AM F38.00001 Dispersion-Aggregation and Wetting-Dewetting Phase Transitions in Mixtures of Polymer Grafted Nanoparticles and a Chemically Dissimilar Polymer Matrix**, TYLER MARTIN, U Colorado, KATRINA MONGCOPA, U Houston, RANA ASHKAR, PAUL BUTLER, NIST, RAMANAN KRISHNAMOORTI, U Houston, ARTHI JAYARAMAN, U Delaware — Significant efforts have been focused towards controlling morphology of the nanoscale fillers and matrix polymer in polymer nanocomposites as the composite morphology is directly related to the macroscopic properties of that material. For nanocomposites with chemically identical graft and matrix polymers, it is well understood that the polymer grafted particle dispersion to aggregation transition is directly linked to and synonymous with wetting/dewetting of the graft and matrix polymer. Our recent work has focused on exploring composites with chemically different graft and matrix polymers, specifically those with attractive graft-matrix interactions that lead to a dispersed filler state at low temperature and aggregated filler state at high temperatures. We show, using coarse-grained molecular simulations, that the sharp phase transition from dispersed to aggregated states is distinct from the continuous wetting-dewetting transition. The onset of wetting to dewetting occurs at temperatures lower than the dispersion to aggregation transition, and dewetting continues at temperatures above the transition temperature in the aggregated state. Furthermore, the graft and matrix chain composition can be varied to tune the dispersion-aggregation transition temperature and the degree of wetting of the grafted layer. Experiments using SANS and SAXS of deuterated poly(styrene) grafted silica particles in a poly(vinyl methyl ether) matrix show remarkable agreement with our simulations.

**11:27AM F38.00002 Dynamics of associating networks**, SHENGCHANG TANG, Massachusetts Institute of Technology, AXEL HABICHT, Freie Universitt Berlin, MUZHOU WANG, SHUAILI LI, Massachusetts Institute of Technology, SEBASTIAN SEIFFERT, Freie Universitt Berlin, BRADLEY OLSEN, Massachusetts Institute of Technology — Associating polymers offer important technological solutions to renewable and self-healing materials, conducting electrolytes for energy storage and transport, and vehicles for cell and protein deliveries. The interplay between polymer topologies and association chemistries warrants new interesting physics from associating networks, yet poses significant challenges to study these systems over a wide range of time and length scales. In a series of studies, we explored self-diffusion mechanisms of associating polymers above the percolation threshold, by combining experimental measurements using forced Rayleigh scattering and analytical insights from a two-state model. Despite the differences in molecular structures, a universal super-diffusion phenomenon is observed when diffusion of molecular species is hindered by dissociation kinetics. The molecular dissociation rate can be used to renormalize shear rheology data, which yields an unprecedented time-temperature-concentration superposition. The obtained shear rheology master curves provide experimental evidence of the relaxation hierarchy in associating networks.

**11:39AM F38.00003 Tuning the Assembly of Spherical Nanoparticles in Semicrystalline Polymers**, DAN ZHAO, Columbia Univ, JACQUES JESTIN, Laboratoire Lon Brillouin, CEA Saclay, LONGXI ZHAO, SANAT K. KUMAR, Columbia Univ, MOHAMMAD MOHAMMADKHANI, BRIAN C. BENICEWICZ, University of South Carolina — We propose a simple, novel strategy to controlling nanoparticle (NPs) dispersion states in a semi-crystalline polymer matrix exploiting the kinetics of polymer crystallization. The system consists of poly(methyl methacrylate) grafted spherical silica NPs and poly(ethylene oxide) matrices, which are thermodynamically miscible in the melt. We first show that no remarkable change was observed in the spatial dispersion of NPs upon fast crystallization. However, for slow crystallization, both TEM and X-ray/neutron scattering reveal that the system starts to be organized in a “layer-by-layer” architecture, where the NPs are aligned in the amorphous phases intercalated by the crystalline lamellar phases. More importantly, we have found that the resulting “sheet-like” NP morphology gives rise to a 2-fold increase in the storage modulus but without compromising the fracture toughness of the neat polymer. These results open pathways for creating in-situ biomimetic hierarchical structures with improved mechanical properties through a simple, single-step crystallization processing, which could lead to new applications for this largest class of commercially relevant polymeric materials.

**11:51AM F38.00004 Direct measurement of the critical pore size in a polymer membrane**, MARK ILTON, CHRISTIAN DIMARIA, KARI DALNOKI-VERESS, Department of Physics & Astronomy, McMaster University, Hamilton, Ontario, Canada, L8S 4M1 — The formation of pores is an important process in cellular membranes. Here we use freestanding polymer films as model membranes to study the stability of nucleated pores. Polymer membranes with pores of varying size are patterned using a lithographic technique. The membranes are heated above their glass transition temperature to allow viscous flow to occur. Pores with a radius larger than a critical value grow, while pores smaller than the critical radius are observed to shrink and eventually close. Remarkably, holes that are close enough to the critical radius neither grow nor shrink, even though the film is in the melt state. A simple model which takes into account the energy cost of having additional surface area at the edge of a pore describes the experiments with no free parameters. Biological membranes have an additional energetic cost of forming a pore, which we mimic using a lamellar-forming diblock copolymer. Indeed, we find that the critical pore radius is increased when pore formation is frustrated by molecular architecture.

**12:03PM F38.00005 Pinpointing the onset of mechanical rejuvenation in a polymer glass by monitoring segmental dynamics before and after a constant strain rate pulse<sup>1</sup>**, KELLY HEBERT, JOSH RICCI, KELLY SURALIK, M.D. EDIGER, Univ of Wisconsin, Madison — Over time, dynamics in polymer glasses become slower through physical aging; it is thought that post-yield mechanical deformation may reverse the effects of physical aging in what has been termed “rejuvenation”. We have monitored segmental dynamics in a poly(methyl methacrylate) glass before and after reversing constant strain rate pulses of varying magnitude to explore the onset of mechanical rejuvenation. We find that the segmental dynamics in the glass is unperturbed after pulses to  $\varepsilon/\varepsilon_{\text{yield}} = 0.6$  or less. For pre-yield pulses of higher magnitude, we find evidence of rejuvenation, which is indicated by faster dynamics after the pulse. We find that full rejuvenation only occurs at a strain of  $\varepsilon/\varepsilon_{\text{yield}} = 3$  or higher. This work is qualitatively consistent with recent simulations of Smessaert and Rottler and additionally shows quantitative agreement with predictions from the theory of Chen and Schweizer. However, in spite of observed enhanced dynamics on a molecular level, we find that large pre-yield pulses do not alter the mechanical response of the polymer during subsequent deformation. We explore the apparent contradiction between the macroscopic mechanical and molecular-level dynamical response of the glass to deformation.

<sup>1</sup>We are thankful for funding from NSF-DMR (1404614)

**12:15PM F38.00006 High resolution imaging of the dynamics of nanoparticles in/on liquids**, PAUL KIM, ALEXANDER RIBBE, THOMAS RUSSELL, DAVID HOAGLAND, Univ of Mass - Amherst — Electron microscopy for the study of nanoscale structure and dynamics in solvated soft materials has only recently been proposed, and since this technique requires high vacuum, significant challenges must be confronted. Specimens can be encapsulated in vacuum-sealed devices for TEM but this approach is not without difficulties, including beam damage, cumbersome specimen handling, and propensity for wall artifacts. Here, we report an alternative SEM approach, obviating need for a liquid cell by exploiting the nonvolatility of ionic liquids, which is illustrated by visualizations of nanoscale dynamics for two solvated systems, dispersed nanospheres and nanorods in/on thin, free-standing IL films. The translational and rotational Brownian of these nanoparticles were quantitatively tracked. In ultra-thin films, a striking and unanticipated dynamical pairing of the nanospheres was observed, manifesting a balance of capillary and hydrodynamic interactions. Concentrated nanorods were seen to assemble into finite stacks that could be tracked over their entire lifetimes. Broadly applicable to solvated soft nanoscopic materials, the new imaging protocol offers a breakthrough in the study of their structure and dynamics.

**12:27PM F38.00007 Predicting Thermomechanical Responses of Polymer Thin Films and Nanocomposites via an Innovative Coarse-grained Approach**, WENJIE XIA, DAVID HSU, SINAN KETEN, Northwestern University — Understanding and predicting the thermomechanical responses of nanoscale polymer systems are very challenging as their responses are greatly influenced by many factors, such as interfacial energy, filler volume fraction and molecule weight, giving rise to the presence of nanoscale interface and free surface. To overcome these issues, here we employ a novel atomistically informed coarse-grained computational technique, called thermomechanically consistent coarse graining (TCCG), to investigate how the nanoscale interface and free surface influence the elastic modulus (E) and glass transition temperature (T<sub>g</sub>) of polymer films and nanocomposites. By performing tensile tests and nanoindentation simulations, we are able to predict the size dependent elastic properties of polymer films and quantify the length scale of the local mechanical interphase. Finally, taking cellulose nanocrystal (CNC) and poly(methyl-methacrylate) (PMMA) nanocomposites as a relevant model system, we present a multi-scale framework built upon our CG approach to allow the prediction of T<sub>g</sub> of nanocomposite as a function of interfacial energy and filler volume fractions by drawing the analogy between thin film and nanocomposites. Our established multi-scale framework is validated by recent experiments and breaks new ground in predicting, without any empirical parameters, key structure-property relationships for polymer nanomaterials.

**12:39PM F38.00008 Nanoparticle Order through Entropic Confinement**, REN ZHANG, Univ of Akron, BONGJOON LEE, Carnegie Mellon University, CHRISTOPHER STAFFORD, JACK DOUGLAS, NIST, MICHAEL BOCKSTALLER, Carnegie Mellon University, ALAMGIR KARIM, Univ of Akron — As has been addressed in colloidal science, visual order transitions can be achieved with entropy contributions alone. Herein, entropy-driven ordering of nanoparticle (NP) structures is generated where entropy increase and visual order are achieved simultaneously. We study an "athermal" NP-polymer blends where NPs are densely grafted with polymer brush of the same chemical composition as the polymer matrix. Visual order of the NPs is induced by geometrically confining the thin film blends with meso-scale topographic patterns. When the residual layer thickness of the patterned blend films approaches the nanoparticle dimension, exclusive segregation of NPs to less confining imprinted mesa region occurs. This preferential segregation of NPs, defined by partition coefficient  $K = 0$ , is attributed to purely entropic penalty, where  $K$  denotes the particle density ratio at highly confined residual layer to that at mesa region. We further demonstrate  $K$  is fully tunable and even invertible with increasing matrix chain dimension. The associated entropic free energy change ( $\Delta F = -\ln K$ ) is calculated to explain NP segregation preference. Accordingly, variation of residual layer thickness and polymer matrix molecule size can both affect NP distribution among patterned thick and thin regions.

**12:51PM F38.00009 Design of Bicontinuous Donor/Acceptor Morphologies for Use as Organic Solar Cell Active Layers**, DYLAN KIPP, Univ of Texas, Austin, JORGE MOK, RAFAEL VERDUZCO, Rice Univ, VENKAT GANESAN, Univ of Texas, Austin — Two of the primary challenges limiting the marketability of organic solar cells are i) the smaller device efficiency of the organic solar cell relative to the conventional silicon-based solar cell and ii) the long term thermal instability of the device active layer. The achievement of *equilibrium* donor/acceptor morphologies with the characteristics believed to yield high device performance characteristics could address each of these two challenges. In this work, we present the results of a combined simulations and experiments-based approach to investigate if a conjugated BCP additive can be used to control the self-assembled morphologies taken on by conjugated polymer/PCBM mixtures. First, we use single chain in mean field Monte Carlo simulations to identify regions within the conjugated polymer/PCBM composition space in which addition of copolymers can lead to bicontinuous equilibrium morphologies with high interfacial areas and nanoscale dimensions. Second, we conduct experiments as directed by the simulations to achieve such morphologies in the PTB7 + PTB7-*b*-PNDI + PCBM model blend. We characterize the results of our experiments via a combination of transmission electron microscopy and X-ray scattering techniques and demonstrate that the morphologies from experiments agree with those predicted in simulations. Accordingly, these results indicate that the approach utilized represents a promising approach to intelligently design the morphologies taken on by organic solar cell active layers.

**1:03PM F38.00010 Predicting the Phase Behavior of Polymer Nanocomposites using Field-Based Simulations<sup>1</sup>**, JASON KOSKI, ROBERT RIGGLEMAN, University of Pennsylvania — Polymer nanocomposites (PNCs) have been shown to improve mechanical, electric, and optical properties, which are not achievable with polymers or nanoparticles alone. The parameter space associated with PNCs is vast and having efficient tools to study and characterize PNCs is critical to understand parameter-structure-property relationships. In recent years, we have extended the powerful polymer field theory framework to capture particle correlations and allow for efficient characterization of PNCs. We have made numerous strides in extending the class of PNC systems that are able to be studied with polymer field theory; namely, nanospheres, nanorods, complex grafted particles, and liquid crystals. In this talk, I provide details in developing this framework and illustrate its potential by demonstrating its applicability to bulk polymer nanocomposite systems where we can relax the mean-field approximation, study systems with several nanoparticles, and systems that can macro- or microphase separate (e.g. polymer blends or block copolymers). I will also discuss recent advances we have made in incorporating dynamics into our framework which has exciting implications in understanding the phase behavior of PNCs.

<sup>1</sup>NSF DMR-1410246

**Tuesday, March 15, 2016 11:15AM - 2:15PM –**

**Session F39 DBIO GSOFT: Cell Motility: From Single Cell to Collective Dynamics II** 342 - Jay Tang, Brown University

**11:15AM F39.00001 Effects of physical factors on the swarming motility of text itPseudomonas aeruginosa**, TIEYAN SI, Harbin Institute of Technology, ZIDONG MA, Brown University, WAI SHING TANG, Chinese University of Hong Kong, ALEXANDER YANG, JAY TANG, Brown University — Many species of bacteria can spread over a semi-solid surface via a particular form of collective motion known as surface swarming. Using *Pseudomonas aeruginosa* as a model organism, we investigate physical factors that either facilitate or restrict the swarming motility. The semi-solid surface is typically formed by 0.5-1% agar containing essential nutrients for the bacterial growth and proliferation. Most bacterial species, including *P. aeruginosa*, synthesize bio-surfactants to aid in swarming. We found addition of exogenous surfactants such as triton into the agar matrix enhances the swarming. In contrast, increasing agar percentage, infusing osmolytes, and adding viscous agents all decrease swarming. We propose that the swarming speed is restricted by the rate of water supply from within the agar gel and by the line tension at the swarm front involving three materials in contact: the air, the bacteria propelled liquid film, and the agar substrate.

**11:27AM F39.00002 Quantifying Spatiotemporal Patterns in the Advancing Front of Twitching Bacterial Colonies**, ERIN SHELTON, MAX GIULIANI, University of Guelph, LORI BURROWS, McMaster University, JOHN DUTCHER, University of Guelph — Type IV pili (T4P) are very thin (5-8 nm in diameter) protein filaments that can be extended and retracted by certain classes of Gram-negative bacteria including *P. aeruginosa* [1]. These bacteria use T4P to move across viscous interfaces, referred to twitching motility. Twitching can occur for isolated cells or in a collective manner [2]. Using a custom-built, temperature and humidity controlled environmental chamber, together with particle image velocimetry and Fourier analysis techniques, we characterized the evolution of the advancing front of expanding colonies. We find that the advancing front consists of finger-like protrusions consisting of many bacteria, with the cells within the expanding colony arranged in a lattice-like pattern. We have characterized the average speed, width and bacterial orientation within the fingers as a function of agar concentration/stiffness. In addition, we have analyzed the motion of individual cells within the fingers at high spatial and temporal resolution. [1] Burrows, L.L. (2012) Annu. Rev. Microbiol. 66: 493520. [2] Semmler, A.B., Whitchurch, C.B., Mattick, J.S. (1999) Microbiology 145: 2863-2873.

**11:39AM F39.00003 Pattern formation in Dictyostelium discoideum aggregates in confined microenvironments<sup>1</sup>**, ADRIEN HALLOU, Department of Engineering, Bioengineering Group, University of Cambridge, Cambridge, UK, PASCAL HERSEN, JEAN-MARC DI MEGLIO, Laboratoire Matière et Systèmes Complexes, UMR CNRS 7057 & Université Paris Diderot, Paris, France, ALEXANDRE KABLA, Department of Engineering, Bioengineering Group, University of Cambridge, Cambridge, UK — Dictyostelium Discoideum (Dd) is often viewed as a model system to study the complex collective cell behaviours which shape an embryo. Under starvation, Dd cells form multicellular aggregates which soon elongate, starting to display an anterior-posterior axis by differentiating into two distinct cell populations; prestalk (front) and prespore (rear) cells zones. Different models, either based on positional information or on differentiation followed up by cell sorting, have been proposed to explain the origin and the regulation of this spatial pattern.

To decipher between the proposed hypotheses, we have developed an experimental platform where aggregates, made of genetically engineered Dd cells to express fluorescent reporters of cell differentiation in either prestalk or prespore cells, are allowed to develop in 20 to 400  $\mu\text{m}$  wide hydrogel channels. Such a setup allows us to both mimic Dd confined natural soil environment and to follow the patterning dynamics using time-lapse microscopy. Tracking cell lineage commitments and positions in space and time, we demonstrate that Dd cells differentiate first into prestalk and prespore cells prior to sorting into an organized spatial pattern on the basis of collective motions based on differential motility and adhesion mechanisms.

<sup>1</sup>A. Hallou would like to thank the University of Cambridge for the award of an "Oliver Gatty Studentship in Biophysical and Colloid Science".

**11:51AM F39.00004 Evolutionary aspects of collective motility in pathogenic bacteria.**, MAXIME DEFORET, JOAO XAVIER, Memorial Sloan-Kettering Cancer Center — Pseudomonas aeruginosa is a pathogenic bacteria that can use its single polar flagellum to swim through liquids. It can move collectively over semisolid surfaces, a behavior called swarming. It can also settle and form surface-attached communities called biofilms that protect them from antibiotics. The transition from single motility (swimming) to collective motility (swarming) is biologically relevant as it enables exploring environments that a single bacterium cannot explore on its own. It is also clinically relevant since swarming and biofilm formation are thought to be antagonistic. We investigate the mechanisms of bacterial collective motility using a multidisciplinary approach that combines mathematical modeling, quantitative experiments, and microbial genetics. We aim to identify how these mechanisms may evolve under the selective pressure of population expansion, and consequently reinforce or hinder collective motility. In particular, we clarify the role of growth rate and motility in invasive populations.

**12:27PM F39.00005 Self-organized, near-critical behavior during aggregation in Dictyostelium discoideum**, GIOVANNA DE PALO, Imperial College London, DARVIN YI, THOMAS GREGOR, Princeton University, ROBERT ENDRES, Imperial College London — During starvation, the social amoeba Dictyostelium discoideum aggregates artfully via pattern formation into a multicellular slug and finally spores. The aggregation process is mediated by the secretion and sensing of cyclic adenosine monophosphate, leading to the synchronized movement of cells. The whole process is a remarkable example of collective behavior, spontaneously emerging from single-cell chemotaxis. Despite this phenomenon being broadly studied, a precise characterization of the transition from single cells to multicellularity has been elusive. Here, using fluorescence imaging data of thousands of cells, we investigate the role of cell shape in aggregation, demonstrating remarkable transitions in cell behavior. To better understand their functional role, we analyze cell-cell correlations and provide evidence for self-organization at the onset of aggregation (as opposed to leader cells), with features of criticality in this finite system. To capture the mechanism of self-organization, we extend a detailed single-cell model of D. discoideum chemotaxis by adding cell-cell communication. We then use these results to extract a minimal set of rules leading to aggregation in the population model. If universal, similar rules may explain other types of collective cell behavior.

**12:39PM F39.00006 ABSTRACT WITHDRAWN —**

**12:51PM F39.00007 Asymmetric Nano/Microtopography Biases Cytoskeletal Dynamics and Promotes Unidirectional Cell Guidance**, XIAOYU SUN, MEGHAN DRISCOLL, CAN GUVEN, SATARUPA DAS, Univ of Maryland-College Park, CAROLE PARENT, National Institute of Health, JOHN FOURKAS, WOLFGANG LOSERT, Univ of Maryland-College Park — Many biological and physiological processes depend upon directed migration of cells, which is typically mediated by chemical or physical gradients or by signal relay. Here we show that cells can be guided in a single preferred direction based solely on local asymmetries in nano/microtopography on subcellular scales. These asymmetries can be repeated, and thereby provide directional guidance, over arbitrarily large areas. The direction and strength of the guidance is sensitive to the details of the nano/microtopography, suggesting that this phenomenon plays a context-dependent role in vivo. We demonstrate that asymmetric nano/microtopography guides the direction of internal actin polymerization waves (esotaxis), and that cells move in the same direction as these waves (microthigmotaxis). This phenomenon is observed both for the pseudopod-dominated migration of the amoeboid Dictyostelium discoideum and for the lamellipod-driven migration of human neutrophils. The conservation of this mechanism across cell types and the asymmetric shape of many natural scaffolds suggests that actin-wave-based guidance is important in biology and physiology.

**1:03PM F39.00008 Limits to Chemically Guided Multicellular Migration**, JULIEN VARENNES, BUMSOO HAN, ANDREW MUGLER, Purdue Univ — Collective cell migration in response to a chemical cue requires both multicellular sensing of chemical gradients and coordinated mechanical action. Examples from morphogenesis and cancer metastasis demonstrate that clusters of migratory cells are extremely sensitive, responding to gradients of less than 1% difference in chemical concentration across a cell body. While the limits to multicellular sensing are becoming known, the ensuing consequences for coherent migration remain poorly understood. We develop a model of multicellular sensing and migration based on the cellular Potts model. Multicellular sensing of noisy chemical gradients is modeled as a process of local excitation and global inhibition (LEGI) among communicating cells. The output of the sensing process is coupled to individual cells polarization to model migratory behavior. We find that larger clusters of cells detect the gradient direction with higher precision and thus achieve stronger polarization bias. At the same time, larger clusters are also accompanied by less coherent collective motion. The trade-off between these two effects leads to an optimally efficient cluster size. We discuss how our results relate to cancer metastasis.

**1:15PM F39.00009 Chemotaxis and Actin Oscillations<sup>1</sup>**, EBERHARD BODENSCHATZ, HSIN-FANG HSU, MPI Dynamics and Self-Organization, JOSE NEGRETE, MPI Physics of Complex Systems, CARSTEN BETA, MPI Dynamics and Self-Organization, ALAIN PUMIR, ENS Lyon, AZAM GHOLAMI, MARCO TARANTOLA, CHRISTIAN WESTENDORF, VLADIMIR ZYKOV, MPI Dynamics and Self-Organization — Recently, self-oscillations of the cytoskeletal actin have been observed in Dictyostelium, a model system for studying chemotaxis. Here we report experimental results on the self-oscillation mechanism and the role of regulatory proteins and myosin II. We stimulate cells rapidly and periodically by using photo un-caging of the chemoattractant in a micro-fluidic device and measured the cellular responses. We found that the response amplitude grows with stimulation strength only in a very narrow region of stimulation, after which the response amplitude reaches a plateau. Moreover, the frequency-response is not constant but rather varies with the strength of external stimuli. To understand the underlying mechanism, we analyzed the polymerization and de-polymerization time in the single cell level. Despite of the large cell-to-cell variability, we found that the polymerization time is independent of external stimuli and the de-polymerization time is prolonged as the stimulation strength increases. Our conclusions will be summarized and the role of noise in the signaling network will be discussed.

<sup>1</sup>German Science Foundation CRC 937

**1:27PM F39.00010 Nanotopography guides and directs cell migration in amoeboid and epithelial cells**, RACHEL LEE, Department of Physics, University of Maryland, College Park, SATARUPA DAS, Institute for Physical Science and Technology, University of Maryland, College Park, MATTHEW HOURWITZ, XIAOYU SUN, Department of Chemistry and Biochemistry, University of Maryland, College Park, Maryland, CAROLE PARENT, Laboratory of Cellular and Molecular Biology, Center for Cancer Research, National Cancer Institute, JOHN FOURKAS, Department of Chemistry and Biochemistry, University of Maryland, College Park, Maryland, WOLFGANG LOSERT, Department of Physics, University of Maryland, College Park — Cell migration plays a critical role in development, angiogenesis, immune response, wound healing, and cancer metastasis. In many cases, cells also move in the context of a matrix of collagen fibers, and the alignment of these fibers can both affect the migration phenotype and guide cells. Here we show that both fast and slow migrating cells – amoeboid HL-60 and epithelial MCF10A – are affected in similar ways by micro/nanostructures with dimensions similar to those of collagen fibers. Cell alignment enhances the efficiency of migration by increasing directional persistence.

**1:39PM F39.00011 Flow-driven waves and sink-driven oscillations during aggregation of Dictyostelium discoideum**<sup>1</sup>, AZAM GHOLAMI, VLADIMIR ZYKOV, Max-Planck Institute for Dynamics and Self-Organization, Goettingen, Germany, OLIVER STEINBOCK, Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL, EBERHARD BODENSCHATZ, Max-Planck Institute for Dynamics and Self-Organization, Goettingen, Germany — The slime mold Dictyostelium discoideum (D.d.) is a well-known model system for the study of biological pattern formation. Under starvation, D.d. cells aggregate chemotactically towards cAMP signals emitted periodically from an aggregation center. In the natural environment, D.d. cells may experience fluid flows that can profoundly change the underlying wave generation process. We investigate spatial-temporal dynamics of a uniformly distributed population of D.d. cells in a flow-through narrow microfluidic channel with a cell-free inlet area. We show that flow can significantly influence the dynamics of the system and lead to a flow-driven instability that initiates downstream traveling cAMP waves. We also show that cell-free boundary regions have a significant effect on the observed patterns and can lead to a new kind of instability. Since there are no cells in the inlet to produce cAMP, the points in the vicinity of the inlet lose cAMP due to advection or diffusion and gain only a little from the upstream of the channel (inlet). In other words, there is a large negative flux of cAMP in the neighborhood close to the inlet, which can be considered as a sink. This negative flux close to the inlet drives a new kind of instability called sink-driven oscillations.

<sup>1</sup>Financial support of the MaxSynBio Consortium is acknowledged.

**1:51PM F39.00012 Texture sensing of cytoskeletal dynamics in cell migration**, SATARUPA DAS, Institute for Physical Science and Technology, University of Maryland, College Park, RACHEL LEE, Department of Physics, University of Maryland, College Park, MATTHEW J. HOURWITZ, XIAOYU SUN, Department of Chemistry and Biochemistry, University of Maryland, College Park, CAROLE PARENT, Center for Cancer Research, NCI, NIH, 37 Convent Drive, Bethesda, JOHN T. FOURKAS, Department of Chemistry and Biochemistry, University of Maryland, College Park, WOLFGANG LOSERT, Department of Physics, University of Maryland, College Park — Migrating cells can be directed towards a target by gradients in properties such as chemical concentration or mechanical properties of the surrounding microenvironment. In previous studies we have shown that micro/nanotopographical features on scales comparable to those of natural collagen fibers can guide fast migrating amoeboid cells by aligning actin polymerization waves to such nanostructures. We find that actin microfilaments and microtubules are aligned along the nanoridge topographies, modulating overall cell polarity and directional migration in epithelial cells. This work shows that topographic features on a biologically relevant length scale can modulate migration outcomes by affecting the texture sensing property of the cytoskeleton.

**2:03PM F39.00013 Influence of electric field on cellular migration**<sup>1</sup>, ISABELLA GUIDO, EBERHARD BODENSCHATZ, Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany — Cells have the ability to detect continuous current electric fields (EFs) and respond to them with a directed migratory movement. Dictyostelium discoideum (D.d.) cells, a key model organism for the study of eukaryotic chemotaxis, orient and migrate toward the cathode under the influence of an EF. The underlying sensing mechanism and whether it is shared by the chemotactic response pathway remains unknown. Whereas genes and proteins that mediate the electric sensing as well as that define the migration direction have been previously investigated in D.d. cells, a deeper knowledge about the cellular kinematic effects caused by the EF is still lacking. Here we show that besides triggering a directional bias the electric field influences the cellular kinematics by accelerating the movement of cells along their path. We found that the migratory velocity of the cells in an EF increases linearly with the exposure time. Through the analysis of the PI3K and Phg2 distribution in the cytosol and of the cellular adherence to the substrate we aim at elucidating whereas this speed up effect in the electric field is due to either a molecular signalling or the interaction with the substrate.

<sup>1</sup>This work is part of the MaxSynBio Consortium which is jointly funded by the Federal Ministry of Education and Research of Germany and the Max Planck Society.

**Tuesday, March 15, 2016 11:15AM - 2:03PM –**

**Session F40 GSNP DCMF: Leo Kadanoff Session II / GSNP Student Awards** 343 - Susan Coppersmith, Bulbul Chakraborty, University of Wisconsin, Brandeis University

**11:15AM F40.00001 Fractions, trees and unfinished business.**, BORIS SHRAIMAN, KITP, UC Santa Barbara — In this talk, mourning the loss of a teacher and a dear friend, I would like to share some unfinished thoughts loosely connecting - via Farey fraction trees - Kadanoff's study of universality of quasi-periodic route to chaos with the effort to understand universal features of genealogical trees.

**11:27AM F40.00002 A potential mechanism for a singular solution of the Euler Equations**, MICHAEL BRENNER, Harvard University, SAHAND HORMOZ, California Institute of Technology, ALAIN PUMIR, ENS Lyon — We describe a potential mechanism for a singular solution of the Euler equation. The mechanism involves the interaction of vortex filaments, but occurs sufficiently quickly and at small enough scales that it could have plausibly evaded experimental and computational detection. Scaling estimates for the characteristics of this solution will be presented, as well as numerical simulations of the initial stages.

**11:39AM F40.00003 Nonlinear dynamics of a strongly driven single spin solid state qubit**<sup>1</sup>, S. N. COPPERSMITH, University of Wisconsin-Madison, Madison, WI 53706, USA, THIBAUT JULLIEN, P. SCARLINO, E. KAWAKAMI, QuTech and Kavli Institute of Nanoscience, TU Delft, Lorentzweg 1, 2628 CJ Delft, The Netherlands, D. R. WARD, D. E. SAVAGE, M. G. LAGALLY, MARK FRIESEN, M. A. ERIKSSON, University of Wisconsin-Madison, Madison, WI 53706, USA, L. M. K. VANDERSYPEN, QuTech and Kavli Institute of Nanoscience, TU Delft, Lorentzweg 1, 2628 CJ Delft, The Netherlands — This talk will discuss how dynamical systems theory can yield new insight into some exotic behavior found in experiments on strongly driven quantum spins in silicon/silicon-germanium heterostructures. Spin resonance experiments were performed by using ac voltages to drive an electron wavefunction in a strong magnetic field gradient. Nontrivial dependence of the resonance frequency on applied power, including the observation of multiple resonant frequencies at one power, are shown to be consistent with frequency-dependent attenuation in the high-frequency lines. The method of analysis is very similar to that presented in the course on nonlinear dynamics that Leo Kadanoff developed at the University of Chicago in the early 1990's.

<sup>1</sup>This work was supported in part by ARO (W911NF-12-0607). Development and maintenance of the growth facilities used for fabricating samples is supported by DOE (DE-FG02-03ER46028). This research utilized NSF-supported shared facilities at UW-Madison.

**11:51AM F40.00004 Learning in a noisy environment: a Lyapunov equation approach**, SARA A SOLLA, Northwestern University, YARDEN COHEN, Weizmann Institute of Science, PREDRAG CVITANOVIC, Georgia Institute of Technology — Consider a behavioral task described as a finite time trajectory through a  $d$ -dimensional space, segmented in  $K$  time steps, and thus fully specified by a vector  $X$  in the  $n = dK$  dimensional state space of possible trajectories. Consider the dynamics of learning a desired target trajectory  $X^*$ . In the vicinity of  $X^*$ , the learning dynamics at the  $t$ -th discrete learning time step can be linearized to  $Y_{t+1} = MY_t + \xi_t$ , where,  $Y_t = X_t - X^*$  and  $\xi$  is independent Gaussian noise of zero mean and covariance  $\Delta$ . The balance between contracting dynamics and noise leads to an asymptotic covariance  $Q$  that obeys the Lyapunov equation  $Q = MQM^T + \Delta$ . Given  $Q$ , how can the unknown deterministic component  $M$  be estimated the presence of noise? We propose the use of systematic target perturbations  $X^* \rightarrow X^* + \epsilon V_j$ , with unit vectors  $V_j$ ,  $1 \leq j \leq n$  that span the space  $X$ . We argue, convincingly if not rigorously, that the linear response to these perturbations fully characterizes the asymptotic dynamics of the learning process. We illustrate the method by analyzing networks of neurons with either intrinsic or extrinsic noise, at time resolutions that span from spike timing to spiking rates.

**12:03PM F40.00005 ABSTRACT WITHDRAWN** —

**12:15PM F40.00006 Nonlinear dynamics, Waddington landscape and stem cells**, CHAO TANG, Peking University — There are hundreds of different cell types (skin, neuron, muscle, etc.) in human body, all derived from the stem cell and all have the same genetic information. About 60 years ago, Waddington speculated that the different cell types correspond to different minima in a landscape emerged from genetic interactions. Recently, biologists succeeded in transforming one cell type to another by perturbing the genetic interactions in a cell. I will discuss the experiments and a mathematical model of a set of such cell type transformations in mice, in which we can see an actual example of the Waddington landscape and ways to alter it to facilitate cell type transformation – in particular, to reprogram a differentiated cell back into a stem cell.

**12:27PM F40.00007 From Glaciers to Icebergs**, WENDY ZHANG<sup>1</sup>, University of Chicago — I will describe works from a collaboration between physics and glaciology that grew out of interactions at the *Computations in Science* seminar Leo Kadanoff organized at the University of Chicago. The first project considers the interaction between ocean waves and Antarctic ice shelves, large floating portions of ice formed by glacial outflows. Back-of-envelope calculation and seismic sensor data suggest that crevasses may be distributed within an ice shelf to shield it from wave energy. We also examine numerical scenarios in which changes in environmental forcing causes the ice shelf to fail catastrophically. The second project investigates the aftermath of iceberg calving off glacier terminus in Greenland using data recorded via time-lapse camera and terrestrial radar. Our observations indicate that the mangle of icebergs within the fjord experiences widespread jamming during a calving event and therefore is always close to being in a jammed state during periods of terminus quiescence. Joint work with Jason Amundson, Ivo R. Peters, Julian Freed Brown, Nicholas Guttenberg, Justin C Burton, L. Mac Cathles, Ryan Cassotto, Mark Fahnestock, Kristopher Darnell, Martin Truffer, Dorian S. Abbot and Douglas MacAyeal.

<sup>1</sup>Kadanoff Session DCMF

**12:39PM F40.00008 Multifractals, random walks and Arctic sea ice**<sup>1</sup>, SAHIL AGARWAL, Yale University, JOHN WETTLAUER, Yale University and Nordic Institute of Theoretical Physics (NORDITA) — We examine the long-term correlations and multifractal properties of daily satellite retrievals of Arctic sea ice albedo, extent, and ice velocity for decadal periods. The approach harnesses a recent development called Multifractal Temporally Weighted Detrended Fluctuation Analysis (MF-TW DFA), which exploits the intuition that points closer in time are more likely to be related than distant points. In both data sets we extract multiple crossover times, as characterized by generalized Hurst exponents, ranging from synoptic to decadal. The method goes beyond treatments that assume a single decay scale process, such as a first-order autoregression, which cannot be justifiably fit to these observations. The ice extent data exhibits white noise behavior from seasonal to bi-seasonal time scales, whereas the clear fingerprints of the short (weather) and long ( $\sim 7$  and 9 year) time scales remain, the latter associated with the recent decay in the ice cover. Thus, long term persistence is reentrant beyond the seasonal scale and it is not possible to distinguish whether a given ice extent minimum/maximum will be followed by a minimum/maximum that is larger or smaller in magnitude. The ice velocity data show long term persistence in auto covariance.

<sup>1</sup>NASA Grant NNN13ZDA001N-CRYO and Swedish Research Council Grant No. 638-2013-9243

**12:51PM F40.00009 Phase transition to turbulence in a pipe**<sup>1</sup>, NIGEL GOLDENFELD<sup>2</sup>, University of Illinois at Urbana-Champaign — Leo Kadanoff taught us much about phase transitions, turbulence and collective behavior. Here I explore the transition to turbulence in a pipe, showing how a collective mode determines the universality class. Near the transition, turbulent puffs decay either directly or through splitting, with characteristic time-scales that exhibit a super-exponential dependence on Reynolds number. Direct numerical simulations reveal that a collective mode, a so-called zonal flow emerges at large scales, activated by anisotropic turbulent fluctuations, as represented by Reynolds stress. This zonal flow imposes a shear on the turbulent fluctuations that tends to suppress their anisotropy, leading to a Landau theory of predator-prey type, in the directed percolation universality class. Stochastic simulations of this model reproduce the functional form and phenomenology of pipe flow experiments. Talk based on work performed with Hong-Yan Shih and Tsung-Lin Hsieh.

<sup>1</sup>This work was partially supported by the National Science Foundation through grant NSF-DMR-1044901.

<sup>2</sup>Kadanoff Session

**1:03PM F40.00010 Material Flows in an Active Nematic Liquid Crystal**, STEPHEN DECAMP, Brandeis University —

**1:15PM F40.00011 Lie Algebraic Analysis of Thin Film Marangoni Flows: Multiplicity of Self-Similar Solutions** , ZACHARY NICOLAOU, Nicolaou —

**1:27PM F40.00012 Order-to-chaos transition in the hardness of random Boolean satisfiability problems** , MELINDA VARGA, University of Notre Dame —

**1:39PM F40.00013 Hamiltonian-Based Model to Describe the Nonlinear Physics of Cascading Failures in Power-Grid Networks** , YANG YANG, Northwestern University —

**1:51PM F40.00014 Cell fate reprogramming by control of intracellular network dynamics** , JORGE G.T. ZANUDO , Pennsylvania State University —

**Tuesday, March 15, 2016 11:15AM - 2:15PM —**

**Session F41 DBIO GSNP GSOFT: Maximum Entropy Models: A Promising Link Between Statistical Physics, Inference, and Biology** 344 - Gasper Tkacik, IST Austria

**11:15AM F41.00001 Learning probabilities from random observables in high dimensions: the maximum entropy distribution and others** , TOMOYUKI OBUCHI<sup>1</sup>, Tokyo Institute of Technology, SIMONA COCCO, Laboratoire de Physique Statistique de l'Ecole Normale Supérieure, REMI MONASSON, Laboratoire de Physique Théorique de l'Ecole Normale Supérieure — We consider the problem of learning a target probability distribution over a set of  $N$  binary variables from the knowledge of the expectation values (with this target distribution) of  $M$  observables, drawn uniformly at random. The space of all probability distributions compatible with these  $M$  expectation values within some fixed accuracy, called version space, is studied. We introduce a biased measure over the version space, which gives a boost with the entropy of the distributions and with an arbitrary 'temperature'. The choice of the temperature allows us to interpolate between the flat measure over all the distributions and the pointwise measure concentrated at the maximum entropy distribution. Using the replica method we compute the volume of the version space and other quantities of interest, such as the distance  $R$  between the target distribution and the center-of-mass distribution over the version space. Some phase transitions are found, corresponding to qualitative improvements in the learning of the target distribution and to the decrease of the distance  $R$ . However, the distance  $R$  does not vary with the temperature, meaning that the maximum entropy distribution is not closer to the target distribution than any others.

<sup>1</sup>I am a member of one of the reciprocal societies, The Physical Society of Japan (JPS), and put the ID of JPS above.

**11:27AM F41.00002 Semiparametric energy-based models of systems exhibiting criticality** , JAN HUMPLIK, GASPER TKACIK, Institute of Science and Technology Austria — Over the last decade, several empirical studies have found evidence that many biological and natural systems exhibit critical fluctuations analogous to those observed during second-order phase transitions in equilibrium systems. In many cases, these fluctuations were shown to be equivalent to a thermodynamic version of Zipf's law—if the system is sufficiently large, then a log-log plot of the probability of a state vs. its rank yields a straight line with slope  $-1$ . Because the origin of critical fluctuations cannot be traced to a unique mechanism, it is important that data-driven phenomenological models of natural systems are flexible enough so as to easily capture any kind of criticality. Here we study a class of models with exactly this property. This class consists of energy-based models in which the exponential Boltzmann factor is replaced by an arbitrary nonlinear function. We demonstrate the usefulness of our method by modeling the spiking activity of a population of retinal neurons, and the distribution of light intensities in small patches of natural images. In light of recent work on models with hidden variables, the proposed method can separate interactions induced by an unknown fluctuating environment from interactions intrinsic to the system.

**11:39AM F41.00003 From Maximum Entropy Models to Non-Stationarity and Irreversibility<sup>1</sup>** , RODRIGO COFRE, Department of Theoretical Physics, University of Geneva, Switzerland, BRUNO CESSAC, Inria, Neuromathcomp team, CESAR MALDONADO, Centro de Modelamiento Matemático, Universidad de Chile —

The maximum entropy distribution can be obtained from a variational principle. This is important as a matter of principle and for the purpose of finding approximate solutions. One can exploit this fact to obtain relevant information about the underlying stochastic process. We report here in recent progress in three aspects to this approach.

1- Biological systems are expected to show some degree of irreversibility in time. Based on the transfer matrix technique to find the spatio-temporal maximum entropy distribution, we build a framework to quantify the degree of irreversibility of any maximum entropy distribution.

2- The maximum entropy solution is characterized by a functional called Gibbs free energy (solution of the variational principle). The Legendre transformation of this functional is the rate function, which controls the speed of convergence of empirical averages to their ergodic mean. We show how the correct description of this functional is determinant for a more rigorous characterization of first and higher order phase transitions.

3- We assess the impact of a weak time-dependent external stimulus on the collective statistics of spiking neuronal networks. We show how to evaluate this impact on any higher order spatio-temporal correlation.

<sup>1</sup>RC supported by ERC advanced grant "Bridges", BC: KEOPS ANR-CONICYT, Renvision and CM: CONICYT-FONDECYT No. 3140572

**11:51AM F41.00004 Learning Maximal Entropy Models from finite size datasets: a fast Data-Driven algorithm allows to sample from the posterior distribution.<sup>1</sup>** , ULISSE FERRARI, Institut de la Vision, Sorbonne Universités, UPMC, INSERM U968, CNRS, UMR 7210, Paris, F-75012, France. — A maximal entropy model provides the least constrained probability distribution that reproduces experimental averages of an observables set. In this work we characterize the learning dynamics that maximizes the log-likelihood in the case of large but finite datasets. We first show how the steepest descent dynamics is not optimal as it is slowed down by the inhomogeneous curvature of the model parameters space. We then provide a way for rectifying this space which relies only on dataset properties and does not require large computational efforts. We conclude by solving the long-time limit of the parameters dynamics including the randomness generated by the systematic use of Gibbs sampling. In this stochastic framework, rather than converging to a fixed point, the dynamics reaches a stationary distribution, which for the rectified dynamics reproduces the posterior distribution of the parameters. We sum up all these insights in a "rectified" Data-Driven algorithm that is fast and by sampling from the parameters posterior avoids both under- and over-fitting along all the directions of the parameters space. Through the learning of pairwise Ising models from the recording of a large population of retina neurons, we show how our algorithm outperforms the steepest descent method.

<sup>1</sup>This research was supported by a grant from the Human Brain Project (HBP CLAP)

**12:03PM F41.00005 UniEnt: uniform entropy model for the dynamics of a neuronal population**<sup>1</sup>, DAMIAN HERNANDEZ LAHME, Department of Physics, Emory University, ILYA NEMENMAN, Department of Physics and Department of Biology, Emory University — Sensory information and motor responses are encoded in the brain in a collective spiking activity of a large number of neurons. Understanding the neural code requires inferring statistical properties of such collective dynamics from multicellular neurophysiological recordings. Questions of whether synchronous activity or silence of multiple neurons carries information about the stimuli or the motor responses are especially interesting. Unfortunately, detection of such high order statistical interactions from data is especially challenging due to the exponentially large dimensionality of the state space of neural collectives. Here we present UniEnt, a method for the inference of strengths of multivariate neural interaction patterns. The method is based on the Bayesian prior that makes no assumptions (uniform a priori expectations) about the value of the entropy of the observed multivariate neural activity, in contrast to popular approaches that maximize this entropy. We then study previously published multi-electrode recordings data from salamander retina, exposing the relevance of higher order neural interaction patterns for information encoding in this system.

<sup>1</sup>This work was supported in part by grants JSMP/220020321 and NSF/IOS/1208126.

**12:15PM F41.00006 Modeling the Mass Action Dynamics of Metabolism with Fluctuation Theorems and Maximum Entropy.**, WILLIAM CANNON, DENNIS THOMAS, DOUGLAS BAXTER, JEREMY ZUCKER, GARRETT GOH, Pacific Northwest National Laboratory — The laws of thermodynamics dictate the behavior of biotic and abiotic systems. Simulation methods based on statistical thermodynamics can provide a fundamental understanding of how biological systems function and are coupled to their environment. While mass action kinetic simulations are based on solving ordinary differential equations using rate parameters, analogous thermodynamic simulations of mass action dynamics are based on modeling states using chemical potentials. The latter have the advantage that standard free energies of formation/reaction and metabolite levels are much easier to determine than rate parameters, allowing one to model across a large range of scales. Bridging theory and experiment, statistical thermodynamics simulations allow us to both predict activities of metabolites and enzymes and use experimental measurements of metabolites and proteins as input data. Even if metabolite levels are not available experimentally, it is shown that a maximum entropy assumption is quite reasonable and in many cases results in both the most energetically efficient process and the highest material flux.

**12:27PM F41.00007 On the sufficiency of pairwise interactions in maximum entropy models of networks**<sup>1</sup>, ILYA NEMENMAN, Emory University, LINA MERCHAN, Savannah State University — Biological information processing networks consist of many components, which are coupled by an even larger number of complex multivariate interactions. However, analyses of data sets from fields as diverse as neuroscience, molecular biology, and behavior have reported that observed statistics of states of some biological networks can be approximated well by maximum entropy models with only pairwise interactions among the components. Based on simulations of random Ising spin networks with p-spin ( $p \geq 2$ ) interactions, here we argue that this reduction in complexity can be thought of as a natural property of some densely interacting networks in certain regimes, and not necessarily as a special property of living systems.

<sup>1</sup>This work was supported in part by James S. McDonnell Foundation grant No. 220020321

**12:39PM F41.00008 Insights in connecting phenotypes in bacteria to coevolutionary information.**<sup>1</sup>, RYAN CHENG, Rice University, FARUCK MORCOS, University of Texas at Dallas, RYAN HAYES, University of Michigan, RODNEY HELM, University of Houston, HERBERT LEVINE, JOSE ONUCHIC, Rice University — It has long been known that protein sequences are far from random. These sequences have been evolutionarily selected to maintain their ability to fold into stable, three-dimensional folded structures as well as their ability to form macromolecular assemblies, perform catalytic functions, etc. For these reasons, there exist quantifiable mutational patterns in the collection of sequence data for a protein family arising from the need to maintain favorable residue-residue interactions to facilitate folding as well as cellular function. Here, we focus on studying the correlated mutational patterns that give rise to interaction specificity in bacterial two-component signaling (TCS) systems. TCS proteins have evolved to be able to preferentially bind and transfer a phosphate group to their signaling partner while avoiding phosphotransfer with non-partners. We infer a Potts model Hamiltonian governing the correlated mutational patterns that are observed in the sequence data of TCS partners and apply this model to recently published in vivo mutational data. Our findings further support the notion that statistical models built from sequence data can be used to predict bacterial phenotypes as well as engineer interaction specificity between non-partner TCS proteins.

<sup>1</sup>This research has been supported by the NSF INSPIRE award (MCB-1241332) and by the CTBP sponsored by the NSF (Grant PHY- 1427654)

**12:51PM F41.00009 Computational Amide I Spectroscopy for Refinement of Disordered Peptide Ensembles: Maximum Entropy and Related Approaches**, MICHAEL REPERT, Massachusetts Inst of Tech-MIT, ANDREI TOKMAKOFF, University of Chicago — The structural characterization of intrinsically disordered peptides (IDPs) presents a challenging biophysical problem. Extreme heterogeneity and rapid conformational interconversion make traditional methods difficult to interpret. Due to its ultrafast (ps) shutter speed, Amide I vibrational spectroscopy has received considerable interest as a novel technique to probe IDP structure and dynamics. Historically, Amide I spectroscopy has been limited to delivering global secondary structural information. More recently, however, the method has been adapted to study structure at the local level through incorporation of isotope labels into the protein backbone at specific amide bonds. Thanks to the acute sensitivity of Amide I frequencies to local electrostatic interactions—particularly hydrogen bonds—spectroscopic data on isotope labeled residues directly reports on local peptide conformation. Quantitative information can be extracted using electrostatic frequency maps which translate molecular dynamics trajectories into Amide I spectra for comparison with experiment. Here we present our recent efforts in the development of a rigorous approach to incorporating Amide I spectroscopic restraints into refined molecular dynamics structural ensembles using maximum entropy and related approaches. By combining force field predictions with experimental spectroscopic data, we construct refined structural ensembles for a family of short, strongly disordered, elastin-like peptides in aqueous solution.

**1:03PM F41.00010 Coevolutionary modeling of protein sequences: Predicting structure, function, and mutational landscapes**, MARTIN WEIGT, Université Pierre et Marie Curie, Paris — Over the last years, biological research has been revolutionized by experimental high-throughput techniques, in particular by next-generation sequencing technology. Unprecedented amounts of data are accumulating, and there is a growing request for computational methods unveiling the information hidden in raw data, thereby increasing our understanding of complex biological systems. Statistical-physics models based on the maximum-entropy principle have, in the last few years, played an important role in this context. To give a specific example, proteins and many non-coding RNA show a remarkable degree of structural and functional conservation in the course of evolution, despite a large variability in amino acid sequences. We have developed a statistical-mechanics inspired inference approach - called Direct-Coupling Analysis - to link this sequence variability (easy to observe in sequence alignments, which are available in public sequence databases) to bio-molecular structure and function. In my presentation I will show, how this methodology can be used (i) to infer contacts between residues and thus to guide tertiary and quaternary protein structure prediction and RNA structure prediction, (ii) to discriminate interacting from non-interacting protein families, and thus to infer conserved protein-protein interaction networks, and (iii) to reconstruct mutational landscapes and thus to predict the phenotypic effect of mutations. References [1] M. Figliuzzi, H. Jacquier, A. Schug, O. Tenaillon and M. Weigt "Coevolutionary landscape inference and the context-dependence of mutations in beta-lactamase TEM-1", Mol. Biol. Evol. (2015), doi: 10.1093/molbev/msv211 [2] E. De Leonardi, B. Lutz, S. Ratz, S. Cocco, R. Monasson, A. Schug, M. Weigt "Direct-Coupling Analysis of nucleotide coevolution facilitates RNA secondary and tertiary structure prediction", Nucleic Acids Research (2015), doi: 10.1093/nar/gkv932 [3] F. Morcos, A. Pagnani, B. Lunt, A. Bertolino, D. Marks, C. Sander, R. Zecchina, J.N. Onuchic, T. Hwa, M. Weigt, "Direct-coupling analysis of residue co-evolution captures native contacts across many protein families", Proc. Natl. Acad. Sci. 108, E1293-E1301 (2011).

**1:39PM F41.00011 Phase transitions in Hidden Markov Models<sup>1</sup>**, JOHN BECHHOEFER, EMMA LATHOUWERS, Simon Fraser Univ — In *Hidden Markov Models* (HMMs), a Markov process is not directly accessible. In the simplest case, a two-state Markov model emits one of two symbols at each time step. We can think of these symbols as noisy measurements of the underlying state. With some probability, the symbol implies that the system is in one state when it is actually in the other. The ability to judge which state the system is in sets the efficiency of a Maxwell demon that observes state fluctuations in order to extract heat from a coupled reservoir. The *state-inference problem* is to infer the underlying state from such noisy measurements at each time step. We show that there can be a phase transition in such measurements:<sup>2</sup> for measurement error rates below a certain threshold, the inferred state always matches the observation. For higher error rates, there can be continuous or discontinuous transitions to situations where keeping a memory of past observations improves the state estimate. We can partly understand this behavior by mapping the HMM onto a 1d random-field Ising model at zero temperature. We also present more recent work that explores a larger parameter space and more states.

<sup>1</sup>Research funded by NSERC, Canada

<sup>2</sup>John Bechhoefer, *New J. Phys.* **17**, 075003 (2015).

**1:51PM F41.00012 Distinguishing cell type using epigenotype<sup>1</sup>**, THOMAS WYTOCK, ADILSON E MOTTER, Dept. Physics and Astronomy, Northwestern University — Recently, researchers have proposed that unique cell types are attractors of their epigenetic dynamics including gene expression and chromatin conformation patterns. Traditionally, cell types have been classified by their function, morphology, cytochemistry, and other macroscopically observable properties. Because these properties are the result of many proteins working together, it should be possible to predict cell types from gene expression or chromatin conformation profiles. In this talk, I present a maximum entropy approach to identify and distinguish cell type attractors on the basis of correlations within these profiles. I will demonstrate the flexibility of this method through its separate application to gene expression and chromatin conformation datasets. I show that our method out-performs other machine-learning techniques and uncorrelated benchmarks. We adapt our method to predict growth rate from gene expression in *E. coli* and *S. cerevisiae* and compare our predictions with those from metabolic models. In addition, our method identifies a nearly convex region of state-space associated with each cell type attractor basin. Estimates of the growth rate and attractor basin make it possible to rationally control gene regulatory networks independent of a model.

<sup>1</sup>This research was supported by NSF-GRFP, NSF-GK12, GAANN, and Northwestern's NIH-NIGMS Molecular Biophysics Training Grant

**2:03PM F41.00013 Can simple interactions capture complex features of neural activity underlying behavior in a virtual reality environment?**, LEENOY MESHULAM, JEFFREY GAUTHIER, CARLOS BRODY, DAVID TANK, WILLIAM BIALEK, Princeton University — The complex neural interactions which are abundant in most recordings of neural activity are relatively poorly understood. A prime example of such interactions can be found in the *in vivo* neural activity which underlies complex behaviors of mice, imaged in brain regions such as hippocampus and parietal cortex. Experimental techniques now allow us to accurately follow these neural interactions in the simultaneous activity of large neuronal populations of awake behaving animals. Here, we demonstrate that pairwise maximum entropy models can predict a surprising number of properties of the neural activity. The models, that are constrained with activity rates and interactions between pairs of neurons, are well fit to the activity 'states' in the hippocampus and cortex of mice performing cognitive tasks while navigating in a virtual reality environment.

**Tuesday, March 15, 2016 11:15AM - 2:15PM —**

**Session F42 DPOLY: Polymer Assembly I** 345 - Sangwoo Lee, Rensselaer Polytechnic Institute

**11:15AM F42.00001 Chain exchange kinetics of block copolymer micelles in ionic liquids**, YUANCHI MA, TIMOTHY LODGE, University of Minnesota — The chain exchange kinetics of block copolymer micelles has been studied using time-resolved small-angle neutron scattering (TR-SANS), a key tool in determining the average micelle composition in contrast-matched solvents. In this work, PMMA-*block*-PnBMA was selected as the model block copolymer, which has a LCST behavior in the common ionic liquids, [EMIM][TFSI] and [BMIM][TFSI]. We examined the chain exchange kinetics of three PMMA-*block*-PnBMA copolymers, with identical PMMA block length ( $M_{\text{PMMA}} = 25000$ ) and different PnBMA block lengths ( $M_{\text{PnBMA}} = 24000, 35000$  and  $53000$ ); the Flory-Huggins interaction parameter ( $\chi$ ) between the core (PnBMA) and the solvent were varied by mixing [EMIM][TFSI] and [BMIM][TFSI] in different ratios. We found that the relaxation of the initial segregation of h- and d- micelles followed the same form with the time as previously developed by our group. Assuming that single chain expulsion is the rate limiting step, the thermal barrier was found to depend linearly on the core block length ( $N_{\text{core}}$ ). Furthermore, the effect of  $\chi$  on the chain exchange kinetics will also be discussed.

**11:27AM F42.00002 Self-assembly of Coordination Macroions — the Effect of Small Polymer Chains<sup>1</sup>**, HUI LI, TIANBO LIU, University of Akron, ALEX ZHUKHOVITSKIY, JEREMIAH JOHNSON, Massachusetts Institute of Technology — In the presence of small simple counterions, macroions with modest charge density could self-assemble into one-layer hollow spherical structures. The driving force to form this vesicle-like structure is considered as counter-ion mediated attractions. On the other hand, overall hydrophilic transition metal-organic macrocations, consisting of hydrophobic ligands (pyridine-based) and hydrophilic palladium (Pd) metal ions, can be used as nanosized macrocations. One of the positively charged coordination macroions, Pd<sub>12</sub>L<sub>24</sub> (Pd = Pd (II), L = (1,3-di(pyridin-4-yl)benzene), is famous for its controllable and precise assembly structure and possible functional sites. By functionalizing the organic ligand with polymer ethylene glycol (PEG), the macroions could possess larger size thus lower charge density. Detecting their self-assembled structures will tell the difference of their solution behavior as well as the discrepancy of macroion clusters. In summary, the small non-charged PEG chains have been observed to reduce the surface charge density, and furthermore, significantly change the solution behavior.

<sup>1</sup>National Science Foundation (CHE1305756)

**11:39AM F42.00003 Simulation and Numerical Modeling of the Self-assembly of an Optoelectronic Peptide**, RACHAEL MANSBACH, ANDREW FERGUSON, Univ of Illinois - Urbana — We report molecular dynamics simulations of the self-assembly of synthetic  $\pi$ -conjugated oligopeptides into optoelectronic nanostructures. The electronic properties provide the basis for an array of organic electronic devices, such as light-emitting diodes, field-effect transistors, and solar cells. Control of the structure, stability, and kinetics of self-assembled organic electronics by tuning monomer chemistry and environmental conditions presents a powerful route to the fabrication of biocompatible designer materials. We have performed coarse-grained simulations of the self-assembly of several hundred peptides over microsecond time scales to probe the morphology and kinetics of aggregation with molecular-level detail. We have subsequently used this simulation data to parameterize a kinetic aggregation model based on Smoluchowski coagulation theory to enable prediction of aggregation dynamics on millisecond time scales. These numerical models are now being integrated into a multi-physics model of peptide aggregation in a microfluidic flow cell developed by our experimental collaborators to model the self-assembly of diverse peptide architectures under tailored flow-fields for the fabrication of biocompatible assemblies with defined morphology and optoelectronic function.

## 11:51AM F42.00004 Complexation Between Cationic Diblock Copolymers and Plasmid DNA

, SEYOUNG JUNG, THERESA REINEKE, TIMOTHY LODGE, Univ of Minnesota - Twin Cities — Deoxyribonucleic acids (DNA), as polyanions, can spontaneously bind with polycations to form polyelectrolyte complexes. When the polycation is a diblock copolymer with one cationic block and one uncharged hydrophilic block, the polyelectrolyte complexes formed with plasmid DNA (pDNA) are often colloiddally stable, and show great promise in the field of polymeric gene therapy. While the resulting properties (size, stability, and toxicity to biological systems) of the complexes have been studied for numerous cationic diblocks, the fundamentals of the pDNA-diblock binding process have not been extensively investigated. Herein, we report how the cationic block content of a diblock influences the pDNA-diblock interactions. pDNA with 7164 base pairs and poly(2-deoxy-2-methacrylamido glucopyranose)-block-poly(N-(2-aminoethyl) methacrylamide) (PMAG-b-PAEMA) are used as the model pDNA and cationic diblock, respectively. To vary the cationic block content, two PMAG-b-PAEMA copolymers with similar PMAG block lengths but distinct PAEMA block lengths and a PAEMA homopolymer are utilized. We show that the enthalpy change from pDNA-diblock interactions is dependent on the cationic diblock composition, and is closely associated with both the binding strength and the pDNA tertiary structure.

## 12:03PM F42.00005 Complexation of $AB^+$ , $AB^+C$ , $ACB^+$ , and $A(B^+-stat-C)$ block copolymer micelles with poly(styrene sulfonate) as models for tunable gene delivery vectors

, JENNIFER LAASER, YAMING JIANG, ELISE LOHMANN, THERESA REINEKE, TIMOTHY LODGE, University of Minnesota — We investigate the complexation of poly(styrene sulfonate) with micelles with mixed cationic/hydrophilic coronas as models for tunable gene delivery vectors. The micelles are self-assembled from  $AB^+$ ,  $AB^+C$ ,  $ACB^+$ , and  $A(B^+-stat-C)$  block polymer architectures, where the hydrophobic A blocks (poly(styrene)) form the micelle cores, and the cationic B blocks (poly(dimethylamino ethyl methacrylate)) and hydrophilic, nonionic C blocks (poly(poly(ethylene glycol) methyl ether methacrylate)) form the coronas. We find that hydrophilic units do not change the colloidal stability of the complexes, and complexes based on all four micelle architectures form broad, multimodal size distributions. While complexes based on the  $AB^+$ ,  $AB^+C$ , and  $ACB^+$  polymer architectures are kinetically trapped at low ionic strength, however, those based on the  $A(B^+-stat-C)$  architecture rapidly rearrange into single-micelle complexes when the linear polyanion is in excess. This suggests that the randomly-placed hydrophilic units break up the ion pairing between the cationic and anionic chains and promote formation of over-charged complexes. Design of the micelle architecture may thus provide a powerful way control the structure and stability of micelle-polyelectrolyte complexes for gene delivery applications.

## 12:15PM F42.00006 Computational Insight into Solvent Effects on Conformation and Assembly of Structured Ionic Polymer<sup>1</sup>

, MANJULA SENANAYAKE, DIPAK ARYAL, DVORA PERAHIA, Clemson University, GARY GREEST, Sandia National Laboratories — Structured ionomers are in the core of numerous current and potential new applications including clean energy, water purification membranes and sensors. The ability to facilitate ions and solvents transport is a key to their function and is controlled by their structure. One effective path for structural control is tuning their conformation by solvent interactions. Here, the conformation and association of an ABCBA co-polymer where C is a randomly sulfonated polystyrene with sulfonation fractions  $f = 0$  to 0.55, B is poly (ethylene-r-propylene), and A is poly (t-butyl styrene), in n-propanol are studied by molecular dynamic simulation. In contrast to the collapsed conformation of the ionizable block in hydrophobic solvents, we find that it remains swollen. Similar to hydrophobic solutions the co-polymers aggregate to form an ionizable core surrounded by extended hydrophobic chains. In contrast to the “locked-in” ionizable segments observed in cyclohexane/heptane, here the ionic clusters remain dynamic.

<sup>1</sup>Supported in part by DOE Grant No. DE-SC007908

## 12:27PM F42.00007 Continuous monitoring of structural dynamics in polymer assemblies.

, JOSE RAFAEL GUZMAN SEPULVEDA<sup>1</sup>, JINAN DENG<sup>2</sup>, JIYU FANG<sup>3</sup>, ARISTIDE DOGARIU<sup>4</sup>, Univ of Central Florida — Due to their flexibility, optical methods are preferred approaches for monitoring the dynamics and mechanical properties of scattering systems such as polymer solutions, colloidal suspensions, and complex media in general. In particular, their potential noninvasiveness is critical for the passive assessment of dynamic processes. Practical implementations however suffer sometimes from limitations due to effects such as multiple scattering or strong attenuation. Here we introduce an optical technique that overcomes some of these limitations and permits accessing the dynamics of complex colloidal systems under realistic conditions and inherent external influences. This interferometric technique operates based on the coherence-gated isolation of single scattering and allows for the spatially-resolved evaluation of the system's dynamics in optically isolated picoliter-sized volumes. This effective isolation permits a fully passive characterization of nonstationary dynamic processes in complex systems including aggregation and self-assembling, sedimentation, structural evolution and phase transitions, interface dynamics, and dynamics in inhomogeneous or stratified solvents.

<sup>1</sup>CREOL, The College of Optics and Photonics.

<sup>2</sup>Department of Materials Science and Engineering, The College of Optics and Photonics.

<sup>3</sup>Department of Materials Science and Engineering, The College of Optics and Photonics.

<sup>4</sup>CREOL, The College of Optics and Photonics.

## 12:39PM F42.00008 Inclusion Kinetics of Polyrotaxanes

, HIDEAKI YOKOYAMA, SHOKO TAKAHASHI, KOHZO ITO, The University of Tokyo, NORIFUMI YAMADA, High Energy Accelerator Research Organization, KEK — Inclusion complex (IC) formation of  $\alpha$ -cyclodextrin ( $\alpha$ -CD) and poly(ethylene glycol) (PEG) brush in water was investigated by Surface Plasmon Resonance Spectroscopy (SPR), neutron reflectometry (NR) and grazing incident wide angle X-ray scattering (GISANS). Spontaneous IC formation of  $\alpha$ -CD with PEG (polyrotaxanes) is believed to be due to hydrophobic interaction between the hydrophobic interior of  $\alpha$ -CD and PEG; however, the detail of the IC formation kinetics has not been observed because IC formation results in aggregation and precipitation of the complex. SPR revealed that IC formation occurs after induction period, which often appears in crystallization. When concentration of  $\alpha$ -CD solution is 10%, IC consisting randomly oriented  $\alpha$ -CD polycrystal appeared. In contrast, when the concentration of  $\alpha$ -CD solution is 5%, a uniform 10-nm-thick IC layer with  $\alpha$ -CD stacked perpendicular to the substrate appeared. 10-nm-thick IC was also found in the diluted PEG brush in contact with a 10%  $\alpha$ -CD solution. The characteristic 10-nm-thick layer is related to the folded crystalline structure of  $\alpha$ -CD on PEG brush. Such crystallization was proved to be the main driving force for IC formation.

## 12:51PM F42.00009 Crystallization in Micellar Cores: confinement effects and dynamics

, REIDAR LUND, THOMAS ZINN, Department of Chemistry, University of Oslo, LUTZ WILLNER, Forschungszentrum Jlich, DEPARTMENT OF CHEMISTRY, UNIVERSITY OF OSLO TEAM, FORSCHUNGSZENTRUM JILICH COLLABORATION — It is well known that liquids confined to small nanoscopic pores and droplets exhibit thermal behavior very different from bulk samples. Here we demonstrate that n-alkanes forming 2-3 nm small micellar cores are considerably affected by confinement in analogue with hard confined systems. We study micelles form by self-assembly of a series of well-defined n-Alkyl-PEO polymers in aqueous solutions [1]. By using small-angle X-ray scattering (SAXS), densimetry and differential scanning calorimetry (DSC), we show that n-alkane exhibit a first-order phase transition i.e. melting. Correlating the structural and thermodynamic data, we find that a melting depression can be accurately described by the Gibbs-Thomson equation [2]. The effect of core crystallinity on the molecular exchange kinetics is investigated using time-resolved small-angle neutron scattering (TR-SANS) [3-6]. We show that there are considerable entropic and enthalpic contributions from the chain packing that affect the kinetic stability of micelles. [7] T. Zinn *et al.*, *Soft Matter*, 2014, **10**, 5212. [2] T. Zinn, L. Willner and R. Lund, *Phys. Rev. Lett.* **113** (2014) 238305. [3] R. Lund, L. Willner, D. Richter, *Adv. Polym. Sci.* **204** (2013) 51. [5] R. Lund *et al.* *Phys. Rev. Lett.*, 2006, **96**, 068302. [6] S.-H. Choi *et al.* *Phys. Rev. Lett.* **104** (2010) 1. [7] T. Zinn, L. Willner, V. Pipich, D. Richter and R. Lund, *ACS Macro Lett.*, 2015, **4**, 651-655.

**1:03PM F42.00010 Assembly, Conformation, and Thermodynamics of Star-Branched Poly(N-isopropylacrylamide) (PNIPAM) in Solution**, MICHAEL J. A. HORE, XIAOLONG LANG, WILLIAM R. LENART, Case Western Reserve University — The synthetic route and molecular architecture of poly(N-isopropylacrylamide) (PNIPAM) affects its assembly and thermoresponsive behavior. Here, the structure and assembly of star-branched PNIPAM is studied in water using a new model based on the random phase approximation (RPA), and small-angle neutron scattering (SANS) for  $f = 3, 4$ , and 6 arm star polymers, synthesized using either click chemistry, RAFT, or ATRP. Unlike linear PNIPAM, we find that for star-branched polymers, the radius of gyration scales with the degree of polymerization  $N$  as  $R_g \sim N^{0.65}$  indicating physical excluded volume effects in the polymer chain conformation.  $R_g$  decreases monotonically as the system temperature approaches the lower critical solution temperature (LCST). Interestingly, PNIPAM chains begin to associate well below the LCST, depending on whether the polymers were synthesized via ATRP or RAFT, and a strong structure factor peak can be observed as  $T$  increases. Finally, the Flory-Huggins interaction parameters between PNIPAM and water are extracted from the scattering data, and indicate that molecular architecture does not substantially influence the interaction between water and PNIPAM. These observations are compared to recent studies in the literature.

**1:15PM F42.00011 Monodisperse Block Copolymer Particles with Controllable Size, Shape, and Nanostructure.**, JAE MAN SHIN, Department of Chemical and Biomolecular Engineering, KAIST, YONGJOO KIM, Department of Material Science and Engineering, KAIST, BUMJOON KIM, Department of Chemical and Biomolecular Engineering, KAIST, PNEL TEAM — Shape-anisotropic particles are important class of novel colloidal building block for their functionality is more strongly governed by their shape, size and nanostructure compared to conventional spherical particles. Recently, facile strategy for producing non-spherical polymeric particles by interfacial engineering received significant attention. However, achieving uniform size distribution of particles together with controlled shape and nanostructure has not been achieved. Here, we introduce versatile system for producing monodisperse BCP particles with controlled size, shape and morphology. Polystyrene-*b*-polybutadiene (PS-*b*-PB) self-assembled to either onion-like or striped ellipsoid particle, where final structure is governed by amount of adsorbed sodium dodecyl sulfate (SDS) surfactant at the particle/surrounding interface. Further control of molecular weight and particle size enabled fine-tuning of aspect ratio of ellipsoid particle. Underlying physics of free energy for morphology formation and entropic penalty associated with bending BCP chains strongly affects particle structure and specification.

**1:27PM F42.00012 Shape-designed single-polymer micelles: a proof-of-concept simulation<sup>1</sup>**, BRIAN MOTHS, THOMAS A. WITTEN, University of Chicago — Much effort has been directed towards self-assembling nanostructures. Strong, local interactions between specific building blocks often determine these structures (e.g., globular proteins). We seek to produce designed structures that are instead determined by collective effects of weak interactions (e.g., surfactant self-assembly). Such structures may reversibly change conformation or disassemble in response to changing solvent conditions, and, being soft, have potential to adapt to fluctuating or unknown application-imposed shape requirements. Concretely, we aim to realize such a structure in the form of a single polymer micelle—an amphiphilic polymer exhibiting a condensed, phase-segregated conformation when immersed in solvent. Connecting all amphiphiles into a single chain provides geometric constraints controlling the surface curvature profile, thus dictating a non-trivial shape. We present 2D Monte Carlo simulation results demonstrating the feasibility of such soft, shape-designed micelles. Preliminary results demonstrate a stable concave “dimple” in a micelle composed of a single A-B multiblock linear copolymer. We discuss both current limitations on shape robustness and effects of block asymmetry, block molecular weights and overall chain length on micelle shape.

<sup>1</sup>This work was supported in part by the National Science Foundation’s MRSEC Program under Award Number DMR-1420709

**1:39PM F42.00013 Mechanism of polymer nanoparticle formation by nanoprecipitation**, CHEN ZHAO, TINGTING LI, EDWARD VAN KEUREN, Georgetown Univ — Nanoprecipitation method is a simple and convenient way to produce nanoparticles from polymers in solution. The control of nanoparticle size and size distribution plays a pivotal role in the use of nanoprecipitation for drug delivery. We investigated various factors and initial conditions that affect the particle size, such as the initial solute concentration, solvent/non-solvent ratio and the molecular weight of the polymer samples. The results shed light on the mechanisms of particle formation and phase separation which occurs in nanoprecipitation. Spinodal decomposition, which takes place as a result of a quench to a sufficiently high supersaturation, is believed to be the main mechanism that governs the phase separation. In addition, the glass transition of the polymers will also be a key factor that contributes to the thermodynamics and kinetics of the phase separation and the resulting particle size and morphology.

**1:51PM F42.00014 Assembly and Structural Evolution of Micelleplexes**, YAMING JIANG, DUSTIN SPROUSE, JENNIFER LAASER, THERESA REINEKE, TIMOTHY LODGE, University of Minnesota-Twin Cities — Cationic micelles complex with DNA to form micelleplexes, which are attractive vehicles for gene delivery. We investigate the formation and structural evolution of micelleplexes in buffered solutions. The micelles are composed of poly((2-dimethylamino)ethyl methacrylate)-block-poly(*n*-butyl methacrylate). The formation of the micelleplexes is monitored via turbidimetric titration. With DNA oligomers, solutions of the complexes are homogeneous until near the charge neutral point, at which point the complexes precipitate. With plasmid DNA, more than a stoichiometric amount of DNA is needed to reach the inhomogeneous region, which suggests that binding is partially inhibited. This inhibition is not fully relieved when the plasmid DNA is linearized, suggesting that the stiffness of the DNA is the main source of the inhibition. With micelles in excess, the micelleplexes formed at low ionic strength exhibit bimodal size distributions and remain stable in solution. With DNA in excess, soluble micelleplexes aggregate over time and precipitate. We explain the structural evolution of the micelleplexes as an interplay between kinetic trapping and thermodynamic equilibrium, and compare the results for DNA with those for a flexible polyanion.

**2:03PM F42.00015 Soft Patchy Particles of Block Copolymers from Interface-Engineered Emulsions**, YONGJOO KM, KANG HEE KU, Korea Adv Inst of Sci & Tech, GI-RA YI, Sungkyunkwan University, YEON SIK JUNG, BUMJOON J. KIM, Korea Adv Inst of Sci & Tech — We report a simple and practical method for creating colloidal patchy particles with a variety of three-dimensional shapes via the evaporation-induced assembly of polystyrene-*b*-poly(4-vinylpyridine) (PS-*b*-P4VP) block copolymer (BCP) in an oil-in-water emulsion. Depending on the particle volume, a series of patchy particles in the shapes of snowmen, dumbbells, triangles, tetrahedra, and raspberry can be prepared, which are then precisely tuned by modulating the interfacial interaction at the particle/water interface using a mixture of two different surfactants. In this talk, theoretic calculations of free energy of the system based on the strong segregation theory (SST) will be mainly discussed to support the experimental observation of various soft patchy particles and identified the underlying principles of their formation with tunable 3D structures.

**Tuesday, March 15, 2016 11:15AM - 1:51PM —**  
**Session F43 GSNP GSOF: Jamming and the Glass Transition II** 346 - Paolo Sibani

**11:15AM F43.00001 Jamming vs Caging in Three Dimensional Jamming Percolation** , YAIR SHOKEF, NIMROD SEGALL, EIAL TEOMY, Tel Aviv University — We study a three-dimensional kinetically-constrained lattice-gas model [1], in which the ability of a particle to move depends on the occupation of neighboring sites in an orientational manner. The kinetic rules are constructed such that chains of permanently-frozen particles reach an infinite length at the critical density of directed percolation. Thus at this critical density the system undergoes a jamming transition, above which there is a finite fraction of jammed particles. We demonstrate that the three-dimensional mesh-like structure of the one-dimensional jammed chains enables the free particles to propagate through the holes in this mesh. This diffusive motion is terminated at a second critical density above which all particles are caged. The largest and second largest clusters of dynamically-connected sites exhibit singularities at both densities. Thus our model assists in separating between the two distinct phenomena of jamming and caging. [1] A. Ghosh, E. Teomy and Y. Shokef, Europhys. Lett. 106, 16003 (2014).

**11:27AM F43.00002 Relation between structure of blocked clusters and relaxation dynamics in kinetically constrained models** , EIAL TEOMY, YAIR SHOKEF, Tel Aviv University — In a liquid all the particles are mobile, while in a glass only some of them are mobile at any given time. Although overall the structure is amorphous in both cases, the difference is that in glasses there are local structures that inhibit the movement of particles inside them. We investigate the size of these structures by considering the minimum number of particles that need to move before a specific particle can move. In kinetically-constrained models this structural property, the mean culling time, is easy to find by iteratively culling mobile particles from a snapshot of the system. We use the Kob-Andersen, Fredrickson-Andersen, and the spiral models, which are either lattice gases in which a particle may hop to a nearby site if its local environment satisfies some constraint, or Ising-like models in which a spin, representing regions of high and low mobility, can flip if its environment satisfies some constraint. We compare these structural properties to the dynamics in these models by measuring the persistence time, which is the average time it takes a particle to move for the first time. We find an algebraic relation between the mean culling time and the persistence time, with a model-dependent exponent.

**11:39AM F43.00003 Growing Hyperuniformity of Bidisperse Soft Discs on Approach to Jamming** , ANTHONY CHIECO, CARL GOODRICH, ANDREA LIU, DOUGLAS DURIAN, University of Pennsylvania — We study the development of hyperuniformity in simulated systems of bidisperse soft discs as the packing fraction  $\phi$  is increased from below to above jamming, using the real-space spectrum of hyperuniformity disorder lengths,  $h(L)$ . For a set of randomly placed  $L \times L$  measuring windows,  $h(L)$  specifies the distance from the window boundaries over which fluctuations are important; for liquid-like systems,  $h(L)$  scales like  $L$ ; but for strongly hyperuniform systems,  $h(L) = h_e$  is constant. We use two preparation protocols, one rapidly-quenches a system by immediately minimizing particle overlap and the other allows particles to move under low temperature thermal driving. Above jamming, both systems become strongly hyperuniform as signified by  $h(L) \rightarrow R_{small}/5$  at large  $L$ . Below jamming, but near the transition, the behavior of  $h(L)$  at small  $L$  is just like above jamming. But for larger  $L$ ,  $h(L)$  breaks away and grows in a protocol-dependent fashion. In general, thermal systems are more uniform than quenched systems, as signified by smaller hyperuniformity disorder lengths. And the development of hyperuniformity happens simultaneously with the onset of jamming.

**11:51AM F43.00004 Crossover from facilitation to hopping in a colloidal glass-former** , SHREYAS GOKHALE, Indian Inst of Science, RAJESH GANAPATHY, K HIMA NAGAMANASA<sup>1</sup>, Jawaharlal Nehru Centre for Advanced Scientific Research, A K SOOD, Indian Inst of Science — Despite extensive research, it remains to be established whether glass formation is a fundamentally thermodynamic or dynamic phenomenon. In particular, it is not yet clear whether structural relaxation is dominated by the correlated motion of localized excitations, as postulated by the dynamical facilitation (DF) theory, or by the collective hopping of groups of particles, as envisioned by various thermodynamic approaches. Here, by analyzing data from experiments on dense colloidal suspensions, we critically compare the role of facilitation and hopping in governing structural relaxation in glass-forming liquids. In particular, we investigate the spatial organization of localized excitations within clusters of most mobile particles as well as their partitioning into shell-like and core-like regions. Our study reveals the existence of a dynamical crossover from a facilitation dominated regime at low area fractions to one dominated by collective hopping close to the glass transition. Our findings strongly suggest that glass formation is thermodynamic in origin.

<sup>1</sup>Currently at the Center for Soft and Living Matter, UNIST, Republic of Korea

**12:03PM F43.00005 Measuring Temperaturelike State Variables in History-Dependent Jammed Granular Systems** , EPHRAIM BILILIGN, KAREN DANIELS, North Carolina State University — Granular systems are athermal, thus a complete statistical mechanics framework must be based on a set of macroscopic state variables which excludes temperature. One leading theory incorporates a stress-based ensemble, and predicts a Boltzmann-like distribution of the force-moment tensor with respect to the conjugate, temperature-like variable, angoricity. We experimentally test this theory on a static, bidisperse, two-dimensional packing of discs. Basal friction is eliminated by floating the discs on a sub-fluidizing upflow of air, and the packings are subjected to either uniaxial compression or simple shear. We simultaneously measure the contact forces acting on each disc using photoelasticity. These measurements are repeated over many configurations of discs by dilating and rearranging the system, and the angoricity is computed as a function of the confining pressure. In particular, we test the predicted linear relationship between angoricity and pressure. Comparison to prior results and numerical simulations also suggests a history-dependent angoricity, an undesirable feature in the proposed state variable.

**12:15PM F43.00006 Universal, non-Debye scaling in the density of states for jammed amorphous systems** , ERIC CORWIN, Univ of Oregon, ALEXIS PONCET, cole Normale Suprieure — The presence of anomalous modes in amorphous packings close to jamming is well known: the density of states of packings close to jamming goes to a constant at low frequency. But the scaling at higher densities is still unclear. Naively, one might expect to find simple Debye scaling. However, newly available theories for systems thought to belong to the same universality class as jamming predict anomalous, non-Debye scaling, but are only strictly applicable to the infinite dimensional case. Do these (mean-field) predictions bring some information about finite-dimensional systems? Here we study packings of soft spheres in dimensions 3 through 7 and show that indeed, far from jamming, we find a universal non-Debye scaling in the density of states, consistent with the mean-field predictions.

**12:27PM F43.00007 Nonconvex optimization and jamming**<sup>1</sup> , YOAV KALLUS, Santa Fe Institute — Recent work on the jamming transition of particles with short-range interactions has drawn connections with models based on minimization problems with linear inequality constraints and a concave objective. These properties reduce the continuous optimization problem to a discrete search among the corners of the feasible polytope. I will discuss results from simulations of models with and without quenched disorder, exhibiting critical power laws, scaling collapse, and protocol dependence. These models are also well-suited for study using tools of algebraic topology, which I will discuss briefly.

<sup>1</sup>Supported by an Omidyar Fellowship at the Santa Fe Institute

### 12:39PM F43.00008 Configurational entropy of glass-forming systems from graph isomorphism

, YUXING ZHOU, SCOTT MILNER, The Pennsylvania State University — The configurational entropy plays a central role in the thermodynamic scenarios of glass transition, such as Adam-Gibbs theory and random first-order transition theory. By definition, the configurational entropy  $S_c$  is the difference between the entropy of liquid and the vibrational entropy with structural rearrangement restricted, both of which can be obtained by means of thermodynamic integration. On the other hand,  $S_c$  is essentially a measure of the number of basins in the energy landscape, and therefore it can also be estimated by explicitly enumerating inherent structures. To this end, we first coarse-grain the vibrational motions by mapping configurations to Voronoi diagrams and then categorize them using canonical labelling. The Voronoi graph entropy is calculated as  $S_G/k_B = -\sum p_i \log(p_i)$ , where  $p_i$  is the probability of finding distinct graph  $i$ . We find for an  $n$ -particle subsystem of glass-forming hard-disk/sphere fluids,  $S_G(n)$  scales linearly with  $n$ , and  $S_c$  can be estimated from the slope.

### 12:51PM F43.00009 Suppression of the threshold of a granular solid by mechanical fluctuations

, AXELLE AMON, Université Rennes 1, ADELIN PONS, THIERRY DARNIGE, PMMH, ESPCI, Université Paris 6 & 7, JÉRÔME CRASSOUS, Université Rennes 1, ERIC CLÉMENT, PMMH, ESPCI, Université Paris 6 & 7 — For a granular material, when the ratio between the shear stress and the confining pressure is smaller than the Mohr-Coulomb threshold, the system can be considered as a solid. Nevertheless, a long-term creep is observed in this solid phase in stress imposed experiments. We present recent experimental and theoretical results demonstrating that the superposition of tiny modulations to the imposed stress are sufficient to change the response of the system from a logarithmic creep to a linear one even deep in the jammed phase. We give a theoretical interpretation of this fluidization without invoking an effective temperature due to a mechanical noise. We interpret our observations as a secular effect, i.e. a ratcheting process which is revealed only on very long times. We show that a local fluidity model is sufficient to interpret fully our experimental observations.

### 1:03PM F43.00010 Fast magnetic resonance imaging of the internal impact response of dense granular suspensions

, CHRISTOPH MLLER, Laboratory for Energy Science and Engineering, ETH Zurich, ALEXANDER PENN, Laboratory for Energy Science and Engineering, ETH Zurich and Institute for Biomedical Engineering, University and ETH Zurich, KLAAS P. PRUESSMANN, Institute for Biomedical Engineering, University and ETH Zurich — Dense granular suspensions exhibit a number of intriguing properties such as discontinuous shear-thickening and the formation of dynamic jamming fronts when impacted by a solid. Probing non-intrusively these phenomena experimentally in full three-dimensional systems is, however, highly challenging as suspensions are commonly opaque and thus, not accessible optically. Here we report the development and implementation of a fast magnetic resonance imaging (MRI) methodology allowing us to image the internal dynamics of dense granular suspensions at high temporal resolutions. An important facet of this work is the implementation of parallel MRI using tailored multi-channel receive hardware and the optimization of magnetic properties (susceptibility and NMR relaxivity) of the liquid phase. These two improvements enable us to utilize fast single-shot pulse sequences while yielding sufficient signal intensity at temporal resolutions of less than 50 ms. Furthermore, using motion-sensitive MR pulse sequences we are able to image bulk motion within the system and the response of dense granular suspensions to fast impacts.

### 1:15PM F43.00011 Local fluctuations in the relaxation rate in a glassy system

, RAJIB PANDIT, Ohio University, ELIJAH FLENNER, Colorado State University, HORACIO E. CASTILLO, Ohio University — We numerically study the equilibrium dynamics of a glass-forming binary hard-sphere mixture, for different packing fractions. We extract a correlator that probes the integrated fluctuations in the local relaxation rate in the system. We find that the strength of this correlator at  $t = \tau_\alpha$  (the  $\alpha$ -relaxation time) grows with packing fraction approximately as a power of  $\tau_\alpha$ . We also find that for a fixed packing fraction, the correlator grows as a power of time, for very long times, with an exponent that depends on the packing fraction. This exponent probes the time correlations of the relaxation rate fluctuations. We find that the exponent is around 3 for very low packing fractions, and gradually decreases to a value below 2 as the glass transition is approached. We conclude that a description of fluctuations in terms of local relaxation rates is only applicable at long times and for packing fractions close to the glass transition.

### 1:27PM F43.00012 Finite temperature mechanical instability in disordered lattices

, LEYOU ZHANG, XIAOMING MAO, Univ of Michigan - Ann Arbor — Mechanical instability takes different forms in various ordered and disordered systems, and little is known about how thermal fluctuations affect different classes of mechanical instabilities. We develop an analytic theory involving renormalization of rigidity and coherent potential approximation that can be used to understand finite-temperature mechanical stabilities in various disordered systems. We used this theory to study two disordered lattices: randomly diluted triangular lattice and randomly braced square lattice. These two lattices belong to two different universality classes as they approach mechanical instability at  $T = 0$ . We show that thermal fluctuations stabilize both lattices. In particular, the triangular lattice displays a critical regime in which the shear modulus scales as  $G \sim T^{1/2}$ , whereas the square lattice shows  $G \sim T^{2/3}$ . We discuss generic scaling laws for finite  $T$  mechanical instabilities and relate to experimental systems including jamming and glass transitions.

### 1:39PM F43.00013 Scaling theory for the jamming transition

, CARL GOODRICH, Harvard University, ANDREA LIU, University of Pennsylvania, JAMES SETHNA, Cornell University — We propose a scaling ansatz for the elastic energy of a system near the critical jamming transition in terms of three relevant fields: the compressive strain  $\Delta\phi$  relative to the critical jammed state, the shear strain  $\epsilon$ , and the inverse system size  $1/N$ . We also use  $\Delta Z$ , the number of contacts relative to the minimum required at jamming, as an underlying control parameter. Our scaling theory predicts new exponents, exponent equalities and scaling collapses for energy, pressure and shear stress that we verify with numerical simulations of jammed packings of soft spheres. It also yields new insight into why the shear and bulk moduli exhibit different scalings; the difference arises because the shear stress vanishes as  $1/\sqrt{N}$  while the pressure approaches a constant in the thermodynamic limit. The success of the scaling ansatz implies that the jamming transition exhibits an emergent scale invariance, and that it should be possible to develop a renormalization-group theory for jamming.

## Tuesday, March 15, 2016 11:15AM - 2:15PM –

Session F44 GQI: Gravity and Quantum Information 347 - Caslav Brukner, IQOQI, Austrian Academy of Sciences; Faculty of Physics, University of Vienna

### 11:15AM F44.00001 Constraining Dark Energy in Table-Top Quantum Experiments

, HOLGER MUELLER, UC Berkeley — If dark energy is a light scalar field, it might interact with normal matter. The interactions, however, are suppressed in the leading models, which are thus compatible with current cosmological observations as well as solar-system and laboratory studies. Such suppression typically relies on the scalar's interaction with macroscopic amounts of ordinary matter but can be bypassed by studying the interaction with individual particles.<sup>1</sup> Using an atom interferometer, we have placed tight constraints on so-called chameleon models, ruling out interaction parameters smaller than  $2.3 \times 10^{-5}$ , while  $M \sim 1$  or larger would lead to conflict with macroscopic experiments.<sup>2</sup> In order to close this gap, we have already increased the sensitivity hundredfold and are expecting a new constraint soon. Purpose-built experiments in the lab or on the international space station will completely close the gap and rule out chameleons and other theories such as symmetrons or  $f(R)$  gravity.

<sup>1</sup>C. Burrage, E. J. Copeland, E. A. Hinds, Probing dark energy with atom interferometry. J. Cosmol. Astropart. Phys. **2015**, 042 (2015).

<sup>2</sup>P. Hamilton, M. Jaffe, P. Haslinger, Q. Simmons, H. Müller, and J. Khoury, Atom-interferometry constraints on dark energy. Science **349**, 849 (2015).

**11:51AM F44.00002 Gravity and Quantum Mechanics<sup>1</sup>** , MILES BLENOWE, Dept. of Physics and Astronomy, Dartmouth College, Hanover NH 03755 — The emergence of the macroscopic classical world from the microscopic quantum world is commonly understood to be a consequence of the fact that any given quantum system is open, unavoidably interacting with unobserved environmental degrees of freedom that will cause initial quantum superposition states of the system to decohere, resulting in classical mixtures of either-or alternatives. A fundamental question concerns how large a macroscopic object can be placed in a manifest quantum state, such as a center of mass quantum superposition state, under conditions where the effects of the interacting environmental degrees of freedom are reduced (i.e. in ultrahigh vacuum and at ultralow temperatures). Recent experiments have in fact demonstrated manifest quantum behavior in nano-to-micron-scale mechanical systems. Gravity has been invoked in various ways as playing a possible fundamental role in enforcing classicality of matter systems beyond a certain scale. Adopting the viewpoint that the standard perturbative quantization of general relativity provides an effective description of quantum gravity that is valid at ordinary energies, we show that it is possible to describe quantitatively how gravity as an environment can induce the decoherence of matter superposition states. The justification for such an approach follows from the fact that we are considering laboratory scale systems, where the matter is localized to regions of small curvature. As with other low energy effects, such as the quantum gravity correction to the Newtonian potential between two ordinary masses, it should be possible to quantitatively evaluate gravitationally induced decoherence rates by employing standard perturbative quantum gravity as an effective field theory; whatever the final form the eventual correct quantum theory of gravity takes, it must converge in its predictions with the effective field theory description at low energies.

<sup>1</sup>Research supported by the National Science Foundation (NSF) and the Foundational Questions Institute (FQXi).

**12:27PM F44.00003 Bidirectional holographic codes and sub-AdS locality<sup>1</sup>** , ZHAO YANG, PATRICK HAYDEN, XIAOLIANG QI, Stanford Univ — Tensor networks implementing quantum error correcting codes have recently been used as toy models of the holographic duality which explicitly realize some of the more puzzling features of the AdS/CFT correspondence. These models reproduce the Ryu-Takayanagi entropy formula for boundary intervals, and allow bulk operators to be mapped to the boundary in a redundant fashion. These exactly solvable, explicit models have provided valuable insight but nonetheless suffer from many deficiencies, some of which we attempt to address in this talk. We propose a new class of tensor network models that subsume the earlier advances and, in addition, incorporate additional features of holographic duality, including: (1) a holographic interpretation of all boundary states, not just those in a "code" subspace, (2) a set of bulk states playing the role of "classical geometries" which reproduce the Ryu-Takayanagi formula for boundary intervals, (3) a bulk gauge symmetry analogous to diffeomorphism invariance in gravitational theories, (4) emergent bulk locality for sufficiently sparse excitations, and the ability to describe geometry at sub-AdS resolutions or even flat space.

<sup>1</sup>David and Lucile Packard Foundation

**12:39PM F44.00004 An extension to Galilean relativity gives rise to quantum mechanics framework** , SIMON BERKOVICH<sup>1</sup>, The George Washington University — The presented scheme for quantum mechanics appeared from considering Cellular Automaton Universe in view of the hidden energy associated with the property of inertia [1]. Galilean relativity states that all inertial frames are equivalent. Our consideration reveals one seemingly small exception - the original frame of reference for the material formations of the Cellular Automaton infrastructure is not isotropic. This frame of reference has a distinctive direction as long as elementary particles of matter are generated by cellular automaton relocations. As a result, Cellular Automaton Universe basically complying with the laws of macrophysics for bulk bodies, could exhibit peculiar characteristics for microphysics. Why the states of microobjects are described by complex numbers is obscure. The observables are presented by real numbers through corresponding macro manipulations. In the inertial frame with unidirectional anisotropy isolated particles are characterized by two numbers; magnitude of their velocity and inclination angle to motion direction. So, these quantum states are mapped to a complex Hilbert space with zero vector representing bulk bodies. The effect of spin may be associated with the sign of the inclination angle trending separations for Stern-Gerlach output and Pauli Principle. [1]Simon Berkovich, Law of inertia and the primal energy in the cellular automaton universe , Journal of Energy Challenges and Mechanics, vol.2(2015), issue 2, pp. 62-67

<sup>1</sup>Emeritus

**12:51PM F44.00005 Asymptotically Limitless Quantum Energy Teleportation via Qudit Probes<sup>1</sup>** , GUILLAUME VERDON-AKZAM, Institute for Quantum Computing - University of Waterloo, EDUARDO MARTIN-MARTINEZ, Institute for Quantum Computing - Perimeter Institute - University of Waterloo, ACHIM KEMPF, Perimeter Institute - Institute for Quantum Computing - University of Waterloo — We propose a modified Quantum Energy Teleportation (QET) scheme that uses arbitrary-dimensional qudit probes and polynomially localized Hamiltonians. We find that with an appropriate scaling of parameters, the teleported energy scales with the teleportation distance more favourably than the nonlocal tails of the Hamiltonians. We show that by allowing the exchange of arbitrary amounts of information between agents and in a suitable limit, an arbitrarily large amount of energy can be teleported through a massless quantum field.

<sup>1</sup>arXiv:1510.03751 - E.M-M and AK acknowledge funding from the NSERC Discovery program.

**1:03PM F44.00006 Relativistic Quantum Communication and the Structure of Spacetime** , EDUARDO MARTIN-MARTINEZ, University of Waterloo and Perimeter Institute — We study the transmission of information and correlations through quantum fields in cosmological backgrounds. With this aim, we make use of quantum information tools to quantify the classical and quantum correlations induced by a quantum massless scalar field in two particle detectors, one located in the early universe (Alice's) and the other located at a later time (Bob's). In particular, we focus on two phenomena: a) the consequences on the transmission of information of the violations of the strong Huygens principle for quantum fields, and b) the analysis of the field vacuum correlations via correlation harvesting from Alice to Bob. We will study a standard cosmological model first and then assess whether these results also hold if we use other than the general relativistic dynamics. As a particular example, we will study the transmission of information through the Big Bounce, that replaces the Big Bang, in the effective dynamics of Loop Quantum Cosmology. We show that much more information reaches us through timelike channels (not mediated by real photons) than it is carried by rays of light, which are usually regarded as the only carriers of information.

**1:15PM F44.00007 Einstein's Equivalence Principle and Universal Decoherence in Massive Composite Quantum Systems** , BELINDA PANG, YANBEI CHEN, Caltech — We demonstrate that in matter wave interferometry, the presence of a uniform gravitational field acting on massive particles with internal degrees of freedom will lead to dephasing and a loss of visibility in the interference pattern, as also shown by previous authors. However, unlike the previous authors, we argue that this is not a universal decoherence mechanism in the sense that any quantum information is lost, and furthermore, that the quantum interference is recoverable. This is a key distinction, because irreversible effects such as decoherence on a quantum system due to uniform gravity implies a violation of Einstein's Equivalence Principle (EEP) in the quantum regime. We show that the dephasing result can be recovered by considering an accelerating observer measuring a freely propagating system, and can be simply understood in terms of the difference in the internal state dependent time of arrival of particles to the screen. One can contrive detection schemes that adjust the path lengths of particles to compensate for this difference and recover the full visibility, while coupling to no additional degrees of freedom. Therefore, the dephasing is an observer dependent effect. EEP is not violated, and uniform gravity is not a mechanism for universal decoherence.

**1:27PM F44.00008 Complete Sets of Solutions in Quantum Mechanics and their Connection with Gravity**, RAFAEL SIERRA, Southern Methodist University — In typical non-relativistic quantum mechanical theory, solutions which are not normalizable are thrown away on the basis of being non-physical. The author does not contend that these solutions exist or are physically reasonable, but, these solutions do introduce interesting physics that can serve to connect the force of gravity with the laws of thermodynamics in a shockingly intimate way. The author will discuss the necessary extensions to the formalism of Schrodinger in order to better deal with and make sense of these solutions. In particular, some time will be devoted to the notion of entropy in systems involving these solutions. For particles sufficiently spaced-out, the second law of thermodynamics will yield dynamics that resemble classical expectations for gravity. Ultimately, gravity will be presented as a force necessary for the preservation of the second law of thermodynamics. Gravity and statistical mechanics will become connected at the quantum domain, provided the quantum domain is enlarged to include wave functions that are generally considered unreasonable.

**1:39PM F44.00009 Geodesics and Acceleration in Influence Theory**, JAMES WALSH, KEVIN KNUTH, University at Albany (SUNY) — Influence theory is concerned with a foundational approach where it is assumed that particles influence one another in a discrete one-to-one fashion. This results in a partially ordered set of influence events, called the influence network, where particles are represented by totally ordered chains of events. Information physics considers physical laws to result from consistent quantification of physical phenomena. Knuth and Bahreyni (2014) demonstrated that the mathematics of spacetime emerges from consistent quantification of influence events by embedded coordinated observers. Knuth (2014) showed that in 1+1 dimensions observer-based predictions about a free (uninfluenced) particle result in the Dirac equation. Here, we show that when a particle in 1+1 dimensions is influenced, it is uniquely and consistently described in terms of relativistic acceleration for constant rate of influence and in general obeys equations of the form of the geodesic equations of general relativity. This suggests that Influence Theory can also account for forces (like gravity), which give rise to well-known relativistic effects such as time dilation.

**1:51PM F44.00010 Gravity and Quantum Theory Unified**, GARY WARREN, None — Historic arguments against Aether theories disappear if the Aether is a 4D compressible hyperfluid in which each particle is our observation of a hypervortex, formed in and comprised of hyperfluid. Such Aether resolves “spooky action at a distance” which allows unification of gravity and quantum theory. Light is transverse waves in free space (away from hypervortices) in the hyperfluid. Their detailed behavior is why we observe a curved 3D Lorentz universe – a slice through the 4D hypervortex. Meanwhile, detailed hypervortex behavior, including faster-than-light longitudinal waves in and along hypervortices, explain quantum phenomena. A particular Lagrangian for such a hyperfluid regenerates Maxwell’s equations, plus an equation for gravity, and an equation for electric charge. Couplings among these equations generate a discrete spectrum of hypervortex solutions that we observe as a spectrum of particles. Gravity results from gradients in the fluid density near vortices. Observed clock rates depend on fluid density, and vortex motion thus intertwining gravity, clock rates and quantum phenomena. Implied experiments will be discussed.

**2:03PM F44.00011 Geometry and dynamics of emergent spacetime from entanglement spectrum**, HIROAKI MATSUEDA, Sendai National College of Technology — We examine geometry and dynamics of classical spacetime derived from entanglement spectrum for 1D lattice free fermions. The spacetime is a kind of canonical parameter space defined by the Fisher information metric. The spectrum has exponential family form like thermal probability. Then, the metric is given by the second derivative of the Hessian potential that can be identified with the entanglement entropy. We emphasize that the canonical parameters are nontrivial functions of partial system size by the truncation, filling fraction of fermions, and time. We find that the emergent geometry becomes anti-de Sitter spacetime with imaginary time, and a radial axis as well as spacetime coordinates appears spontaneously. We also find that the information of the UV limit of the original fermions lives in the boundary of the anti-de Sitter spacetime. These findings strongly suggest that the Hessian potential for free fermions has enough geometrical meaning associated with gauge-gravity correspondence.

**Tuesday, March 15, 2016 11:15AM - 2:03PM –**  
**Session F45 GQI: Adiabatic Quantum Computation and Quantum Annealing: Energy Landscapes, Speedup and Embedding** 348 - Daniel Lidar, Univ. of Southern California

**11:15AM F45.00001 Quantum Annealing at Google: Recent Learnings and Next Steps**, HARTMUT NEVEN, Google — Recently we studied optimization problems with rugged energy landscapes that featured tall and narrow energy barriers separating energy minima. We found that for a crafted problem of this kind, called the weak-strong cluster glass, the D-Wave 2X processor achieves a significant advantage in runtime scaling relative to Simulated Annealing (SA). For instances with 945 variables this results in a time-to-99%-success-probability  $10^9$  times shorter than SA running on a single core. When comparing to the Quantum Monte Carlo (QMC) algorithm we only observe a pre-factor advantage but the pre-factor is large, about  $10^6$  for an implementation on a single core. We should note that we expect QMC to scale like physical quantum annealing only for problems for which the tunneling transitions can be described by a dominant purely imaginary instanton. We expect these findings to carry over to other problems with similar energy landscapes. A class of practical interest are k-th order binary optimization problems. We studied 4-spin problems using numerical methods and found again that simulated quantum annealing has better scaling than SA. This leaves us with a final step to achieve a wall clock speedup of practical relevance. We need to develop an annealing architecture that supports embedding of k-th order binary optimization in a manner that preserves the runtime advantage seen prior to embedding.

**11:51AM F45.00002 Ground States of Random Spanning Trees on a D-Wave 2X<sup>1</sup>**, J.S. HALL, Mississippi State University, L. HOBL, RWTH Aachen University, Julich Supercomputing Centre, M.A. NOVOTNY, Mississippi State University, KRISTEL MICHIELSEN, Julich Supercomputing Centre, RWTH Aachen University — The performances of two D-Wave 2 machines (476 and 496 qubits) and of a 1097-qubit D-Wave 2X were investigated. Each chip has a Chimera interaction graph  $\mathcal{G}$ . Problem input consists of values for the fields  $h_j$  and for the two-qubit interactions  $J_{i,j}$  of an Ising spin-glass problem formulated on  $\mathcal{G}$ . Output is returned in terms of a spin configuration  $\{s_j\}$ , with  $s_j = \pm 1$ . We generated random spanning trees (RSTs) uniformly distributed over all spanning trees of  $\mathcal{G}$ . On the 476-qubit D-Wave 2, RSTs were generated on the full chip with  $J_{i,j} = -1$  and  $h_j = 0$  and solved one thousand times. The distribution of solution energies and the average magnetization of each qubit were determined. On both the 476- and 1097-qubit machines, four identical spanning trees were generated on each quadrant of the chip. The statistical independence of these regions was investigated. In another study, on the D-Wave 2X, one hundred RSTs with random  $J_{i,j} \in \{-1, 1\}$  and  $h_j = 0$  were generated on the full chip. Each RST problem was solved one hundred times and the number of times the ground state energy was found was recorded. This procedure was repeated for square subgraphs, with dimensions ranging from  $7 \times 7$  to  $11 \times 11$ .

<sup>1</sup>Supported in part by NSF grants DGE-0947419 and DMR-1206233. D-Wave time provided by D-Wave Systems and by the USRA Quantum Artificial Intelligence Laboratory Research Opportunity.

**12:03PM F45.00003 Instantons and scaling of the transitions rates in Quantum Monte Carlo simulations of thermally-assisted quantum tunneling in spin systems<sup>1</sup>**, VADIM SMELYANSKIY, Google, ZHANG JIANG, Stinger Ghaffarian Technologies, Inc., SERGIO BOIXO, SERGEI ISSAKOV, Google, GUGLIELMO MAZZOLA, MATTHIAS TROYER, Swiss Federal Institute of Technology in Zurich, HARTMUT NEVEN, Google — We study analytically and numerically the dynamics of the quantum Monte Carlo (QMC) algorithm to simulate thermally-assisted tunneling in mean-field spin models without conservation of total spin. We use Kramers escape rate theory to calculate the scaling of the QMC time with the problem size to simulate the tunneling transitions. We develop path-integral instanton approach in coherent state and Suzuki-Trotter representations to calculate the escape rate and most probable escape path in QMC dynamics. Analytical results are in a good agreement with numerical studies. We identify the class of models where the exponent in the scaling of the QMC time is the same as that in physical tunneling but the pre-factor depends very significantly on the QMC path representation. We propose the classes of problems where QMC can fail to simulate tunneling efficiently.

<sup>1</sup>The work of GM and MT has been supported by the Swiss National Science Foundation through the National Competence Center in Research QSIT and by ODNI, IARPA via MIT Lincoln Laboratory Air Force Contract No. FA8721-05-C-0002.

**12:15PM F45.00004 Validating the solutions of the D-Wave quantum annealers through graph mirroring<sup>1</sup>**, DILINA PERERA, J.S. HALL, M.A. NOVOTNY, Mississippi State University — D-Wave quantum annealers seek to find the ground states of Ising spin glasses. The problem Hamiltonian is formulated as an undirected graph that can be embedded into the devices native disordered Chimera graph structure. However, depending on the complexity of the problem and the specifications of the annealing schedule, the device may not necessarily find the global minimum during a given annealing process. We present a method, which we call answer checking, that enhances the expectation that the solution provided by the device is the true ground state of the problem. The underlying principle is to embed a mirrored graph  $G'$  of the original graph  $G$ , and connect the two graphs via ferromagnetic/antiferromagnetic couplers. This allows one to rule out solutions for the composite graph that do not comply with the underlying mirror symmetry inherent to the true ground state, which in turn, reduces the uncertainty associated with the solutions. Using the 1097 qubit D-Wave 2X, we test this approach by applying it to a range of problems, including random spanning trees and generally allowed graphs  $G$ .

<sup>1</sup>Supported in part by Pacific Northwest National Laboratory. D-Wave time provided by USRA.

**12:27PM F45.00005 Quantum Annealing for Constrained Optimization**, ITAY HEN, FEDERICO SPEDALIERI, Information Sciences institute, USC — Recent advances in quantum technology have led to the development and manufacturing of experimental programmable quantum annealers that could potentially solve certain quadratic unconstrained binary optimization problems faster than their classical analogues. The applicability of such devices for many theoretical and practical optimization problems, which are often constrained, is severely limited by the sparse, rigid layout of the devices' quantum bits. Traditionally, constraints are addressed by the addition of penalty terms to the Hamiltonian of the problem, which in turn requires prohibitively increasing physical resources while also restricting the dynamical range of the interactions. Here we propose a method for encoding constrained optimization problems on quantum annealers that eliminates the need for penalty terms and thereby removes many of the obstacles associated with the implementation of these. We argue the advantages of the proposed technique and illustrate its effectiveness. We then conclude by discussing the experimental feasibility of the suggested method as well as its potential to boost the encodability of other optimization problems.

**12:39PM F45.00006 Embedding parameters for Quantum Annealing**, DAVIDE VENTURELLI, NASA Ames Research Center — Many optimization problems are defined on highly connected graphs and many interesting physical spin-glass systems are featuring long-range interactions. One method to solve for the optimum/ground state is quantum annealing (QA). Most architectures for QA devices, manufactured or proposed, are based on optimizing Hamiltonians having spins connected in a non-complete graph, with nodes with a small maximum degree, compared to the requirements. To overcome this limitation 'embedding' is employed: the native graph is tiled with ferromagnetic chains of spins that now are meant to represent the logical binary variables. While it is known how the strength of the ferromagnetic bonds can ensure that the classical Ising ground state of the embedded system can be univocally mapped to the ground state of the original system, there is very little study on the impact of these parameters on QA. Programmers have taken conservative choices for the parameters and the common practices can be improved. Starting from the physics of connected ferromagnetic Ising chains, we will review several parameter choices and discuss previous and new results obtained on the D-Wave 2X machine, on carefully designed problems that allow to isolate and evaluate the role of connectivity in embedded systems.

**12:51PM F45.00007 Systematic and Deterministic Graph-Minor Embedding of Cartesian Products of Complete Graphs**, ARMAN ZARIBAFIYAN, DOMINIC J.J. MARCHAND, SEYED SAEED CHANGIZ REZAEI, 1QBit — The limited connectivity of current and next-generation quantum annealers motivates the need for efficient graph-minor embedding methods. The overhead of the widely used heuristic techniques is quickly proving to be a significant bottleneck for real-world applications. To alleviate this obstacle, we propose a systematic deterministic embedding method that exploits the structures of both the input graph of the specific combinatorial optimization problem and the quantum annealer. We focus on the specific case of the Cartesian product of two complete graphs, a regular structure that occurs in many problems. We first divide the problem by embedding one of the factors of the Cartesian product in a repeatable unit. The resulting simplified problem consists of placing copies of this unit and connecting them together appropriately. Aside from the obvious speed and efficiency advantages of a systematic deterministic approach, the embeddings produced can be easily scaled for larger processors and show desirable properties with respect to the number of qubits used and the chain length distribution.

**1:03PM F45.00008 Simulating highly nonlocal Hamiltonians with less nonlocal Hamiltonians<sup>1</sup>**, YIGIT SUBASI, CHRISTOPHER JARZYNSKI, University of Maryland at College Park — The need for Hamiltonians with many-body interactions arises in various applications of quantum computing. However, interactions beyond two-body are difficult to realize experimentally. Perturbative gadgets were introduced to obtain arbitrary many-body effective interactions using Hamiltonians with two-body interactions only. Although valid for arbitrary  $k$ -body interactions, their use is limited to small  $k$  because the strength of interaction is  $k$ 'th order in perturbation theory. Here we develop a nonperturbative technique for obtaining effective  $k$ -body interactions using Hamiltonians consisting of at most  $l$ -body interactions with  $l < k$ . This technique works best for Hamiltonians with a few interactions with very large  $k$  and can be used together with perturbative gadgets to embed Hamiltonians of considerable complexity in proper subspaces of two-local Hamiltonians. We describe how our technique can be implemented in a hybrid (gate-based and adiabatic) as well as solely adiabatic quantum computing scheme.

<sup>1</sup>We gratefully acknowledge financial support from the Lockheed Martin Corporation under contract U12001C.

**1:15PM F45.00009 Crushing runtimes in adiabatic quantum computation with Energy Landscape Manipulation (ELM): Application to Quantum Factoring** , NIKE DATTANI, Kyoto University, RICHARD TANBURN, OLIVER LUNT, Oxford University — We introduce two methods for speeding up adiabatic quantum computations by increasing the energy between the ground and first excited states. Our methods are even more general. They can be used to shift a Hamiltonian's density of states away from the ground state, so that fewer states occupy the low-lying energies near the minimum, hence allowing for faster adiabatic passages to find the ground state with less risk of getting caught in an undesired low-lying excited state during the passage. Even more generally, our methods can be used to transform a discrete optimization problem into a new one whose unique minimum still encodes the desired answer, but with the objective function's values forming a different landscape. Aspects of the landscape such as the objective function's range, or the values of certain coefficients, or how many different inputs lead to a given output value, can be decreased \*or\* increased. One of the many examples for which these methods are useful is in finding the ground state of a Hamiltonian using NMR. We apply our methods to an AQC algorithm for integer factorization, and the first method reduces the maximum runtime in our example by up to 754%, and the second method reduces the maximum runtime of another example by up to 250%.

**1:27PM F45.00010 On universal adiabatic quantum computation** , ARI MIZEL, Laboratory for Physical Sciences — We give a careful proof that ground state quantum computation can efficiently simulate universal gate model quantum computation. The proof allows for general gate model quantum computations; no restrictions are required on qubit geometry or on the locality of two-qubit gates. Our lower-bound technique may have more general application.

**1:39PM F45.00011 Quantum Annealing and Many-Body Localization<sup>1</sup>** , NOAH BRAY-ALI, Joint Quantum Institute, University of Maryland, College Park and National Institute of Standards and Technology, Gaithersburg, MD 20899 — The quantum phase transition separating the Ising spin glass from the quantum paramagnet phase in one-dimension is many-body localized. We study quantum annealing across this transition using the recently developed, dynamical strong-disorder renormalization group approach. The probability of successful adiabatic quantum computation of the spin glass ground-state obeys a universal scaling function of system size, anneal rate, and strength of disorder, which we obtain. Measurement of this universal scaling behavior in a quantum annealing device, for example, would be the first direct test of the activated dynamics of a many-body localized quantum phase transition.

<sup>1</sup>Support provided by National Research Council Post-Doctoral Research Associateship

**1:51PM F45.00012 Bifurcation-based adiabatic quantum computation with a nonlinear oscillator network** , HAYATO GOTO, Toshiba Corporation — The dynamics of nonlinear systems qualitatively change depending on their parameters, which is called bifurcation. A quantum-mechanical nonlinear oscillator can yield a quantum superposition of two oscillation states, known as a Schrödinger cat state, via its bifurcation with a slowly varying parameter. Here we propose a quantum computer comprising such quantum nonlinear oscillators, instead of quantum bits, to solve hard combinatorial optimization problems. The nonlinear oscillator network finds optimal solutions via quantum adiabatic evolution, where nonlinear terms are increased slowly, in contrast to conventional adiabatic quantum computation or quantum annealing. To distinguish them, we refer to the present approach as bifurcation-based adiabatic quantum computation. Our numerical simulation results suggest that quantum superposition and quantum fluctuation work effectively to find optimal solutions.

**Tuesday, March 15, 2016 11:15AM - 2:15PM –**

**Session F46 GIMS: Instrumentation III: Scattering, Diffraction, Imaging** 311 - Dennis Mills, Argonne National Laboratory

**11:15AM F46.00001 What is the diffraction limit? From Airy to Abbe using direct numerical integration.** , Y. M. CALM, J. M. MERLO, M. J. BURNS, K. KEMPA, M. J. NAUGHTON<sup>1</sup>, Boston College — The resolution of a conventional optical microscope is sometimes taken from Airy's point spread function (PSF),  $0.61\lambda/NA$ , and sometimes from Abbe,  $\lambda/2NA$ , where  $NA$  is the numerical aperture<sup>2</sup>, however modern fluorescence and near-field optical microscopies achieve spatial resolution far better than either of these limits<sup>3</sup>. There is a new category of 2D metamaterials called planar optical elements (POEs), which have a microscopic thickness ( $< \lambda$ ), macroscopic transverse dimensions ( $> 100\lambda$ ), and are composed of an array of nanostructured light scatterers. POEs are found in a range of micro- and nano-photonics technologies<sup>4</sup>, and will influence the future optical nanoscopy. With this pretext, we shed some light on the 'diffraction limit' by numerically evaluating Kirchhoff's scalar formulae (in their exact form) and identifying the features of highly non-paraxial, 3D PSFs. We show that the Airy and Abbe criteria are connected, and we comment on the design rules for a particular type of POE: the flat lens.

<sup>1</sup>This work is supported by the W. M. Keck Foundation.

<sup>2</sup>J. W. Strutt (Lord Rayleigh), *Phil. Mag.* **8**, 261 (1879)

<sup>3</sup>S. W. Hell, *Science* **316**, 1153 (2007)

<sup>4</sup>A. Kildishev, A. Boltasseva, & V. Shalaev, *Science* **339**, 1289 (2013)

**11:27AM F46.00002 Imaging of Biological Tissues by Visible Light CDI** , DMITRY KARPOV, New Mexico State University, Los Alamos National Laboratory, TOMY DOS SANTOS ROLO, Karlsruhe Institute of Technology, HANNAH RICH, EDWIN FOHTUNG, New Mexico State University, Los Alamos National Laboratory — Recent advances in the use of synchrotron and X-ray free electron laser (XFEL) based coherent diffraction imaging (CDI) with application to material sciences and medicine proved the technique to be efficient in recovering information about the samples encoded in the phase domain. The current state-of-the-art algorithms of reconstruction are transferable to optical frequencies, which makes laser sources a reasonable milestone both in technique development and applications. Here we present first results from table-top laser CDI system for imaging of biological tissues and reconstruction algorithms development and discuss approaches that are complementing the data quality improvement that is applicable to visible light frequencies due to its properties. We demonstrate applicability of the developed methodology to a wide class of soft bio-matter and condensed matter systems. This project is funded by DOD-AFOSR under award No FA9550-14-1-0363 and the LANSCE Professorship at LANL.

**11:39AM F46.00003 A New Experimental Approach in Digital Holographic Microscopy to Insight into Submicron-sized Particle's Scattering Properties.** , NAVA SUBEDI, MATTHEW BERG, Mississippi State University — A novel application of digital holographic microscopy is presented. In this work, a submicron-sized particle is illuminated by two different wavelengths. Then, a special filtering technique is used so that the one wavelength only contributes to form the hologram of the particle in a flow-through, contact-free manner and other to produce the scattering pattern of the illuminating wave in the same plane. Later, an algorithm is applied to separate these two overlapping information. The separated holographic information is used to reconstruct the image of the particle and scattering pattern is used to analyze redistribution of energy on the medium caused by the particle. This information is unique to the particle's shape and size, thus provides the insight into a particle's scattering properties simultaneously with an image of the particle.

**11:51AM F46.00004 HOMER: the Holographic Optical Microscope for Education and Research**<sup>1</sup>, ANALI LUVIANO, Norwich University — Holography was invented in 1948 by Dennis Gabor and has undergone major advancements since the 2000s leading to the development of commercial digital holographic microscopes (DHM). This noninvasive form of microscopy produces a three-dimensional (3-D) digital model of a sample without altering or destroying the sample, thus allowing the same sample to be studied multiple times. HOMER-the Holographic Optical Microscope for Education and Research-produces a 3-D image from a two-dimensional (2-D) interference pattern captured by a camera that is then put through reconstruction software. This 2-D pattern is created when a reference wave interacts with the sample to produce a secondary wave that interferes with the unaltered part of the reference wave. I constructed HOMER to be an efficient, portable in-line DHM using inexpensive material and free reconstruction software. HOMER uses three different-colored LEDs as light sources. I am testing the performance of HOMER with the goal of producing tri-color images of samples. I'm using small basic biological samples to test the effectiveness of HOMER and plan to transition to complex cellular and biological specimens as I pursue my interest in biophysics.

<sup>1</sup>Norwich University

**12:03PM F46.00005 Bayesian Library for the Analysis of Neutron Diffraction Data**<sup>1</sup>, WILLIAM RATCLIFF, NIST - National Institute of Standards & Technology, JOSEPH LESNIEWSKI, Georgetown University, DYLAN QUINTANA, Carnegie Mellon University — During this talk, I will introduce the Bayesian Library for the Analysis of Neutron Diffraction Data. In this library we use of the DREAM [1] algorithm to effectively sample parameter space. This offers several advantages over traditional least squares fitting approaches. It gives us more robust estimates of the fitting parameters, their errors, and their correlations. It also is more stable than least squares methods and provides more confidence in finding a global minimum. I will discuss the algorithm and its application to several materials. I will show applications to both structural and magnetic diffraction patterns. I will present examples of fitting both powder and single crystal data. [1] Jasper A. Vrugt, Cajo J. F. ter Braak, Martyn P. Clark, James M. Hyman, and Bruce A. Robinson, WATER RESOURCES RESEARCH, VOL. 44, W00B09 (2008)

<sup>1</sup>We would like to acknowledge support from the Department of Commerce and the NSF.

**12:15PM F46.00006 On Polarized Neutron Scattering from a Prototypical NMR Spin-Modulated System**, MICHAEL KOTLARCHYK, GEORGE THURSTON, Rochester Institute of Technology — The potential for utilizing the scattering of polarized neutrons from nuclei whose spin has been modulated using nuclear magnetic resonance (NMR) has previously been considered by Buckingham (1). That work broadly considered the overall feasibility and utility of such experiments with a potential aim, for example, of studying slow structural changes such as those that occur in biological macromolecules. Here, from first principles, we present a more in-depth development of the differential scattering cross-sections that would arise in such measurements from a prototypical and simplified model target system containing non-interacting nuclei with non-zero spins. In particular, we investigate the modulation of the polarized scattering cross-sections following the application of RF pulses that impart initial transverse rotations to selected sets of spin-1/2 nuclei. The aim is to lay the foundation for enhancing scattering signals from chosen nuclei, so as to advance knowledge of macromolecular or liquid structure. (1) A.D. Buckingham, Chem. Phys. Letts. 2003(371):517-521

**12:27PM F46.00007 Phase sensitive small angle neutron scattering**, ERIK BROK, Univ. of Maryland, NIST, CHARLES F MAJKRZAK, KATHRYN KRYCKA, NIST — It is a well-known problem that information about the scattered wave is lost in scattering experiments because the measured quantity is the modulus squared of the complex wave function. This "phase problem" leads to ambiguity in determining the physical properties of the scattering sample. Small angle neutron scattering (SANS) is a useful technique for determining the structure of biomolecules, in particular proteins that cannot be crystallized and studied with x-ray crystallography. However, because the biomolecules are usually suspended in a liquid the observed scattering is an average of all possible orientations, making it difficult to obtain three dimensional structural information. In a proposed method polarized SANS and magnetic nanoparticle references attached to the sample molecules is used to obtain phase sensitive structural information and simultaneously circumvent the problem of orientational averaging (Majkrzak et al. J. Appl. Cryst. 47, 2014) If realized and perfected the technique is very promising for unambiguous determination of the three dimensional structure of biomolecules. We demonstrate the principles of our method and show the first experimental data obtained on a simple test system consisting of core shell magnetic nanoparticles.

**12:39PM F46.00008 Current and Future Scientific Investigations at GP-SANS**, LISA DEBEER-SCHMITT, KATHERINE BAILEY, YURI MELNICHENKO, LILIN HE, KEN LITRELL, Oak Ridge National Lab — The general-purpose small-angle neutron scattering beam line, GP-SANS, in operation since 2007, is optimized for investigation of structures with dimensions from 0.5 to 200 nm. Along with high neutron flux, sample environments can easily be integrated into the beam line providing the user a versatile temperature range from 30 mK to 1600 K. In addition, there are two cryomagnets (horizontal 4.5 T and vertical 8 T), pressure cells, stop flow cell, electrochemical cell, load frames and custom-build equipment available to users allowing for significant flexibility in experimental setup. GP-SANS has supported investigation of a diverse array of intriguing scientific topics, including polymer solutions, gel and blends, colloids, micelles, molecular self-assembly and interactions in complex fluids, microemulsions, spin textures and magnetic domains in novel materials, porosity in geological materials and phase separation, grain growth, and orientation in metallurgical alloys.

**12:51PM F46.00009 Ptychographic coherent x-ray surface scattering imaging**<sup>1</sup>, JONG WOO KIM, ZHANG JIANG, TAO SUN, JIN WANG, Argonne National Lab — Lensless x-ray coherent diffraction imaging enables the determination of nano-scaled structures in physical and biological sciences. Several coherent diffractive imaging (CDI) methods have been developed in both transmission and reflection modes such as Bragg CDI, plane-wave CDI, Fresnel CDI, coherent surface scattering imaging (CSSI) and so on. The grazing-incidence coherent surface scattering (CSSI) technique, which is recently developed by T. Sun et al., takes advantage of enhanced x-ray surface scattering and interference near total external reflection, and thereby overcomes some limitations that the transmission mode have. However, the sample size can be investigated is limited by x-ray beam size because the sample is supposed to be isolated. We incorporated ptychographic algorithm with coherent surface scattering imaging to overcome this limitation and make it more useful and applicable. The ptychographic coherent surface scattering imaging technique enables us to measure 2D roughness of the flat surface such as thin film and silicon wafer regardless of the surface area.

<sup>1</sup>LDRD

**1:03PM F46.00010 Design and Characterization of a Novel Near Field Detector for Three Dimensional X-ray Diffraction**, SCOTT ANNETT, LAWRENCE MARGULIES, Univ of Guelph, DARREN DALE, Cornell High Energy Synchrotron Source, Cornell University, STEFAN KYCIA, Univ of Guelph — Three dimensional x-ray diffraction microscopy (3DXRD) is a powerful technique that provides crystallographic and spatial information of a large number of grains in a sample simultaneously. A key component of a 3DXRD experiment is the near field detector which provides high resolution spatial information of the sample. A novel design for a near field detector was developed and characterized. This design, called the Quad Near Field Detector, utilizes four quadrants, each with a dedicated scintillating phosphor and optical microscope. A novel translation stage for focusing the microscopes was developed, tested, and implemented. The near field detector was calibrated and characterized at the Cornell High Energy Synchrotron Source. A flood field correction was developed for the detector to correct for variations in intensity response. Diffraction data of all four quadrants was able to reproduce the crystal orientation of the ruby calibrant. In conclusion, the design and implementation of the Quad Near Field Detector was a success and will be a useful tool for future 3DXRD experiments.

**1:15PM F46.00011 A novel design of coherent and efficient electron beam-splitter based on quantum interaction-free measurement<sup>1</sup>**, YUJIA YANG, CHUNG-SOO KIM, RICHARD HOBBS, AKSHAY AGARWAL, MIT, PIETER KRUIT, TU Delft, KARL K. BERGGREN, MIT — We propose the design and theoretical analysis of a novel coherent and efficient electron beam-splitter utilizing quantum interaction-free measurement. A coherent electron beam-splitter is a necessary component in electron interferometry, electron holography, and recently emerging quantum electron optics. For most of these applications, a coherent, highly efficient, lossless, and two-port beam-splitter is preferred, which currently available electron beam-splitters cannot readily provide. Our electron beam-splitter design combines a weak phase grating with a resonator. Beam-splitting is achieved by passing the electron beam through the weak phase grating multiple times in the resonator. The beam-splitting ratio is controlled by the number of passes through the grating. Higher-order diffractions can be suppressed by inserting an aperture in the diffraction plane. The loss introduced by the aperture can be arbitrarily low according to quantum interaction-free measurement, thus enabling a lossless, two-port electron beam-splitter. Moreover, this novel design is not limited to electron optics, and can be generalized to light, atom, and molecular optics.

<sup>1</sup>This work is funded by Gordon and Betty Moore Foundation.

**1:27PM F46.00012 High-brightness electron beams for ultrafast electron microdiffraction and imaging**, TIANYIN SUN, FARAN ZHOU, KISEOK CHANG, ZHENSHENG TAO, JOE WILLIAMS, CHONG-YU RUAN, Michigan State University, MSU UEM COLLABORATION — Currently the ultrafast electron diffraction has achieved sub-picosecond temporal resolution and atomic resolution. However, direct ultrafast imaging of a nanometer scale specimen through coherent single-particle diffraction has not been achieved largely due to insufficient intensity when tuned to a coherence length that matches the size of the specimen under the projected phase space density. Utilizing a recently implemented high-brightness electron source with flexible optical design, we test the performance of ultrafast electron microdiffraction and coherence imaging. We demonstrate the feasibilities of single-shot microdiffraction on a single micrometer-sized domain in Highly Ordered Pyrolytic Graphite (HOPG) and coherent diffractive imaging of 10 nm scale charge-ordered domain structures in single-crystal complex materials, as validated by the measured brightness at the sample plane. These initial results show that source-limited performance even from a sub-relativistic electron beamline can drastically improve the current performance of ultrafast electron imaging and diffraction.

**1:39PM F46.00013 Imaging Acoustic Phonon Dynamics on the Nanometer-Femtosecond Spatiotemporal Length-Scale with Ultrafast Electron Microscopy**, DAYNE PLEMMONS<sup>1</sup>, DAVID FLANNIGAN<sup>2</sup>, University of Minnesota — Coherent collective lattice oscillations known as phonons dictate a broad range of physical observables in condensed matter and act as primary energy carriers across a wide range of material systems. Despite this omnipresence, analysis of phonon dynamics on their ultrashort native spatiotemporal length scale — that is, the combined nanometer (nm), spatial and femtosecond (fs), temporal length-scales — has largely remained experimentally inaccessible. Here, we employ ultrafast electron microscopy (UEM) to directly image discrete acoustic phonons in real-space with combined nm-fs resolution. By directly probing electron scattering in the image plane (as opposed to the diffraction plane), we retain phase information critical for following the evolution, propagation, scattering, and decay of phonons in relation to morphological features of the specimen (i.e. interfaces, grain boundaries, voids, ripples, etc.). We extract a variety of morphologically-specific quantitative information from the UEM videos including phonon frequencies, phase velocities, and decays times. We expect these direct manifestations of local elastic properties in the vicinity of material defects and interfaces will aid in the understanding and application of phonon-mediated phenomena in nanostructures.

<sup>1</sup>Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN, 55455, USA

<sup>2</sup>Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN, 55455, USA

**1:51PM F46.00014 Dark-Field Scanning Transmission Ion Microscopy *via* Direct Detection of Transmitted Helium Ions with a Multichannel Plate**, TAYLOR WOEHL, RYAN WHITE, ROBERT KELLER, Material Measurement Laboratory, National Institute of Standards and Technology — A multichannel plate was used as an ion sensitive transmission detector in a commercial helium ion microscope for annular dark-field imaging of nanomaterials, i.e. scanning transmission ion microscopy. In contrast to previous transmission helium ion microscopy approaches that used secondary electron conversion holders, our new approach directly detects transmitted helium ions on an annular detector. Monte Carlo simulations are used to predict detector collection angles at which annular dark-field images with atomic number contrast are obtained. We demonstrate atomic number contrast imaging *via* scanning transmission ion imaging of silica-coated gold nanoparticles and magnetite nanoparticles. While the resolution of this transmission technique is limited by beam broadening in the substrate, we image magnetite nanoparticles with high contrast on a relatively thick silicon nitride substrate. We expect this new approach to annular dark-field scanning transmission ion microscopy will open avenues for more quantitative ion imaging techniques, such as direct mass-thickness determination, and advance fundamental understanding of underlying ion scattering mechanisms leading to image formation.

**2:03PM F46.00015 Structure of deuterated liquid n-butanol by neutron diffraction and molecular dynamics simulations**, VIVIANA CRISTIGLIO, Institut Laue Langevin, Grenoble, MIGUEL ANGEL GONZALEZ, GABRIEL JULIO CUELLO, Institut Laue Langevin, Grenoble, FRANCE, CARLOS CABRILLO, CSIS, Instituto de Estructura de la Materia, Madrid, SPAIN, LUIS CARLOS PARDO, ALVARO SILVA-SANTISTEBAN, ETSEIB, Universitat Politècnica de Catalunya, Barcelona, SPAIN — Aliphatic alcohols are the simpler molecular liquids possessing a polar hydroxylic group and a nonpolar alkyl tail. While the structure of the smallest alcohols has been relatively well studied, no much attention has been paid to the temperature dependence of the pre-peak observed before the main diffraction peak. The role of H-bonding in causing this feature and the direct relation between the number of C atoms and their distance were discovered very early, suggesting a liquid picture constituted of straight chains joined by H-bonds with the formation of mesoscopic size clusters. X-rays and neutron diffraction measurements showed that the height of the pre-peak associated with the formation of H-bonds increases with temperature. To explain this counterintuitive effect, a complete diffraction study using two neutron diffractometers D4 and D16 (ILL, Grenoble, France) allowing to cover the range 0.01-23 Å<sup>-1</sup> and exploring a temperature range from 100 K (glassy butanol) to 400 K (moderately supercritical conditions) has been conducted. Molecular Dynamics simulations using the OPLS-AA potential were also carried out as a function of temperature and compared to experiment. Experimental and numerical results of liquid n-butanol and its glassy transition will be presented.

**Tuesday, March 15, 2016 11:15AM - 12:39PM —**  
**Session F47 APS: Sexual and Gender Diversity Issues in Physics C-LGBT Ad Hoc Committee**  
**Report 312 - Monica Plisch, APS**

**11:15AM F47.00001 Report of the APS Ad-Hoc Committee on LGBT Issues Presentation of Findings and Recommendations**, MICHAEL FALK, Johns Hopkins University — In 2014 the Executive Officer of the American Physical Society (APS), Kate Kirby, created an Ad-Hoc Committee on LGBT Issues (C-LGBT) charged with reporting on the obstacles to inclusion of LGBT physicists, a term which for the purpose of this report refers to persons who self-identify as lesbian, gay, bisexual, transgender, queer, questioning, intersex, or asexual, as well as other sexual and gender minorities. The full charge was as follows: “The committee will advise the APS on the current status of LGBT issues in physics, provide recommendations for greater inclusion, and engage physicists in laying the foundation for a more inclusive physics community. ?More specifically, the committee will investigate LGBT representation in physics, assess the educational and professional climate in physics, recommend changes in policies and practices that impact LGBT physicists, and address other issues that affect inclusion.” We will present the findings and recommendations of the C-LGBT final report, and a panel discussion will be held following the presentation to discuss the future of APS efforts toward LGBT inclusion in physics.

**11:51AM F47.00002 Panel Discussion : Report of the APS Ad-Hoc Committee on LGBT Issues**, TIM ATHERTON, Tufts University, RAMON BARTHELEMY, APS/AIP Science & Technology Fellow, American Association for the Advancement of Science, SAVANNAH GARMON, Osaka Prefecture University, KYLE REEVES, University of North Carolina, APS AD-HOC COMMITTEE ON LGBT ISSUES TEAM — Following the presentation of the findings and recommendations of the APS Ad-Hoc Committee on LGBT Issues (C-LGBT) by Committee Chair Michael Falk, a panel discussion will be held featuring several members of the committee. The discussion will focus on how APS can best ensure the recommendations of the committee are carried out in a timely fashion and other ideas on future APS efforts toward LGBT inclusion in physics. Discussion topics will also include the research and other input that shaped the committee's findings and recommendations.

**Tuesday, March 15, 2016 11:15AM - 2:15PM –**  
**Session F48 GQI: Quantum Gates in Superconducting Circuits** 349 - Jerry Chow, IBM T.J. Watson Research Center

**11:15AM F48.00001 High-fidelity resonator-induced phase gate with single-mode squeezing**, SHRUTI PURI, Dpartement de Physique, Universit de Sherbrooke, ALEXANDRE BLAIS, Dpartement de Physique, Universit de Sherbrooke and Canadian Institute for Advanced Research — Despite recent breakthroughs in the demonstration of small-scale quantum error correction, reaching the fidelity required for fault tolerance with entangling gates still remains a challenge. We propose a protocol to increase the fidelity of a two-qubit resonator induced phase gate by using a off-resonant narrowband squeezing drive. For this gate, two superconducting transmon qubits are dispersively coupled to a microwave resonator. By off-resonantly driving the resonator, a controlled-Z gate can be implemented between the qubits [1]. However, photons leaving the resonator reveal the qubit which-path information leading to decoherence. We show that driving the resonator with a field squeezed at an optimal angle and strength erases the qubit which-path information and consequently increases the gate fidelity. We find that, under realistic conditions and modest squeezing power, it is possible to implement a high-fidelity two-qubit controlled-Z gate with short gate times. [1] A. W. Cross and J. M. Gambetta Phys Rev A 91, 032325 (2015).

**11:27AM F48.00002 Characterization of the resonator induced phase gate<sup>1</sup>**, ANTONIO MEZZACAPO, H. PAIK, M. O. SANDBERG, D. T. MCCLURE, B. ABDO, O. E. DIAL, A. W. CROSS, A. D. CORCOLES, S. SHELDON, E. MAGESAN, S. J. SRINIVASAN, J. M. CHOW, J. M. GAMBETTA, IBM T.J. Watson Research Center, Yorktown Heights, NY 10598, USA, D. BOGORIN, B. L. T. PLOURDE, Department of Physics, Syracuse University, Syracuse, New York, 13244 - 1130, USA — The Resonator induced phase (RIP) gate is a versatile microwave gate that can perform collective qubit operations. We characterize the performance of the RIP gate using various drive powers and detunings in a 4-qubit superconducting system. We find a good agreement between the experimental results and the theoretical predictions in the gate rate and minimum gate time. The minimum gate time is limited by residual photons in the bus cavity caused by a non-adiabatic response to the drive. We measure the multi-qubit interactions and analyze how the rates depend on the cavity-qubit coupling and the detuning to the drive and how these interactions can be used for quantum information processing.

<sup>1</sup>We acknowledge support from IARPA under contract W911NF-10-1-0324

**11:39AM F48.00003 Demonstrating Multi-Qubit Operations in a Superconducting 3D circuit QED Architecture<sup>1</sup>**, HANHEE PAIK, M.O. SANDBERG, A. MEZZACAPO, D. T. MCCLURE, B. ABDO, O.E. DIAL, A.W. CROSS, A.D. CORCOLES, S. SHELDON, E. MAGESAN, S.J. SRINIVASAN, J.M. GAMBETTA, J.M. CHOW, IBM T. J. Watson Research Center, Yorktown Heights, NY 10598 USA, D. BOGORIN, B.L.T. PLOURDE, Department of Physics, Syracuse University, Syracuse, NY 13244, USA — We present our recent results on multi-qubit operations in a superconducting 3D circuit QED (cQED) system using a resonator-induced phase (RIP) gate. In our system, four qubits are coupled by a single bus resonator. The RIP gate is implemented by applying a microwave pulse to the bus that performs entangling operations. We demonstrate controlled-phase gates using RIP on 2-qubit subsystems with gate fidelities between 95%-97% evaluated by randomized benchmarking. Via a multi-qubit echo scheme, we perform isolated two-qubit interactions in the full 4-qubit system to generate a GHZ state.

<sup>1</sup>We acknowledge support from IARPA under contract W911NF-10-1-0324

**11:51AM F48.00004 Understanding and improving the cross resonance gate in superconducting qubits<sup>1</sup>**, SARAH SHELDON, EASWAR MAGESAN, JERRY M. CHOW, JAY M. GAMBETTA, IBM T.J. Watson Research Center — We present improvements in both theoretical understanding and experimental implementation of the cross resonance (CR) gate that have led to shorter two qubit gatetimes and interleaved randomized benchmarking fidelities exceeding 99%. The CR gate is an all-microwave two qubit gate offers that does not require tunability and is therefore well suited to quantum computing architectures based on 2D superconducting qubits. The performance of the gate has previously been hindered by long gatetimes and fidelities averaging 96-97%. We have developed a calibration procedure that accurately measures the full CR Hamiltonian. The resulting measurements agree with theoretical analysis of the gate and also elucidate the error terms that have previously limited the gate fidelity. The increase in fidelity that we have achieved was accomplished by introducing a second microwave drive tone on the target qubit to cancel unwanted components of the CR Hamiltonian.

<sup>1</sup>This work is supported by ARO under contract W911NF-14-1-0124.

**12:03PM F48.00005 High-fidelity single-shot three-qubit gates via machine learning<sup>1</sup>**, EHSAN ZAHEDINEJAD, JOYDIP GHOSH, BARRY C. SANDERS, University of Calgary — Three-qubit quantum gates play a crucial role in quantum error correction and quantum information processing. Here I discuss how to generate policies for quantum control to design three-qubit gates namely, Toffoli, Controlled-Not-Not and Fredkin gates for an architecture of nearest-neighbor-coupled superconducting artificial atoms. The resulted fidelity for each gate is above the 99.9% which is the threshold fidelity for fault-tolerant quantum computing. We test our policy in the presence of decoherence-induced noise as well as show its robustness under random external noise. The three-qubit gates are designed via our machine learning algorithm called Subspace-Selective Self-Adaptive Differential Evolution (SuSSADE).

<sup>1</sup>NSERC, AITF and University of Calgarys Eyes High Fellowship Program

**12:15PM F48.00006 All-microwave cavity-mediated three-qubit gate between superconducting qubits**, SOPHIA ECONOMOU, ED BARNES, Department of Physics, Virginia Tech — While single-qubit and entangling two-qubit operations are universal for quantum computing, in practice the availability of a single-shot multi-qubit entangling gate can be faster and of higher fidelity. For the case of three qubits coupled to a common cavity mode, we show that a high fidelity, fast CCZ gate can be implemented. Our proposal is based on partial spectrum engineering and pulse shaping. Because our approach does not rely on frequency selectivity, instead driving more than one transitions simultaneously, our three-qubit gate can be achieved on a timescale comparable to that of a two-qubit gate. Our protocol generalizes our recently introduced SWIPHT two-qubit gates.

**12:27PM F48.00007 Tunable coupling between fixed-frequency superconducting transmon qubits, Part I: Concept, design, and prospects<sup>1</sup>**, STEFAN FILIPP, IBM Research - Zurich, 8803 Rueschlikon, Switzerland, DAVID C. MCKAY, EASWAR MAGESAN, ANTONIO MEZZACAPPO, JERRY M. CHOW, JAY M. GAMBETTA, IBM TJ Watson Research Center, Yorktown Heights, NY, USA — The controlled realization of qubit-qubit interactions is essential for both the physical implementation of quantum error-correction codes and for reliable quantum simulations. Ideally, the fidelity and speed of corresponding two-qubit gate operations is comparable to those of single qubit operations. In particular, in a scalable superconducting qubit architecture coherence must not be compromised by the presence of additional coupling elements mediating the interaction between qubits. Here we present a coupling method between fixed-frequency transmon qubits based on the frequency modulation of an auxiliary circuit coupling to the individual transmons. Since the coupler remains in its ground state at all times, its coherence does not significantly influence the fidelity of consequent entangling operations. Moreover, with the possibility to create interactions along different directions, our method is suited to engineer Hamiltonians with adjustable coupling terms. This property can be utilized for quantum simulations of spins or fermions in transmon arrays, in which pairwise couplings between adjacent qubits can be activated on demand.

<sup>1</sup>We acknowledge support from ARO under contract W911NF-14-1-0124.

**12:39PM F48.00008 Tunable coupling between fixed-frequency superconducting transmon qubits, Part II: Implementing a two-qubit XX-90 gate**, DAVID C. MCKAY, IBM T.J. Watson Research Center, Yorktown Heights NY, USA, STEFAN FILIPP, IBM Research Zurich, 8803 Rueschlikon, Switzerland, ANTONIO MEZZACAPPO, EASWAR MAGESAN, JERRY M. CHOW, JAY M. GAMBETTA, IBM T.J. Watson Research Center, Yorktown Heights NY, USA — In this talk we will present a two-qubit gate implemented in a tunable coupling architecture which consists of a flux-tunable qubit ("coupler") coupling two fixed-frequency transmons ("qubits"). In this architecture, a resonant SWAP (XX+YY) interaction is generated between the qubits when the coupler is modulated at the qubit frequency difference, typically a few hundred MHz. This interaction has a number of advantages, in particular, it only requires AC flux control and can resonantly address individual qubit pairs. Here we present a protocol which realizes the XX-90 gate based on this interaction. This gate has the specific characteristic that it takes any of the four basis states ( $|00\rangle, |10\rangle, |01\rangle, |11\rangle$ ) to Bell states. We demonstrate gate fidelities greater than 96% characterized by state tomography and randomized benchmarking. Looking forward, this gate is a prime candidate for implementing the surface code because it can couple highly coherent qubits which are spaced far apart in frequency thereby minimizing crosstalk and collisions. This work is supported by ARO under contract W911NF-14-1-0124.

**12:51PM F48.00009 Gatemon Benchmarking and Two-Qubit Operation<sup>1</sup>**, LUCAS CASPARIS, THORVALD LARSEN, MICHAEL OLSEN, KARL PETERSSON, FERDINAND KUEMMETH, PETER KROGSTROP, JESPER NYGARD, CHARLES MARCUS, Center for Quantum Devices and Station Q Copenhagen, Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark — Recent experiments have demonstrated superconducting transmon qubits with semiconductor nanowire Josephson junctions<sup>2,3</sup>. These hybrid gatemon qubits utilize field effect tunability singular to semiconductors to allow complete qubit control using gate voltages, potentially a technological advantage over conventional flux-controlled transmons. Here, we present experiments with a two-qubit gatemon circuit. We characterize qubit coherence and stability and use randomized benchmarking to demonstrate single-qubit gate errors of  $\sim 0.5\%$  for all gates, including voltage-controlled  $Z$  rotations. We show coherent capacitive coupling between two gatemons and coherent SWAP operations. Finally, we perform a two-qubit controlled-phase gate with an estimated fidelity of  $\sim 91\%$ , demonstrating the potential of gatemon qubits for building scalable quantum processors.

<sup>1</sup>We acknowledge financial support from Microsoft Project Q and the Danish National Research Foundation.

<sup>2</sup>G. de Lange et al., Physical Review Letters **115**, 127002 (2015).

<sup>3</sup>T. W. Larsen, K. D. Petersson et al., Physical Review Letters **115**, 127001 (2015).

**1:03PM F48.00010 Dephasing-induced Leakage in Superconducting Qubits**, FREDERICK STRAUCH, Williams College — Superconducting quantum devices such as the transmon or xmon are described as weakly anharmonic oscillators with multiple energy levels, the lowest two of which constitute a qubit. Quantum logic operations using these devices typically involve states outside of the qubit subspace; residual population in such states is known as leakage. While control methods are known to eliminate leakage from ideal devices, I will show that dephasing limits the effectiveness of these methods and discuss the implications of this dephasing-induced leakage for quantum information processing.

**1:15PM F48.00011 Suppressing Leakage in High Fidelity Single Qubit Gates for Superconducting Qubits<sup>1</sup>**, Z. CHEN, J. KELLY, C. QUINTANA, UC Santa Barbara, R. BARENDTS, Google, Santa Barbara, B. CAMPBELL, UC Santa Barbara, Y. CHEN, Google, Santa Barbara, B. CHIARO, A. DUNSWORTH, UC Santa Barbara, A.G. FOWLER, E. LUCERO, E. JEFFREY, A. MEGGRANT, J. MUTUS, M. NEELEY, Google, Santa Barbara, C. NEILL, P.J.J. O'MALLEY, UC Santa Barbara, P. ROUSHAN, D. SANK, Google, Santa Barbara, A. VAINSENER, J. WENNER, T. WHITE, UC Santa Barbara, A.N. KOROTKOV, UC Riverside, J.M. MARTINIS, UC Santa Barbara and Google, Santa Barbara — Recent results show that superconducting qubits are approaching the threshold for fault tolerant quantum error correction. However, leakage into non-qubit states remains a significant hurdle because leakage errors are highly detrimental for error correction schemes such as the surface code. I will demonstrate that with a simple addition to DRAG pulse shaping, leakage can be suppressed to the  $10^{-5}$  level while simultaneously maintaining  $10^{-3}$  gate fidelity. I will also show that the remaining leakage errors are due to heating of the qubit, suggesting further avenues for improvement.

<sup>1</sup>The work was supported by Google Inc., and by the NSFGRF under Grant No. DGE 1144085

**1:27PM F48.00012 Circuit design implementing longitudinal coupling: a scalable scheme for superconducting qubits**, SUSANNE RICHER, DAVID DIVINCENZO, JARA Institute for Quantum Information, RWTH Aachen University, D-52056 Aachen, Germany — We present a circuit construction for a new fixed-frequency superconducting qubit and show how it can be scaled up to a grid with strictly local interactions. The circuit QED realization we propose implements  $\sigma_z$ -type coupling between a superconducting qubit and any number of  $LC$  resonators. The resulting *longitudinal coupling* is inherently different from the usual  $\sigma_x$ -type *transverse coupling*, which is the one that has been most commonly used for superconducting qubits. In a grid of fixed-frequency qubits and resonators with a particular pattern of always-on interactions, coupling is strictly confined to nearest and next-nearest neighbor resonators<sup>1</sup>; we note that just four distinct resonator frequencies, and only a single unique qubit frequency, suffice for the scalability of this scheme. There is never any direct coupling between the qubits. A controlled phase gate between two neighboring qubits can be realized with microwave drives on the qubits, without affecting the other qubits. This fact is a supreme advantage for the scalability of this scheme.

<sup>1</sup>P.-M. Billangeon et al., *Phy. Rev. B* 91:094517, 2015

**1:39PM F48.00013 Controllable frequency comb generation in a tunable superconducting coplanar waveguide resonator**<sup>1</sup>, J. Q. YOU, SHUAIPENG WANG, YIPU WANG, DENGKE ZHANG, XIAOQING LUO, ZHEN CHEN, Quantum Physics and Quantum Information Division, Beijing Computational Science Research Center, TIEFU LI, Institute of Microelectronics, Department of Micro and Nanoelectronics, Tsinghua University — Frequency combs have attracted considerable interest because they are extremely useful in a wide range of applications, such as optical metrology and high precision spectroscopy. Here we report the design and characterization of a controllable frequency comb generated in a tunable superconducting coplanar waveguide resonator in the microwave regime. Both the center frequency and teeth density of the comb are precisely controllable. The teeth spacing can be adjusted from Hz to MHz. The experimental results can be well explained via theoretical analysis.

<sup>1</sup>This work is supported by the NSAF Grant No. U1330201, the NSFC Grant No. 91421102, and the MOST 973 Program Grant Nos. 2014CB848700 and 2014CB921401.

**1:51PM F48.00014 Design and Measurement of a Tunable Thin-Film LC Resonator for Coupling to Superconducting Circuits**, C. J. BALLARD, R. P. BUDOYO, K. D. VOIGT, S. K. DUTTA, C. J. LOBB, F. C. WELLSTOOD, University of Maryland-College Park — We have designed and measured a tunable lumped element LC resonator for coupling to transmon qubits. We use an rf SQUID loop as a variable inductive element that shunts the inductor of the resonator and produces a shift in the resonator frequency that depends on the flux applied to the loop. In order to achieve a balanced response, we shunt the inductor with two single junction SQUID loops. Each junction has a critical current of approximately 300pA, which is small enough to prevent multiple trapped flux states. We tune the effective inductance of the loops by using a split, gradiometric modulation coil that is well isolated from the cavity at the resonance frequency. Our resonator is made of thermally evaporated aluminum on a sapphire substrate and has a resonance frequency of 5.3 GHz. It is mounted inside a 3D microwave cavity that has a TE101 frequency of 6.3 GHz.

**2:03PM F48.00015 Quantization of lumped elements electrical circuits revisited**, KEVIN LALUMIERE, ALIREZA NAJAFI-YAZDI, Anyon Systems Inc. — In 1995, the Les Houches seminar of Michel Devoret introduced a method to quantize lumped elements electrical circuits [1]. This method has since been formalized using the matricial formalism, in particular by G. Burkard [2,3]. Starting from these seminal contributions, we present a new algorithm to quantify electrical circuits. This algorithm unites the features of Devoret's and Burkard's approaches. We minimize the set of assumptions made so that the method can treat directly most electrical circuits. This includes circuits with resistances, mutual inductances, voltage and current sources. We conclude with a discussion about the choice of the basis in which the Hamiltonian operator should be written, an issue which is often overlooked. [1] M. H. Devoret, Les Houches, Session LXIII, 1995 [2] G. Burkard et al., *Phys. Rev. B*, 69, 064503, 2004 [3] F. Solgun, Ph.D. Dissertation, RWTH Aachen, 2015

## Tuesday, March 15, 2016 11:15AM - 2:39PM —

Session F50 DAMOP: Non-Equilibrium Physics with Cold Atoms Hilton Baltimore Holiday Ballroom 1 - Joe Britton, NIST

**11:15AM F50.00001 The Way to Phase Space Crystals**<sup>1</sup>, LINGZHEN GUO, MARTHALER MICHAEL, GERD SCHÖN, Karlsruhe Institute of Technology (KIT) — A novel way to create a band structure of the quasienergy spectrum for driven systems is proposed based on the discrete symmetry in phase space. The system, e.g., an ion or ultracold atom trapped in a potential, shows no spatial periodicity, but it is driven by a time-dependent field. Under rotating wave approximation, the system can produce a periodic lattice structure in phase space. The band structure in quasienergy arises as a consequence of the  $n$ -fold discrete periodicity in phase space induced by this driving field. We propose explicit models to realize such a phase space crystal and analyze its band structure in the frame of a tightbinding approximation. The phase space lattice differs fundamentally from a lattice in real space, because its coordinate system, i.e., phase space, has a noncommutative geometry. The phase space crystal opens new ways to engineer energy band structures, with the added advantage that its properties can be changed in situ by tuning the driving fields parameters.

<sup>1</sup>Carl-Zeiss Stiftung

**11:27AM F50.00002 Floquet topological systems in the vicinity of level crossings: Reservoir induced coherence of the Floquet density matrix and steady-state entropy production**<sup>1</sup>, HOSSEIN DEGHANI, ADITI MITRA, New York University — Results are presented for a Floquet topological system for the case where the separation between quasi-energy levels becomes small, and in particular, comparable to the coupling strength to an external reservoir. For this case, even at steady-state, the reduced density matrix in the Floquet basis has non-zero off-diagonal elements, with the strength of the off-diagonal elements increasing as one approaches the level crossings. The steady-state reduced density matrix has oscillations at integer multiples of the periodic drive, and a Fourier decomposition allows the extraction of the occupation of the Floquet quasi-energy levels, which also depends on the coupling to the reservoir. The lack of detailed balance is quantified in terms of an entropy production rate.

<sup>1</sup>Supported by US Department of Energy, Office of Science, Basic Energy Sciences, under Award No. DE-SC0010821

### 11:39AM F50.00003 A quantum resonance catastrophe for a periodically driven impurity

, SEBASTIAN EGGERT, Univ Kaiserslautern, DANIEL THUBERG, SEBASTIÁN REYES, Pontificia Universidad Católica de Chile — There has been much interest in creating novel quantum states through active dynamic manipulations (quenches and driving) in a variety of state-of-the-art systems, such as molecular electronics, ultra-cold quantum gases, nanodot arrays, and photonic crystals. We now consider the transport in an extended one-dimensional array of coupled quantum sites which is periodically driven at one impurity location by using an exact solution with help of the Floquet theory. While a static potential barrier is known to always allow transport via tunneling, a corresponding time-periodic impurity shows resonances at special driving frequencies where the transmission is completely blocked. We find that even for an infinitesimally small periodic perturbation there is a breakdown of conductance. Such a quantum resonance catastrophe occurs when the frequency is tuned to couple to bound states just outside the band. Our results show an abundance of tuning possibilities for the transmission and the width of the resonance with frequency, potential barrier and particle energy, leading to versatile opportunities in the design of switches.

### 11:51AM F50.00004 Stroboscopic Symmetry-Protected Topological Phases

, LUIZ SANTOS, UIUC, THOMAS IADECOLA, CLAUDIO CHAMON, Boston University — Symmetry-protected topological (SPT) phases of matter have been the focus of many recent theoretical investigations, but controlled mechanisms for engineering them have so far been elusive. In this talk, I demonstrate that by driving interacting spin systems periodically in time and tuning the available parameters, one can realize lattice models for bosonic SPT phases in the limit where the driving frequency is large. We provide concrete examples of this construction in one and two dimensions, and discuss signatures of these phases in stroboscopic measurements of local observables. Phys. Rev. B 92, 125107 (2015); arXiv:1503.07871

### 12:03PM F50.00005 Statistical Transmutation in Periodically Driven Optical Lattices<sup>1</sup>

, TIGRAN SEDRAKYAN, W. I. Fine Theoretical Physics Institute, University of Minnesota, Joint Quantum Institute, University of Maryland - College Park, VICTOR GALITSKI, Joint Quantum Institute, University of Maryland - College Park, ALEX KAMENEV, W. I. Fine Theoretical Physics Institute, University of Minnesota — We show that interacting bosons in a periodically driven two dimensional (2D) optical lattice may effectively exhibit fermionic statistics. The phenomenon is similar to the celebrated Tonks-Girardeau regime in 1D. The Floquet band of a driven lattice develops the moat shape, i.e., a minimum along a closed contour in the Brillouin zone. Such degeneracy of the kinetic energy favors fermionic quasiparticles. The statistical transmutation is achieved by the Chern-Simons flux attachment similar to the fractional quantum Hall case. We show that the velocity distribution of the released bosons is a sensitive probe of the fermionic nature of their stationary Floquet state.

<sup>1</sup>This work was supported by the PFC-JQI (T.S.), USARO and Simons Foundation (V.G.), and DOE contract DE-FG02-08ER46482 (A.K.)

### 12:15PM F50.00006 Driven impurity in an ultracold 1D Bose gas with intermediate interaction strength

, JEAN-SEBASTIEN CAUX, University of Amsterdam, STEVE SIMON, University of Oxford, CLAUDIO CASTELNOVO, University of Cambridge — We study a single impurity driven by a constant force through a 1D Bose gas using a Lieb-Liniger based approach. Our calculation is exact in the interaction amongst the particles in the Bose gas, and is perturbative in the interaction between the gas and the impurity. In contrast to previous studies of this problem, we are able to handle arbitrary interaction strength for the Bose gas. We find very good agreement with recent experiments [Phys. Rev. Lett. 103, 150601 (2009)].

### 12:27PM F50.00007 The anomalous Floquet-Anderson insulator as a non-adiabatic quantized charge pump.

, PARAJ TITUM, Institute for Quantum Information and Matter, Caltech, Pasadena, California 91125, USA, EREZ BERG, The Weizmann Institute of Science, Rehovot, 76100, Israel, MARK S. RUDNER, Niels Bohr International Academy and Center for Quantum Devices, University of Copenhagen, 2100 Copenhagen, Denmark, GIL REFAEL, Institute for Quantum Information and Matter, Caltech, Pasadena, California 91125, USA, NETANEL H. LINDNER, Physics Department, Technion, 320003 Haifa, Israel — Periodically driven quantum systems provide a novel and versatile platform for realizing topological phenomena. Among these are analogs of topological insulators and superconductors, attainable in static systems; however, some of these phenomena are unique to the periodically driven case. Here, we show that disordered, periodically driven systems admit an anomalous two dimensional phase, whose quasi-energy spectrum consists of chiral edge modes that coexist with a fully localized bulk - an impossibility for static Hamiltonians. This unique situation serves as the basis for a new topologically-protected non-equilibrium transport phenomenon: quantized non-adiabatic charge pumping. We identify the bulk topological invariant that characterizes the new phase (which we call the anomalous Floquet Anderson Insulator, or AFAI). We provide explicit models which constitute a proof of principle for the existence of the new phase. Finally, we present evidence that the disorder-driven transition from the AFAI to a trivial, fully localized phase is in the same universality class as the quantum Hall plateau transition.

### 12:39PM F50.00008 Exact nonadiabatic steering of quantum particles between arbitrary instantaneous eigenstates of time-dependent Hamiltonians

, RAFAEL HIPOLITO, PAUL GOLDBART, Georgia Institute of Technology — We consider a system governed by a Hamiltonian  $H[R_n]$  that depends on a set of parameters  $R_n(t)$  that can be varied with time. We address the task of steering this system between a pair of eigenstates, one corresponding to  $H[R_n(t_i)]$ , the other to  $H[R_n(t_f)]$ . For any parameter history connecting  $R_n(t_i)$  and  $R_n(t_f)$ , we formulate a measure of success with this task, based on a path-integral expression for the overlap between the time-evolved initial state (as driven by  $H[R_n(t)]$ ) and the final state, which is obtained by integrating out the system degrees of freedom but which retains a dependence on the parameter history  $R_n(t)$ . We discuss various settings in which this program may be carried out with perfect accuracy, by optimizing the measure of success with respect to the parameter history. The task may be accomplished over timescales that are much shorter than simple adiabaticity would require and are on the order of the intrinsic timescale of the system dynamics. For illustration, we consider the example of a particle (possibly with internal freedoms) that is confined by a harmonic potential having time-varying center, curvature and squeezing parameters, for which we determine the parameter history required to steer the particle with perfect accuracy.

### 12:51PM F50.00009 Geodesic paths for quantum many-body systems<sup>1</sup>

, MICHAEL TOMKA, TIAGO SOUZA, STEVE ROSENBERG, MICHAEL KOLODRUBETZ, ANATOLI POLKOVNIKOV, Boston University — The quantum length is a distance between parameter-dependent eigenstates of an adiabatically driven quantum system. Its associated metric has many intriguing properties, for example it is related to the fidelity susceptibility, an important quantity in the study of quantum phase transitions. The metric also appears as the leading adiabatic correction of the energy fluctuations of a quantum system and gives rise to a time-energy uncertainty principle and a geometric interpretation of time. The adiabatic response of an open quantum system can as well be expressed through this metric. Further, the quantum length introduces the notion of Riemannian geometry to the manifold of eigenstates and hence allows one to define geodesics in parameter space. We study the geodesics in parameter space of certain quantum many-body systems, emerging from this quantum distance. These geodesic paths provide a well-defined optimal control protocol on how to drive the systems parameters in time, to get from one eigenstate to another. Generating optimal evolution plays a central role in quantum information technology, adiabatic quantum computing and quantum metrology.

<sup>1</sup>Swiss National Science Foundation (SNSF)

**1:03PM F50.00010 Hysteresis of Current in Noninteracting Atomic Fermi Gases in Optical Ring Potentials**, MEKENA METCALF, CHIH-CHUN CHIEN, CHEN-YEN LAI, Univ of California - Merced — Hysteresis is a ubiquitous phenomenon, which can be found in magnets, superfluids, and other many-body systems. Although interactions are present in most systems exhibiting hysteresis, here we show the current of a non-interacting Fermi gas in an optical ring potential produces hysteresis behavior when driven by a time-dependent artificial gauge field and subject to dissipation. Fermions in a ring potential threaded with flux can exhibit a persistent current when the system is in thermal equilibrium, but cold-atoms are clean and dissipation for reaching thermal equilibrium may be introduced by an external, thermal bath. We use the standard relaxation approximation to model the dynamics of cold-atoms driven periodically by an artificial gauge field. A competition of the driven time and the relaxation time leads to hysteresis of the mass current, and work done on the system, as a function of the relaxation time, exhibits similar behavior as Kramers transition rate in chemical reaction and one-dimensional thermal transport.

**1:15PM F50.00011 On Exact Solutions of Novel Multistate Landau-Zener Problems.**<sup>1</sup>, ANIKET PATRA, EMIL YUZBASHYAN, Rutgers University — A multistate Landau-Zener (MLZ) Hamiltonian is used to model numerous non-equilibrium experiments involving cold atoms, quantum dots and quantum dot molecules. We recently showed that all the known MLZ problems either reduce to the  $2 \times 2$  Landau Zener problem or belong to a family of mutually commuting Hamiltonians (that are polynomial in time).<sup>2</sup> Based on this classification we identify previously unknown MLZ problems, explicitly obtain their solutions and discuss relevant experimental scenarios.

<sup>1</sup>Supported in part by the David and Lucile Packard Foundation.

<sup>2</sup>A. Patra and E. A. Yuzbashyan, J. Phys. A: Math. Theor. **48**, 245303 (2015).

**1:27PM F50.00012 Adiabaticity in a dimerised optical lattice site with increasing laser intensity**, SCOTT TAYLOR, CHRIS HOOLEY, University of St Andrews, UK — Recent experiments attempting to simulate magnetic phenomena with cold atoms in optical lattices rely on systems of a few atoms in dimerised lattice sites. These atoms may be manipulated by deformations of the lattice potential, which often need to be adiabatic, but must also happen quickly. We consider such a system of two fermions in a time-dependent double well potential, described by a two-site Hubbard model with time-dependent hopping and interaction energies. The adiabaticity of the following process is analysed: the system is prepared in the ground state of a shallow potential, which is smoothly transformed to a deep potential over some period of time. Experimentally, this corresponds to ramping up the intensity of the lasers generating the lattice. We present numerical and analytical results, demonstrating principles to design fast, adiabatic ramp profiles.

**1:39PM F50.00013 Non-equilibrium dynamics of a quantum gas in a box**, ZORAN HADZIBABIC, University of Cambridge — For the past two decades harmonically trapped ultracold atomic gases have been used with great success to study both equilibrium and non-equilibrium many-body physics in a flexible experimental setting. Recently, we achieved the first atomic Bose-Einstein condensate in an essentially uniform potential of an optical-box trap<sup>1</sup>, which has opened new possibilities for closer connections with other many-body systems and the theories that rely on the translational symmetry of the system. I will present our recent experiments on non-equilibrium phenomena in this system, including the study of the Kibble-Zurek dynamics of spontaneous symmetry breaking in a quenched homogeneous gas<sup>2</sup>.

<sup>1</sup>A. L. Gaunt et al., Phys. Rev. Lett. **110**, 200406 (2013)

<sup>2</sup>N. Navon et al., Science **347**, 167 (2015)

**2:15PM F50.00014 Spin diffusion in ultracold spin-orbit coupled <sup>40</sup>K gas**, T. YU, M. W. WU, Univ of Sci & Tech of China — We investigate the steady-state spin diffusion for ultracold spin-orbit coupled <sup>40</sup>K gas by the kinetic spin Bloch equation approach. It is found that the behaviors of the steady-state spin diffusion are determined by three characteristic lengths in the system: the mean free path, the Zeeman oscillation length and the spin-orbit coupling oscillation length. It is further revealed that by tuning the scattering strength, the system can be divided into *five* regimes, in which the behaviors of the spacial evolution of the steady-state spin polarization shows different dependencies on the scattering strength, Zeeman field and spin-orbit coupling strength. These rich behaviors of the spin diffusions in different regimes are hard to be understood in the framework of the simple drift-diffusion model or the direct inhomogeneous broadening picture in the literature. However, almost all these rich behaviors can be well understood by means of our *modified* drift-diffusion model and/or *modified* inhomogeneous broadening picture. Specifically, several anomalous features of the spin diffusion are revealed, which are in contrast to those obtained from *both* the simple drift-diffusion model and the direct inhomogeneous broadening picture.

**2:27PM F50.00015 Prediction of the expansion velocity of ultracold 1D quantum gases for integrable models**, ZHONGTAO MEI, University of Cincinnati, LEV VIDMAR, FABIAN HEIDRICH-MEISNER, Ludwig-Maximilians-Universitaet Muenchen, CARLOS BOLECH, University of Cincinnati — In the theory of Bethe-ansatz integrable quantum systems, rapidities play an important role as they are used to specify many-body states. The physical interpretation of rapidities going back to Sutherland is that they are the asymptotic momenta after letting a quantum gas expand into a larger volume rendering it dilute and noninteracting. We exploit this picture to calculate the expansion velocity of a one-dimensional Fermi-Hubbard model by using the distribution of rapidities defined by the initial state [1]. Our results are consistent with the ones from time-dependent density-matrix renormalization. We show in addition that an approximate Bethe-ansatz solution works well also for the Bose-Hubbard model. Our results are of interests for future sudden-expansion experiments with ultracold quantum gases. [1] Z. Mei et al., arXiv:1509.00828

## Tuesday, March 15, 2016 11:15AM - 2:15PM –

Session F51 FIAP: 2DEG and Quantum Hall Effect Hilton Baltimore Holiday Ballroom 2 - Mansour Shayegan, Princeton University

**11:15AM F51.00001 Reorientation of quantum Hall stripes within a partially filled Landau level**, Q. SHI, M.A. ZUDOV, University of Minnesota, J.D. WATSON, G.C. GARDNER, M.J. MANFRA, Purdue University — We investigate the effect of the filling factor on transport anisotropies, known as stripes, in high Landau levels of a two-dimensional electron gas. We find that at certain in-plane magnetic fields, the stripes orientation is sensitive to the filling factor within a given Landau level. This sensitivity gives rise to the emergence of stripes away from half-filling while orthogonally-oriented, native stripes reside at half-filling. We attribute this switching of the anisotropy axes within a single Landau level to a strong dependence of the native symmetry breaking potential on the filling factor.

### 11:27AM F51.00002 Magnetic Response Functions in Landau Levels , YANG GAO, QIAN NIU, UT Austin —

We propose a new quantization scheme which generates Landau levels consistent with the zero-field magnetic response functions from the semiclassical theory. It reproduces the Onsager's rule in the leading order, and re-formulates corrections to the Berry phase and magnetic moment effect in terms of one single magnetic response: the zero-field magnetization. It can yield higher order corrections by including successively magnetic susceptibility and higher order magnetic response functions. In application, it can be easily applied to obtain Landau levels in lattice models. Moreover, it provides an experimental method of measuring different magnetic response functions directly from the measurement of Landau level fan diagram or Hofstadter spectrum.

### 11:39AM F51.00003 Hall Potential Distribution in Anti-Hall bar Geometry<sup>1</sup> , VINICIO TARQUINI,

TALBOT KNIGHTON, ZHE WU, JIAN HUANG, Wayne State University, LOREN PFEIFFER, KEN WEST, Princeton — A high quality system has been fabricated in an Anti-Hall bar geometry, by opening a  $1.4 \times 2.0$  mm rectangular window using wet etching in the middle of a  $2.4 \times 3.0$  mm two-dimensional high-mobility ( $\mu = 2.6 \times 10^6$  cm<sup>2</sup>/(V·s)) hole system confined in a 20 nm wide (100) GaAs quantum well. Topologically this system is equivalent to a normal Hall bar even though there is an extra set of edges in the center. This configuration allows us to probe the Hall potential distribution in relation to the formation of edge channels. The Quantum Hall measurements at 30 mK show a standard behavior of the outer edges. At each Hall plateau the inner edge becomes an equipotential and the Hall voltage between the inner and outer edges exhibits a drastic asymmetry for the upper and lower arms of the sample. At various integer fillings, depending on the chirality, the voltage drop across one of the arms measures 0 while the drop across the other one is equal to the Hall voltage. This behavior will be explained in terms of the dynamical process of forming the edge channels which also will account for the more irregular behavior of the Hall potential in more disordered systems.

<sup>1</sup>NSF DMR-1410302

### 11:51AM F51.00004 Finite-wavevector Electromagnetic Response in Quantum Hall Systems: Lattice Corrections and Signatures of Hall Viscosity , FENNER HARPER, THOMAS JACKSON, RAHUL ROY, Univ of

California - Los Angeles — It has recently been shown that the electromagnetic response of a quantum Hall fluid at finite wavevector includes a dependence on the Hall viscosity, raising the possibility of measuring this quantity in an experiment. We present a new, quantum mechanical derivation of this relationship and extend the result to include lattice corrections, which may be significant in a real sample. We find that these corrections have a universal structure whose form depends only on the symmetries of the underlying lattice, and provide numerical estimates for cases of experimental interest. Finally, we consider the Hall viscosity of lattice models more generally and discuss our results in this broader context.

### 12:03PM F51.00005 Insulating States in the Integer Quantum Hall Regime<sup>1</sup> , TALBOT KNIGHTON,

Wayne State University, ALESSANDRO SERAFIN, National High Magnetic Field Laboratory, ZHE WU, VINICIO TARQUINI, Wayne State University, J. F. XIA, NEIL SULLIVAN, National High Magnetic Field Laboratory, LOREN PFEIFFER, KEN WEST, Princeton University, JIAN HUANG, Wayne State University — Quantum Hall measurements are performed at temperatures 20-300 mK in high quality *p*-type GaAs quantum well systems having mobility  $\mu = 4 \times 10^6$  cm<sup>2</sup>/V·s for density  $5 \times 10^{10}$  cm<sup>-2</sup>. We report a series of insulating phases appearing at or near integer filling factors  $\nu \geq 1$ . The DC resistance demonstrates a maximum of 25M $\Omega$ , much larger than the quantum resistance  $h/e^2$ , with threshold transport behavior at low currents around 10 pA at low temperatures. The threshold diminishes upon heating up to 200 mK, consistent with a finite temperature melting of bubble phases or Wigner crystal. Additionally, these peaks have a complex electrical impedance for AC signals, with large phase shifts down to 1Hz. In this regime, the ac impedance of the two chiral edges show distinct correlated characteristics.

<sup>1</sup>NSF DMR-1410302

### 12:15PM F51.00006 Geometry of Landau Level without Galilean or Rotational Symmetry<sup>1</sup> ,

YU SHEN, F. D. M. HALDANE, Department of Physics, Princeton University, Princeton NJ 08544-0708 — The integer quantum Hall effect is usually modeled using Galilean-invariant or rotationally-invariant Landau levels. However, these are not generic symmetries of electrons moving in a crystalline background. We explicitly break both symmetries by considering an inversion-symmetric Hamiltonian with quartic terms. We carry out exact diagonalization numerically with a truncated Hilbert space, and define an emergent metric  $g_{ab}^n$  for each Landau level as the expectation value of a bilinear form in momentum. With an appropriate choice of the guiding center coherent state, the Landau level wavefunctions are holomorphic functions of  $z^*$  times a Gaussian (this is distinct from a well-known property of rotationally-invariant lowest-Landau-level wavefunctions). We show that the zeroes of the wavefunction define a "topological spin  $s_n$ ", with its original definition as an "intrinsic angular momentum" no longer valid without rotational symmetry. This is now related to the number of zeroes  $n$  encircled by the classical orbit by  $s_n = n + \frac{1}{2}$ . Finally we introduce a mass tensor  $m_{ab}^n$  for each Landau level using a Lagrangian formalism. We conclude that topological and geometric information can be extracted without resort to Galilean or Rotational symmetries.

<sup>1</sup>This work is partly supported by DOE grant No. DE-SC0002140 and the W. M. Keck Foundation.

### 12:27PM F51.00007 Quantum Hall states in strained InAs heterostructures<sup>1</sup> , JESSE KANTER,

FRANCESCA ARESE LUCINI, ALEXANDRA DUBOY, The Graduate Center, City College, City University of New York, T.D. MISHIMA, M.B. SANTOS, University of Oklahoma, JAVAD SHABANI, The Graduate Center, City College, City University of New York — In a recent development it was realized that non-Abelian quasiparticles, parafermion zero-modes emerge at an interface between a superconductor and two dimensional electron system (2DES) in the quantum Hall regime. [1]. Unlike widely used GaAs systems, surface level pinning in InAs could allow for fabrication of transparent contacts to superconductors. However, no fractional quantum Hall state has been observed in InAs quantum wells so far. Whether this is due to the type of disorder present in the quantum well is not clear. In this work, we study the transport and dingle mobility of 2DEs confined to strained InAs quantum wells as a function of electron density and spacer thickness to the surface. We compare our results to early observation of fractional quantum Hall states in GaAs. [1] R. S. K. Mong, et al. Phys. Rev. X 4, 011036 (2014)

<sup>1</sup>This material is based upon work supported by the NSF under Grant No. DMR-1207537

### 12:39PM F51.00008 Universal response of quantum hall states to lattice curvature , RUDRO BISWAS,

Department of Physics, Purdue University, DAM SON, Kadanoff Center for Theoretical Physics, University of Chicago — In this talk I shall present general results for the response of quantum Hall states to points of singular real-space curvature. The salient results are that (i) points of singular curvature bind an excess fractional charge and (ii) bound states appear in the inter-Landau level energy gap whose energies are universal functions of bulk parameters and the curvature. Time permitting, I will comment on the implications of these results.

**12:51PM F51.00009 Microwave Spectroscopic Observation of Multiple Phase Transitions of Bilayer Electron Solids in a Wide Quantum Well**, LLOYD ENGEL, ANTHONY HATKE, National High Magnetic Field Laboratory, YANG LIU, MANSOUR SHAYEGAN, LOREN PFEIFFER, KEN WEST, KIRK BALDWIN, Princeton University — For a single-layer two dimensional electron system, the fractional quantum Hall effect (FQHE) series terminates to form an insulating phase (IP) for Landau filling factor  $\nu < 1/5$ . In a wide quantum well the charge distribution can separate into two layers as density increases resulting in a modification of the IP onset to  $\nu < 1/2$  [1]. The IP is understood as an electron solid pinned by residual disorder. The solid exhibits a microwave pinning mode resonance, which is due to pieces of the solid oscillating within the disorder potential. We have previously observed that the microwave pinning mode spectra reveal phase transitions between different types of solid within the terminating IP [2]. In this talk we extend our studies of microwave spectroscopic measurements of a wide quantum well by investigating these phase transitions in the presence of an in-plane magnetic field. Applying an in-plane field forces the system to be more bilayer-like and for small tilt angles we find that the transitions move to higher  $\nu$ . However, at sufficiently high angles the resonance onset extends above  $\nu = 1/2$  and the  $\nu$  of the transitions saturate. [1] Manoharan et al., Phys. Rev. Lett. 77, 1813 (1996). [2] A. T. Hatke et al., Nature Commun. 6, 7071 (2015).

**1:03PM F51.00010 Dicke Model for Quantum Hall Systems**, YUSUKE HAMA, RIKEN, MOHAMMAD FAUZI, Tohoku University, KAE NEMOTO, National Institute of Informatics, YOSHIRO HIRAYAMA, Tohoku University, ZYUN EZAWA, RIKEN — Quantum Hall (QH) systems comprise of many-body electron spins and nuclear spins. They are weakly coupled with nuclear spins through the hyperfine interaction so that electron spin dynamics is scarcely affected by the nuclear spins. The dynamics of the QH systems, however, may drastically change when the nuclear spins interact with low energy collective excitation modes of the electron spins. In connection with this, the nuclear spin relaxation measurement have revealed novel behaviors in the canted antiferromagnetic phase in the total filling factor two bilayer QH systems [1,2]. Here, we theoretically study the interaction between the nuclear spins and the linear dispersing Nambu-Goldstone mode mediated by the hyperfine interaction. We show that such interaction is effectively represented by the Dicke model, and predict that collective spin phenomena realized in quantum optical systems are also observed in the QH systems [3]. References: [1] N. Kumada et al., Science 313, 329 (2006). [2] M. H. Fauzi et al., Phys. Rev. B 90, 235308 (2014). [3] Y. Hama et al., arXiv:1510.04792v1.

**1:15PM F51.00011 Large-filling-factor giant Shubnikov-de Haas oscillations in the ultrahigh-mobility two-dimensional GaAs/AlGaAs electron system**, ZHUO WANG, RAMESH.G. MANI, GEORGIA STATE UNIVERSITY, WERNER WEGSCHEIDER, ETH Zurich — The observation of microwave-induced zero-resistance states (ZRS) produced new interest in transport studies of very high filling factors in the high mobility GaAs/AlGaAs 2D electron system. In particular, there has been interest in the study of the overlap of such ZRS with high filling factor quantum Hall effect.[1] Ref. 1 reported different phase relations between oscillatory resistances at high filling factors. In an effort to clarify the observations, we examine the influence of a dc current bias on the lineshape of oscillatory resistances in the ultrahigh-mobility two-dimensional GaAs/AlGaAs electron system. With increasing dc current bias, a change is also observed in the characteristic lineshape of the SdH oscillations. To quantify the change, we carry out lineshape fits of the oscillatory resistance obtained at different dc bias. In this talk, we will summarize the results of the study. [1] R. G. Mani, W. B. Johnson, V. Umansky, V. Narayanamurti, and K. Ploog, Phys. Rev. B 79, 205320 (2009).

**1:27PM F51.00012 Landau-level mixing, floating-up extended states, and scaling behavior in a GaAs-based two-dimensional electron system containing self-assembled InAs dots<sup>1</sup>**, CHI-TE LIANG, CHIEH-WEN LIU, CHIEH-I LIU, Graduate Institute of Applied Physics, National Taiwan University, Taipei, Taiwan 106, R.O.C., GIL-HO KIM, Sungkyunkwan University, Korea, C. F. HUANG, 2nd Patent Division, Intellectual Property Office, Ministry of Economic Affairs, Taipei, Taiwan 106, R.O.C., DA-REN HANG, Department of Materials and Optoelectronic Science, National Sun Yat-sen University, Kaohsiung, Taiwan 804, R.O.C., D. A. RITCHIE, Cavendish Laboratory, University of Cambridge, United Kingdom — Temperature-driven flow lines corresponding to Landau level filling factor  $\nu = 2 \sim 4$  were studied in the  $\sigma_{xx} - \sigma_{xy}$  plane in a GaAs-based two-dimensional electron system with self-assembled InAs dots. In the insulator-quantum Hall (I-QH) transition resulting from the floating-up extended states, the flow diagram showed the validity of the scaling and we observed the expected semicircle. On the other hand, the curve  $\sigma_{xx}(\sigma_{xy})$  in the low-field insulator demonstrated the existence of Landau-level mixing. By decreasing the effective disorder, we found that such flow lines can leave the I-QH regime and follow the scaling for the plateau transition between  $\nu = 4$  and 2. The semicircle in the observed I-QH transition, in fact, originated from the distortion on the plateau-transition curve due to Landau-level mixing. Our study showed the importance of the level-mixing effects to the scaling and semicircle law as the extended states float up.

<sup>1</sup>We thank the MOST, Taiwan (grant number: MOST 104-2622-8-002 -003) for financial support.

**1:39PM F51.00013 Probing the excited subband dispersion of holes confined to GaAs wide quantum wells<sup>1</sup>**, INSUN JO, YANG LIU, H. DENG, M. SHAYEGAN, L. N. PFEIFFER, K. W. WEST, K. W. BALDWIN, Dept. of Electrical Engineering, Princeton University, Princeton, NJ08544, USA, R. WINKLER, Dept. of Physics, Northern Illinois University, DeKalb, IL 60115, USA — Owing to the strong spin-orbit coupling and their large effective mass, the two-dimensional (2D) holes in modulation-doped GaAs quantum wells provide a fertile test bed to study the rich physics of low-dimensional systems. In a wide quantum well, even at moderate 2D densities, the holes start to occupy the excited subband, a subband whose dispersion is very unusual and has a non-monotonic dependence on the wave vector. Here, we study a 2D hole system confined to a 40-nm-thick (001) GaAs quantum well and demonstrate that, via the application of both front and back gates, the density can be tuned in a wide range, between  $\sim 1$  and  $2 \times 10^{11} \text{ cm}^{-2}$ . Using Fourier analysis of the low-field Shubnikov-de Haas oscillations, we investigate the population of holes and the spin-orbit interaction induced spin-splitting in different subbands. We discuss the results in light of self-consistent quantum calculations of magneto-oscillations.

<sup>1</sup>Work support by the DOE BES (DE-FG02-00-ER45841), the NSF (Grants DMR-1305691 and MRSEC DMR-1420541), the Gordon and Betty Moore Foundation (Grant GBMF4420), and Keck Foundation for experiments, and the NSF Grant DMR-1310199 for calculations.

**1:51PM F51.00014 Formation of a helical channel in a 2D system in a quantum Hall regime<sup>1</sup>**, ALEKSANDR KAZAKOV, Purdue University, V. KOLKOVSKY, Z. ADAMUS, G. KARCEWSKI, T. WOJTOWICZ, Institute of Physics, Polish Academy of Sciences, LEONID ROKHINSON, Purdue University — A two-dimensional system with reconfigurable network of one-dimensional p-wave superconducting channels is a perfect platform to perform braiding of non-Abelian excitations. Such channels can be realized in CdTe:Mn quantum wells in a quantum Hall effect regime, where counterpropagating edge states with opposite spin polarization can be formed by electrostatic gating. These edges form helical channels similar to the edges of 2D topological insulators and, coupled to a superconductor, should support non-Abelian excitations. While long channels are localized at low temperatures, we found that resistance in short ( $\sim 6 \mu\text{m}$ ) helical channels remains finite at low temperatures. Transport data and resistance scaling with channel length will be presented.

<sup>1</sup>Work supported by ONR, National Science Centre (Poland) and Foundation for Polish Science

**2:03PM F51.00015 Enhanced thermopower of gate-induced ZnO two-dimensional electron gas<sup>1</sup>**, SUNAO SHIMIZU, RIKEN CEMS, MOHAMMAD S. BAHRAMY, RIKEN CEMS, University of Tokyo, TAKAHIKO IIZUKA, University of Tokyo, SHIMPEI ONO, RIKEN CEMS, CRIEPI, KAZUMOTO MIWA, CRIEPI, YOSHINORI TOKURA, YOSHIHIRO IWASA, RIKEN CEMS, University of Tokyo — Control of dimensionality has proven to be an effective way to manipulate the electronic properties of materials, thereby enabling exotic quantum phenomena, such as superconductivity<sup>2</sup>, quantum Hall effects, and valleytronic effects<sup>3</sup>. Another example is thermoelectricity, which has been proposed to be favorably controllable by reducing the dimensionality<sup>4</sup>. We report the thermopower in a gate-induced two-dimensional electron gas (2DEG) formed at the surface of ZnO. Combining electric double layer transistor experiments and realistic tight-binding calculations, it is shown that, for a wide range of carrier densities, the 2DEG channel comprises a single subband, and its effective thickness can be reduced to several nanometers at sufficiently high gate biases. We demonstrate that the thermopower of the 2DEG region is significantly higher than that of bulk ZnO. Our approach opens up a novel route to exploit the peculiar behavior of 2DEG electronic states and realize thermoelectric devices with advanced functionalities.

<sup>1</sup>This work was supported by JSPS KAKENHI Grant Numbers 24224009, 25000003, 26288115, 26820298.

<sup>2</sup>Q. Y. Wang *et al.*, Chinese Phys. Lett. **29**, 037402 (2012).

<sup>3</sup>K. F. Mak *et al.*, Science **344**, 1489 (2014).

<sup>4</sup>L. D. Hicks and M. S. Dresselhaus, Phys. Rev. B **47**, 12727 (1993).

## Tuesday, March 15, 2016 11:15AM - 1:51PM – Session F52 GERA FIAP: Physics of Batteries II Hilton Baltimore Holiday Ballroom 3 -

**11:15AM F52.00001 First principles studies of structure stability and lithium intercalation of ZnCo2O4**, YANNING ZHANG, Chengdu Green Energy and Green Manufacturing Technology RD Center, WEIWEI LIU, Beijing Computational Science Research Center, BEIJING COMPUTATIONAL SCIENCE RESEARCH CENTER TEAM — Among the metal oxides, which are the most widely investigated alternative anodes for use in lithium ion batteries (LIBs), binary and ternary transition metal oxides have received special attention due to their high capacity values. ZnCo2O4 is a promising candidate as anode for LIB, and one can expect a total capacity corresponding to 7.0 - 8.33 mol of recyclable Li per mole of ZnCo2O4. Here we studied the structural stability, electronic properties, lithium intercalation and diffusion barrier of ZnCo2O4 through density functional calculations. The calculated structural and energetic parameters are comparable with experiments. Our theoretical studies provide insights in understanding the mechanism of lithium ion displacement reactions in this ternary metal oxide.

**11:27AM F52.00002 First-principles investigations of ionic conduction in Li and Na borohydrides**, JOEL VARLEY, TAE-WOOK HEO, KEITH RAY, STANIMIR BONEV, BRANDON WOOD, Lawrence Livermore Natl Lab — Recent experimental studies have identified a family of alkali borohydride materials that exhibit superionic transition temperatures approaching room temperature and ionic conductivities exceeding 0.1 S/cm<sup>-1</sup>, making them highly promising solid electrolytes for next-generation batteries. Despite the rapid advances in improving the superionic conductivity in these materials, an understanding of the exact mechanisms driving the transport remains unknown. Here we use *ab initio* molecular dynamics calculations to address this issue by characterizing the diffusivity of the Li and Na species in a representative set of closoborane ionic conductors. We investigate both the Na and Li-containing borohydrides with icosahedral (B<sub>12</sub>H<sub>12</sub>) and double-capped square antiprism (B<sub>10</sub>H<sub>10</sub>) anion species and discuss the trends in ionic conductivity as a function of stoichiometry and the incorporation of various dopants. Our results support the borohydrides as a subset of a larger family of very promising solid electrolytes and identify strategies to improving the conductivity in these materials. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

**11:39AM F52.00003 Defect Physics and Ionic conduction in Solid Electrolyte Interphase for Lithium Ion Batteries<sup>1</sup>**, JIE PAN, YANG-TSE CHENG, University of Kentucky, YUE QI, Michigan State University — The ionic conduction through the solid electrolyte interphase (SEI) is important to the rate capability of the battery. The origin of ionic conduction in the SEI is defect formation and transport. In this study, we developed a theoretical method based on density functional theory to calculate the ionic conductivity in LiF, an important SEI component, in contact with electrode materials. Seventeen native defects with their relevant charge states were investigated to determine the dominant defects on various electrodes. The contacted electrode serves as a Li reservoir with adjustable Li chemical potential ( $\mu_{Li}$ ) for defect formation. The formation energy and diffusion barrier of defects were mapped to ionic conductivity by the Nernst-Einstein relationship. The main defect is Schottky pair in the intrinsic region and Li ion vacancy in the p-type region. The ionic conductivity is calculated to be approximately 10<sup>-31</sup> S/cm when LiF is in contact with an anode but it can increase to 10<sup>-12</sup> S/cm on a cathode. Comparing with other SEI components, the ionic conductivity is very low in LiF if it is coated on an anode surface. However, due to the low concentration of electronic carriers, LiF can act as a good passivation layer on the electrode and prevent further electrolyte decomposition.

<sup>1</sup>This work is supported by Department of Energy and National Science Foundation.

**11:51AM F52.00004 First Principles Study of Electrochemical and Chemical Stability of the Solid Electrolyte-Electrode Interfaces in All-Solid-State Li-Ion Batteries<sup>1</sup>**, YIZHOU ZHU, XINGFENG HE, YIFEI MO, Department of Materials Science and Engineering, Univ of Maryland-College Park — All-solid-state Li-ion battery is a promising next-generation energy-storage technology. Using novel ceramic solid electrolyte materials, all-solid-state battery has advantages of intrinsic safety and high energy density compared to current Li-ion batteries based on organic liquid electrolyte. However, the power density achieved in all-solid-state battery is still unsatisfactory. The high interfacial resistance at electrode-electrolyte interface is one of the major limiting factors. Here we demonstrated a computational approach based on first principles calculation to systematically investigate the chemical and electrochemical stability of solid electrolyte materials, and provide insightful understanding of the degradation and passivation mechanisms at the interface. Our calculation revealed that the intrinsic stability of solid electrolyte materials and solid electrolyte-electrode interfaces is limited and the formation of interphase layers are thermodynamically favorable. Our study demonstrated a computational scheme to evaluate the electrochemical and chemical stability of the solid interfaces. Our newly gained understanding provided principles for developing solid electrolyte materials with enhanced stability and for engineering interfaces in all-solid-state Li-ion batteries.

<sup>1</sup>This work was supported by Office of Energy Efficiency and Renewable Energy (DE-EE0006860).

**12:03PM F52.00005 Using Defects in Materials to Store Energy: a Theoretical Study**, I-TE LU, MARCO BERNARDI, Department of Applied Physics and Materials Science, California Institute of Technology — We study the energy stored by defects in materials using density functional theory (DFT) calculations. Leveraging experimental data to estimate the energy density of defects, expressed as the defect formation energy per unit volume (units of MJ/L) or weight (units of MJ/kg), we identify candidates for high energy density storage, including tungsten, diamond, graphite, silicon, and graphene. DFT calculations are applied to these materials to study the formation energy of vacancies, interstitials, and Frenkel pairs. Our results indicate that the energy density stored by defects in these materials, with experimentally accessible non-equilibrium defect concentrations, can be higher than that of common energy storage technologies such as lithium batteries and supercapacitors. We discuss storage of solar energy and electrical energy (through ion bombardment) using defects.

**12:15PM F52.00006 Strain-induced tuning of surface energy, electron conductivity, and reduction drive in spinel  $\text{LiMn}_2\text{O}_4$  cathodes<sup>1</sup>**, IVAN SCIVETT, GILBERTO TEOBALDI, University of Liverpool —  $\text{LiMn}_2\text{O}_4$  (LMO) implementation in rechargeable Li-ion batteries (LIBs) for stationary storage is hampered by the limited lifetime of the material and its interfaces, starting from the Solid Electrolyte Interphase [1,2]. Recent experiments [2] and Density Functional Theory (DFT) simulations [3] indicate that the formation and effectiveness of the SEI on LMO are related to the surface orientation and reduction drive. In this context, we analyse the role of geometrical strain for the relative energy, magnetic ordering and the reduction drive of several LMO surfaces. DFT simulations reveal LMO surfaces to be markedly sensitive to geometrical strain. Strain lower than 10% can induce insulator-metal and ferromagnetic-antiferromagnetic transitions, alter the relative energy of LMO surfaces, and induce changes as large as 1.0 eV in the surface chemical potential, thence reduction drive. Prompted by advances in the synthesis of metal-oxide core-shell nanostructures [4], use of strained LMO coating as SEI-formation agent is put forward towards engineering of longer lived SEI on LMO substrates.

1. JCPD 2012, 116, 9852-9861
2. J. Am. Chem. Soc. 2010, 132, 15268-15276
3. J. Phys. Chem. C 2015, 119, 21358-21368
4. ACS Nano 2012, 6, 5531

<sup>1</sup>EU FP7 project SIRBATT (Ref. 608502, end date: August 2016)

**12:27PM F52.00007 Atomic dynamics in  $\text{PrBaCo}_2\text{O}_6$** , ELVIS SHOKO, UDO SCHWINGENSCHLOGL, King Abdullah University of Science and Technology, Thuwal, 23955-6900 — We have used a combination of lattice dynamics and *ab initio* molecular dynamics (MD) to study atomic dynamics in  $\text{PrBaCo}_2\text{O}_6$ , a prototype material for a large class of layered compounds of both fundamental and technological interest. With the layered structure as the framework for understanding the dynamics, our analysis reveals clear signatures of this structural motif in the overall atomic dynamics, especially for O atoms. In particular, we find that O atom dynamics in the PrO layer is predominantly in-plane (*ab*-plane) in contrast to the predominantly out-of-plane dynamics in the  $\text{CoO}_2$  layer. This finding suggests that the oxide ionic conductivity is dominated by the O atoms in the PrO layer. Additionally, we find sharp low-energy modes below 20 meV for both Ba and Pr atoms, reminiscent of rattler modes known for reducing thermal conductivity in cage compounds.

**12:39PM F52.00008  $\text{MnO}_2$  Encapsulated Electrospun  $\text{TiO}_2$  Nanofibers: A Strategic Approach towards the Development of Aqueous Electrolyte Based Asymmetric Supercapacitors**, MUHAMED SHAREEF, Kansas State University, MILAN PALEI, TIRUPATTUR NATARAJAN SRINIVASAN, Indian Institute of Technology Madras, GURPREET SINGH, Kansas State University — An aqueous electrolyte based asymmetric supercapacitor was designed from  $\text{MnO}_2$  coated  $\text{TiO}_2$  nanofibers which were prepared by electrospinning and post hydrothermal process. The core shell fiber architecture exhibit highest specific capacitance of 868 F/g in aqueous  $\text{Na}_2\text{SO}_4$  electrolyte as compared to the similar structures. The Asymmetric supercapacitor (ASC) fabricated based on these core shell fibers demonstrates large voltage window of 2.6 V which is one of the widest voltage window among aqueous electrolyte based asymmetric supercapacitors. In addition, the ASC delivers large specific capacitance and energy density as revealed by the electrochemical studies. The thin  $\text{MnO}_2$  shell, of thickness 6 nm, contributes to the extraordinary electrochemical performance for charge storage by redox reaction and intercalation mechanisms, while the anatase phase  $\text{TiO}_2$  core provides an easy pathway for electronic transport with additional electrochemical stability over thousands of charge discharge cycles.

**12:51PM F52.00009 Helically coiled carbon nanotube forests for use as electrodes in supercapacitors**, ANTHONY CHILDRESS, KEVIN FERRI, RAMAKRISHNA PODILA, APPARAO RAO, Clemson Univ — Supercapacitors are a class of devices which combine the high energy density of batteries with the power delivery of capacitors, and have benefitted greatly from the incorporation of carbon nanomaterials. In an effort to improve the specific capacitance of these devices, we have produced binder-free electrodes composed of helically coiled carbon nanotube forests grown on stainless steel current collectors with a performance superior to traditional carbon nanomaterials. By virtue of their helicity, the coiled nanotubes provide a greater surface area for energy storage than their straight counterparts, thus improving the specific capacitance. Furthermore, we used an Ar plasma treatment to increase the electronic density of states, and thereby the quantum capacitance, through the introduction of defects.

**1:03PM F52.00010 High-Energy-Density Cost-Effective Graphene Supercapacitors**, VLADIMIR SAMUILOV, YING YING MU, NADER HEDAYAT, Department of Materials Science and Engineering, SUNYSB, VYACHESLAV SOLOVYOV, Graphene ESD, SENSOR CAT AT STONY BROOK TEAM — We introduce a cost-effective graphene platelet composite material as a replacement of an expensive reduced graphene oxide for electrodes in high energy density supercapacitors. We have tested a low size supercapacitor prototypes with the graphene platelets electrodes and newly developed polymer-gel  $\text{Li}^+$  ion electrolyte. We discuss the ways how to increase the capacitance and the energy densities of the supercapacitor significantly. A working prototype for testing the concept of the high voltage supercapacitor has been developed as well. The first test done up to 10 V showed excellent performance of the multi-cell multi-layer high voltage test assembly.

**1:15PM F52.00011 Dipolar self-consistent field theory for ionic liquids between charged plates: Effects of dielectric contrast between cation and anion under external electrostatic fields<sup>1</sup>**, ISSEI NAKAMURA, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences — We develop a new dipolar self-consistent field theory (DSCFT) for both incompressible and compressible ionic liquids under external electrostatic fields. Our theory accounts for the difference between the dipole moments and the molecular volumes of the cation and anion, and the double layer caused by the strong association of the ions with the electrodes. To date, few theoretical studies have considered the dielectric contrast between the cation and anion. Thus, our study focuses on the effect of the dielectric inhomogeneity on the ion distribution and the capacitance. Our theory shows that the capacitance changes with the applied voltage in agreement with experimental observations. Importantly, the dielectric contrast and the difference in molecular volumes between the cation and anion have equal effects on the magnitude of the capacitance. We also consider compressible ionic liquids by developing a hybrid of DSCFT combined with Monte Carlo simulations. We then demonstrate that the hard-core nature of the ions causes oscillations in the density profile and dielectric value near the charged plates. Accordingly, the dielectric constants derived from the classical theories of Onsager and Kirkwood are shown to be gross approximations of the true situation in nanochannels.

<sup>1</sup>National Natural Science Foundation of China (21474112)

## 1:27PM F52.00012 Theoretical Investigation of oxides for batteries and fuel cell applications

PANCHAPAKESAN GANESH, ANDREW A. LUBIMTSEV, JANAKIRAMAN BALACHANDRAN, Center for Nanophase Materials Sciences, ORNL — I will present theoretical studies of Li-ion and proton-conducting oxides using a combination of theory and computations that involve Density Functional Theory based atomistic modeling, cluster-expansion based studies, global optimization, high-throughput computations and machine learning based investigation of ionic transport in oxide materials. In Li-ion intercalated oxides, we explain the experimentally observed (Nature Materials 12, 518522 (2013)) 'intercalation pseudocapacitance' phenomenon, and explain why  $Nb_2O_5$  is special to show this behavior when Li-ions are intercalated (J. Mater. Chem. A, 2013, 1, 14951-14956), but not when Na-ions are used. In addition, we explore Li-ion intercalation theoretically in  $VO_2(B)$  phase, which is somewhat structurally similar to  $Nb_2O_5$  and predict an interesting role of site-trapping on the voltage and capacity of the material, validated by ongoing experiments. Computations of proton conducting oxides explain why Y-doped  $BaZrO_3$ , one of the fastest proton conducting oxide, shows a decrease in conductivity above 20% Y-doping. Further, using high throughput computations and machine learning tools we discover general principles to improve proton conductivity. Acknowledgements: LDRD at ORNL and CNMS at ORNL

## 1:39PM F52.00013 Atomic-Scale Mechanisms for Electrolyte Decomposition in Li-ion Battery Cathodes<sup>1</sup>

MALLORY FUHST, University of Michigan Department of Applied Physics, DONALD SIEGEL, University of Michigan Department of Mechanical Engineering — Li-ion batteries using high energy density  $LiCoO_2$  (LCO) intercalation cathodes are known to generate gaseous species inside the cell, which can lead to venting flammable solvent vapor. It has been hypothesized that reactions at the cathode/electrolyte interface catalyze the production of these gaseous species. To elucidate the underlying reaction mechanism, first principles calculations were used to model interactions between LCO surfaces and Ethylene Carbonate (EC), a commonly used solvent in Li-ion batteries. A Metropolis Monte Carlo algorithm was used to identify likely low energy adsorption configurations for EC on the (10-14) surface of LCO. Several of these geometries were further analyzed with DFT. The thermodynamics and kinetics of EC decomposition were evaluated for plausible reaction pathways and associated various solvent decomposition mechanisms, such as hydrogen abstraction. Preliminary results indicate that hydrogen abstraction may lead to the spontaneous decomposition of EC into CO and other adsorbed species at the surface.

<sup>1</sup>This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. DGE 1256260

**Tuesday, March 15, 2016 11:15AM - 2:15PM –**

**Session F53 DCP: DCP Plyler and Jankunis Prize Session** Hilton Baltimore Holiday Ballroom 4 -

## 11:15AM F53.00001 Earle K. Plyler Prize for Molecular Spectroscopy & Dynamics: Photochemistry of Phenol: A Full-Dimensional Semiclassical Simulation<sup>1</sup>

DONALD TRUHLAR, University of Minnesota, Minneapolis, MN — This lecture will present a simulation of the photodissociation of phenol that is made possible by combining four methods in a complementary way: (1) the fourfold way for generating diabatic electronic states, based on diabatic molecular orbitals and configurational uniformity; (2) anchor points reactive potentials for fitting the 33-dimensional diabatic potentials; (3) coherent switches with decay of mixing for multistate dynamics governed by coupled potential energy surfaces, including density matrix coherence and decoherence; (4) army ants tunneling, including electronically nonadiabatic tunneling. By combining all these methods, one can thoroughly sample an ensemble of trajectories with potential energy surfaces and couplings that include multireference dynamic electron correlation. By including army ants tunneling, the trajectory simulation of phenol photodissociation dynamics based on accurate full-dimensional anchor-points reactive potential surfaces and state couplings successfully reproduces the experimentally observed bimodal total kinetic energy release spectra. Analysis of the trajectories uncovers an unexpected dissociation pathway. The new method for including tunneling in full-dimensional molecular dynamics simulations is general, and it can also be used for electronically adiabatic processes.

<sup>1</sup>My coauthors in this work are Xuefei Xu, Jingjing Zheng, and Ke R. Yang. This work was supported in part by U.S. Department of Energy, Office of Basic Energy Sciences, under SciDAC grant no. DE-SC0008666.

## 11:51AM F53.00002 Jankunas Doctoral Dissertation Award: Attosecond science with recolliding electrons

PETER KRAUS, University of California, Berkeley — Measuring the motion of valenceshell electrons in molecules is one of the main research thrusts in modern ultrafast science. The process of highharmonic generation (HHG), the conversion of many infrared photons into one XUV photon, relies on the laserdriven ionization, acceleration and precisely timed recombination in a strong laser field. The frequencies emitted upon recollision can be uniquely mapped to a transit time of the electron in the continuum thus providing attosecond temporal and Angstrom spatial resolution encoded in the HHG spectrum. In this talk we present experiments that utilize these capacities of HHG for following a coherent valenceshell electron current in nitric oxide on the femtosecond time scale in a classical pumpprobe experiment. Furthermore, we use the intrinsic time resolution of the HHG process to measure attosecond timescale electron dynamics: The motion of an electron hole across a molecular chain after ionization in spatially oriented iodoacetylene molecules.

## 12:27PM F53.00003 Multi-Configuration Pair-Density Functional Theory

LAURA GAGLIARDI, Department of Chemistry, University of Minnesota — We have recently developed a new theoretical framework, called Multiconfiguration Pair-Density Functional Theory (MC-PDFT), [1] which combines multiconfigurational wave functions with a generalization of density functional theory (DFT). In this talk I will describe the basic principles of the theory and I present our latest results with MC-PDFT on spectroscopy, [2] charge-transfer systems [3] and molecules containing transition metals [4].

[1] G. Li Manni, R. K. Carlson, S. Luo, D. Ma, J. Olsen, D. G. Truhlar, and L. Gagliardi, Multi-Configuration Pair-Density Functional Theory, *J. Chem. Theory Comput.*, **10** (9), 2014 pp 3669-3690

[2] C. E. Hoyer, L. Gagliardi, and D. G. Truhlar, Multiconfiguration Pair-Density Functional Theory Spectral Calculations Are Stable to Adding Diffuse Basis Functions, *J. Phys. Chem. Lett.*, (6), 2015, pp 4184-4188

[3] S. Ghosh, A. L. Sonnenberger, C. E. Hoyer, D. G. Truhlar, and L. Gagliardi, Multiconfiguration Pair-Density Functional Theory Outperforms Kohn-Sham Density Functional Theory and Multireference Perturbation Theory for Ground-State and Excited-State Charge Transfer, *J. Chem. Theory Comput.*, **11** (8), 2015, pp 3643-3649

[4] R. K. Carlson, D. G. Truhlar, and L. Gagliardi, Multiconfiguration Pair-Density Functional Theory: A Fully Translated Gradient Approximation and Its Performance for Transition Metal Dimers and the Spectroscopy of  $Re_2Cl_8^{2-}$ , *J. Chem. Theory Comput.*, **11** (9), 2015, pp 4077-4085

**1:03PM F53.00004 MN15-L and MN-15: New Kohn-Sham Density Functionals with Board Accuracy for Main-Group and Transition Metal Chemistry and Noncovalent Interactions<sup>1</sup>**, HAOYU YU, Department of Chemistry, University of Minnesota, XIAO HE, East China Normal University, DONALD G. TRUHLAR, University of Minnesota, DONALD G. TRUHLAR TEAM — The accuracy of Kohn-Sham density functional theory depends on the exchange-correlation functional. Local functionals depending on only the density ( $\rho$ ), density gradient (grad), and possibly kinetic energy density ( $\tau$ ) have been popular because of their low cost and simplicity, but the most successful functionals for chemistry have involved nonlocal Hartree-Fock exchange (hybrid functionals). We have designed a new meta gradient approximation called MN15-L and a new hybrid meta gradient approximation called MN15 and tested them systematically for 17 absolute atomic energies, 51 noncovalent interaction energies, 56 data on transition metal atoms and molecules, and for 298 other atomic and molecular energetic data, including main-group and transition metal bond energies, ionization potentials, proton affinities, reaction barrier heights, hydrocarbon thermochemistry, excitation energies, and isomerization energies. When compared with 84 previous density MN15 and MN15-L give respectively the smallest and second smallest mean unsigned errors (MUEs, in kcal/mol) on all 422 data with errors for the 4 subsets above being: MN15: 6, 0.26, 4.4, 1.6; MN15-L: 7, 0.45, 4.3, 2.0. Third best: M06: 4, 0.35, 7.7, 2.2. Best previous local functional: M06-L: 7, 0.42, 6.0, 3.5. Other popular functionals: B3LYP: 18, 0.82, 8.2, 4.3; HSE06: 33, 0.58, 8.8, 3.6; TPSS: 18, 0.89, 7.25, 5.0; PBE, 47, 0.88, 9.1, 6.0. MN15-L also performs well for solid-state cohesive energies.

<sup>1</sup>This research is supported by the U.S. Department of Energy and inorganic catalyst design center from university of Minnesota.

**1:15PM F53.00005 Density functionals from deep learning**, JEFFREY MCMAHON, Department of Physics and Astronomy, Washington State University — Density-functional theory is a formally exact description of a many-body quantum system in terms of its density; in practice, however, approximations to the universal density functional (DF) are necessary. Machine learning has recently been proposed as a novel approach to discover such a DF (or components of it)<sup>1</sup>. Conventional machine learning algorithms, however, are limited in their ability to process data in their raw form, leading to invariance and/or sensitivity issues. In this presentation, an alternative approach based on deep learning will be demonstrated<sup>2</sup>. Deep learning allows computational models that are capable of discovering intricate structure in large and/or high-dimensional data sets with multiple levels of abstraction, and do not suffer from the aforementioned issues. Results from the application of this approach to the prediction of the kinetic-energy DF of noninteracting electrons will be presented. Using theoretical results from computer science, a connection between the underlying model and the theorems of Hohenberg and Kohn will also be suggested.

<sup>1</sup>J. C. Snyder, M. Rupp, K. Hansen, K.-R. Müller, and K. Burke, *Phys. Rev. Lett.* **108**, 253002 (2012).

<sup>2</sup>J. M. McMahon, *Submitted* (2015).

**1:27PM F53.00006 Enhancing Linear-Scaling DFT for Extended Systems via a QM/QM Fragment Approach**, LAURA RATCLIFF, Argonne National Laboratory, LUIGI GENOVESE, CEA Grenoble, STEPHAN MOHR, Barcelona Supercomputing Center, THIERRY DEUTSCH, CEA Grenoble — We recently introduced a minimal basis approach to the wavelet-based BigDFT code, wherein a minimal set of localized support functions are expressed in an underlying wavelet basis and optimized to reflect their chemical environment. This not only forms the basis of an accurate linear-scaling DFT approach, allowing systems of 10,000 atoms or more to be treated with modest computational resources, but also facilitates the straightforward definition of a fragment approach. Such an approach can reduce the computational cost by an order of magnitude while also offering additional flexibility. We have previously demonstrated the suitability of a molecular fragment approach for the treatment of environmental effects within the context of constrained DFT and have now also expanded the method to include the treatment of extended, periodic systems. In this talk we will describe the extended fragment approach and present examples of its application to large defect systems, as well as offering a perspective on future directions for the treatment of very large systems, such as an embedded approach.

**1:39PM F53.00007 Complex wet-environments in electronic-structure calculations<sup>1</sup>**, GIUSEPPE FISICARO, University of Basel, LUIGI GENOVESE, Laboratoire de simulation atomistique (L-Sim), SP2M, INAC, CEA-UJF, OLIVIERO ANDREUSSI, Institute of Computational Science, Università della Svizzera Italiana & THEOS-MARVEL École Polytechnique Fédérale de Lausanne, NICOLA MARZARI, THEOS-MARVEL École Polytechnique Fédérale de Lausanne, STEFAN GOEDECKER, University of Basel — The computational study of chemical reactions in complex, wet environments is critical for applications in many fields. It is often essential to study chemical reactions in the presence of an applied electrochemical potentials, including complex electrostatic screening coming from the solvent. In the present work we present a solver to handle both the Generalized Poisson and the Poisson-Boltzmann equation. A preconditioned conjugate gradient (PCG) method has been implemented for the Generalized Poisson and the linear regime of the Poisson-Boltzmann, allowing to solve iteratively the minimization problem with some ten iterations. On the other hand, a self-consistent procedure enables us to solve the Poisson-Boltzmann problem. The algorithms take advantage of a preconditioning procedure based on the BigDFT Poisson solver for the standard Poisson equation. They exhibit very high accuracy and parallel efficiency, and allow different boundary conditions, including surfaces. The solver has been integrated into the BigDFT and Quantum-ESPRESSO electronic-structure packages and it will be released as an independent program, suitable for integration in other codes. We present test calculations for large proteins to demonstrate efficiency and performances.

<sup>1</sup>This work was done within the PASC and NCCR MARVEL projects. Computer resources were provided by the Swiss National Supercomputing Centre (CSCS) under Project ID s499. LG acknowledges also support from the EXTMOS EU project.

**1:51PM F53.00008 Investigating the Self-assembled Structure of Polycyclic Aromatic Hydrocarbons Using Two Dimensional Infrared Spectroscopy**, JENEE D. CYRAN, Max Planck Institute of Polymer Research, AMBER T. KRUMMEL, Colorado State University — Self-assembly mechanisms are required for many biological and material processes, such as chlorophyll in photosynthesis, the tobacco mosaic virus and in the formation of molecular crystals. The self-assembly process can be favorable in the case of formation of nanoparticles for electronic devices. However, self-assembly processes, such as asphaltene nanoaggregation, can be unwarranted. Studying the structure of self-assembled supramolecules is important to understand how to mimic or inhibit the formation of the nanoaggregates. In this research, we studied the monomer and self-assembled structure of two polycyclic aromatic hydrocarbons (PAHs), lumogen orange and violanthrone-79, using two-dimensional infrared spectroscopy (2D IR). The carbonyl stretching and the ring breathing vibrational modes were used as vibrational probes. For violanthrone-79, a local mode basis and an electrostatic coupling model were applied to three nanoaggregate structures; parallel, antiparallel, and 28 degrees rotation. The experimental and simulated 2D IR spectra are best represented by majority of the antiparallel configuration with some angular distribution. For lumogen orange, vibrational cross peaks appear as the concentration is increased from a monomer to a nanoaggregate. The 2D IR cross peaks indicate vibrational coupling, which relates directly to the nanoaggregate structure. Comparison between the self-assembled structure of lumogen orange and violanthrone-79 can determine the role of side chains in the nanoaggregate structure.

**2:03PM F53.00009 Reversible electro-strain coupling in K-doped BaTiO<sub>3</sub><sup>1</sup>**, SHI LIU, Geophysical Laboratory, Carnegie Institution of Washington, RONALD E. COHEN, Geophysical Laboratory, Carnegie Institution of Washington and Department für Geo- und Umweltwissenschaften, Ludwig-Maximilians-Universität — Ferroelectric materials that possess a spontaneous polarization have a wide range of applications. Coupled with a non-180° polarization switching, the strain of a ferroelectric crystal will change, due to the exchange of nonequal crystallographic axes. The field-induced large electro-strain coupling accompanied by non-180° domain switching, however, is usually an one-time effect, because the system lacks the driving force to recover to its original state, thus limiting its usefulness. It is suggested that defect dipoles introduced by dopant-vacancy pairs could serve as the driving force for reversible domain switching. However, there is still a lack of first-principles-supported microscopic understanding of the role of defect dipoles in reversible domain switching. In this work, we explore the intrinsic effects of K-dopants and oxygen vacancy on the 90° polarization switching in the prototypical ferroelectric BaTiO<sub>3</sub> with density functional theory. The interplay between polar defect dipole, vacancy concentration and electromechanical properties is investigated. We find that defect dipoles could drive the system back to its original state spontaneously after the electric field is turned off.

<sup>1</sup>S.L. is supported by Carnegie Institution for Science and R.E.C is supported by ONR.

## **Tuesday, March 15, 2016 11:15AM - 2:15PM –**

**Session F54 GERA: Materials for Sustainable Development** Hilton Inner Harbor Holiday Ballroom 5 - Talat Rahman, University of Central Florida

**11:15AM F54.00001 Materials for sustainable development**, MARTY GREEN, NIST —

**11:51AM F54.00002 Teaching Sustainability in Materials Science and Engineering (and Beyond).**, R. LESAR, Department of Materials Science and Engineering, Iowa State University — Since 2008 we have been teaching various aspects of sustainability to undergraduate students at Iowa State University. In our first courses we introduced the ideas of sustainability in the context of global development. These courses were taught mostly to engineering students and took primarily a technical view of sustainability, both in the class room and on the ground in Africa. Since 2010, however, our focus has been on a course that presents a very broad view of sustainability to a highly diverse set of students from all parts of the University. This course presents interesting challenges owing to the breadth of the material and the rather large range of technical knowledge and skills (especially in mathematics) of the students. Our goals are to guide the students to a better understanding of the challenges of sustainability given the many constraints. Since there is a clear need for broadly creating a more informed view of sustainability, this course is the focus of today's talk. In it we will present our basic objectives for the course and our approach to covering the broad and disparate range of material. Having taught the course six (and a fraction) times, we will also comment on what we feel works well and what is still evolving.

In collaboration with K.M. Bryden, Department of Mechanical Engineering, Iowa State University and A.Hallam, Department of Economics, Iowa State University

**12:27PM F54.00003 Room temperature Creep and Elastic Anisotropy of LaCoO<sub>3</sub> based perovskites**, NINA ORLOVSKAYA, University of Central Florida — LaCoO<sub>3</sub> is the parent compound of the La<sub>1-x</sub>Ca<sub>x</sub>CoO<sub>3-δ</sub> system that is a mixed electronic and oxide-ion conductor of technical interest for oxygen separation membranes, the cathode of solid oxide fuel cells, oxygen sensors, and catalysis. Its high-temperature properties, such as electronic-ionic conductivity, electrochemical performance, and catalytic activity, have been studied to a great extent, while the mechanical behavior of the lanthanum cobaltites is still not completely understood. LaCoO<sub>3</sub>-based ceramics do not demonstrate elastic deformation during loading, but rather exhibit ferroelastic behavior with non-linearity and hysteresis, which provides time, temperature and loading rate dependent deformation. The goal of this research was to investigate room temperature creep at different stresses in polycrystalline ferroelastic LaCoO<sub>3</sub> based perovskites under compression. The attempt was made to identify the most important parameters which affect creep strain over different time periods. New phenomenological approach of ferroelastic creep was developed to describe mechanical behavior of cobaltites. Simple analytical expression was obtained to estimate equilibrium strain at given stress. Driving force of ferroelastic switching was defined for loading and unloading and the expression was proposed that allowed calculations of characteristic time for domain switching from driving force. The anisotropy of elastic behavior of the cobaltites was also studied.

**1:03PM F54.00004 Sustainable materials for catalysis**, JUDITH YANG, University of Pittsburgh —

**1:39PM F54.00005 The Next Fifty Years: Electricity, Storage and Sustainability**, ELIZABETH A. KOCS, University of Illinois at Chicago — Energy since the industrial revolution has been marked by historic transitions in sources, carriers and impacts, with each transition requiring a fifty-year time scale. Sustainability and clean energy, emergent themes with origins in the 1970s, are receiving increasing attention as climate change becomes more urgent. Transportation and the electricity grid, which account for nearly two thirds of carbon emissions, are ready for transitions to cleaner and more sustainable operation driven by electricity storage. The development of the lithium-ion battery and prospects for next generation beyond lithium-ion technology with the potential to electrify transportation and accelerate the deployment of renewable wind and solar will be discussed. The energy storage frontier: lithium ion batteries and beyond, George Crabtree, Elizabeth Kocs, Lynn Trahey, MRS Bulletin 40, 1067 (2015) Energy, society and science: the next fifty years, George Crabtree, Elizabeth Kocs, Thomas Alaan, Futures 58, 53 (2014)

## **Tuesday, March 15, 2016 11:15AM - 2:15PM –**

**Session F55 DBIO GSOFT: Brain Morphology and Mechanics: From Cortex Folding to Neuronal Growth to Compression Stiffening** Hilton Baltimore Holiday Ballroom 6 - Jennifer Schwartz, Syracuse University

**11:15AM F55.00001 How does the cortex get its folds? The role of tension-based morphogenesis**, DAVID VAN ESSEN, Washington University in St Louis — The cerebral cortex is a sheet-like structure that is convoluted to varying degrees in different species and, for human cortex, shows remarkable variability across individuals – even in identical twins. This talk will discuss key biological events and physical forces involved in how the cortex gets its folds. The early stages of cortical morphogenesis are established by exquisitely regulated patterns of cellular proliferation and migration that place the right numbers of cells in an appropriate starting configuration. A major focus will be on the proposed role of mechanical tension in the next stages of morphogenesis. Does tension along apical dendrites of cortical pyramidal cells help make the cortex a sheet? Does tension along long-distance axons cause the cortex to fold? These are attractive but controversial ideas. I will suggest ways in which physicists can contribute critical models and analyses that may help distinguish the relative contributions of several mechanisms (differential proliferation, buckling of the cortical sheet, and tension-based cortical folding). Physicists can also help in evaluating the degree to which cortical circuits reflect principles of compact wiring and the putative role of tension-based morphogenesis in wiring length minimization.

**11:51AM F55.00002 Gyrfication from constrained cortical expansion** , TUOMAS TALLINEN, University of Jyväskylä — The convolutions of the human brain are a symbol of its functional complexity. But how does the outer surface of the brain, the layered cortex of neuronal gray matter get its folds? In this talk, we ask to which extent folding of the brain can be explained as a purely mechanical consequence of unpatterned growth of the cortical layer relative to the sublayers. Modeling the growing brain as a soft layered solid leads to elastic instabilities and the formation of cusped sulci and smooth gyri consistent with observations across species in both normal and pathological situations. Furthermore, we apply initial geometries obtained from fetal brain MRI to address the question of how the brain geometry and folding patterns may be coupled via mechanics.

**12:27PM F55.00003 Elastic instabilities in a layered cerebral cortex: A revised axonal tension model for cortex folding**<sup>1</sup> , J. M. SCHWARZ, Department of Physics, Syracuse University — Despite decades of research, there is still no consensus regarding the mechanism(s) driving cerebral cortex folding. Two different mechanisms—axonal tension based on efficient wiring of the neurons and differential growth-induced buckling—are the prevailing hypotheses, though quantitative comparison with data raises issues with both of them. I will present a model for the elasticity of the cerebral cortex as a layered material with bending energy along the layers and elastic energy between them. The cortex is also subjected to axons pulling from the underlying white matter. Above a critical threshold force, a 'flat' cortex configuration becomes unstable and periodic undulations emerge, i.e. a buckling instability occurs, to presumably initiate folds in the cortex. This model builds on the original axonal tension model for cortex folding based on the efficient wiring of neurons but with no buckling mechanism and allows one to understand why small mice brains exhibit no folds, while larger human brains do. Finally, an estimate of the bending rigidity constant for the cortex can be made based on the critical wavelength to quantitatively test this revised axonal tensional model.

<sup>1</sup>This work was done in collaboration with Oksana Manyuhina and David Mayett.

**1:03PM F55.00004 Effects of surface asymmetry on neuronal growth**<sup>1</sup> , CRISTIAN STALL, Tufts University, Physics and Astronomy — Understanding the brain is of tremendous fundamental importance, but it is immensely challenging because of the complexity of both its architecture and function. A growing body of evidence shows that physical stimuli (stiffness of the growth substrate, gradients of various molecular species, geometry of the surrounding environment, traction forces etc.) play a key role in the wiring up of the nervous system. I will present a systematic experimental and theoretical investigation of neuronal growth on substrates with asymmetric geometries and textures. The experimental results show unidirectional axonal growth on these substrates. We demonstrate that the unidirectional bias is imparted by the surface ratchet geometry and quantify the geometrical guidance cues that control neuronal growth. Our results provide new insight into the role played by physical cues in neuronal growth, and could lead to new methods for stimulating neuronal regeneration and the engineering of artificial neuronal tissue.

<sup>1</sup>We acknowledge support from NSF through CBET 1067093

**1:39PM F55.00005 COMPRESSION STIFFENING OF BRAIN AND ITS EFFECT ON MECHANONSENSING BY GLIOMA CELLS** , KATARZYNA POGODA, Institute of Nuclear Physics, Polish Academy of Sciences — The stiffness of tissues, often characterized by their time-dependent elastic properties, is tightly controlled under normal condition and central nervous system tissue is among the softest tissues. Changes in tissue and organ stiffness occur in some physiological conditions and are frequently symptoms of diseases such as fibrosis, cardiovascular disease and many forms of cancer. Primary cells isolated from various tissues often respond to changes in the mechanical properties of their substrates, and the range of stiffness over which these responses occur appear to be limited to the tissue elastic modulus from which they are derived. Our goal was to test the hypotheses that the stiffness of tumors derived from CNS tissue differs from that of normal brain, and that transformed cells derived from such tumors exhibit mechanical responses that differ from those of normal glial cells. Unlike breast and some other cancers where the stroma and the tumor itself is substantially stiffer than the surrounding normal tissue, our data suggest that gliomas can arise without a gross change in the macroscopic tissue stiffness when measured at low strains without compression. However, both normal brain and glioma samples stiffen with compression, but not in elongation and increased shear strains. On the other hand, different classes of immortalized cells derived from human glioblastoma show substantially different responses to the stiffness of substrates *in vitro* when grown on soft polyacrylamide and hyaluronic acid gels. This outcome supports the hypothesis that compression stiffening, which might occur with increased vascularization and interstitial pressure gradients that are characteristic of tumors, effectively stiffens the environment of glioma cells, and that *in situ*, the elastic resistance these cells sense might be sufficient to trigger the same responses that are activated *in vitro* by increased substrate stiffness.

**2:00PM - 2:00PM** –  
Session G1 Poster Session I (Tuesday, 2:00 pm - 5:00 pm) Exhibit Hall EF -

**G1.00001 APPLICATIONS** –

**G1.00002 Simple thermal treatment for the size control of pore arrays in a polystyrene colloidal crystal films**<sup>1</sup> , RYAN M. JAMIOLKOWSKI<sup>2</sup>, Pennsylvania Muscle Institute, University of Pennsylvania, Philadelphia, PA, USA, SHANE A. FIORENZA<sup>3</sup>, Department of Physics, West Chester University of Pennsylvania, West Chester, PA, USA, KEVIN CHEN, ALYSSA M. TATE, Pennsylvania Muscle Institute, University of Pennsylvania, Philadelphia, PA, USA, SHAWN H. PFEIL, Department of Physics, West Chester University of Pennsylvania, West Chester, PA, USA, YALE E. GOLDMAN, Pennsylvania Muscle Institute, University of Pennsylvania, Philadelphia, PA, USA — Nanosphere Lithography (NSL) offers an attractive route to fabricating periodic structures with nanoscale features, without e-beam or deep UV lithography. In particular, it is uniquely suited to the low cost fabrication of large repeated arrays pores or pillars created by taking advantage of the interstitial spaces in close-packed monolayers of nano to micro-scale beads. However pore size, shape, and spacing cannot be controlled independently. We present both a robust method for producing large, approximately 1 cm<sup>2</sup>, hexagonally close packed monolayer films of 1 micron diameter polystyrene beads on glass substrates, and thermal treatment of these films near the glass temperature, T<sub>g</sub>, of polystyrene to modify the pore size. This builds on earlier work showing that pore size can be modified for colloidal crystals formed at a liquid gas interface [2]. These processes promise a simple, reproducible, and low cost route to periodic pore arrays for nano-phonic applications such as zero mode waveguides (ZMWs)

<sup>1</sup>Funding: F30 AI114187 (RMJ), R01-GM080376 (YEG)

<sup>2</sup>co-first author

<sup>3</sup>co-first author

**G1.00003 Synthesis of Novel Birnessite Type  $\text{MnO}_2$  Nanochains by Electrospinning and their Application as Supercapacitor Electrodes**, MUHAMED SHAREEF, Kansas State University, MILAN PALEI, SAMERENDER HANU-MANTHA RAO, TIRUPATTUR NATARAJAN, Indian Institute of Technology Madras, GURPREET SINGH, Kansas State University — A first time method for the synthesis of continuous nanochains by employing electrospinning and post processes are reported with theoretic support. High aspect ratio electrospun PAN nanofibers were stabilized in air at a specific heating rate followed by functionalization in aqueous  $\text{KMnO}_4$  solution. The composite membrane was calcined in air in order to remove polymer skeleton along with reduction of  $\text{KMnO}_4$  into  $\text{MnO}_2$ . The highly crystalline and phase pure birnessite type  $\text{MnO}_2$  nanochains were characterized by different microscopic and spectroscopic techniques. Electrochemical studies of these nanochains were carried out using three electrode and two electrode set up with 0.5 M  $\text{Na}_2\text{SO}_4$  aqueous electrolyte. A possible mechanism for the formation of nanochains was also explained

**G1.00004 Spin torque resonant vortex core expulsion for an efficient radio-frequency detection scheme**, V. CROS, A.S. JENKINS, R. LEBRUN, P. BORTOLOTTI, E. GRIMALDI, Unit Mixte de Physique CNRS/Thales, Univ. Paris-Sud, Univ. Paris-Saclay, S. TSUNEGI, H. KUBOTA, K. YAKUSHIJI, A. FUKUSHIMA, S. YUASA, Spintronic Research Center, AIST — It has been proposed by Tulapurkar et al.[1ref] that a high frequency detector based on the so called spin-diode effect in spin transfer oscillators could eventually replace conventional Schottky diodes, due to their nanoscale size, frequency tunability, and large output sensitivity. Although a promising candidate for ICT applications, the output voltage generated from this effect is consistently low. Here we present a scheme for a new type of spintronics-based high frequency detector based on the expulsion of the vortex core of a magnetic tunnel junction. The resonant expulsion of the core leads to a large and sharp change in resistance associated with the difference in magnetoresistance between the vortex ground state and the final C-state, which is predominantly in either the parallel or anti-parallel direction relative to the polariser layer [2]. Interestingly, this reversible effect is independent of the incoming rf current amplitude, offering a compelling perspective for a fast real-time rf threshold detector. REF : EU FP7 grant (MOSAIC No. ICT-FP7-317950 is acknowledged. [1] Tulapurkar et al. Nature 438, 339, [2] A.S. Jenkins et al., Nat. Nanotech (2015)

**G1.00005 Physics Incubator at Kansas State University**, BRET FLANDERS, AMITABHA CHAKRABARTI, Kansas State University — Funded by a major private endowment, the physics department at Kansas State University has recently started a physics incubator program that provides support to research projects with a high probability of commercial application. Some examples of these projects will be discussed in this talk. In a parallel effort, undergraduate physics majors and graduate students are being encouraged to work with our business school to earn an Entrepreneurship minor and a certification in Entrepreneurship. We will discuss how these efforts are promoting a “culture change” in the department. We will also discuss the advantages and the difficulties in running such a program in a Midwest college town.

**G1.00006 Radiation Pattern and Scattering Properties of Optical Antennas<sup>1</sup>**, ZEYAN XU, University of Texas at Dallas, KEVIN MESSER, ELI YABLONOVITCH, University of California, Berkeley — When light emitting devices (e.g. LEDs) are coupled with optical antennas of the same resonance frequency, their spontaneous emission rate can be enhanced drastically. The ultimate goal is to have the rate of spontaneous emission faster than the stimulated emission so that the LEDs would be as fast as lasers and enable us to achieve energy efficient interconnects for on-chip communication. In this project, we built multiple optical setups to experimentally measure the far field radiation pattern, light scattering properties and photoluminescence of a series of optical antennas. We also used Lumerical FDTD software to theoretically simulate the structure and found out that the simulated results agree with experimental values. As the longitudinal length increased, the spectrum shifted towards higher wavelengths on the spectrum. Also, by studying the radiation patterns of the optical antennas, we are able to understand their strengths as a function of direction, and how the geometrical shape contribute to the shape of radiation patterns. Understanding the radiation pattern and the scattering spectrum of optical antennas will enable us to design devices with specific requirements on radiational directions and resonance frequencies for optical antennas.

<sup>1</sup>This work was funded by National Science Foundation Award ECCS-0939514.

**G1.00007 Visible WGM emissions from rare earth ion doped ZnO microspheres**, FABITHA K, Research scholar, M S RAMACHANDRA RAO, Professor — ZnO is known to be an ideal candidate for short wavelength range opto-electronic device applications due to its wide and direct bandgap (3.37 eV) and high excitonic binding energy (60 meV). Apart from the UV emission at ~380 nm (free exciton emission) ZnO also possesses a broad emission band centered at ~530 nm which is expected to be originated from the oxygen vacancy (Vo) defects. In rare earth (RE) ion doped ZnO, emissions originate from the 4f levels of RE ions will be obtained in addition to the characteristic emissions of ZnO. Small micro/nanostructures made of ZnO with high crystalline quality show unique characteristics in light emission, especially in lasing applications. A micro/ nanostructured ZnO crystal generally has a wurtzite structure with a natural hexagonal cross section, which serves as a WGM lasing micro cavity owing to its high reflective index (~2). However, there exists a potential optical loss at corners of hexagons; therefore, an isotropic structure like spheres may be a better candidate to achieve efficient light confinement. In our work, highly smooth micro spheres with different diameters were grown. Raman spectroscopy measurements confirm the hexagonal wurtzite structure of ZnO, SEM and AFM studies shows the smooth surfaced spheres. WGM lasing characteristics of ZnO spheres have been investigated using optical pumping with 488 nm laser in a micro-PL system. Details of the results will be presented.

**G1.00008 Title: Development of Single photon Quantum Optical Experiments using Type-I and Type-II Spontaneous Parametric Down Conversion**, ANDREW LAUGHARN, SEYFOLLAH MALEKI, Union College — We constructed a quantum optical apparatus to control and detect single photons. We generated these photons via Type-I and Type-II spontaneous parametric down conversion by pumping a GaN laser (405nm) incident on a BBO crystal. We detected the two down converted photons (810nm), denoted signal and idler, in coincidence so as to measure and control single photons. We implemented a coincidence counting unite onto an Altera DE2 board and used LabView for data acquisition. We used these photon pairs to demonstrate quantum entanglement and indistinguishability using multiple optical experiments.

**G1.00009 High speed Infrared imaging method for observation of the fast varying temperature phenomena**, REZA MOGHADAM, KAMBIZ ALAVI, University of Texas at Arlington Department of Electrical Engineering, BAOHONG YUAN, University of Texas at Arlington Department of Biomedical Engineering — With new improvements in high-end commercial R&D camera technologies many challenges have been overcome for exploring the high-speed IR camera imaging. The core benefits of this technology is the ability to capture fast varying phenomena without image blur, acquire enough data to properly characterize dynamic energy, and increase the dynamic range without compromising the number of frames per second. This study presents a noninvasive method for determining the intensity field of a High Intensity Focused Ultrasound Device (HIFU) beam using Infrared imaging. High speed Infrared camera was placed above the tissue-mimicking material that was heated by HIFU with no other sensors present in the HIFU axial beam. A MATLAB simulation code used to perform a finite-element solution to the pressure wave propagation and heat equations within the phantom and temperature rise to the phantom was computed. Three different power levels of HIFU transducers were tested and the predicted temperature increase values were within about 25% of IR measurements. The fundamental theory and methods developed in this research can be used to detect fast varying temperature phenomena in combination with the infrared filters.

**G1.00010 Room temperature lasing in GeSn alloys: A path to CMOS-compatible infrared lasers**, ZAIRUI LI, YUN ZHAO, Electro-Optics Program, University of Dayton, Dayton, OH, JAMES GALLAGHER, JOS MENNDEZ, Department of Physics, Arizona State University, Tempe, AZ, JOHN KOUVETAKIS, Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ, IMAD AGHA, JAY MATHEWS, Electro-Optics Program, University of Dayton, Dayton, OH and Department of Physics, University of Dayton, Dayton, OH — *h —abstract—* The semiconductor industry has been pushing silicon photonics development for many years, resulting in the realization of many CMOS-compatible optoelectronic devices. However, one challenge that has not been overcome is the development of Si-based lasers. Recently, GeSn alloys grown on Si have shown much promise in the field of infrared optoelectronics. These alloy films are compatible with CMOS processing, have band gaps in the infrared, and the band structure of GeSn can be tuned via Sn concentration to induce direct band gap emission. In this work, we report on room temperature lasing in optically-pumped waveguides fabricated from GeSn films grown epitaxially on Si(100) substrates. The waveguides were defined using standard UV photolithography and dry-etched in a Cl plasma. The end facets were mirror polished, and Al was deposited on one facet to enhance cavity quality. The waveguides were optically-pumped using a 976nm wavelength solid-state laser, and the corresponding emission was measured. The dependence of the emission power on the pump power shows a clear transition between spontaneous and stimulated emission, thereby demonstrating room temperature lasing.

**G1.00011 Field-induced activation of metal oxide semiconductor for low temperature flexible transparent electronic device applications**, PUSHPA RAJ PUDASAINI, JOO HYON NOH, ANTHONY WONG, AMADA HAGLUND, The University of Tennessee, THOMAS ZAC WARD, Materials Science and Technology Division, ORBL, Oak Ridge, TN 37831, USA, DAVID MANDRUS<sup>1</sup>, PHILIP RACK<sup>2</sup>, The University of Tennessee — Amorphous metal-oxide semiconductors have been extensively studied as an active channel material in thin film transistors due to their high carrier mobility, and excellent large-area uniformity. Here, we report the athermal activation of amorphous indium gallium zinc oxide semiconductor channels by an electric field-induced oxygen migration via gating through an ionic liquid. Using field-induced activation, a transparent flexible thin film transistor is demonstrated on a polyamide substrate with transistor characteristics having a current ON-OFF ratio exceeding 10<sup>8</sup>, and saturation field effect mobility of 8.32 cm<sup>2</sup>/(V.s) without a post-deposition thermal treatment. This study demonstrates the potential of field-induced activation as an athermal alternative to traditional post-deposition thermal annealing for metal oxide electronic devices suitable for transparent and flexible polymer substrates.

<sup>1</sup>Materials Science and Technology Division, ORBL, Oak Ridge, TN 37831, USA

<sup>2</sup>Center for Nanophase Materials Sciences, ORNL, Oak Ridge, TN 37831, USA

**G1.00012 Dependence of superconducting properties of NbN thin films on sputtering parameters**,<sup>1</sup> TRUPTI KHAIRE, FAUSTIN CARTER, JUNJIA DING, CHRYSTIAN POSADA, AMY BENDER, GENSHENG WANG, VOLODYMYR YEFREMENKO, JOHN PEARSON, Argonne National Laboratory, STEVE PADIN, University of Chicago, CLARENCE CHANG, AXEL HOFFMANN, VALENTYN NOVOSAD, Argonne National Laboratory, SPT3G COLLABORATION — Recently, there has been growing interest in utilizing NbN, TiN, NbTiN thin films in superconducting device applications (e.g. detectors for CMB, mm and sub-mm astronomy). In this work, we have fabricated NbN superconducting thin films by DC reactive magnetron sputtering of Nb in the presence of argon and nitrogen gases. We found that the critical temperature of NbN films is sensitive to various deposition parameters like nitrogen flow rate, target voltage, base pressure, RF substrate bias, and the substrate temperature. By studying each of these factors we have been able to create highly reproducible NbN thin films. We obtained a T<sub>c</sub> of 15.25±0.25 K for 300 nm thick NbN film grown on silicon substrate at modest temperature of 250 °C in the presence of RF substrate bias. We are also investigating the microwave properties of these NbN films at temperatures well below 50 mK by fabricating quarter wavelength CPW resonators out of NbN and characterizing their frequency shifts and quality factors as functions of temperature and power. In this work we present the results of these analyses.

<sup>1</sup>This work was supported by BES-DOE grant DE-AC02-06CH11357

**G1.00013 Nano crystalline palladium disposable electrode development for electrochemical spectroscopy application**<sup>1</sup>, WEI CHEN, Natl Chiao Tung Univ, CHIEN-HAO SU, Cheeshin Technology Co., PENG-JEN CHEN, Natl Chiao Tung Univ, KUO-CHEN HSU, Cheeshin Technology Co., CHIA-CHING CHANG, Natl Chiao Tung Univ, CHEESHIN TECHNOLOGY CO. COLLABORATION — Electrochemical spectroscopy is a highly sensitive and selective detection method to revealing the intermolecular interaction. Gold electrode provides excellent charge transfer property and has been widely used in electrochemical analysis. However, gold electrode is expensive. Moreover, it is time consuming and complicated to regenerate a reaction active gold electrode. Therefore, a ready-to-use electrode is highly desired for electrochemical analysis. In this study, we have developed a novel nano-crystalline palladium (Pd) film electrode which is deposited on flexible polyethylene terephthalate (PET) by sputtering. This Pd electrode is as good as well prepared gold electrode both in cyclic voltammetry (CV) and electric impedance spectroscopy (EIS) due to its highly dispersive {1 1 1} facets-exposed nanocrystalline Pd on high quality. By using this ready-to-use Pd film electrode, the interactions between DNA and drugs can be detected at sub-nanogram level.

<sup>1</sup>This research is supported by MOST 104-2622-M-009-002 -CC2; Corresponding author: Chia-Ching Chang; ccchang01@faculty.nctu.edu.tw

**G1.00014 Nanopore gating with an anchored polymer in a switching electrolyte bias**<sup>1</sup>, CRAIG WELLS, INING JOU, DMITRIY MELNIKOV, MARIA GRACHEVA, Clarkson Univ — We theoretically study the interaction between a tethered, negatively charged polymer chain of varying lengths and a solid state membrane with a nanopore when subject to a time-dependent applied electrolyte bias. Brownian dynamics is used to describe the movement of a biomolecule interacting with a membrane immersed in an electrolyte solution. With the help of an applied electrolyte bias, we can control polymer's equilibrium position, extending it inside the pore for a sufficiently positive bias. We find that the amount of time a polymer takes to enter and extend inside a nanopore in a positive bias increases nearly linearly with the chain length, corresponding to an electrically driven process. The time it takes for the chain to exit the pore, however, increases nearly quadratically with chain length, corresponding to a diffusion process. Understanding the dynamical behavior of the tethered polymer chain will facilitate further advances in this area of nanotechnology.

<sup>1</sup>NSF DMR and CBET Grant No. 1352218

**G1.00015 Nanoindentation of Chitosan Doped with Silver Nanoparticles**, MATTHEW PALUMBO, ALEM TEKLU, NARAYANAN KUTHIRUMMAL, Coll of Charleston, NICOLE LEVI-POLYACHENKO, Wake Forest, DEPARTMENT OF PHYSICS AND ASTRONOMY, COLLEGE OF CHARLESTON COLLABORATION, DEPARTMENT OF PLASTIC AND RECONSTRUCTIVE SURGERY, WAKE FOREST UNIVERSITY HEALTH SCIENCES COLLABORATION — Imaging and spectroscopic analysis via nanoindentation was performed with the Nanosurf EasyScan2 AFM on the pure and silver doped chitosan samples allowing for a more localized determination of their stiffness, hardness, and reduced Young's modulus. The pure chitosan sample was tested to have a stiffness of 0.367 N/m, a hardness of 1.12 GPa, and a reduced Young's modulus of 30.5 MPa. The film with 5mg Ag nanoparticle per gram of chitosan was tested on the boundaries between the chitosan and Ag nanoparticles to show an increase in stiffness of about 4.6% at 0.384 N/m, an increase in hardness of about 5.4% at 1.18 GPa, and an increase in the reduced Young's modulus of about 5.0% at 3.2 MPa in comparison to the pure chitosan sample. On the other hand, upon increasing the doping to 10mg Ag nanoparticle per gram of chitosan showed a decrease in stiffness of about 6.3% at 0.344 N/m, a decrease in hardness of about 27.0% at 0.820 GPa, and a decrease in the reduced Young's modulus of about 6.0% at 28.7 MPa in comparison to the pure chitosan sample. Obviously, films doped with 5mg Ag nanoparticle per gram of chitosan provided the composites with improved mechanical strength compared to chitosan alone.

**G1.00016 Thin film metallic sensors in an alternating magnetic field for magnetic nanoparticle hyperthermia cancer therapy**, Z. A. HUSSEIN, Z. BOEKELHEIDE, Lafayette College — In magnetic nanoparticle hyperthermia in an alternating magnetic field for cancer therapy, it is important to monitor the temperature in situ. This can be done optically or electrically, but electronic measurements can be problematic because conducting parts heat up in a changing magnetic field. Microfabricated thin film sensors may be advantageous because eddy current heating is a function of size, and are promising for further miniaturization of sensors and fabrication of arrays of sensors. Thin films could also be used for in situ magnetic field sensors or for strain sensors. For a proof of concept, we fabricated a metallic thin film resistive thermometer by photolithographically patterning a 500Å Au/100Å Cr thin film on a glass substrate. Measurements were taken in a solenoidal coil supplying 0.04 T (rms) at 235 kHz with the sensor parallel and perpendicular to the magnetic field. In the parallel orientation, the resistive thermometer mirrored the background heating from the coil, while in the perpendicular orientation self-heating was observed due to eddy current heating of the conducting elements by Faradays law. This suggests that metallic thin film sensors can be used in an alternating magnetic field, parallel to the field, with no significant self-heating.

**G1.00017 Effect of pore's geometry on the electroosmotic flow and nanoparticle dynamics in the nanopore**<sup>1</sup>, ZACHERY HULINGS, DMITRIY MELNIKOV, MARIA GRACHEVA, Clarkson University — We theoretically study how the electroosmotic fluid velocity in a charged cylindrical nanopore in a solid state membranes depends on the pore's geometry, electrolyte concentration, and applied electrolyte bias. We find that in long pores, the fluid velocity follows the classical von Smoluchowski result for an infinite pore with a maximum along the pore axis. However, when the pore's length is comparable to its diameter, the velocity profile develops a local minimum along the pore axis with a maximum value near the membrane walls. The minimum becomes more pronounced when the electrolyte concentration and/or applied bias become larger. We attribute this effect to the inhomogeneous electric field distribution in the nanopore with the field along the axis of the pore being smaller than along the pore's walls due to the effects of access resistance on each side of the channel. We also investigate repercussions of such a velocity profile on the transport of a nanoparticle through the nanopore.

<sup>1</sup>NSF DMR and CBET Grant No. 1352218

**G1.00018 Thermocouples in an alternating magnetic field (AMF) for studying magnetic nanoparticle hyperthermia**, S. HARTZELL, Z. BOEKELHEIDE, Lafayette College — Magnetic nanoparticle hyperthermia, a method of cancer therapy, is currently a subject of active research. A critical parameter during therapy or laboratory research is the temperature of the system (tissue or nanoparticle suspension). Thermocouples are affordable and ubiquitous temperature sensors which could be used in this capacity; however, their metallic nature results in self-heating due to eddy currents when placed in an AMF. This presentation will quantitatively discuss calculations and measurements of the self-heating of three common types of thermocouples. Type T, K, and E thermocouples of both thin (40 gauge) and thick (20 gauge) wires were tested in a range of applied magnetic field magnitudes (235 kHz, 0-0.4 T rms). Among the thermocouples, all three types demonstrated large self-heating in 20 gauge wires. For the 40 gauge wires, type K showed large self-heating, while type T showed small but significant self-heating and type E showed no significant self-heating in comparison to the background. Our results indicate that thin type E thermocouples can be accurately used as temperature sensors in an AMF environment similar to the one used here, and type T thermocouples may be appropriate under conditions with lower magnetic field strength or frequency.

## **G1.00019 SEMICONDUCTORS —**

**G1.00020 Quantum Generation Dynamics of Coherent Phonon in Semiconductors: Transient and Nonlinear Fano Resonance**, YOHEI WATANABE, Grad. School of PAS. Univ. Tsukuba, KEN-ICHI HINO, MUNEAKI HASE, NOBUYA MAESHIMA, Div. of PAS. Univ. Tsukuba — The coherent phonon (CP) generation is one of the representative phenomena induced by ultrashort pulsed laser. In particular, in the initial stage of the CP generation in lightly *n*-doped Si, the vestige of Fano resonance (FR) manifested in a flash was observed in time-resolved spectroscopy experiments, in which it was speculated that this phenomenon results from the birth of transient polaronic quasiparticles composed of electrons and phonons strongly interacting each other [1]. This study is aimed at constructing a fully-quantum-mechanical model for the CP generation and tracking the origin of the transient FR. We calculate two physical quantities in both of polar and non-polar semiconductors such as GaAs and undoped Si. One is a retarded longitudinal susceptibility which allows one to calculate a transient induced photoemission spectrum. The other is the Fourier-transform of LO-phonon displacement into frequency domain. We have succeeded in showing that the transient FR is exclusively caused in Si in harmony with the experiments, though, not observed in GaAs [2]. [1] M. Hase, M. Kitajima, A. M. Constantinescu and H. Petek, Nature 426, 51 (2003). [2] Y. Watanabe, K. Hino, M. Hase and N. Maeshima, Phys. Rev. B (submitted), arXiv:1510.00263.

**G1.00021 Transition Metal and Vacancy Defect Complexes in Phosphorene**, MUKUL KABIR, ROHIT BABAR, Department of Physics, Indian Institute of Science Education and Research, Pune 411008, India — Inducing magnetic moment in otherwise nonmagnetic two-dimensional semiconducting materials is the first step to design spintronic material. Here, we study the adsorption of transition-metals on pristine and defected phosphorene, within density functional theory. We predict that increased transition-metal diffusivity on the pristine phosphorene would hinder controlled magnetism. In contrast, point-defects anchor the transition-metal to reduce metal diffusivity. The di-vacancy complex is more important in this context due to their increased thermodynamic stability over the mono-vacancy. For most cases, the defect-transition metal complexes retain the intrinsic semiconducting properties, and induce a local moment. We provide a simple microscopic model which describe the local moment of these transition metal and defect complexes.

## G1.00022 Magnetotransport in Pulsed Laser Deposited Manganese Doped Lead Sulfide Films

, GAURAB RIMAL, KESHAB SARKOTA, Department of Physics & Astronomy, University of Wyoming, ARTUR MAKSYMOW, LEONARD SPINU, Advanced Materials Research Institute, University of New Orleans, WENYONG WANG, JINKE TANG, Department of Physics & Astronomy, University of Wyoming — Diluted magnetic semiconductors (DMS) have been proposed as promising candidates for spintronic applications. Most research in this field has been confined to III-V and II-VI semiconductor system. There are reports on IV-VI semiconductors, however reports on lead sulfide (PbS) based DMS is limited. We study the transport, magnetic and structural properties of manganese doped lead sulfide (Mn:PbS) films produced by pulsed laser deposition (PLD). The films are found to show hopping transport at low temperature. Low temperature magnetoresistance (MR) studies show that the sign of MR can be changed by application of gate voltage. The magnetic properties of the films were also studied which showed ferromagnetic behavior at room temperature.

## G1.00023 Towards thermally induced spin accumulation in Fe/GaAs structures<sup>1</sup>, THOMAS WAGNER,

Department of Materials Science and Metallurgy, University of Cambridge, Cambridge, UK, KAMIL OLEJNIK, Institute of Physics ASCR, Praha, Czech Republic, JAMES HAIGH, Hitachi Cambridge Laboratory, Cambridge, UK, ANDREW IRVINE, Cavendish Laboratory, University of Cambridge, Cambridge, UK, SYLVAIN MARTIN, Hitachi Cambridge Laboratory, Cambridge, UK, RICHARD CAMPION, School of Physics and Astronomy, University of Nottingham, Nottingham, UK, JOERG WUNDERLICH, Hitachi Cambridge Laboratory, Cambridge, UK — We study non-local spin valves of semiconductor-ferromagnetic metal hybrid systems [1]. The epitaxially grown samples consist of a low doped GaAs transport channel with ultrathin Fe top contacts. Magnetic fields applied along the easy and hard axis show spin-valve and Hanle-type curves, respectively. The latter can be used to determine the spin-dephasing time in our samples [2]. We further investigate the potential of non-local spin valves for electrical detection of thermally induced spin accumulation in semiconductors. Thermal spin injection is driven by temperature gradients across interfaces between ferromagnetic and non-magnetic materials [3]. Common ways to establish the required temperature gradients are Joule heating and absorption of focused laser light. We present finite-element simulations of the temperature profile expected in our microdevices. This is of interest in the emerging field of spin caloritronics.

[1] X. Lou *et al.*, Nat. Phys. 3, 197-202 (2007)

[2] K. Olejnik, *et al.*, Phys. Rev. Lett. 109, 076601 (2012)

[3] A. Slachter, *et al.*, Nat. Phys. 6, 879-882 (2010)

<sup>1</sup>We acknowledge funding by the European Union under grant agreement 316657 (SpinIcur)

## G1.00024 Spin-orbit coupling in InSb semiconductor nanowires: physical limits for majorana states<sup>1</sup>, GUILHERME SIPAHI, TIAGO DE CAMPOS, Universidade de So Paulo, SUNY at Buffalo, PAULO E. FARIA JUNIOR, Universidade de So Paulo,

Universitt Regensburg, MARTIN GMITRA, Universitt Regensburg, IGOR ZUTIC, SUNY at Buffalo, JAROSLAV FABIAN, Universitt Regensburg — The search for Majorana fermions is a hot subject nowadays [1]. One of the possibilities for their realization is the use of semiconductor nanowires and p-type superconductors coupled together. Following this path, the first step is the determination of realistic band structures of these wires including spin-orbit effects. To consider the spin-orbit effects, its common to use models that take into account only the first conduction band. Although these reduced models have been successfully used to determine some physical properties, a more realistic description of the spin-orbit coupling between the bands is required to further investigate possible ways to realize the Majorana fermions. In this study we use a state of the art 14 band k.p formalism together with the envelope function approach [2] to determine the band structure of InAs semiconductor nanowires and analyze how the quantum confinement change the coupling between the bands. As a result we have extracted the effective masses and the spin-orbit splitting for a large range of nanowire radial sizes and for several conduction bands that can be used in effective models. [1] J. Alicea, Rep. Prog. Phys. 75, 076501 (2012). [2] P. E. Faria Junior and G. M. Sipahi, J. Appl. Phys. 10, 10, 103716 (2012).

<sup>1</sup>FAPESP (No. 2011/19333-4, No. 2012/05618-0 and No. 2013/23393-8), CNPq (No. 246549/2012-2 and No. 149904/2013-4), CAPES(PVE 88881.068174/2014-01) and DFG SFB 689

## G1.00025 Effect of magnetic polaron for acceptor bound exciton in CdTe:Dy crystals, PETRO BUKIVSKIY, YURIY GNATENKO, ANATOLII BUKIVSKII, Institute of Physics of National Academy of Sciences of Ukraine, ROMAN GAMERNYK, Lviv

National University — We investigated low temperature ( $T = 4.2$  K) photoluminescence (PL) spectra and temperature dependence ( $T = 1.8 - 40$  K) of excitonic PL for CdTe doped by dysprosium. Dysprosium concentration was  $10^{20} \text{ cm}^{-3}$ . We detected the effect of magnetic polaron for acceptor bound excitons. Theoretical analysis of temperature dependency of emission energy of these excitons was performed. The calculations based on Spalek-Deitl-Kossut theory gave us an opportunity to estimate the magnetic polaron energy  $\varepsilon_p$  and its temperature dependence  $\varepsilon_p(T)$  in  $T = 1.8$  to  $40$  K temperature range. In addition, we calculated the temperature dependence of contributions of mean exchange field and thermodynamic fluctuations of magnetization to the spin splitting value  $\Delta$ . Also, we calculated the temperature dependence of probability distribution function  $P(\Delta, T)$  of the spin splitting value for acceptor bound excitons. It was found that calculated total contributions of mean exchange field and thermodynamic fluctuations of magnetization to spin splitting value is in good agreement with experimental data.

## G1.00026 Hematite nanoribbons based on (110) and (104) surfaces and their unusual character<sup>1</sup>

, PRABATH WANAGURU, JIAO AN, QIMING ZHANG, The University of Texas at Arlington — Atomically thin hematite nanoribbons based on (110) and (104) surfaces are studied systematically by first-principles methods. Calculations have performed using the GGA+U approach and structures were fully relaxed to identify the geometric, electronic and magnetic properties. The studied hematite nanoribbons are formed by cutting the atomically-thin hematite nanosheets along their [100] and [010] directions. The (110) surface based nanoribbons show definite tunable semiconducting character while one type of the (104) based nanoribbons display surface modifications or bending nature indicating pseudo-Jahn-Teller effect. The remaining type of (104) based nanoribbons show built-in oxygen vacancy on one edge despite preserving the stoichiometry and introduces the half-metallicity into the nanoribbons at larger widths. We will present the optimized structures, their electronic properties and energetics in detail.

<sup>1</sup>This research is supported by NSF SusChEM Program (Award DMR-1306291).

## G1.00027 Optimized Energy Transfer from Electron-hole pairs to Eu ions in GaN, RUOQIAO

WEI, NATALIE HERNANDEZ, Lehigh University, BRANDON MITCHELL, University of Mount Union, YASUFUMI FUJIWARA, Osaka University, VOLKMAR DIEROLF, Lehigh University — Europium doped Gallium Nitride (GaN:Eu) has demonstrated potential for the red-emitting active layer in nitride-based light emitting diodes. Under above band gap excitation, the red emission was shown to increase due to the optimization of crystal growth conditions. This suggests that excitation efficiency had been improved, which would imply that the energy transfer from electron-hole pairs to Eu ions occurred on a faster time-scale. To test this assumption, we performed time-resolved spectroscopy measurements, under ps-scale time resolution, on samples with a variety of co-dopants and growth conditions. Results show that the energy is transferred on a time scale faster than ns and the excitation efficiency is influenced by the various growth parameters and co-dopants.

**G1.00028 Free-carrier absorption from shallow donors in transparent conducting oxides<sup>1</sup>**, ANDREW SHAPIRO, PHILIP WEISER, MICHAEL STAVOLA, Lehigh University — An experimental study of the free-carrier absorption in a few transparent conducting oxides (TCO's) has been performed to compare the strength of the absorption in different hosts and its dependence on wavelength and temperature. The goal of our work is to make the IR absorption arising from free carriers a quantitative tool for characterizing the conductivity of doped TCO's.

<sup>1</sup>Supported by NSF Grant DMR 1160756

**G1.00029 Structural and electronic properties of amorphous ternary and quaternary oxide semiconductors<sup>1</sup>**, K. NOCONA SANDERS, RABI KHANAL, JULIA E. MEDVEDEVA, Missouri University of Science and Technology — Amorphous structures of several multi-cation wide-bandgap oxides (In-Ga-Zn-O, In-Sc-O, In-Y-O, and In-La-O) were obtained via first-principles molecular dynamics liquid-quench approach using different cooling rates and different oxygen and metal compositions. A detailed comparison of the structural properties, namely, the distribution of metal-oxygen (M-O) and metal-metal (M-M) distances, bond angles, and coordination, allows us to determine how the MO polyhedra network is affected by the crystalline-to-amorphous transition. Furthermore, the role of oxygen non-stoichiometry in defect formation is investigated. Specifically, local structural defects associated with severe distortions in the metal-oxygen polyhedra, such as under-coordinated metal and oxygen atoms, or M-M bonds, appear in the electronic band structure of amorphous oxides. Both carrier-generating defects and carrier trapping/scattering defects are identified. The results help determine the optimal composition and preparation conditions (i.e., oxygen partial pressure, deposition temperature) in order to achieve the desired properties of the technologically-appealing amorphous oxide semiconductors.

<sup>1</sup>NSF-MRSEC

**G1.00030 Anomalous Magneto-Optical Behavior of Rare Earth Doped Gallium Nitride<sup>1</sup>**, ANDREW HELBERS, Department of Physics, Lehigh University, BRANDON MITCHELL, Department of Physics and Astronomy, University of Mt. Union, NATHANIEL WOODWARD, U.S. Army Research Laboratory, VOLKMAR DIEROLF, Department of Physics, Lehigh University — We have observed unusual magneto-optical properties in rare earth doped gallium nitride. Specifically, the reversal of a magnetic field applied parallel to the c-axis produces unexpected, marked differences in luminescence spectra in several of our samples. Notably, relative emission strengths of Zeeman-split lines from the rare earth ions appear to change when the field is reversed. These effects were not observed in rare earth doped lithium niobate and lithium tantalate, which are also hexagonal and polar. Measurements for erbium doped gallium nitride suggest that these asymmetries seem to be linked to the degree of ferromagnetism of the samples. Results are presented showing these differences. The symmetry of the observed effects requires a perturbation of the RE states with a screw like symmetry. We explore whether this may be accomplished by defects such as threading dislocations.

<sup>1</sup>The work related to ferroelectric materials was supported by NSF grant (DMR-1008075).

**G1.00031 Optical and Electrical Studies of Gamma-Irradiated AlGaIn/GaN High Electron Mobility Transistors**, ANUPAMA YADAV, ELENA FLITSIYAN, LEONID CHERNYAK, Department of Physics, University of Central Florida, Orlando, USA, SHIHYUN AHN, FAN REN, Department of Chemical Engineering, University of Florida, Gainesville, USA, STEPHEN PEARTON, Department of Materials Science and Engineering, University of Florida, Gainesville, USA, IGOR LUBOMIRSKY, SERGEY KHODOROV, Department of Materials and Interfaces, Weizmann Institute of Science, Rehovot, Israel — The impact of <sup>60</sup>Co gamma-irradiation on n-channel AlGaIn/GaN High Electron Mobility Transistors (HEMTs) was studied by means of temperature dependent Cathodoluminescence (CL) and Electron Beam Induced Current (EBIC) technique. Increase in diffusion length after low dose of gamma-irradiation ( $\leq 200$  Gy) is consistent with the decrease in the CL intensity. The observed effect is explained via the mechanism involving trapping of Compton electrons on irradiation induced nitrogen vacancies. For high dose ( $>200$  Gy), diffusion length was observed to decrease which is presumably associated with the mobility degradation. It is shown that calculated activation from the EBIC and CL measurements follows exactly the same trend, which implies that same underlying phenomenon is responsible for observed findings. In addition, DC current-voltage measurements were conducted on the devices in order to relate the material's fundamental properties to the device performance.

**G1.00032 Computational modelling of the Li effects on the electronic structure of porous silicon<sup>1</sup>**, MARÍA LUCERO GOMEZ-HERRERA, Facultad de Ingeniería Universidad Autónoma de Querétaro C. P. 76000, México Querétaro, ÁLVARO MIRANDA DURÁN, ALEJANDRO TREJO BAÑOS, MIGUEL CRUZ IRISSON, Instituto Politécnico Nacional, ESIME Culhuacán, Av. Santa Ana 1000 C, P. 04918 México D. F. — This work analyses the effects of Li impurities on the electronic structure of pSi by means of the density functional theory with the generalized gradient approximation and the supercell scheme. The porous structures were modeled by removing atoms in the [001] direction of an otherwise perfect Si crystal. All surface dangling bonds were saturated with H atoms. To model the Li impurities some H atoms are replaced with Li atoms at the surface. Results show additional bands around the Fermi level with the insertion of a single Li atom on the pore surface, which suggests a trap-like state of localized charge. With increasing concentration of surface Li the band gap gradually decreases approaching to a metallic behavior. This results could be important to the application of pSi in Li-ion batteries

<sup>1</sup>This work was partially supported by CONACYT infrastructure project 252749

**G1.00033 Tuning the electronic band-gap of fluorinated 3C-silicon carbide nanowires<sup>1</sup>**, ÁLVARO MIRANDA DURÁN, ALEJANDRO TREJO BAÑOS, ESIME-Culhuacán, Instituto Politécnico Nacional, Av. Santa Ana 1000, 04430 México D.F., México, LUIS ANTONIO PÉREZ, Instituto de Física, Universidad Nacional Autónoma de México, Apartado Postal 20-364, 01000 México D.F., México, MIGUEL CRUZ IRISSON, ESIME-Culhuacán, Instituto Politécnico Nacional, Av. Santa Ana 1000, 04430 México D.F., México — The possibility of control and modulation of the electronic properties of silicon carbide nanowires (SiCNWs) by varying the wire diameter is well known. SiCNWs are particularly interesting and technologically important, due to its electrical and mechanical properties, allowing the development of materials with specific electronic features for the design of stable and robust electronic devices. Tuning the band gap by chemical surface passivation constitutes a way for the modification of the electronic band gap of these nanowires. We present, the structural and electronic properties of fluorinated SiCNWs, grown along the [111] crystallographic direction, which are investigated by first principles. We consider nanowires with six diameters, varying from 0.35 nm to 2.13 nm, and eight random covering schemes including fully hydrogen- and fluorine terminated ones. Gibbs free energy of formation and electronic properties were calculated for the different surface functionalization schemes and diameters considered. The results indicate that the stability and band gap of SiCNWs can be tuned by surface passivation with fluorine atoms

<sup>1</sup>This work was supported by CONACYT infrastructure project 252749 and UNAM-DGAPA-PAPIIT IN106714. A.M. would like to thank for financial support from CONACyT-Retención. Computing resources from project SC15-1-IR-27 of DGTIC-UNAM are acknowledged

**G1.00034 Excitonic photoluminescence lifetimes in PbI<sub>2</sub> nanoclusters for PbCdI<sub>2</sub> semiconductor materials**, ANATOLII BUKIVSKII, YURIY GNATENKO, YURI PIRYATINSKI, Institute of Physics of National Academy of Sciences of Ukraine, BEES TEAM — We investigated excitonic photoluminescence (PL) spectra and kinetics of PL decays for various wavelengths for Pb<sub>1-x</sub>Cd<sub>x</sub>I<sub>2</sub> solid solutions (X = 0.2, X = 0.3, X = 0.4, X = 0.5, X = 0.7). Earlier we had shown that by approximation of the experimental data with stretched exponential function and applying the inverse Laplace transformation to this function we can estimate the average time constant  $\langle\tau\rangle$  of the PL decay. Now, instead of measuring single kinetics for several wavelengths, we performed Time Resolved Emission Scanning continuously for all of the self-trapped excitons emission ranges. We developed analytical software that enables us to calculate both the average time constant  $\langle\tau\rangle$  of the decay and average lifetime  $\tau$  of the emission process. This software also enables us to calculate distribution of rate constants  $H(k)$  for each concentration for each wavelength. By using the demo version of Edinburgh Instruments FAST software, we also calculated continuous distribution of time constants of PL kinetics in Pb<sub>1-x</sub>Cd<sub>x</sub>I<sub>2</sub> solid solutions. These distributions show the presence of three different components of the PL signal, which are time-separated. These results strongly correlate with obtained spectral data.

**G1.00035 Evidence of iridescence in TiO<sub>2</sub> nanostructures. A probably photonic effect**, RAFAEL REY-GONZALEZ<sup>1</sup>, HEIDY P. QUIROZ<sup>2</sup>, CLAUDIA BARRERA-PATIO<sup>3</sup>, ANDERSON DUSSAN<sup>4</sup>, Universidad Nacional de Colombia, GRUPO DE OPTICA E INFORMACION CUANTICA COLLABORATION, GRUPO DE MATERIALES NANOESTRUCTURADOS Y SUS APLICACIONES COLLABORATION — In this work, we present a study of optical properties of titanium dioxide nanotubes (TiO<sub>2</sub>). Nanotubes were obtained by electrochemical anodization method, using ethylene glycol solutions containing different amounts of water and fluoride. A complex structure is observed between nanotubes and Ti foils on surface when nanotubes are released from the sheet. These forms can be associated with replicas or marks in surface of the Ti foil. The optical response of replicas is studied by Uv-Vis spectrophotometry using white light and varying the angle of the incident light. Absorbance measurements reveal that these replicas exhibit a shift towards lower values of lambda when the angle of the incident light increases of 20° to 60°. These changes may be associated with iridescent effects in this material. The concavity of the replicas in association with air could be generating photonic-like effects. Using a 2D model of replicas - air system, the photonic band structures are found through a plane wave approach. Correlations between photonic properties and iridescent effects are explored.

<sup>1</sup>Grupo de Optica e Informacion Cuantica

<sup>2</sup>Grupo de Materiales Nanoestructurados y sus Aplicaciones

<sup>3</sup>Grupo de Optica e Informacion Cuantica

<sup>4</sup>Grupo de Materiales Nanoestructurados y sus Aplicaciones

**G1.00036 ABSTRACT MOVED TO L29.00015 —**

**G1.00037 ABSTRACT WITHDRAWN —**

**G1.00038 Simple Screened Hydrogen Model of Excitons in Two-Dimensional Materials**, THOMAS OLSEN, SIMONE LATINI, FILIP RASMUSSEN, KRISTIAN THYGESEN, Tech Univ of Denmark — We present a generalized hydrogen model for the binding energies ( $E_B$ ) of excitons in two-dimensional (2D) materials that sheds light on the fundamental differences between excitons in two and three dimensions. In contrast to the well-known hydrogen model of three-dimensional (3D) excitons, the description of 2D excitons is complicated by the fact that the screening cannot be assumed to be local. We show that one can consistently define an effective 2D dielectric constant by averaging the screening over the extend of the exciton. For an ideal 2D semiconductor this leads to a simple expression for  $E_B$  that only depends on the excitonic mass and the 2D polarizability  $\alpha$ . The model is shown to produce accurate results for 51 transition metal dichalcogenides. Remarkably, over a wide range of polarizabilities the expression becomes independent of the mass and we obtain  $E_B^{2D} \approx 3/(4\pi\alpha)$ , which explains the recently observed linear scaling of exciton binding energies with band gap. It is also shown that the model accurately reproduces the non-hydrogenic Rydberg series in WS<sub>2</sub> and can account for screening from the environment.

**G1.00039 Measurement of Exciton Binding Energy of Monolayer WS<sub>2</sub>**<sup>1</sup>, XI CHEN<sup>2</sup>, BAIREN ZHU, XIAODONG CUI, The University of Hong Kong — Excitonic effects are prominent in monolayer crystal of transition metal dichalcogenides (TMDCs) because of spatial confinement and reduced Coulomb screening. Here we use linear differential transmission spectroscopy and two-photon photoluminescence excitation spectroscopy (TP-PLE) to measure the exciton binding energy of monolayer WS<sub>2</sub>. Peaks for excitonic absorptions of the direct gap located at K valley of the Brillouin zone and transitions from multiple points near  $\Gamma$  point of the Brillouin zone, as well as trion side band are shown in the linear absorption spectra of WS<sub>2</sub>. But there is no gap between distinct excitons and the continuum of the interband transitions. Strong electron-phonon scattering, overlap of excitons around  $\Gamma$  point and the transfer of the oscillator strength from interband continuum to exciton states make it difficult to resolve the electronic interband transition edge even down to 10K. The gap between excited states of the band-edge exciton and the single-particle band is probed by TP-PLE measurements. And the energy difference between 1s exciton and the single-particle gap gives the exciton binding energy of monolayer WS<sub>2</sub> to be about 0.71eV.

<sup>1</sup>The work is supported by Area of excellency (AoE/P-04/08), CRF of Hong Kong Research Grant Council(HKU9/CRF/13G) and SRT on New Materials of The University of Hong Kong

<sup>2</sup>First and second authors listed contribute equally in the work.

**G1.00040 ABSTRACT WITHDRAWN —**

**G1.00041 ABSTRACT WITHDRAWN —**

**G1.00042 Metal to insulator quantum-phase** RHODES, ZHENGUANG LU, DMITRY SMIRNOV, EFSTRATIOS MANOUSAKIS, FL-32310, USA, AMBER MCCREARY, SIMIN FENG, MAURICO TERRONE, MADAN DUBEY, U.S. Army Research Laboratory, Adelphi, MD 20783, USA, TERRONES, Dept. of Physics, RPI, NY 12180, USA — ReS<sub>2</sub> a layer-independent material for optoelectronic applications. Here, we present an overall evaluation of transport properties. ReS<sub>2</sub> behaves as an *n*-type semiconductor with an intrinsic carrier mobility surpassing 1000 cm<sup>2</sup>/Vs. Semiconducting behavior is observed at low electron densities *n*, but at high values of *n* the material exhibits a metallic *T*<sup>2</sup>-dependence. The electric-field induced metallic state observed in MoS<sub>2</sub> is reproduced in ReS<sub>2</sub> through a scaling analysis of the conductivity as a function of *T* and *n*, we find that the transition is driven by electronic correlations.

<sup>1</sup>Supported by U.S. Army Research Office MURI Grant No. W911NF-11-1-0001

**G1.00043 Finite two-dimensional electron gas in a patterned semiconductor system<sup>1</sup>**, ORION CIFTJA, VICTORIA LIVINGSTON, ELSA THOMAS, SETH SAGANTI, Prairie View AM University — On various occasions, fabrication of a two-dimensional semiconductor quantum dot leads to a small system of electrons confined in a domain that is not circular and may have a pronounced square (or rectangular) shape. In this work we consider a square-shaped semiconductor quantum dot configuration and treat the system of electrons as a finite two-dimensional electron gas. Within this framework, we adopt a Hartree-Fock approach and study the properties of a small two-dimensional system of electrons confined in a finite square region. We calculate the energy for various finite systems of fully spin-polarized (spinless) electrons interacting with a Coulomb potential. The results give a fairly accurate picture of how the energy of the finite system evolves towards the bulk value as the size of the system increases. The calculations for a square domain are challenging since expressions depend in each component of particle's position and not the radial distance from the center of the square-shaped semiconductor quantum dot. Therefore, we also consider a possible circularly symmetric approximation to the problem. We assess the quality of this approximation and discuss instances where its use is not only desirable, but also accurate.

<sup>1</sup>This research was supported in part by U.S. Army Research Office (ARO) Grant No. W911NF-13-1-0139 and National Science Foundation (NSF) Grant No. DMR-1410350.

**G1.00044 Strain Engineered Direct-indirect Band Gap Transition and its Mechanism in 2D Phosphorene.**, XIHONG PENG, QUN WEI, ANDREW COPPLE, Arizona State University — Phosphorene, a two-dimensional puckered honeycomb structure of black phosphorus, showed promising properties for applications in nano-electronics. In this work, we report strain effect on the electronic band structure of phosphorene, using first principles density-functional theory (DFT) including standard DFT and hybrid functional methods. It was found that phosphorene can withstand a tensile strain up to 30%. The band gap of phosphorene experiences a direct-indirect-direct transition when axial strain is applied. The origin of the gap transition was revealed and a general mechanism was developed to explain energy shifts with strain according to the bond nature of near-band-edge electronic orbitals. Effective masses of carriers in the armchair direction are an order of magnitude smaller than that of the zigzag axis indicating the armchair direction is favored for carrier transport. Ref: X.-H. Peng, Qun Wei, A. Copple, Phys. Rev. B 90, 085402 (2014).

**G1.00045 STM study on the structures of SnSe surfaces<sup>1</sup>**, TAE HOON KIM, SANG-UI KIM, TRINH THI LY, ANH TUAN DUONG, SUNGLAE CHO, Department of Physics, EHSRC, and BRL, Univ of Ulsan, S. H. RHIM, Department of Physics and EHSRC, Univ of Ulsan, JUNGDAE KIM, Department of Physics, EHSRC, and BRL, Univ of Ulsan — SnSe is a 2 dimensional layered material, and each layer is coupled by van der Waals forces allowing very easy cleaving though the layer surfaces. SnSe has been studied for various potential applications because of its high stability and elemental abundance in earth. Recently, it was also reported that bulk SnSe has an excellent thermoelectric property of  $ZT=2.6$  at 923 K along the b axis (Zhao et al, Nature 508 373 (2014)). The surface of a single crystal SnSe was studied via a home-built low temperature scanning tunneling microscopy (STM). Clear atomic images of SnSe surfaces were observed at the filled and empty state measurements, and detail atomic structures were analyzed by comparing with DFT simulations. We found that the atomic image of SnSe surfaces measured by STM is not trivial to understand. Only Sn atoms were visible on STM topographic images for the both of filled and empty state probing.

<sup>1</sup>This work was supported by the National Research Foundation of Korea(NRF) [Nos. NRF-2013R1A1A1A1008724, NRF-2009-0093818, and NRF-2014R1A4A1071686]

**G1.00046 STM study on the surface defects of SnSe induced by thermal annealing<sup>1</sup>**, TRINH THI LY, SANG-UI KIM, TAE HOON KIM, ANH TUAN DUONG, SUNGLAE CHO, Department of Physics, EHSRC, and BRL, Univ of Ulsan, S. H. RHIM, Department of Physics and EHSRC, Univ of Ulsan, JUNGDAE KIM, Department of Physics, EHSRC, and BRL, Univ of Ulsan — SnSe is a IV - VI semiconductor with 0.86 eV gap, and a single crystal SnSe usually exhibits a p-type characteristic. SnSe is one of 2D layered materials, and it has attracted researchers' attentions due to excellent physical properties for future applications. In particular, exceptionally high ZT value ( $ZT = \sim 2.6$  at 923 K) was reported for SnSe single crystal (Zhao et al, Nature 508 373 (2014)). Even though many researches on SnSe have proposed the possibilities of various applications so far, surprisingly little information is available regarding the microscopic structure of SnSe surfaces. We conducted a systematic study on the surface defect of SnSe induced by thermal annealing via a home-built low temperature scanning tunneling microscopy (STM). Various defects were characterized by STM/STS, and we found that Sn vacancy is a dominating intrinsic defect. The size of vacancy was changed after annealing process in UHV at different temperatures.

<sup>1</sup>This work was supported by the National Research Foundation of Korea(NRF) [Nos. NRF-2013R1A1A1A1008724, NRF-2009-0093818, and NRF-2014R1A4A1071686]

**G1.00047 Polarization-dependent photocurrents in polar stacks of van der Waals solids<sup>1</sup>**, SONGCI LI, Univ of Washington, YULI LYANDA-GELLER, Purdue University, ANTON ANDREEV, Univ of Washington — Monolayers of semiconducting van der Waals solids, such as transition metal dichalcogenides (TMDs), acquire significant electric polarization normal to the layers when placed on a substrate or in a heterogeneous stack. This causes linear coupling of electrons to electric fields normal to the layers. Irradiation at oblique incidence at frequencies above the gap causes interband transitions due to coupling to both normal and in-plane ac electric fields. The interference between the two processes leads to sizable in-plane photocurrents and valley currents. The direction and magnitude of currents is controlled by light polarization and is determined by its helical or nonhelical components. The helicity-dependent ballistic current arises due to asymmetric photo generation. The non-helical current has a ballistic contribution (dominant in sufficiently clean samples) caused by asymmetric scattering of photoexcited carriers, and a side-jump contribution. Magneto-induced photocurrent is due to the Lorentz force or due to intrinsic magnetic moment related to Berry curvature.

<sup>1</sup>This work was supported by the U. S. Department of Energy Office of Science, Basic Energy Sciences under awards number DE-SC0010544 (YLG) and DE-FG02-07ER46452 (S. L. and A. A.)

**G1.00048 Anisotropic diffusion of oxygen on a few layers of black phosphorous.**, HECTOR NOE FERNANDEZ-ESCAMILLA, VCTOR HUGO GONZALEZ-CHVEZ, UNIVERSIDAD AUTNOMA DE NUEVO LEN, EDUARDO MARTNEZ-GUERRA, ANDRS GARAY-TAPIA, Centro de Investigacin en Materiales Avanzados, EDGAR MARTNEZ-GUERRA, UNIVERSIDAD AUTNOMA DE NUEVO LEN — Recently, phosphorene has also been scored well as a functional material for two-dimensional electronic and optoelectronic devices. That is, because in contrast to graphene, black phosphorous has an inherent, direct and appreciable band gap that can be modulated with the numbers of layers. However, the presence of exposed lone pairs at the surface makes phosphorous very reactive to air and humidity and consequently, degradation of its properties. No such fundamental explanation have been made, thus corresponding first principle predictions to evaluate diffusion of O over and along a mono- and a few layers are indispensable. Energy barriers and the mechanisms of oxygen diffusion on mono- and a few layer of black phosphorous were calculated using the NEB(Nudge Elastic band) method as implemented in Quantum Espresso. The electronic states are expanded in plane waves with kinetic-energy cutoffs of 25 and 200 Ry for the wave function and charge density, respectively. Also, as the H<sub>2</sub>O and O<sub>2</sub> are polar molecules, spin-polarized calculations have been carried out. We evaluated the diffusion barriers for O<sub>2</sub> and H<sub>2</sub>O on phosphorene along zigzag, armchair and intermediated directions. Our calculations show that diffusion of O is preferred on zigzag directions and dissociation of O<sub>2</sub> is favored as a result of energy gains of about 2 eV. Also, apparently diffusion pathways are blocked along layers.

**G1.00049 Effect of the electric field on buckled and puckered arsenene.** , VICTOR HUGO CHAVEZ, HECTOR NOE FERNANDEZ-ESCAMILLA, EDGAR MARTNEZ-GUERRA, UNIVERSIDAD AUTONOMA DE NUEVO LEON — With the emergence of new 2D materials, more recently phosphorene, arsenene appears as a new candidate to be explored for electronic devices. We have studied the stability of arsenene pristine and the effect of a transversal electric field on its electronic properties. The calculations were performed using the SIESTA code, with the GGA exchange-correlation functional in the PBE form. We have used numerical atomic orbitals as the basis set for the valence wavefunctions employing a double  $\zeta$ -polarized basis. We use the Perdew-Becke pseudopotential for an As atom that includes the scalar-relativistic effect and Troullier-Martins parametrization. We adopt the Monkhorst-Pack scheme for k-point sampling of Brillouin zone integrations with 25 25 1 and 25 25 1 for the buckled/planar and puckered systems, respectively. We found that buckled and puckered arsenenes are stable and posses indirect gap. The effect of the electric field on the electronic structure of the buckled arsenene is the modulation of indirect to direct gap, while in puckered arsenene the gap linearly decreases as electric field is increased. This research was supported by Consejo Nacional de Ciencia y Tecnología (Conacyt) under Grant No. 43830-F.

**G1.00050 ABSTRACT WITHDRAWN —**

**G1.00051 ABSTRACT WITHDRAWN —**

**G1.00052 A theoretical study on the thermal oxidation of silicon carbide: Chemical species at the SiO<sub>2</sub>/SiC interface**<sup>1</sup> , NOBUO TAJIMA, The University of Tokyo, TOMOAKI KANEKO, JUN NARA, TAKAHIRO YAMASAKI, TATSUO SCHIMIZU, National Institute for Materials Science, KOICHI KATO, The University of Tokyo, TAKAHISA OHNO, National Institute for Materials Science — Silicon carbide (SiC) is potentially a suitable candidate of the channel materials of power devices since it has wide bandgap, high electron mobility, and thermal conductivity. Furthermore, it is favorable for device fabrication as it can be thermally oxidized to create insulating silicon oxide (SiO<sub>2</sub>) layer. However, the SiC devices of current technology do not show acceptable performance because of a defective nature of the created SiO<sub>2</sub>/SiC stacking structure, which causes problems such as channel mobility degradation, threshold voltage increase, and leakage current. The origins of the defective nature are not understood so far, though it is presumed that they are rather concentrated at the interface. In the present study, we have performed first principles calculations to know the chemical species possibly produced at the oxide interface of thermally oxidized SiC. The First principles simulation code PHASE/0 (<http://www.ciss.iis.u-tokyo.ac.jp/riss/english/project/device/>) was used in the theoretical calculations.

<sup>1</sup> A portion of this research was supported by the grant from MEXTs project and carried out in partnership with the University of Tokyo

**G1.00053 Preparation and study of Titanium Nitride films by reactive sputtering and an investigation of target poisoning during the process.**<sup>1</sup> , TAREQUE AZIZ, ABDUL RUMAIZ, Brookhaven Natl Lab — Titanium Nitride (TiN<sub>x</sub>) thin films were prepared by reactive dc sputtering in presence of Ar-N<sub>2</sub> plasma. The thin films were grown on Quartz and pure Si surfaces. The Ar-N<sub>2</sub> content ratio was gradually varied while the substrate and the Titanium target were kept at room temperature. Structural properties, optical and electrical properties of the thin films were studied by using X-ray Photoelectron Spectroscopy (XPS) and XRD and 4 probe resistivity measurement. Target poisoning of the Ti target was also studied by varying reactive gas concentration and measuring the target current. A study of target current vs growth rate of the films was performed to investigate the onset of "poison" mode. Although there was an insignificant drop in plasma current, we noticed a drop in the deposition rate. This result was tested against Monte Carlo simulations using SRIM simulations. Effects of annealing on the crystallinity and the sheet resistance will also be discussed.

<sup>1</sup> The work has been supported by BSA,DOE

**G1.00054 Optimization of metamorphic buffers for molecular epitaxial growth of high quality AlInSb/InSb quantum structures** , YINQIU SHI, WIN, Department of Physics and Astronomy, DENISE GOSSELINK, WIN, Department of Electrical and Computer Engineering, KAVEH GHARAVI, IQC, Department of Physics and Astronomy, JONATHAN BAUGH, IQC, Department of Chemistry, ZBIGNIEW WASILEWSKI, WIN, Department of Electrical and Computer Engineering, University of Waterloo, Canada — Strong spin-orbit interaction in InSb quantum wells and wires makes them attractive candidates for the realization of Majorana bound states. Molecular beam epitaxy (MBE) is the best tool to obtain these structures but lack of suitable substrates demands development of low dislocation density, smooth metamorphic buffer layers, lattice matched to the InAlSb/InSb material system. Here we present a comparative study of MBE growth of such buffers on GaAs substrates oriented in [001] crystallographic direction and [001] offcut 2° towards [100]. 1 $\mu$ m-thick AlSb nucleation buffers were grown on both substrates with optimized growth conditions. The high density of surface terraces on the offcut substrates effectively suppressed the formation of undesirable hillocks, typical of growth on [100] substrates. Further lattice constant grading and dislocation filtering was achieved through repetitions of Al<sub>0.24</sub>In<sub>0.76</sub>Sb interlayers in the Al<sub>0.12</sub>In<sub>0.88</sub>Sb matrix. Surface morphology evolved quite differently through these stages of metamorphic buffer preparation on both types of substrates, resulting in up to 50nm-high hillocks for the on-orientation substrates and hillock-free morphology for 2° off substrates. Mechanism of hillock suppression is discussed.

**G1.00055 Epitaxial aluminum on hybridized InAs/GaSb quantum wells** , BING-BING TONG, TING-XIN LI, XIAO-YANG MU, CHI ZHANG, RUI-RUI DU, Peking University — Hybridized InAs/GaSb quantum wells (QW) are approved the existence of helical edge channels. According to the theoretical prediction, the combination with superconductor will lead to superconducting topological phase and realization of Majorana bound state (MBS). Besides, InAs/GaSb material shows a low Schottky barrier to superconductor, and high quality of superconductor-topological insulator interface will result in hard induced gap. In recent report [1], under low temperature of substrate, there is a good lattice match between InAs nanowire and Al in the same direction. In our lab, we perform aluminum epitaxy on the in-situ cleaved InAs/GaSb QW with similar methods in our ultra-high vacuum STM system. After metal epitaxy, the Al layer can be selectively etched for fabricating the superconductor-topological insulator junction devices. [1] P. Krogstrup, N. L. B. Ziino, W. Chang, S. M. Albrecht, M. H. Madsen, E. Johnson, J. Nygård, C. M. Marcus, T. S. Jespersen, Nature Materials 14, 400 (2015).

**G1.00056 Synthesis and Analysis of MnTiO<sub>3</sub> Thin Films on ITO Coated Glass Substrates**<sup>1</sup> , EMERICK MARTIN, MEHMET-ALPER SAHINER, Seton Hall Univ — Perovskites like Manganese Titanium Oxide have interesting chemical properties that may be advantageous to the development of p-n junction photovoltaic cells. Due to the limited understanding behind the compound, it is essential to know the characteristics of it when it is deposited in thin film form. The cells were created using pulsed laser deposition method for two separate mediums (first layers after ITO). ZnO was deposited onto ITO glass for the first sample. For the second sample, a layer of pure Molybdenum was deposited onto the ITO glass. The MnTiO<sub>3</sub> was then deposited onto both samples. There was a target thickness of 1000 Angstroms, but ellipsometry shows that, for the Mo based sample, that film thickness was around 1500 Angstroms. There were inconclusive results for the ZnO based sample. The concentration of active carriers was measured using a Hall Effect apparatus for the Mo based sample. The XRD analyses were used to confirm the perovskite structure of the films. Measurements for photoelectric conversion efficiency were taken using a Keithley 2602 SourceMeter indicated low values for efficiency. The structural information that is correlated with the low electrical performance of this sample will be discussed.

<sup>1</sup> SHU-NJSGC Summer 2015 Fellowship

**G1.00057 The Study of the Thermoelectric Properties of Phase Change Materials<sup>1</sup>** , MING YIN, MOHAMMED ABDI, ZIBUSISU NOIMANDE, GODWIN MBAMALU, Benedict College, DHEYAA ALAMEERI, TIMIR DATTA, University of South Carolina — We study thermoelectric property that is electrical phenomena occurring in conjunction with the flow of heat of phase-change materials (PCM) in particular GeSbTe (GST225). From given sets of material parameters, COMSOL Multiphysics heat-transfer module is used to compute maps of temperature and voltage distribution in the PCM samples. These results are used to design an apparatus including the variable temperature sample holder set up. An Arbitrary/ Function generator and a circuit setup is also designed to control the alternation of heaters embedded on the sample holder in order to ensure sequential back and forward flow of heat current from both sides of the sample. Accurate values of potential differences and temperature distribution profiles are obtained in order to compute the Seebeck coefficient of the sample. The results of elemental analysis and imaging studies such as XRD, UV-VIS, EDEX and SEM of the sample are obtained. Factors affecting the thermoelectric properties of phase change memory are also discussed.

<sup>1</sup>NNSA/ DOD Consortium for Materials and Energy Studies

**G1.00058 Electron Density and Capacitance at the interface of Au-ZnO Based Schottky Diode** , CHIN-SHENG WU, Yuan Ze university, Taiwan — ZnO with wide direct band gap (3.37 eV) is a well-known and an interesting compound semiconducting material, which have been used for the fabrication of optical, electrical, and piezoelectric devices such as light emitting diodes, solar cells. Schottky diodes are associated with quicker switching and lower turn on voltages compared to p-n junction diodes. J-V characteristics exhibit nonlinear rectifying behavior with threshold voltage of 2.1 V. The barrier heights were found to be 0.61 eV. The measured capacitance for the Schottky junction depends on the reverse bias potential and frequency. At the lower frequencies the capacitance has the higher values due to the trapping occurred at the interface through the surface roughness and lattice mismatch. We perform model potential calculation with quantum well around the interface. Model potentials allow some degree of freedom in the design of the emitted wavelength through adjustment of the energy levels. We apply the various well width  $w$  and barrier height  $V$  in order to match the device information made by Willander. Solving the Schrödinger equation with exchange- correlation energy and effective mass of electrons will produce values of the energy levels and states. The variational barrier heights result in the change of the electron density This accounts for the excessive capacitance at the interface of Schottky diode.

**G1.00059 Electronic structure and magnetism in partially gated graphene nano-ribbons** , RITA MAJI, JOYDEEP BHATTACHARJEE, NATIONAL INSTITUTE OF SCIENCE EDUCATION AND RESEARCH, BHUBANESWAR, ODISHA, INDIA — Properties of 3-coordinated carbon networks evolve upon physical or chemical functionalization depending on the resultant modification to  $\pi$ -conjugation and its interplay with the anti-ferromagnetic (AFM) correlation between unpaired  $2p_z$  electrons at nearest neighbor (nn) sites. Although the former generally dominates the latter in determining the ground state, we propose it to be possible to enhance and modify nn magnetic correlations by inducing non-uniform density of electrons through application of bias partially within a periodic unit. Using tight-binding based mean-field Hubbard model and the DFT based first principles calculations, we show in ZGNRs as well as AGNRs, a systematic emergence of nn ferromagnetic (FM) correlation and spin-separation within and in the vicinity of positively biased region in a unit-cell, as an intermediate phase, as the ground state evolves from AFM to non-magnetic as a function of bias voltage. The associated evolution of the degenerate band-structure from direct to indirect is also punctuated by lifting of degeneracy coinciding exactly with the appearance of nn FM correlation and accommodating energy windows for half-metallic transport. In ZGNR such localization driven nn FM correlation leads to non-trivial edge magnetism and band-structure.

**G1.00060 Effective multiband Hamiltonian for InAs in wurtzite phase<sup>1</sup>** , PAULO E. FARIA JUNIOR, TIAGO CAMPOS, CARLOS M. O. BASTOS, GUILHERME M. SIPAHI, University of Sao Paulo, MARTIN GMITRA, JAROSLAV FABIAN, University of Regensburg — Recent advances in nanostructure growth techniques allowed the synthesis of new III-V compounds with wurtzite crystal structure[1]. Although ab initio band structures for these new wurtzite materials can be found in the literature[2], we still lack multiband models and parameter sets that can be simply used to investigate, for instance, quantum confinement effects. In this study, we calculated the ab initio band structure of bulk InAs wurtzite and developed a multiband k.p Hamiltonian to describe the energy bands around the energy gap. In order to correctly describe the spin splitting effects we included the k-dependent spin-orbit term, often neglected in literature. We showed that our model is very robust to describe the important features of the band structure and also the spin splittings with great agreement to the ab initio values. [1] P. Caroff et al., Nat. Nanotechnol. 4, 50 (2009). [2] A. De and C. E. Pryor, PRB 81, 155210 (2010).

<sup>1</sup>CNPq (149904/2013-4 and 88887.110814/2015-00), CAPES PVE (88881.068174/2014-01), DFG SFB 689 and FAPESP (2012/05618-0)

**G1.00061 Magneto-Electronic Energy Spectra of Monolayer Tinene** , S. C. CHEN, Center for Micro/Nano Science and Technology, National Cheng Kung University, F. L. SHYU, Department of Physics, Chinese Military Academy, J. Y. WU, Department of Physics, National Cheng Kung University, C. W. CHIU, Department of Physics National Kaohsiung Normal University, C.H. LEE, Institute of Applied Physics, National Chengchi University, M. F. LIN, Department of Physics, National Cheng Kung University — The novel magnetic quantization in monolayer tinene, being closely related to the  $sp^3$  bondings, spin-orbital coupling and magnetic field, is investigated by the generalized tight-binding model. The feature-rich two groups of low-lying LLs, which are, respectively, dominated by the  $2p_z$  orbitals and  $(2p_x, 2p_y)$  orbitals, are revealed near the Fermi level simultaneously. They are very different in the spatial distributions, state degeneracy, spin configurations and  $B_z$ -dependence. The  $B_z$ -dependent energy spectra might be approximated by the simple relationships. The splittings of LLs in the second groups are due the effects of magnetic fields. The unique magnetic-electronic properties in tinene are absent in graphene, silicene and germanene. The predicted magneto-electronic energy spectra could be directly verified by the STS measurements.

**G1.00062 Ab-Initio Computations of Electronic and Related Properties of cubic Lithium Selenide ( $Li_2Se$ )** , ABDOULAYE GOITA, Department of Electrical Engineering, Southern University and AM College, Baton Rouge, LA 70813, USA, IFEANYI H. NWIGBOJI, Department of Computational Science, University of Texas at El Paso, El-Paso, TX 79968 USA, YURIY MALOZOVSKY, DIOLA BAGAYOKO, Department of Physics, Southern University and AM College, Baton Rouge, LA 70813, USA — We present theoretical predictions, from ab-initio, self-consistent calculations, of electronic and related properties of cubic lithium selenide ( $Li_2Se$ ). We employed a local density approximation (LDA) potential and the linear combination of atomic orbitals (LCAO). We performed the computations following the Bagayoko, Zhao, and Williams (BZW) method, as enhanced by Ekuma and Franklin (BZW-EF). Our results include electronic energies, total and partial densities of states, effective masses, and the bulk modulus. The theoretical equilibrium lattice constant is 5.882 Å. We found cubic  $Li_2Se$  to have a direct band gap of 4.363 eV (prediction), at  $\Gamma$ . This gap is 4.065 eV for a room temperature lattice constant of 6.017 Å. The calculated bulk modulus is 31.377 GPa. Acknowledgments: This work was funded in part by the National Science Foundation (NSF) and the Louisiana Board of Regents, through LASIGMA [Award Nos. EPS- 1003897, NSF (2010-15)-RII-SUBR] and NSF HRD-1002541, the US Department of Energy – National, Nuclear Security Administration (NNSA) (Award No. DE- NA0002630), LaSPACE, and LONI-SUBR.

**G1.00063 Ab-initio Density Functional Theory (DFT) Studies of Electronic, Transport, and Bulk Properties of Sodium Oxide ( $\text{Na}_2\text{O}$ ).** , DANIEL POLIN, Department of Physics New York University, New York, NY 10003, USA, JOSHUA ZIEGLER, Department of Physics Case Western Reserve University, Cleveland, OH 44106, USA., YURIY MALOZOVSKY, DIOLA BAGAYOKO, Department of Physics Southern University and AM College, Baton Rouge, LA 70813, USA — We present the findings of *ab-initio* calculations of electronic, transport, and structural properties of cubic sodium oxide ( $\text{Na}_2\text{O}$ ). These results were obtained using density functional theory (DFT), specifically a local density approximation (LDA) potential, and the linear combination of Gaussian orbitals (LCGO). Our implementation of LCGO followed the Bagayoko, Zhao, and Williams method as enhanced by the work of Ekuma and Franklin (BZW-EF). We describe the electronic band structure of  $\text{Na}_2\text{O}$  with a direct band gap of 2.22 eV. Our results include predicted values for the electronic band structure and associated energy eigenvalues, the total and partial density of states (DOS and pDOS), the equilibrium lattice constant of  $\text{Na}_2\text{O}$ , and the bulk modulus. We have also calculated the electron and holes effective masses in the  $\Gamma$  to L,  $\Gamma$  to X, and  $\Gamma$  to K directions. Acknowledgments: This work was funded in part by the National Science Foundation (NSF) and the Louisiana Board of Regents, through LASiGMA [Award Nos. EPS- 1003897, NSF (2010-15)-RII-SUBR] and NSF HRD-1002541, the US Department of Energy – National, Nuclear Security Administration (NNSA) (Award No. DE- NA0002630), LaSPACE, and LONI-SUBR.

**G1.00064 Auger recombination in InGaN/GaN** , CHI-CHAN HUANG, WEN-CHING CHAO, WEI-SHENG CHEN, ANTARYAMI MOHANTA, DER-JUN JANG, Department of Physics, National Sun Yat-sen University — The radiative and nonradiative recombination of In-GaN/GaN samples were studied by time-resolved photoluminescence apparatus and time-integrated photoluminescence by photoexcitation with laser pulses of temporal resolution of 100 ps and energies of 3.0 and 4.5 eV. We found that the Shockley-Read-Hall and Auger coefficients derived from the analysis of TRPL using the rate equation of carrier concentration were much larger than those derived from the time-integrated PL photoexcited with various numbers of carrier concentration. We will discuss the discrepancy.

**G1.00065 Effect of GaAs spacer layer thickness on optical properties of multi-stacked InAs/GaAs quantum dots** , CHIA-HSIANG WANG, ANTARYAMI MOHANTA, DER-JUN JANG, FU-YU WANG, Department of Physics, National Sun Yat-sen University, J. S. WANG, Department of Physics, Chung Yuan Christian University — Effect of GaAs spacer layer thickness ( $d_{\text{GaAs}}$ ) on multi-stacked InAs/GaAs quantum dots are investigated by photoluminescence (PL) and excitation wavelength ( $\lambda_{\text{exc}}$ ) dependent pump-probe reflection spectroscopy. Dominance of light hole transition in the PL spectra is observed at smaller  $d_{\text{GaAs}}$  (<15 nm). Double maxima  $(\Delta R/R)_1$  and  $(\Delta R/R)_2$  appear in the differential reflection spectra (DRS) at intermediate  $\lambda_{\text{exc}}$  beyond which positive to negative reversal of the DRS is observed due to dominating effect of inter band absorption in InAs wetting layer. The  $\lambda_{\text{exc}}$  at which double maxima occur, and the positive to negative reversal starts is found to be dependent on  $d_{\text{GaAs}}$ .

**G1.00066 Observation of weak carrier localization in green emitting InGaN/GaN multi-quantum well structure** , WEN-CHING CHAO, ANTARYAMI MOHANTA, TSU-CHIANG YEN, WEI-SHENG CHEN, DER-JUN JANG, Department of Physics, National Sun Yat-sen University — Green emitting InGaN/GaN multi-quantum well samples were investigated using photoluminescence (PL) and time-resolved photoluminescence (TRPL) spectroscopy. Weak carrier localization with characteristic energy of ~12 meV due to an inhomogeneous distribution of In in the InGaN quantum well (QW) layer is observed. The temperature dependence of the PL peak energy exhibits S-shape phenomenon and is comparatively discussed within the framework of the Varshni's empirical formula. The full width at half maximum (FWHM) of the PL emission band shows an increasing-decreasing-increasing behavior with increasing temperature arising from the localized states caused by potential fluctuations. The radiative life time,  $\tau_r$ , extracted from the TRPL profile shows  $\sim T^{3/2}$  dependence on temperature above 200 K, which confirms the absence of the effect of carrier localization at room temperature.

**G1.00067 The carrier recombination in  $\text{ZnO}/\text{Al}_2\text{O}_3$  superlattice** , KO MAI, WEI-SHENG CHEN, TSU-CHIANG YEN, DER-JUN JANG, YUNG-SUNG CHEN, Department of Physics, National Sun Yat-sen University — The optical properties of  $\text{ZnO}/\text{Al}_2\text{O}_3$  superlattice are studied by a time-correlated single-photon counting apparatus with temporal resolution of 150 ps using laser pulses of energy 4.5 eV from a Ti:sapphire laser. Photoluminescence emission around 550 nm is clear evident for photoexcitation with energies of 3.0 and 4.5 eV. The differences of the widths of the PL spectrum and lifetimes of carrier recombination are compared for both photoexcitation and are explained by the spatial overlap of the carriers inside the superlattices.

**G1.00068 Quantum Interference, Geometric-phase Effects, and Semiclassical Transport in Quantum Hall Systems at Low Magnetic Fields** , CHUN-FENG HUANG, 2nd Patent Division, Intellectual Property Office, Ministry of Economic Affairs, Taipei, Taiwan 106, R.O.C., I.-H. TSAI, Department of Mathematics, National Taiwan University, Taipei, Taiwan, R. O. C. — It is well-established how the quantum interference induces strong localization leading to quantum Hall effect at high enough magnetic fields. Decreasing the magnetic fields, however, the localization strength can be reduced and the semiclassical magneto-oscillations following Shubnikov-de Haas formula appear in most quantum Hall systems. To understand the transport properties as the localization strength becomes weak, our team has investigated the magneto-resistance in some quantum Hall systems at low magnetic fields. Under the semiclassical transport, the crossing points in Hall plateaus showed Landau-band quantization and microwave-induced heating demonstrated the band-edge equivalence important to Landau-level addition transformation [1-2]. We note that such equivalence is consistent with the edge universality based on the random matrices of Wigner type, and the Landau-band quantization can be explained by considering geometric phase effects. From our study, some quantum Hall features can survive as the semiclassical transport reveals the insufficient localization. [1] Solid State Commun. 141, 17 (2007). [2] Solid State Commun. 156, 45 (2013).

**G1.00069 Stability of composite fermion states in Chern insulators<sup>1</sup>** , PAWEŁ POTASZ, BLAZEJ JAWOROWSKI, wroclaw university of technology — We analyze an existence of composite fermion (CF) states in fractional Chern insulators (FCI) using exact diagonalization. The consider Chern insulator models for spinless fermions exhibit a signature of CF states at 2/5 and 3/7 filling factors. Evidences of fractional quantum Hall type phases for a region in a parameter space with larger energy gap are shown by looking at momenta of the n-fold degenerate ground state, spectral flow, quasihole excitation spectrum, and entanglement spectra. We analyze stability of phases as a function of model parameters showing strong correlation with flatness of Berry curvature.

<sup>1</sup>The authors acknowledges partial financial support from the sources granted for science development in the years 2013-2016, Grant No. IP2012 007372

**G1.00070 Multi-state magnetoresistance in ferromagnet/organic-ferromagnet/ferromagnet junctions.**<sup>1</sup>, GUICHAO HU, Shandong Normal University, SHIJIE XIE, Shandong University — Organic ferromagnets (OFs) are fascinating in the field of organic spintronics, since they combine both the ferromagnetic and organic properties. The utilization of OFs in the design of organic spintronic is promising to generate some novel effects [1-4]. Here, we designed an organic spin valve by sandwiching the OF between two ferromagnets. By calculating the spin-dependent transport property, we found that the current through the device strongly depends on the alignment of the magnetization orientation of the electrodes and the OF. The spin-related electron tunneling between the ferromagnetic electrodes suffers a further spin selection from the spin-polarized states of the central OF. This work indicates a realization of four-state magnetoresistance based on OFs, which may be manipulated by a magnetic field to control the magnetization orientations of the ferromagnets and the OF. [1] G. C. Hu, M. Y. Zuo, Y. Li, J. F. Ren, and S. J. Xie, Appl. Phys. Lett. 104, 033302 (2014). [2] G. C. Hu, H. Wang, J. F. Ren, S. J. Xie, and C. Timm, Org. Electron. 15, 118 (2014). [3] G. C. Hu, K. L. He, A. Saxena, and S. J. Xie, J. Chem. Phys. 129, 234708 (2008). [4] G. C. Hu, Y. Guo, J. H. Wei, and S. J. Xie, Phys. Rev. B 75, 165321 (2007).

<sup>1</sup>Support from the NSF of China is acknowledged.

**G1.00071 Theoretical study on electronic structure of bathocuproine: Renormalization of the band gap in the crystalline state and the large exciton binding energy**<sup>1</sup>, SUSUMU YANAGISAWA, Department of Physics and Earth Sciences, Univ. of the Ryukyus, SHIN-NO-SUKE HATADA, YOSHITADA MORIKAWA, Department of Precision Science and Technology, Osaka Univ. — Bathocuproine (BCP) is a promising organic material of a hole blocking layer in organic light-emitting diodes or an electron buffer layer in organic photovoltaic cells. The nature of the unoccupied electronic states is a key characteristic of the material, which play vital roles in the electron transport. To elucidate the electronic properties of the molecular or crystalline BCP, we use the GW approximation for calculation of the fundamental gap, and the long-range corrected density functional theory for the molecular optical absorption. It is found that the band gap of the BCP single crystal is 4.39 eV, and it is in agreement with the recent low-energy inverse photoemission spectroscopy measurement. The polarization energy is estimated to be larger than 1 eV, demonstrating the large polarization effects induced by the electronic clouds surrounding the injected charge. The theoretical optical absorption energy is 3.68 eV, and the exciton binding energy is estimated to be 0.71 eV, implying the large binding in the electron-hole pair distributed around the small part of the molecular region.

<sup>1</sup>This work was supported by the Grants-in-Aid for Young Scientists (B) (No. 26810009), and for Scientific Research on Innovative Areas "3D Active-Site Science" (No. 26105011) from Japan Society for the Promotion of Science.

**G1.00072 Magneto-conductance of hybrid quantum ring**, NAMMEE KIM, HEESANG KIM, DAE-HAN PARK, Soongsil University — Magneto-conductance behaviors of hybrid magnetic-electric quantum rings are studied. The hybrid magnetic-electric quantum rings are formed by spatially in-homogeneous distributions of magnetic fields and the additional antidot electrostatic potential. Electrons are both magnetically and electrostatically confined to the plane. Electronic structures of hybrid magnetic-electric quantum rings and two terminal conductance taking into account the resonant backscattering via the magnetic edge channels are shown including comparison with the case of a conventional electric quantum ring with uniform external magnetic field.

**G1.00073 Local current-voltage characteristic of thin film ferroelectric SrTiO<sub>3</sub>**, ANDREW JOHNSON, Hope College, RYAN COTTIER, NIKOLETA THEODOROPOLU, Texas State University, JOSHUA VEAZEY, Grand Valley State University — Certain thin-film ferroelectric oxide-semiconductor heterostructures allow for reversible, local changes in conductivity, with potential applications including non-volatile memory devices. Force microscopy techniques were used to investigate the impact of the ferroelectric polarization state on local conductive properties of ferroelectric SrTiO<sub>3</sub> (STO) thin films deposited by molecular beam epitaxy onto both p- and n-type Si(001) substrates. Under certain conditions, local current voltage (I-V) curves exhibited pronounced hysteresis under forward bias. These characteristics are not, however, well-correlated with the polarization state of the ferroelectric STO. Alternative explanations for the current hysteresis are presented. This work was generously supported by the Hope College Department of Physics Frissel Research Fund, and the National Science Foundation under NSF-MRI Grant No. CHE-1126462. Support by the NSF-Career grant, DMR-1255629 is gratefully acknowledged. Portions of this work were conducted in the CMP group facilities at Michigan State University; we would like to gratefully acknowledge R. Loloee and the MSU physics department for their support.

**G1.00074 Resonant Transmission through Serially Connected Hexagonal Nanorings with Magnetic Flux Effects**<sup>1</sup>, ERIC HEDIN, YONG JOE, Ball State University — Nanostructures composed of six quantum dots (QDs) connected in a ring are linked together in a linear chain with each ring separated by a coupling segment from adjoining rings. A tight-binding model is used to obtain the electron transmission through an arbitrary number of rings in series as a function of energy, external magnetic field, coupling parameters, and QD site energy values. Modifications of the transmission band structure as a function of external field, due to the Aharonov-Bohm and Zeeman effects, demonstrate control over the conductance properties of the linear chain of nano-rings. Resonant transmission effects (with electron energy equal to the QD site energy values) show a complex dependence upon an interplay of magnetic flux, inter-ring coupling, and the strength of the coupling between the ring system and the external leads. For specific values of lead and ring couplings, nearly full transmission (ballistic transport) is seen to occur across a broad energy range, independent of the number of rings in series.

<sup>1</sup>Partially supported by BSU ASPIRE program

**G1.00075 Achieving Thermodynamic Limit of Subthreshold Slope in Nanoscale Schottky Barrier MOSFET with Pillar Structure Inserted**<sup>1</sup>, JUNG-YONG LEE, SUNGCHUL JUNG, KIBOG PARK, Ulsan Natl Inst of Sci & Tech — As the device size decreases continuously by scaling in the current Si CMOS technology, subthreshold slope which is related to device operation and leakage current becomes more and more important. Especially, the drain induced barrier lowering (DIBL) modulation for improving subthreshold slope in metal/oxide/metal field effect transistor (MOSFET) is difficult to achieve. We propose a new device structure, edge-over Schottky Barrier MOSFET (EO-SB-MOSFET), which shows low DIBL and subthreshold slope approaching the thermodynamic limit of 60 mV/DEC at room temperature. EO-SB-MOSFET has a pillar structure which elongates the transistor channel by forming it over the edge of pillar. Hence, EO-SB-MOSFET has a much longer channel compared with planar MOSFET in the same pitch. We performed 2-dimensional TCAD modeling on an EO-SB-MOSFET with channel lateral size of 6.5 nm and pillar height of 36 nm. The TCAD modeling predicts DIBL of ~5 mV/V, subthreshold slope of ~61.3 mV/DEC, and off-state current of ~0.1 nA/μm at drain bias 0.5 V. It is also noticed that the subthreshold slope gets further close to the thermodynamic limit as the pillar height increases.

<sup>1</sup>Supported by NRF in South Korea (2013R1A1A2007070)

## **G1.00076 Study of quantum transport in a magnetic wire<sup>1</sup> , SANKALPA GHOSH<sup>2</sup>, PUJA MONDOL, ANKIP KUMAR,**

Physics Department, Indian Institute of Technology, Delhi, ALAIN NOGARET<sup>3</sup>, Department of Physics, University of Bath, Bath BA2 7AY, UK, HARVEY BEERE, DAVID RITCHIE, Cavendish Laboratory, University of Cambridge, CB3 0HE, UK — Spatially varying magnetic fields lead to some very interesting physics for two dimensional electron gas. In this work we present some recent results based on the experimental observation of edge states confined by magnetic potentials and their dependence on the strength of the magnetic field strength as well as electrostatic gate voltage. By numerically integrating Schrödinger Equation we explain the behavior of such magneto-electric edge states in such two dimensional electron gas.

<sup>1</sup>UGC UKIERI Thematic Partnership

<sup>2</sup>Principal Indian Investigator

<sup>3</sup>Principal UK Investigator

## **G1.00077 UNDERGRADUATE RESEARCH —**

**G1.00078 Flexo-Electro-Optical Properties of Fullerene-C(Buckyballs) Suspended in 4'-Pentyl-4-Biphenyl (5CB)** , JONATHAN FOUST, ANGELO VISCO, RIZWAN MAHMOOD, Slippery Rock Univ — We have investigated electro optical properties of a widely studied liquid crystal (5CB) when fullerene C-60 (buckyballs) is suspended in various concentrations as a function of temperature. Under a polarizing microscope, we have observed disclination (defect) points at the sites of buckyballs suggesting a strong interaction between the two components. The data indicate a shift in the transition temperature and sudden decrease in dielectric anisotropy ( $\Delta\epsilon$ ) at some critical concentration (~0.15 wt. %) of fullerene. A sudden increase was also observed upon increasing the concentration of buckyballs that remains constant within the experimental uncertainty. **Keywords:** buckyballs, fullerene, liquid crystal, dielectric anisotropy **Acknowledgements:** RM acknowledges the financial support of the Grant Office, Slippery Rock University.

## **G1.00079 ABSTRACT WITHDRAWN —**

**G1.00080 Electrical response of monolayer MoS<sub>2</sub> to vapors of aliphatic alcohols<sup>1</sup>** , PABLO SEPULVEDA, IDALIA RAMOS, University of Puerto Rico-Humacao, CARL NAYLOR, A.T. CHARLIE JOHNSON, University of Pennsylvania, NICHOLAS PINTO, University of Puerto Rico-Humacao — Monolayer MoS<sub>2</sub> crystals were used to sense vapors of Methanol, Ethanol and 1-Propanol. Due to the large surface area, these sensors are expected to show rapid response and recovery times. The current through the sensor was monitored as a function of time with a constant applied voltage. This current decreased in the presence of the sensing gas and recovered upon its removal. Our results show that the response time gets longer as the size of the alcohol increases, but the recovery time stays approximately the same (~20s) regardless of the size of the alcohol. The sensitivity was also seen to decrease as the size of the alcohol increased. These observations could be associated with the slower diffusion of the larger alcohol molecules into the MoS<sub>2</sub> crystal. The sensors are also fairly robust since the same sensor was used in all of the measurements after annealing in air at 70C for 10 minutes. Additional sensing measurements as a function of gas concentration will also be presented.

<sup>1</sup>This work was supported by NSF under grants DMR-PREM-1523463 and DMR-RUI-1360772.

**G1.00081 Schottky diode based on WS<sub>2</sub> crossed with PEDOT/PSSA<sup>1</sup>** , DELIRIS ORTIZ, NICHOLAS PINTO, University of Puerto Rico - Humacao, CARL NAYLOR, A.T. CHARLIE JOHNSON, University of Pennsylvania — An easy technique to fabricate a Schottky diode with WS<sub>2</sub> and PEDOT-PSSA under ambient conditions is presented. WS<sub>2</sub> is an air stable transition metal dichalcogenide semiconductor. When connected as a field effect transistor, WS<sub>2</sub> exhibited n-type behavior with a charge mobility of ~7cm<sup>2</sup>/V-s on SiO<sub>2</sub>. PEDOT/PSSA is a conducting polymer that can be electro-spun to form fibers with a conductivity of ~1 S/cm. In this work we fabricated a Schottky diode by crossing a CVD grown monolayer WS<sub>2</sub> crystal with a single electro-spun PEDOT/PSSA fiber. The resulting diode characteristics were analyzed assuming the standard thermionic emission model of a Schottky junction. Analysis of the results includes the ideality parameter of 4.75, diode rectification ratio ~10, and a turn on voltage of 1.4V. Efforts to investigate if these parameters are tunable with a back gate will also be presented.

<sup>1</sup>This work was supported by NSF-DMR-1523463 and NSF DMR RUI-1360772. ATJ acknowledges support from EFRI 2DARE EFMA-1542879.

**G1.00082 Opto-electronic Properties of Monolayer-Protected Clusters of Au functionalized with a New Fluorescent Ligand** , THOMAS KOUNTZ, Towson University, VIRAJ THANTHIRIGE, Western Michigan University, KEITH REBER, MARY SAJINI DEVADAS, Towson University — Metal nanoclusters are the focus of intense study due to their interesting optical, electronic, and catalytic properties; specifically gold clusters. The applications of gold monolayer-protected clusters (MPCs) are being researched by a series of optical spectroscopic and voltammetric analyses to determine core size, atom-level composition, charge states, and optical/electrical properties. Understanding these fundamental properties is critical for both expansion of applications and creation of new MPCs. The purpose of this study is to expand the applications of gold MPCs, with the attachment of a new coumarin surface ligand - synthesized specifically for this experiment. Our focus in this research is on quantum clusters - specifically Au<sub>25</sub>(C<sub>6</sub>S)<sub>18</sub>. This MPC is researched particularly because of its inherent stability being a magic number cluster. It is created by means of a modified Brust-Schiffrin method. The applications that are influenced include but are not limited to: catalytic activity, solar energy conversion, size-tunable fluorescence, sensors, and optical electronics.

**G1.00083 Crystallization Trends of PEO-b-PCL with Solvent and Temperature Effects** , KRISTI ALLEN, ALLISON CARANDANG, RYAN VAN HORN, Allegheny College — There is a great deal of interest in being able to selectively modify properties of certain polymers. This increases the amount of control that can be exercised over end products in terms of the hydrophobicity or hydrophilicity, transparency, and brittleness and is highly valued in the biomedical industry. In this case, the crystallization trends of the diblock co-polymer poly(ethylene-oxide)-b-poly( $\epsilon$ -caprolactone) (PEO-b-PCL) were observed with the manipulation of solvent and drying temperatures in a variety of samples. The solvents utilized included tetrahydrofuran, chloroform, and toluene. The crystallized samples were scanned via infrared spectroscopy. Results showed highest amounts of PEO crystallization compared to PCL crystallization in toluene while the lowest values were seen in samples in tetrahydrofuran. The chloroform samples fell in the middle. Moderate differences were observed in different molecular weight samples.

**G1.00084 Collective dynamics of non-transitively coupled active oscillators** , ARGHYADIP MUKHERJEE, Indian Institute of Science, PAWAN NANDAKISHORE, SHASHI THUTUPALLI, National Center for Biological Sciences-TIFR, NCBS THEORY TEAM — Non-transitive relations between coupled nonequilibrium units are a central feature of many natural and engineered systems ranging from interacting organismal populations to cells in a tissue. As a generalised abstraction for such interactions, we consider a system comprised of units whose internal degrees of freedom are intertwined to their orientation. Specifically, the individual elements are amplitude-phase oscillators with an orientation which can interact with the oscillation phase. An emergent mean field couples their dynamics causing the mesoscopic orientational order of the oscillators to affect their phase dynamics and vice versa. Here, we report on theoretical and experimental results on the emergent dynamics in a system built from mechanical oscillators. We show that the phase space consists of a rich variety of behaviors ranging from orientationally ordered synchronized states, traveling waves and even states with partial ordering. We briefly discuss the biological context for our abstract physical models.

**G1.00085 Silicon Photomultipliers Characterization** , CHRISTOPHER BOWSER, MARIAN TZOLOV, Lock Haven Univ, NICK BARBI, PulseTor LLC — Low noise and high sensitivity photon detectors such as the Photomultiplier Tube (PMT) are very common instruments used in research and many other applications. The PMTs have drawbacks such as durability, size, and sensitivity to magnetic field which make them unsuitable for some tasks. Silicon Photomultipliers (SiPMs) are compact, solid state detectors with gain close to that of a PMT, which are a promising replacement of a PMT. We have studied two types of SiPMs designed for optimum response in the visible and near-UV spectral range. We have verified the basic electrical parameters of the devices using current-voltage characteristics and impedance spectroscopy in dark. The spectral response was measured in DC mode, which is very simple to realize and still delivers very good sensitivity. We have established the linearity of the photoresponse and the limits at high intensity illumination. The pairing of the SiPMs with several common scintillators was studied with the goal of optimum performance of the SiPM/scintillator pair.

**G1.00086 Fabrication of a three dimensional particle focusing microfluidic device using a 3D printer, PDMS, and glass**<sup>1</sup> , ROBYN COLLETTE, DANIEL ROSEN, KATHRYN SHIRK, Shippensburg University of Pennsylvania — Microfluidic devices have high importance in fields such as bioanalysis because they can manipulate volumes of fluid in the range of microliters to picoliters. Small samples can be quickly and easily tested using complex microfluidic devices. Typically, these devices are created through lithography techniques, which can be costly and time consuming. It has been shown that inexpensive microfluidic devices can be produced quickly using a 3D printer and PDMS. However, a size limitation prohibits the fabrication of precisely controlled microchannels. By using shrinking materials in combination with 3D printing of flow-focusing geometries, this limitation can be overcome. This research seeks to employ these techniques to quickly fabricate an inexpensive, working device with three dimensional particle focusing capabilities. By modifying the channel geometry, colloidal particles in a solution will be focused into a single beam when passed through this device. The ability to focus particles is necessary for a variety of biological applications which requires precise detection and characterization of particles in a sample.

<sup>1</sup>We would like to thank the Shippensburg University Undergraduate Research Grant Program for their generous funding.

**G1.00087 Statistical Modeling of Robotic Random Walks on Different Terrain** , AUSTIN NAYLOR, LAURA KINNAMAN<sup>1</sup>, Morningside College — Issues of public safety, especially with crowd dynamics and pedestrian movement, have been modeled by physicists using methods from statistical mechanics over the last few years. Complex decision making of humans moving on different terrains can be modeled using random walks (RW) and correlated random walks (CRW). The effect of different terrains, such as a constant increasing slope, on RW and CRW was explored. LEGO robots were programmed to make RW and CRW with uniform step sizes. Level ground tests demonstrated that the robots had the expected step size distribution and correlation angles (for CRW). The mean square displacement was calculated for each RW and CRW on different terrains and matched expected trends. The step size distribution was determined to change based on the terrain; theoretical predictions for the step size distribution were made for various simple terrains.

<sup>1</sup>It's Dr. Laura Kinnaman, not sure where to put the Prefix.

**G1.00088 Novel Fabrication of Carbon Spheres Decorated with Nickel Nanoparticles for Supercapacitors**<sup>1</sup> , CESAR NIEVES, Univ of Puerto Rico - Humacao, JOSHUA ROBLES, University of South Florida, NICHOLAS PINTO, IDALIA RAMOS, Univ of Puerto Rico - Humacao, PENN-UPR PARTNERSHIP FOR RESEARCH AND EDUCATION IN MATERIALS COLLABORATION — Carbon spheres (CS) were synthesized by hydrothermal method using a 0.8M aqueous sucrose solution as the carbon source. The starting solution was heated in a stainless steel autoclave at 200°C for 4h to produce carbon spheres with regular shapes having diameters in the range of 1-20 $\mu$ m. Ni-nanoparticles were deposited on the CS surfaces by an electro-less deposition technique. Our work is the first attempt to decorate CS with nickel nanoparticles using this method. The obtained Ni-CS was studied using Scanning Electron Microscopy (SEM), Energy Dispersive Spectroscopy (EDS) and Ultra-Violet/Visible Spectroscopy (UV-Vis). CS decorated with Nickel nanoparticles increase their capacity to conduct a current making them useful in catalysts and in supercapacitors. Conductivity measurements on these Ni decorated CS and their use in supercapacitors will be presented.

<sup>1</sup>This work was supported by NSF under grant NSF-DMR-1523463 (PENN-UPR PREM).

**G1.00089 Utilizing Diffuse Reflection to Increase the Efficiency of Luminescent Solar Concentrators**<sup>1</sup> , SETH BOWSER, SETH WEIBLE, JOEL SOLOMON, JONATHAN SCHRECENGOST, BRUCE WITTMERSHAUS, School of Science, Pennsylvania State University: Erie, The Behrend College — A luminescent solar concentrator (LSC) consists of a high index solid plate containing a fluorescent material that converts sunlight into fluorescence. Utilizing total internal reflection, the LSC collects and concentrates the fluorescence at the plates edges where it is converted into electricity via photovoltaic solar cells. The lower production costs of LSCs make them an attractive alternative to photovoltaic solar cells. To optimize an LSCs efficiency, a white diffusive surface (background) is positioned behind it. The background allows sunlight transmitted in the first pass to be reflected back through the LSC providing a second chance for absorption. Our research examines how the LSCs performance is affected by changing the distance between the white background and the LSC. An automated linear motion apparatus was engineered to precisely measure this distance and the LSCs electrical current, simultaneously. LSC plates, with and without the presence of fluorescent material and in an isolated environment, showed a maximum current at a distance greater than zero. Further experimentation has proved that the optimal distance results from the backgrounds optical properties and how the reflected light enters the LSC.

<sup>1</sup>This material is based upon work supported by the National Science Foundation under Grant Number NSF-ECCS-1306157.

**G1.00090 Improving the Stability of Fluorescent Silver Nanoclusters<sup>1</sup>**, NICHOLAS SWANSON, DANIELLE STANKO, IAN CAMPBELL, BRUCE WITTMERSHAUS, School of Science, Pennsylvania State University: Erie, The Behrend College — The quantum mechanical nature of noble metal nanoparticles results in them having optical properties much different from the bulk metal. Silver nanoclusters (AgNC), groups of 4 to 20 atoms, are characterized by strong optical transitions in the visible part of the spectrum giving them an appearance like fluorescent organic dyes. These nanoclusters can also have fluorescence quantum yields over 90%. Following the analysis of published results of DNA templated nanoclusters, we created a procedure for synthesizing AgNC. The AgNC have a high fluorescence quantum yield but degrade with a lifetime of only a few days when in solution at room temperature. Our goal in this study was to increase the stability of the AgNC towards improving their value as a fluorescent material in various applications, such as luminescent solar concentrators. To increase their stability, we've chosen to modify our procedure by removing oxygen from the solution after the sample has reacted. Oxygen removal caused a significant increase in the stability of the clusters over a given period of time.

<sup>1</sup>This material is based upon work supported by the National Science Foundation under Grant Number NSF-ECCS-1306157.

**G1.00091 Equivalence Principle tests as probes of Modified Newtonian Dynamics**, ALEX POYNEER, JONAS PEREIRA, THOMAS KRAUSE, JAMES OVERDUIN, Towson University — Modified Newtonian dynamics (MOND) has been proposed as a way to reconcile gravitational theory and observational cosmology without the need for large amounts of unseen dark matter. Instead, a change is postulated to the Newtonian limit of standard theory in the regime of very small accelerations. We consider whether it might be possible to constrain this idea using proposed space tests of the Equivalence Principle (EP). Such tests could be sensitive to accelerations as small as  $10^{-18}$  g over 20 orbits.

**G1.00092 Concentration Dependence of Gold Nanoparticles for Fluorescence Enhancement<sup>1</sup>**, JOEL SOLOMON, BRUCE WITTMERSHAUS, School of Science, Pennsylvania State University: Erie, The Behrend College — Noble metal nanoparticles possess a unique property known as surface plasmon resonance in which the conduction electrons oscillate due to incoming light, dramatically increasing their absorption and scattering of light. The oscillating electrons create a varying electric field that can affect nearby molecules. The fluorescence and photostability of fluorophores can be enhanced significantly when they are near plasmonic nanoparticles. This effect is called metal enhanced fluorescence (MEF). MEF from two fluorescence organic dyes, Lucifer Yellow CH and Riboflavin, was measured with different concentrations of 50-nm colloidal gold nanoparticles (Au-NP). The concentration range of Au-NP was varied from 2.5 to 250 pM. To maximize the interaction, the dyes were chosen so their emission spectra had considerable overlap with the absorption spectra of the Au-NP, which is common in MEF studies. If the dye molecules are too close to the surface of Au-NP, fluorescence quenching can occur instead of MEF. To try to observe this difference, silica-coated Au-NP were compared to citrate-based Au-NP; however, fluorescence quenching was observed with both Au-NP.

<sup>1</sup>This material is based upon work supported by the National Science Foundation under Grant Number NSF-ECCS-1306157.

**G1.00093 Local density of states measurements via STM and TS on clean fresh cleaved HOPG and Gold thin films on HOPG under ambient conditions.<sup>1</sup>**, CASEY MOREAN, ROMAN MARIJCZUK, INDRAJITH SENEVIRATHNE, Lock Haven University — Highly Oriented Pyrolytic Graphite (HOPG) has many applications in physics and engineering thus understanding affiliated physical and chemical phenomena is important. This also makes HOPG an important and interesting system to study. This is an investigation of surfaces of HOPG and Au thin films (ranging about 20nm) via Scanning Tunneling Microscopy (STM) and Tunneling Spectroscopy (TS) with a Pt-Ir tip equipped Nanosurf Naio STM. In this investigation, clean fresh cleaved HOPG substrates were used. Surfaces of HOPG and Au sputter deposited at different film thicknesses were imaged via constant current mode to assess the surface consistency and roughness. Consistent atomic resolution images were obtained. The systems were then investigated via TS by applied tip voltage (V) vs. tunneling current (I) curves. These spectroscopic data were then used to assess the local density of states (LDOS) and the surface variation of LDOS. The discussion will attempt to assess the surface electronic environment of these systems in relation to the Au deposition and variation of Au thicknesses on HOPG. Since measurements were carried out in ambient conditions this adds to the complexity which will also be discussed.

<sup>1</sup>Lock Haven University Nanotechnology Program

**G1.00094 Gravity Wave Disturbances in the F-Region Ionosphere Above Large Earthquakes**, MARGIE BRUFF, North Carolina School of Science and Mathematics — The direction of propagation, duration and wavelength of gravity waves in the ionosphere above large earthquakes were studied using data from the Super Dual Auroral Radar Network. Ground scatter data were plotted versus range and time to identify gravity waves as alternating focused and de-focused regions of radar power in wave-like patterns. The wave patterns before and after earthquakes were analyzed to determine the directions of propagation and wavelengths. Conditions were considered 48 hours before and after each identified disturbances to exclude waves from geomagnetic activity. Gravity waves were found travelling away from the epicenter before all six earthquakes for which data were available and after four of the six earthquakes. Gravity waves travelled in at least two directions away from the epicenter in all cases, and even stronger patterns were found for two earthquakes. Waves appeared, on average, 4 days before, persisting 2-3 hours, and 1-2 days after earthquakes, persisting 4-6 hours. Most wavelengths were between 200-300 km. We show a possible correlation between magnitude and depth of earthquakes and gravity wave patterns, but study of more earthquakes is required. This study provides a better understanding of the causes of ionospheric gravity wave disturbances and has potential applications for predicting earthquakes.

**G1.00095 Work function measurements via STM and TS on clean fresh cleaved HOPG and Gold thin films on HOPG under ambient conditions.<sup>1</sup>**, ROMAN MARIJCZUK, CASEY MOREAN, INDRAJITH SENEVIRATHNE, Department of Geology & Physics Lock Haven University — Stability and homogeneity of HOPG has enabled it to be used as a platform for various applications in understanding many physical and chemical phenomena. Novel emergence of graphene as a derivative of graphite also makes HOPG an interesting system to study. This is an ambient investigation of HOPG and Au thin films (ranging about 20nm) surfaces via Scanning Tunneling Microscopy (STM) and Tunneling Spectroscopy (TS) with a Pt-Ir tip equipped Nanosurf Naio STM. In this investigation, clean fresh cleaved HOPG substrates were used. Surfaces of HOPG and Au sputter deposited at different film thicknesses were imaged via constant current mode to assess the surface consistency and roughness. Consistent atomic resolution images were obtained. The same systems were then investigated via TS by tunneling current (I) vs. height (z) curves. These spectroscopic data were then used to assess the localized work function measurements and surface variation of the work function. The discussion will attempt to assess the surface electronic environment of these systems in relation to the Au deposition and variation of Au thickness on HOPG. Ambient measurements will inherently complicate these measurements and the complexities will also be discussed.

<sup>1</sup>Lock Haven University Nanotechnology Program

**G1.00096 Basic atmospheric measurements via Arduino Uno microcontroller with commercially available sensors towards simple real-time weather forecasting for increased classroom engagement**<sup>1</sup>, RYAN ECKEL, MEGHAN TANNER, INDRAJITH SENEVIRATHNE, Lock Haven University Department of Geology and Physics — Makers, engineers and the applied physics community have adapted Arduino microcontrollers due to their versatility, robustness and cost effectiveness. Arduino microcontroller environment coupled with commercially available sensors have been used to systematically measure, record and analyze temperature, humidity and barometric pressure for building a simplified weather station for subsequent educational purposes. This data will become available in classroom settings for real-time analysis towards simple weather forecasting. Setup was assembled via breadboard, wire and simple soldering with an Arduino Uno ATmega328P microcontroller connected to a PC. The microcontroller was programmed with Arduino Software while the bootloader was used to upload the code. Commercial DHT22 humidity and temperature sensor, and BMP180 barometric pressure sensor were used to obtain relative humidity, temperature and the barometric pressure. A weather resistant enclosure protected the system while stable real-time data measurements were obtained, and uploaded onto the PC. The data was used to predict atmospheric conditions and lifting condensation level (LCL). Discussion will focus on capabilities and limitations of these systems and corresponding teaching aspects.

<sup>1</sup>Lock Haven University Nanotechnology Program

**G1.00097 Enhanced low current, voltage, and power dissipation measurements via Arduino Uno microcontroller with modified commercially available sensors.**<sup>1</sup>, MEGHAN TANNER, RYAN ECKEL, INDRAJITH SENEVIRATHNE, Lock Haven University Department of Geology & Physics — The versatility, simplicity, and robustness of Arduino microcontroller architecture have won a huge following with increasingly serious engineering and physical science applications. Arduino microcontroller environment coupled with commercially available sensors have been used to systematically measure, record, and analyze low currents, low voltages and corresponding dissipated power for assessing secondary physical properties in a diverse array of engineering systems. Setup was assembled via breadboard, wire, and simple soldering with an Arduino Uno with ATmega328P microcontroller connected to a PC. The microcontroller was programmed with Arduino Software while the bootloader was used to upload the code. Commercial Hall effect current sensor modules ACS712 and INA169 current shunt monitor was used to measure corresponding low to ultra-low currents and voltages. Stable measurement data was obtained via sensors and compared with corresponding oscilloscope measurements to assess reliability and uncertainty. Sensor breakout boards were modified to enhance the sensitivity of the measurements and to expand the applicability. Discussion of these measurements will focus on capabilities, capacities and limitations of the systems with examples of possible applications.

<sup>1</sup>Lock Haven Nanotechnology Program

**G1.00098 Photocurrent of Photovoltaic Cells**, SETH PEELER, MAX MCINTYRE, RAQUEL COSSEL, CHRIS BOWSER, MARIAN TZOLOV, Lock Haven University of PA — Photovoltaic cells can be used to harness clean, renewable energy from light. Examined in this project were photovoltaic cells based on a bulk heterojunction between PCPDTBT and PCBM sandwiched between an ITO anode and an Al cathode. Current-voltage characteristics and impedance spectra for multiple photovoltaic devices were taken under varying DC electrical bias and different level of illumination. This data was interpreted in terms of an equivalent circuit with linear elements, e.g. capacitance, series resistance, and parallel resistance. A physical interpretation of each circuit element will be presented. The spectral response of the devices was characterized by optical transmission and photocurrent spectroscopy using a spectrometer in the spectral range from 300 to 900 nm. The DC measurements confirmed that the devices are electrically rectifying. The AC measurements allowed modeling of the devices as a dielectric between two electrodes with injection current passing through it. The characteristic peaks for both PCPDTBT and PCBM are clearly visible in both the photocurrent and transmission data. The good correlation between the photocurrent and transmission data indicates photocurrent generation due to absorption in both materials constituting the heterojunction.

**G1.00099 Characterization of the Pseudocapacitive Nature of Surface Bound Prussian Blue Analogues**<sup>1</sup>, DANIEL CLARK, JENNIFER HAMPTON, Hope College — With the increased use of intermittent renewable energy sources, more efficient methods of energy storage must be explored. Electrochemical capacitors provide a larger volumetric charge density than physical capacitors while maintaining fast charge and discharge rates. Prussian Blue analogues (nickel and cobalt hexacyanoferrate) are ideal pseudocapacitors for frequent charge and discharge cycles since the crystalline structure does not physically change during switching, causing less stress on the film. This project examines the charge transfer and diffusion coefficients for nickel and nickel-cobalt thin films modified with potassium hexacyanoferrate. The films were examined using a scanning electron microscope, an atomic force microscope and an electrochemical workstation to determine their composition, topography and pseudocapacitive nature. Preliminary data suggest that nickel-cobalt films have a larger quantity of charge and have a lower diffusion coefficient per charge than nickel films.

<sup>1</sup>This work is supported by the Hope College Nyenhuis Faculty Development Fund, the Hope College Department of Physics Guess Research Fund, and the National Science Foundation under Grants RUI-DMR-1104725, MRI-CHE-0959282, and MRI-CHE-1126462.

**G1.00100 Dealloying NiCo and NiCoCu Alloy Thin Films Using Linear Sweep Voltammetry**<sup>1</sup>, BENJAMIN PEECHER, JENNIFER HAMPTON, Hope College — When electrodeposited into thin films, metals have well-known electrochemical potentials at which they will be removed from the film. These potential differences can be utilized to re-oxidize only certain metals in an alloy, altering the films structure and composition. Here we discuss NiCo and NiCoCu thin films response to linear sweep voltammetry (LSV) as a means of electrochemical dealloying. For each of four different metal ratios, films were dealloyed to various potentials in order to gain insight into the evolution of the film over the course of the LSV. Capacitance, topography, and composition were examined for each sample before and after linear sweep voltammetry was performed. For NiCo films with high percentages of Ni, dealloying resulted in almost no change in composition, but did result in an increased capacitance, with greater increases occurring at higher LSV potentials. Dealloying also resulted in the appearance of large (100–1000 nm) pores on the surface of the film. For NiCoCu films with high percentages of Ni, Cu was almost completely removed from the film at LSV potentials greater than 500 mV. The LSV first removed larger copper-rich dendrites from the films surface before creating numerous nano-pores, resulting in a net increase in area.

<sup>1</sup>This work is supported by an award to Hope College from the HHMI Undergraduate Science Education Program, the Hope College Department of Physics Frissel Research Fund, and the National Science Foundation under Grants RUI-DMR-1104725 and MRI-CHE-0959282.

**G1.00101 Effects of Stress on Corrosion in a Molten Salt Environment**, SAMUEL GIRDZIS, DENNIS MANOS, WILLIAM COOKE, The College of William and Mary — Molten salt is often used as a heat transfer and energy storage fluid in concentrating solar power plants. Despite its suitable thermal properties, molten salt can present challenges in terms of corrosion. Previous studies have focused extensively on mass loss due to molten salt-induced corrosion. In contrast, we have investigated how corrosion begins and how it changes the surface of stainless steel. Samples of alloys including 304 and 316 stainless steel were exposed to the industry-standard NaNO<sub>3</sub>-KNO<sub>3</sub> (60%-40% by weight) mixture at temperatures over 500°C and then analyzed using Hinox, SEM, and TOF-SIMS. We compare the corrosion at grain boundaries to that within single grain surfaces, showing the effect of the increased internal stresses and the weakened passivation layer. Also, we have examined the enhanced corrosion of samples under mechanical stress, simulating the effects of thermal stresses in a power plant.

**G1.00102 Exact and Approximate Solutions for a Class of Cooperative Stochastic Models<sup>1</sup>**, REBECCA MELKERSON, GILLENHAAL BECK, ESTEVAN HALL-MEJIA, SABIN NSHIMYUMUKIZA, Washington and Lee University, CARLOS DA FONSECA, Kuwait University, DAN MAZILU, IRINA MAZILU, Washington and Lee University — We present a class of cooperative sequential adsorption models with evaporation defined on general lattice structures. Using matrix algebra theory to solve the associated master equations, we find the time-dependent probability distributions. We discuss these models in the context of ionic self-assembly of silica nanoparticles in order to also find the time-dependent surface coverage. To test the limits of the matrix theory, we add the possibilities for evaporation either once the surface is fully covered or at intermediate steps. We justify our mathematical models by comparing the results to customized experiments and computer simulations.

<sup>1</sup>Washington and Lee University Summer Research Scholars

**G1.00103 Potential Mapping of an Indium-Tin-Oxide Glass Box in a GEC Reference Cell<sup>1</sup>**, REBECCA KAPLAN, Towson Univ, JORGE CARMONA-REYES, TRUELL HYDE, LORIN MATTHEWS, Baylor University, CASPER PROGRAM TEAM — The use of indium-tin-oxide (ITO) coated boxes, as well as boxes coated with other substances, placed on or floating above the lower electrode in studies using Gaseous Electronics Conference Radio Frequency Reference Cells have increased in interest, as have the use of plain glass boxes. This increase in interest is due to the greater ability to control the confinement forces and in effect create dust chain structures which aid in studies within other areas of physics such as; entropy, kinetic dust temperature, plasma balls and coulomb explosions. Further analysis of the data obtained using these boxes shows what appear to be at least two different regions of confinement inside the boxes as well as some unexpected phenomena related to anomalous values and behavior of the electric field. These areas affect the dust to dust and dust to plasma interactions independently in the separate regions and are therefore of great interest. In this study electric potential and electric field maps created in MatLab with data obtained using two probes mounted on CASPER's S-100 nano-manipulator will be presented, connecting the information obtained from these maps to the behavior of the dust observed for different experimental conditions.

<sup>1</sup>All of this has been made possible by the opportunity and funding from the CASPER program and the National Science Foundation grant number PHY-1262031.

**G1.00104 Deducing Shape of Anisotropic Particles in Solution from Light Scattering: Spindles and Nanorods.**, ILONA TSUPER, DANIEL TERRANO, KIRIL A. STRELETZKY, Cleveland State University, OLGA V. DEMENT'EVA, SERGEY A. SEMYONOV, VICTOR M. RUDOY, Frumkin Institute of Physical Chemistry and Electrochemistry, Moscow, Russia — Depolarized Dynamic Light Scattering (DDLS) enables to measure rotational and translational diffusion of nanoparticles suspended in solution. The particle size, shape, diffusion, and interactions can then be inferred from the DDLS data using various models of diffusion. Incorporating the technique of DDLS to analyze the dimensions of easily imaged elongated particles, such as Iron (III) oxyhydroxide (FeOOH) Spindles and gold Nanorods, allows testing of the models for rotational and translational diffusion of elongated particles in solution. This, in turn, can help to better interpret DDLS data on hard-to-image anisotropic wet systems such as micelles, microgels, and protein complexes. This study focused on FeOOH Spindles and gold nanorod particles. The light scattering results on FeOOH analyzed using the basic model of non-interacting prolate ellipsoids yielded dimensions within 17% of the SEM measured dimensions. The dimensions of gold nanorod obtained from the straight cylinder model of DDLS data provided results within 25% of the sizes that were obtained from TEM. The nanorod DDLS data was also analyzed by a spherocylinder model.

**G1.00105 Developing Affordable Wet-Sample Electron Microscopy Integrated with a Temperature Controlled Sample Holder.**, DANIEL TERRANO, PETRU S. FODOR, KIRIL A. STRELETZKY, Cleveland State University — Scanning electron microscopy (SEM) is widely used to analyze the size, shape and composition of material systems. However, using this tool for analyzing systems such as particles suspended in solution, requires drastic sample alterations, such as precipitation and fixation. Besides altering their environment, this exposes the particles to the harsh conditions within an electron microscope, such as high vacuum and electron beam exposure. To this end, the first goal of this study was to develop methodologies for imaging wet samples using electron microscopy. This is realized by creating a sandwich structure containing the solution of interest between a partially electron transparent window and a silicon substrate. The ability of the developed imaging cells to provide good imaging conditions is demonstrated with a variety of samples including polystyrene spheres, polymeric microgels and spindle shaped nanoparticles. As some of the systems investigated are temperature sensitive, the second goal of the project was to develop a temperature controlled stage that can be integrated with the SEM. In the future this heating stage will be used alongside the wet samples to image microgels above and below their critical solution temperature.

**G1.00106 Deposition of Highly Luminescent Zinc Tungstate Thin Films on Various Substrates**, RASHAD FARRAKHAN, Lock Haven University — Zinc tungstate films have promising applications in small form factor backscatter electron detectors. We are developing a multistep technology for synthesis of these films. Zinc and tungsten were co-sputtered onto substrates through the process of magnetron sputtering. The metallic films were oxidized in a vacuum sealed tube furnace in controlled flow of argon and oxygen at 800 C. The chemical composition of the film was characterized by Energy-Dispersive X-Ray Spectroscopy (EDS). The structure of the film was investigated by Raman Spectroscopy. The photoluminescence quantum efficiency of the films was found to be 60%. Process parameters for obtaining the desired 1-1 ratio of zinc to tungsten in the film is explored through varying factors such as: the composition of the target used in the sputtering, the power and or voltage used in the sputtering process. Our experiments show that zinc tungstate thin films can be deposited on various substrates with good adhesion and mechanical integrity, and still be efficient light emitters.

**G1.00107 ABSTRACT WITHDRAWN —**

**G1.00108 Synthesis of Polymeric Microgels and their Characterization with Light Scattering.**, CHRISTIAN GUNDER, KIRIL A. STRELETZKY, KRISTA FREEMAN, JANNA MINO, Cleveland State University — Polymeric microgels were synthesized in by chemically crosslinking hydroxypropylcellulose (HPC) chains in aqueous solutions of sodium hydroxide at temperatures above the low critical solution temperature (LCST) of HPC. In order to create a narrower size distribution of HPC microgels, surfactant was added. It was found that the LCST of the solution moved from 40C up to 80C with an increase in surfactant concentration from 0 to 12 g/l. Formed microgels were characterized by dynamic light scattering (DLS). Microgel solutions synthesized resulted in reasonably monodispersed nanoparticles with Rh of 90-150 nm below the transition, and Rh of 50-90 nm above the transition. The effect of synthesis temperature and crosslinker concentration on microgel size, polydispersity, and swelling ratio were also studied.

**G1.00109 Monte Carlo and Exact Diagonalization of Copper (II) Trimer Spin Frustrated Systems<sup>1</sup>**, HAILEY X. EGIDO-BETANCOURT, LEONARD W. TER HAAR, CHRISTOPHER N. VARNEY, University of West Florida — We discuss the use and importance of trimer-based systems because of the spin frustration that may arise within extended lattices comprised of trimers. The possible intra- and inter-trimer exchange pathways they possess due to interconnections are evaluated using density functional theory (DFT) to identify the optimal structures that may be used in designing extended lattices. As example, trinuclear Cu<sub>3</sub><sup>2+</sup> cores with each pair of copper atoms bridged by carboxylate ligands have three-fold symmetry. As trimers these structures have the potential to be modeled as a frustrated quantum spin-1/2 system. To analyze the magnetic ground state and topological properties, we utilize exact diagonalization on small clusters and compare with Monte Carlo simulations for a range of system sizes.

<sup>1</sup>Research reported in this abstract was supported by UWF NIH MARC U-STAR 1T34GM110517-01.

**G1.00110 Tensile Strain Effects on the Magneto-transport in Calcium Manganese Oxide Thin Films: Comparison with its Hole-doped Counterpart**<sup>1</sup>, BRIDGET LAWSON, SAMUEL NEUBAUER, ADEEL CHAUDHRY, CACIE HART, NATALIE FERRONE, DAVID HOUSTON, GRACE YONG, RAJESWARI KOLAGANI, Towson University — Magnetoresistance properties of the epitaxial thin films of doped rare earth manganites are known to be influenced by the effect of bi-axial strain induced by lattice mismatch with the substrate. In hole-doped manganites, the effect of both compressive and tensile strain is qualitatively consistent with the expected changes in unit cell symmetry from cubic to tetragonal, leading to Jahn-Teller strain fields that affect the energy levels of Mn<sup>3+</sup> energy levels. Recent work in our laboratory on CaMnO<sub>3</sub> thin films has pointed out that tetragonal distortions introduced by tensile lattice mismatch strain may also have the effect of modulating the oxygen content of the films in agreement with theoretical models that propose such coupling between strain and oxygen content. Our research focuses on comparing the magneto-transport properties of hole-doped manganite LaCaMnO<sub>3</sub> thin films with that of its electron doped counter parts, in an effort to delineate the effects of oxygen stoichiometry changes on magneto-transport from the effects of Jahn-Teller type strain.

<sup>1</sup>Towson University Office of Undergraduate Research, Fisher Endowment Grant and Undergraduate Research Grant from the Fisher College of Science and Mathematics, Seed Funding grant from the School of Emerging technologies and the NSF grant ECCS 112856

**G1.00111 Heat of Combustion of Dried and Undried Coffee**<sup>1</sup>, MATHEW GISO, SAMUEL AMANUEL, Dept. of Phys. & Astro., Union College — Globally, over two billion cups of coffee are consumed per day. During roasting, 15-20% of the weight of the coffee beans is lost. We studied the gasses released during the roasting process using an IR spectrometer and identified the evaporation profile of water as a function of temperature. The heat of combustion (H<sup>o</sup>c) of the beans was also determined using an Isoperibol Oxygen-Bomb calorimeter and the H<sup>o</sup>c of dry beans were determined to be 21.24 0.13 MJ/kg while the H<sup>o</sup>c of the wet beans were determined to be 19.56 0.12 MJ/kg. This study can potentially lead to developing more economical and environmentally friendly techniques of roasting coffee beans.

<sup>1</sup>This work was partially supported by NSF-DMR: 1229142.

**G1.00112 Visualizing Sound: Demonstrations to Teach Acoustic Concepts**, VALERIE RENNOLL, American University — Interference, a phenomenon in which two sound waves superpose to form a resultant wave of greater or lower amplitude, is a key concept when learning about the physics of sound waves. Typical interference demonstrations involve students listening for changes in sound level as they move throughout a room. Here, new tools are developed to teach this concept that provide a visual component, allowing individuals to see changes in sound level on a light display. This is accomplished using a microcontroller that analyzes sound levels collected by a microphone and displays the sound level in real-time on an LED strip. The light display is placed on a sliding rail between two speakers to show the interference occurring between two sound waves. When a long-exposure photograph is taken of the light display being slid from one end of the rail to the other, a wave of the interference pattern can be captured. By providing a visual component, these tools will help students and the general public to better understand interference, a key concept in acoustics.

**G1.00113 Effect of Uniaxial Strain on Band Structure of Multi-layer WS<sub>2</sub>**<sup>\*1</sup>, CONRAD TROHA<sup>2</sup>, DUY LE, TALAT RAHMAN, Univ of Central Florida — The ability to tailor band structure of a multi-layer transition metal dichalcogenide is of interest because it opens up utilizations of the material for various applications. Strain is considered a robust way to alter the electronic structure of a material. We performed calculations, using density functional theory, of band structure of multi-layer WS<sub>2</sub> under the effects of uniaxial strain. We show that the position of the bottom of conduction band (BCB) at  $\Sigma$  moves to higher, and at K to lower, energy levels under the effects of uniaxial tensile strain, making multi-layer WS<sub>2</sub> closer to a direct band gap material. Our results suggest that uniaxial tensile strain can be used to alter band structure of multi-layer WS<sub>2</sub> to achieve higher yield photo luminescence.

<sup>1\*</sup> This work is supported in part by U.S. Department of Energy (DOE DE-FG02-07ER15842)

<sup>2</sup>Presenter

**G1.00114 Complexity and Fly Swarms**, GRANT CATES, JOELLE MURRAY, Linfield College — Complexity is the study of phenomena that emerge from a collection of interacting objects and arises in many systems throughout physics, biology, finance, economics and more. Certain kinds of complex systems can be described by self-organized criticality (SOC). An SOC system is one that is internally driven towards some critical state. Recent experimental work suggests scaling behavior of fly swarms—one of the hallmarks of an SOC system. Our goal is to look for SOC behavior in computational models of fly swarms.

**G1.00115 Gas separation by adsorption in carbon nanohorns.**<sup>1</sup>, ANTON NEKHAI<sup>2</sup>, Rensselaer Polytechnic Institute, SILVINA GATICA, Howard University — Gas separation by adsorption can be accomplished by three basic physical mechanisms: equilibria, kinetics, and steric effects. Equilibrium mechanisms rely on the strength of attraction between gas molecules and their substrate. For example, CO<sub>2</sub> possesses the strongest, attractive interactions with its substrate. As a result, the equilibrium mechanism presents the most plausible strategy to separate carbon dioxide from mixtures. The specification of a sound adsorbent is the key for separation by adsorption. In this paper we investigate carbon nanohorns for selectivity of carbon dioxide over methane. Carbon Nanohorns resemble short, wide, highly defected single-wall nanotubes that end in conical tips ("horns"). In contrast to regular nanotubes that assemble into parallel bundles, nanohorns form spherical aggregates with the nanohorns arranged along radial directions. Using the simulation technique Grand Canonical Monte Carlo (GCMC) we obtained the adsorption isotherms of CH<sub>4</sub> and CO<sub>2</sub> in a 2D array of carbon nanohorns. We estimated the selectivity based on the IAST approximation. We also study the adsorption of argon and neon and compare with experimental results.

<sup>1</sup>We acknowledge support from the Partnership for Reduced Dimension Materials (PRDM), NSF grant No. DMR1205608

<sup>2</sup>Participant at summer REU program at Howard University

**G1.00116 Doped Lanthanum Hafnates as Scintillating Materials for High-Energy Photon Detection**<sup>1</sup>, KAREEM WAHID, MADHAB POKHREL, YUANBING MAO, University of Texas Rio Grande Valley — Recent years have seen the emergence of nanocrystalline complex oxide scintillators for use in X-ray and gamma-ray detection. In this study, we investigate the structural and optical properties of La<sub>2</sub>Hf<sub>2</sub>O<sub>7</sub> nanoparticles doped with varying levels of Eu<sup>3+</sup> or Ce<sup>3+</sup> by use of X-ray diffraction, Raman spectroscopy, scanning electron microscopy, transmission electron microscopy, and optical photoluminescence. In addition, scintillation response under X-ray and gamma-ray exposure is reported.

<sup>1</sup>The authors thank the support from the Defense Threat Reduction Agency (DTRA) of the U.S. Department of Defense (Award HDTRA1-10-1-0114).

**G1.00117 ABSTRACT WITHDRAWN —**

**G1.00118 Controlled, Pulsed Frequency Chirped Laser Light at Large Detuning**, TRACY PALTOO, TANNER GROGAN, BRIAN KAUFMAN, MATTHEW WRIGHT, Adelphi Univ — We have developed a technique to create pulsed, frequency chirped laser light (1 GHz in 5 ns) at large detuning ( $>7$  GHz). Laser light is passed through an electro-optical phase modulator, where the light is modulated with a 7 GHz carrier signal whose frequency is modulated on the nanosecond time scale. The modulated light is passed into a diode laser which becomes injection locked. The injection-locked laser system amplifies and filters the laser light to create a single frequency chirped laser pulse whose detuning is some multiple of the carrier frequency. We have developed the ability to pulse the laser on timescales less than 3 ns and create an arbitrary frequency chirp shape.

**G1.00119 Whispering Gallery Modes Used to Determine the Changing Size of Levitated Aerosol Droplets in a Fluctuating Optical Trap**, ANGELA LUDVIGSEN, LOWELL MCCANN, University of Wisconsin - River Falls — A laser can be used as an optical trap to catch and hold small, transparent objects. Observations of optically trapped aqueous aerosol droplets have demonstrated that the droplet moves between two or more stable positions dependent upon the power of the trapping laser. It is hypothesized that this movement coincides with a resonance between the trapping light and the droplet's surface, called a Whispering Gallery Mode. When this resonance occurs, forces acting on the droplet cause it to move. To investigate this behavior, Raman scattered light from the droplet as well as the droplet's position are measured. The Raman spectrum exhibits a series of peaks resulting from the droplet's spherical shape, referred to as Cavity Enhanced Raman Spectroscopy. The location and spacing of these peaks are known to be related to the diameter and the optical properties of the droplet. From this spectrum, the magnitude of the electric and magnetic fields of the scattered light are calculated. This allows for a precise measurement of the droplet's radius at the moment that the droplet moves between stable positions. After determining the droplet's radius from the spectrum, the effect of varying the intensity of the trapping laser beam on the droplet radius can be investigated.

**G1.00120 Apparatus for the Measurement of Thermoelectric Power<sup>1</sup>**, SHOJI HISHIDA, PEI-CHUN HO, Physics/CSU-Fresno — The Seebeck Effect refers to the electric potential that is established in a material under an imposed temperature gradient. This effect provides a useful tool for characterizing the thermal and electric transport behavior of materials. A measurement probe is under development in order to measure the Seebeck Coefficient (Thermoelectric Power) of a sample over the temperature range from 10 - 300 K in a cryocooler system. The sample is mounted between two platforms: one that is thermally connected with the measurement probe and another that is thermally isolated, referred to as the cold and hot platforms respectively. A  $2k\Omega$  resistance heater on the hot platform is used to establish a temperature gradient across the sample and between the two platforms. A Cernox resistance thermometer measures the temperature of the cold platform, and a Type T differential thermocouple, composed of copper-constantan-copper wires, is used to measure the temperature difference. The probe will be calibrated using the known thermopowers of Nickel, Platinum, and Chromel samples. The performance results of this design will be presented.

<sup>1</sup>Research at CSU-Fresno is supported by NSF DMR-1506677. Shoji Hishida is also supported by the Undergraduate Research Grant at CSU Fresno

**G1.00121 Two Undergraduate Projects for Data Acquisition and Control**, KELLY HIERSCHE, TARA PENA, TANNER GROGAN, MATTHEW WRIGHT, Adelphi Univ — We are designing two separate instruments for use in our undergraduate laboratory. In the first project, a Raspberry Pi is used to simultaneously monitor a large number of current and voltage readings and store them in a database. In our second project, we are constructing our own microcontrollers to work as a general-purpose interface based off work carried out in Review of Scientific Instruments **84**, 103101 (2013). It was designed for low cost and simple construction, making it ideal for undergraduate level work. This circuit has room for two interchangeable daughter boards, giving it the capability to work as a general lab interface, lock-in detector, or waveform generator.

**G1.00122 Anion Photoelectron Spectroscopy of the Homogenous 2-Hydroxypyridine Dimer Electron Induced Proton Transfer System<sup>1</sup>**, ALEXANDRA VLK, SARAH STOKES, Towson University, YI WANG, ZACHARY HICKS, XINXING ZHANG, NICOLAS BLANDO, Johns Hopkins University, ANDREW FROCK, Baltimore Polytechnic Institute, SARA MARQUEZ, KIT BOWEN<sup>2</sup>, Johns Hopkins University, BOWEN LAB JHU TEAM — Anion photoelectron spectroscopic (PES) and density functional theory (DFT) studies on the dimer anion of (2-hydroxypyridine)<sub>2</sub><sup>-</sup> are reported. The experimentally measured vertical detachment energy (VDE) of 1.21eV compares well with the theoretically predicted values. The 2-hydroxypyridine anionic dimer system was investigated because of its resemblance to the nitrogenous heterocyclic pyrimidine nucleobases. Experimental and theoretical results show electron induced proton transfer (EIPT) in both the lactim and lactam homogeneous dimers. Upon electron attachment, the anion can serve as the intermediate between the two neutral dimers. A possible double proton transfer process can occur from the neutral (2-hydroxypyridine)<sub>2</sub> to (2-pyridone)<sub>2</sub> through the dimer anion. This potentially suggests an electron catalyzed double proton transfer mechanism of tautomerization.

<sup>1</sup>Research supported by the NSF grant no. CHE-1360692

<sup>2</sup>Principal Investigator

**G1.00123 Charge Transport and Structural Dynamics in Phosphonium-based Ionic Liquids**, ZACHARIAH VICARS, TYLER COSBY, Univ of Tennessee, Knoxville, YANGYANG WANG, Oak Ridge National Laboratory, KATSUHIKO TSUNASHIMA, Wakayama College, JOSHUA SANGORO, Univ of Tennessee, Knoxville — A series of phosphonium-based ionic liquids are investigated by broadband dielectric spectroscopy, rheology, and differential scanning calorimetry. Varying the molecular structure of the anion leads to significant changes in charge transport and structural dynamics. The results are discussed within the framework and current understanding of anion/cation interactions in determining physicochemical properties of ionic liquids.

**G1.00124 Protein Folding and Self-Organized Criticality**, ARUN BAJRACHARYA, JOELLE MURRAY, Linfield College — Proteins are known to fold into tertiary structures that determine their functionality in living organisms. However, the complex dynamics of protein folding and the way they consistently fold into the same structures is not fully understood. Self-organized criticality (SOC) has provided a framework for understanding complex systems in various systems (earthquakes, forest fires, financial markets, and epidemics) through scale invariance and the associated power law behavior. In this research, we use a simple hydrophobic-polar lattice-bound computational model to investigate self-organized criticality as a possible mechanism for generating complexity in protein folding.

**G1.00125 Construction of a Laser Induced Breakdown Spectroscopy Setup<sup>1</sup>**, JOSEPH MAYS, ANDRIA PALMER, JAMES AMOS, TOM DYNKA, LAZLO UJJ, University of West Florida — Laser Induced Breakdown Spectroscopy (LIBS) is a practical spectroscopy to determine the chemical and atomic composition of materials. The third harmonic output of a Nd:YAG Q-switched laser generating 5ns pulses with 10Hz repetition rate was used to ablate the sample and create a micro-plasma. The emission of the radiating plasma was focused into an optical fiber with 0.22 numerical aperture. The spectra was measured with an Ocean Optics micro spectrometer. A synchronized shutter was used to select single laser pulses. In order to reach the breakdown threshold of the sample using the available energy of the laser pulses ( $<5$  mJ) a beam expander and a parabolic mirror was used for tight focusing. The optical and technical details including the characterization of the system will be presented. LIBS spectra taken from a variety of metal and organic samples show appropriate selectivity for quantitative and qualitative analysis for materials.

<sup>1</sup>UWF NIH MARC U-STAR 1T34GM110517-01, UWF Office of Undergraduate Research

**G1.00126 Assessing the Effectiveness of Gravitational Wave Outreach Video Games in High School Students**, JONATHAN WHEELER, Andrews University — Students and faculty at the Gravitational Wave Group in Birmingham, UK developed a remake of the classic 1972 game of Pong. Black Hole Pong was developed to be used in events such as science fairs as a way to engage children and pique interest in black holes. I present the results of a study which assesses the utility of Black Hole Pong and its successors in raising awareness of gravitational wave research, and in fostering conceptual understanding of astrophysics and gravity. Of particular interest in this study is potential use in high school science classrooms during astrophysics units.

**G1.00127 All-Optical Quasi-Phase Matching of Frequency Doubling Using Counterpropagating Light**<sup>1</sup>, RICHARD CAMUCCIO, RACHEL MYER, ALLISON PENFIELD, ETIENNE GAGNON, AMY LYTLE, Franklin & Marshall College — Nonlinear optical frequency conversion is a useful method for creating coherent light sources with unique capabilities. The main challenge for conversion efficiency of processes like frequency doubling is the chromatic dispersion of the nonlinear medium. Successful techniques for correcting the phase mismatch between the different frequencies are often limited by the type of nonlinear medium that may be used. An all-optical method of quasi-phase matching using counterpropagating light has recently been demonstrated for high-order harmonic generation, an extreme nonlinear process. Sequences of counterpropagating pulses are used to interfere with the harmonic generation process periodically, correcting the phase mismatch and boosting efficiency. We report progress on an experimental investigation of the effect of counterpropagating light on the more commonly used low-order nonlinear optical processes. We present data showing the effects of a single counterpropagating pulse on the efficiency of frequency doubling of a Ti:sapphire ultrafast laser oscillator in beta-Barium Borate.

<sup>1</sup>Research Corporation for Science Advancement (RCSA), Cottrell College Science Award 21084; Franklin & Marshall Hackman Summer Scholars Program

**G1.00128 Phenomenological Modeling for Langmuir Monolayers**<sup>1</sup>, DIMITRI BAPTISTE, DAVID KELLY, TWYMMUN SAFFORD, CHANDRA PRAYAGA, CHRISTOPHER N. VARNEY, AARON WADE, University of West Florida — Experimentally, Langmuir monolayers have applications in molecular optical, electronic, and sensor devices. Traditionally, Langmuir monolayers are described by a rigid rod model where the rods interact via a Leonard-Jones potential. Here, we propose effective phenomenological models and utilize Monte Carlo simulations to analyze the phase behavior and compare with experimental isotherms.

<sup>1</sup>Research reported in this abstract was supported by UWF NIH MARC U-STAR 1T34GM110517-01

**G1.00129 The effect of drainage channels on the hydrodynamic drag of non-colloidal spheres down an inclined plane.**<sup>1</sup>, BRIAN RYU, CHARLES DHONG, JOELLE FRECHETTE, Johns Hopkins University — While it is well known that surface asperities and roughness alter the hydrodynamic drag of a non-colloidal sphere down an inclined plane, less is known about how the hydrodynamic drag is modified if the asperities and roughness are connected through a network of drainage channels, which allows the movement of fluid between asperities. We investigate the rotational and translation motion of spheres on several pairs of surfaces that have the same porosity and asperity size, but one surface has interconnected drainage channels whereas the other does not. These can have direct relevance to lubricated surfaces such as ball bearings in industrial settings, or biological relevance of leucocyte movement across rough surfaces.

<sup>1</sup>Provost's Undergraduate Research Awards, Office of Naval Research, National Science Foundation

**G1.00130 Magnetic and Magnetocaloric Properties in Non-Stoichiometric Gallium Deficient  $\text{Ni}_2\text{MnGa}_{1-x}$  Heusler Alloys**, ALEXANDER MADDEN, MOLLIE CORRIGAN, LINDA BARTON, Rochester Institute of Technology — Magnetic data show that off-stoichiometric gallium deficient Heusler alloys of the form  $\text{Ni}_2\text{MnGa}_{1-x}$  have structural martensite transition temperatures that increase strongly with  $x$ , while their ferromagnetic Curie temperatures remain nearly unchanged. The martensite transition approaches room temperature for  $x = 0.13$ . Samples were prepared by rf induction heating. The influence of quenching and post annealing on magnetic properties, as well as structural grain sizes and magnetic domain structure, were investigated. Since the first order structural phase transition can be adjusted to any convenient temperature, these materials offer intriguing possibilities as magnetic refrigerants. Magnetocaloric properties were investigated by direct measurement of  $\Delta T$  with the application of field  $\Delta H$ .

**G1.00131 First-principles study of low-frequency phonon modes in heterostructures of transition metal dichalcogenides**<sup>1</sup>, NATHAN PRINS, DANNA DORATOTAJ, JIA-AN YAN, Towson University — Transition metal dichalcogenides (TMDs) are layered compounds with weak interlayer interactions and have attracted tremendous attention because of their remarkable electronic, optical and transport properties. Heterostructures made of TMDs offer an additional degree of freedom to tune their electronic properties. In this work, we present a first-principles study of the low-frequency modes in  $\text{WS}_2/\text{MoS}_2$  and  $\text{WSe}_2/\text{MoSe}_2$  heterostructures for various stacking geometry and stacking sequence. Our calculations show that the low-frequency layer shearing modes and layer breathing modes provide a useful way to characterize the stacking geometry of these heterostructures. Finally, the simulated Raman spectra for these heterostructures are discussed.

<sup>1</sup>This work was supported by the FCSM Undergraduate Research Committee, the FCSM Fisher General Endowment and the FDRC grant (OSPR No. 140269) at Towson University.

**G1.00132 ABSTRACT WITHDRAWN —**

**G1.00133 Understanding Binding Peptide Design Using a Synthesis of Residue Physicality and Energetic Frustration**, LENAYA FLOWERS, Department of Physics, University of Houston, SWARNENDU TRIPATHI, MARGARET CHEUNG, Department of Physics, University of Houston and Center for Theoretical Biological Physics, Rice University — The ubiquitous nature of Calmodulin (CaM) allows it to bind to numerous peptides, thus altering the function of a protein complex. Variations in CaMs function are a product of the numerous binding targets (BT) and their significant biological pathways. Given that CaM is a well-studied protein, we have found that certain amino acids in CaMs sequence play an important role in the event of protein binding. 36 CaM binding targets were analyzed to find sequential, physical commonalities. Using the *Frustrometer* (frustrometer.tk), we obtained z-scores (a numerical value for level of frustration) for each amino acids in a given binding target sequence. From those results, we were able to identify which residues show a highly favorable energetic change after binding and those that do not. We have found charged residues show the most prominent change when bound to CaM, these amino acids may provide a critical role in the overall design and function of a CaM-BT complex.

**G1.00134 Weyl semimetal state in TaP: experimental discovery<sup>1</sup>** , PAVEL SHIBAYEV, SU-YANG XU, ILYA BELOPOLSKI, DANIEL S. SANCHEZ, Princeton University, SHUANG JIA, Peking University, HSIN LIN, National University of Singapore, M. ZAHID HASAN, Princeton University, HASAN RESEARCH GROUP TEAM<sup>2</sup> — Despite their extreme rareness in nature, Weyl semimetals provide the first realization of Weyl fermions. After families of tantalum-based (TaAs, TaP) and niobium-based (NbAs, NbP) compounds were recently predicted as Weyl semimetal candidates, our group experimentally realized the Weyl semimetal state in TaP. Angle-resolved photoemission spectroscopy (ARPES) was used to probe the surface features of TaP. Weyl fermion cones and nodes were directly observed in the bulk, and Fermi arcs were observed on the surface. The surface states were found to possess a rich structure, containing topological Fermi arcs and topologically trivial closed contours in the neighborhood of Weyl points. This finding opens up possibilities to study the relationship between trivial and topological surface states on the surface of a Weyl semimetal. By determining the number of chiral edge modes on a closed path enclosing the Weyl node, bulk-boundary correspondence was demonstrated, leading to the establishment of a topologically nontrivial nature of the Weyl semimetal state in TaP.

<sup>1</sup>The work at Princeton and Princeton-led ARPES measurements were supported by the Gordon and Betty Moore Foundations EPiQS Initiative through grant GBMF4547 (Hasan) and by U.S. Department of Energy DE-FG-02-05ER46200.

<sup>2</sup>Research group led by Professor M. Zahid Hasan (Princeton University)

**G1.00135 The effects of impurities and incidence angle on the secondary electron emission of Ni(110)<sup>1</sup>** , HADAR LAZAR, University of Chicago, MARLENE PATINO, University of California, Los Angeles, YEVGENY RAITSES, Princeton Plasma Physics Laboratory, BRUCE KOEL, Department of Chemical and Biological Engineering, Princeton University, CHARLES GENTILE, ELIOT FEIBUSH, Princeton Plasma Physics Laboratory — The investigation of secondary electron emission (SEE) of conducting materials used for magnetic fusion devices and plasma thrusters is important for determining device lifetime and performance. Methods to quantify the secondary electron emission from conducting materials and to characterize the effects that impurities and incidence angles have on secondary electron emission were developed using 4-grid low energy electron diffraction (LEED) optics. The total secondary electron yield from a Ni(110) surface was continuously measured from the sample current as surface contamination increased from reactions with background gases in the ultrahigh vacuum chamber. Auger electron spectroscopy (AES) and temperature programmed desorption (TPD) were used to examine the composition and impurity levels on the Ni(110) surface. The total secondary electron yield was also measured at different incidence angles.

<sup>1</sup>Thank you to the Princeton Plasma Physics Laboratory (PPPL) and the Department of Energy (DOE) for the opportunity to work on this project through the Science Undergraduate Laboratory Internships (SULI).

**G1.00136 Frequency and voltage dependence of series resistance in a solar cell** , ALEXANDER OGLE, THADDEUS COX, JENNIFER HEATH, Linfield College — While admittance measurements of solar cells are typically conducted in reverse or at zero bias, and analyzed using the depletion approximation, the operating point of the solar cell is in forward bias, and the series resistance is often estimated using IV curves with a high forward current. In this mode, the device is no longer in the depletion regime, and the large number of injected minority carriers alter the transport properties significantly. In our Cu(In,Ga)Se<sub>2</sub> devices, we measure negative values of capacitance at high forward bias, which may be linked to injected minority carriers and carrier transport limitations, although our calculations of capacitance may also be influenced by series resistance. In this study, we compare ac and dc measurements of voltage dependent series resistance to try to better understand the negative capacitance signal.

**G1.00137 Improving Qubit Quality Factors Through Exotic Materials** , VICTORIA NORMAN, University of Chicago — In the time since the first qubits were successfully fabricated, the coherence times of superconducting Josephson junction qubits have improved by several orders of magnitude. Yet as the quantum information and computation field moves forward, these coherence times still need further improvement. We are now finding that in some superconducting systems, non-thermal equilibrium quasiparticles are becoming the limiting factor in qubit lifetimes. For SIS superconducting qubits, the T<sub>1</sub> and T<sub>2</sub><sup>\*</sup> values may be improved by the use of materials with higher superconducting band gap, E<sub>G</sub>, for which low values may allow for quasiparticles to break up Cooper pairs more easily, leading to a shorter lifetime. At this time, Al-Al<sub>2</sub>O<sub>3</sub>-Al transmons are very well characterized and understood and will therefore serve as an appropriate baseline with which to compare the more exotic junction materials. Using tantalum and niobium, which have E<sub>G</sub> values of 3 times and 10 times that of aluminum respectively, we expect the T<sub>1</sub> and T<sub>2</sub><sup>\*</sup> values to increase significantly for the Al-Al<sub>2</sub>O<sub>3</sub>-Nb, Al-Al<sub>2</sub>O<sub>3</sub>-Ta, and Ta-Ta<sub>2</sub>O<sub>5</sub>-Nb qubits.

**G1.00138 Development of a cost effective microscope heater stage<sup>1</sup>** , JOSHUA DUGRE, CHANDRA PRAYAGA, AARON WADE, University of West Florida — Utilizing 3D printing technology, a heater stage has been developed and implemented for microscopic systems. Due to the flexibility of 3D printing, the heater stage can be easily modified to fit any sample size with only slight modifications to the heating element being required. The sample in contact with the heating element can also easily be secured in a thermal insulator, such as aluminum foil. The thermal gradient of the heater stage has been recorded to be less than 1°C and has been compared to more expensive designs, and the cost effectiveness of the system has been determined. The system has been tested with a sample of the liquid crystal 8CB in order to determine the exact temperatures of the phase transitions of the crystal to verify that the system is applicable to a wide range of experimental physics.

<sup>1</sup>UWF Quality Enhancement Plan Award

**G1.00139 Van der Waal Interactions in Ultrafine Nanocellulose Aerogels<sup>1</sup>** , BYRON FRITCH, DEREK BRADLEY, TIM KIDD, University of Northern Iowa — Nanocellulose aerogels have shown an ability to be used in many different applications ranging from oil sponges to conductive materials to possibly a low calorie food substitute. Not much is known about the structural and physical property changes that occur when the composition of the aerogel changes. We studied what properties change when the aerogel amounts change, as well as how sticky the aerogels are and how strong they are. The higher concentrations appeared to have more plate-like structures while the lower concentrations had a more fibrous material. These fibers in the low concentrations had a smaller diameter than a human hair. Only the low concentration aerogels were able to stick to a glass surface in the adhesion test, but were able to support a mass much larger than their own. These low concentrations also would stick to your finger when lightly touched. Preliminary tests show that a concentration that is not too low, but not too high, is best for tensile strength. All concentrations were able to hold many times their own mass. Cellulose should be studied more because it is a renewable material and is easily accessed. Nanocellulose is also not environmentally dangerous allowing it to be used in applications involving humans and the environment like noted above.

<sup>1</sup>National Science Foundation grant DMR- 1410496

**G1.00140 ABSTRACT WITHDRAWN —**

**G1.00141 Study of Langmuir and Langmuir-Blodgett Thin films<sup>1</sup>** , ROSS GOODWIN, CHANDRA PRAYAGA, AARON WADE, University of West Florida — Arachidic Acid, Cholesterol, and Stearic Acid thin films were created and studied utilizing the Langmuir method in order to obtain a single molecule or monomolecular layer out of a desired substance at an air-water interface. The phase transitions are observed by measuring the surface pressure vs. area isotherms. Langmuir-Blodgett (LB) films were created on a prepared substrate. The LB film structures were then studied using X-ray Diffraction, and Raman Spectroscopy.

<sup>1</sup>UWF Office of Undergraduate Research Project Award, UWF ITEP-Technology Fee Project Award, UWF Quality Enhancement Plan Award

**G1.00142 Spatially varying geometric phase in classically entangled vector beams of light<sup>1</sup>** , ANDREW KING-SMITH, CODY LEARY, The College of Wooster — We present theoretical results describing a spatially varying geometric (Pancharatnam) phase present in vector modes of light, in which the polarization and transverse spatial mode degrees of freedom exhibit classical entanglement. We propose an experimental setup capable of characterizing this effect, in which a vector mode propagates through a Mach-Zehnder interferometer with a birefringent phase retarder present in one arm. Since the polarization state of a classically entangled light beam exhibits spatial variation across the transverse mode profile, the phase retarder gives rise to a spatially varying geometric phase in the beam propagating through it. When recombined with the reference beam from the other interferometer arm, the presence of the geometric phase is exhibited in the resulting interference pattern.

<sup>1</sup>We acknowledge funding from the Research Corporation for Science Advancement by means of a Cottrell College Science Award.

**G1.00143 Deterministic and Stochastic Modeling of an Artificial Bistable Switch in E. coli** , DANIEL FINKELSTEIN, East Chapel Hill High School and Duke University, NICOLAS BUCHLER, SARGIS KARAPETYAN, Duke University — Networks of mutually interacting genes are common in natural regulatory networks. To better understand these interactions, scientists have recently been constructing artificial genetic networks. Much of the effort is focused on creating genetic oscillators and bistable switches. In this project, we analyzed the possibility to create a bistable switch in E. coli. In this realization of the switch, the Repressor (basic leucine zipper CEBP/alpha) represses the transcription of the Inhibitor (artificial dominant negative 3HF). The Inhibitor, in turn, sequesters the Repressor by binding to it. Using deterministic modeling we identified a range of parameters suitable for bistability. We then analyzed the resulting solutions with the full model taking the reaction rates corresponding to E. coli and the including stochastic nature of gene expression. We have shown that the bistability is not destroyed by stochastic fluctuations if several copies of genes are present. Specifically, taking a realistic number of plasmids (10) we show that the number of proteins in the systems undergoes sizable fluctuations; however, the two states with low and high concentrations of inhibitor stay distinct in the relevant range of parameters.

**G1.00144 Alpha Background Rejection in Bolometer Detectors** , NICHOLAS DEPORZIO, Northeastern Univ, CUORE COLLABORATION — This study presents the modification of bolometer detectors used in particle searches to veto or otherwise reject alpha radiation background and the statistical advantages of doing so. Several techniques are presented in detail – plastic film scintillator vetoes, metallic film ionization vetoes, and Cherenkov radiation vetoes. Plastic scintillator films are cooled to bolometer temperatures and bombarded with 1.4MeV to 6.0MeV alpha particles representative of documented detector background. Quantum dot based liquid scintillator is similarly bombarded to produce a background induced scintillation light. Photomultipliers detect this scintillation light and produce a veto signal. Layered metallic films of a primary metal, dielectric, and secondary metal, such as gold-polyethylene-gold films, are cooled to milli-kelvin temperatures and biased to produce a current signal veto when incident 1.4MeV to 6.0MeV alpha particles ionize conduction paths through the film. Calibration of veto signal to background energy is presented. These findings are extrapolated to quantify the statistical impact of such modifications to bolometer searches. Effects of these techniques on experiment duration and signal-background ratio are discussed.

**G1.00145 Green Chemistry Techniques for Gold Nanoparticles Synthesis** , SARAH A. CANNAVINO, CHRISTY A. KING, DAVON W. FERRARA, Belmont University — Gold nanoparticles (AuNPs) are often utilized in many technological and research applications ranging from the detection of tumors, molecular and biological sensors, and as nanoantennas to probe physical processes. As these applications move from the research laboratory to industrial settings, there is a need to develop efficient and sustainable synthesis techniques. Recent research has shown that several food products and beverages containing polyphenols, a common antioxidant, can be used as reducing agents in the synthesis of AuNPs in solution. In this study, we explore a variety of products to determine which allow for the most reproducible solution of nanoparticles based on the size and shapes of particles present. We analyzed the AuNPs solutions using extinction spectroscopy and atomic force microscopy. We also develop a laboratory activity to introduce introductory chemistry and physics students to AuNP synthesis techniques and analysis.

**G1.00146 Solvent vapor induced morphology variation in thin films of PS-b-PLA copolymers** , LAUREN FOOTE, MAXIMILIAN HERES, THOMAS KINSEY, JOSHUA SANGORO, Univ of Tennessee, Knoxville — Molecular dynamics in thin films of PS-b-PLA copolymers annealed by solvent vapor annealing is investigated using broadband dielectric spectroscopy, atomic force microscopy and ellipsometry. Impact of morphology changes on molecular dynamics are analyzed. The results of this study are discussed within the framework of current understanding of morphology control of copolymer thin films.

**G1.00147 Optical Properties of Silver Nanoparticulate Glasses** , RACHEL N. EVANS, SARAH A. CANNAVINO, CHRISTY A. KING, JOSEPH A. LAMARTINA, ROBERT H. MAGRUDER, DAVON W. FERRARA, Belmont University — The ion exchange method of embedding metal nanoparticles (NPs) into float glass is an often used technique of fabricating colored glasses and graded-index waveguides. The depth and size of NP formation in the glass depends on the concentration and temperature of metal ions in the molten bath. In this study we explore the dichroic properties of silver metal ion exchange restricted to only one side of a glass microscope slide using reflection and transmission spectroscopy and its dependence on temperature, concentration of silver ions, and length of time in the molten bath.

**G1.00148 Simulation of Thin Film Equations on an Eye-Shaped Domain with Moving Boundary<sup>1</sup>** , JOSEPH BROSCHE, TOBIN DRISCOLL, RICHARD BRAUN, University of Delaware — During a normal eye blink, the upper lid moves, and during the upstroke the lid paints a thin tear film over the exposed corneal and conjunctival surfaces. This thin tear film may be modeled by a nonlinear fourth-order PDE derived from lubrication theory. A major stumbling block in the numerical simulation of this model is to include both the geometry of the eye and the movement of the eyelid. Using a pair of orthogonal and conformal maps, we transform a computational box into a rough representation of a human eye where we proceed to simulate the thin tear film equations. Although we give up some realism, we gain spectrally accurate numerical methods on the computational box. We have applied this method to the heat equation on the blinking domain with both Dirichlet and no-flux boundary conditions, in each case demonstrating at least 10 digits of accuracy. We are able to perform these simulations very quickly (generally in under a minute) using a desktop version of MATLAB.

<sup>1</sup>This project was supported by Grant 1022706 (R.J.B., T.A.D., J.K.B.) from the NSF

### **G1.00149 Constructing Dual Beam Optical Tweezers for Undergraduate Biophysics Research**

, BRIAN DAUDELIN, DEVON WEST-COATES, JON DEL'ETOILE, ERIC GROTZKE, THAYAPARAN PARAMANATHAN, Bridgewater State University, MA — Optical tweezing, or trapping, is a modern physics technique which allows us to use the radiation pressure from laser beams to trap micron sized particles. Optical tweezers are commonly used in graduate level biophysics research but seldom used at the undergraduate level. Our goal is to construct a dual beam optical tweezers for future undergraduate biophysical research. Dual beam optical tweezers use two counter propagating laser beams to provide a stronger trap. In this study we discuss how the assembly of the dual beam optical tweezers is done through three main phases. The first phase was to construct a custom compressed air system to isolate the optical table from the vibrations from its surroundings so that we can measure pico-newton scale forces that are observed in biological systems. In addition, the biomaterial flow system was designed with a flow cell to trap biomolecules by combining several undergraduate semester projects. During the second phase we set up the optics to image and display the inside of the flow cell. Currently we are in the process of aligning the laser to create an effective trap and developing the software to control the data collection. This optical tweezers set up will enable us to study potential cancer drug interactions with DNA at the single molecule level and will be a powerful tool in promoting interdisciplinary research at the undergraduate level.

### **G1.00150 Landau Damping in a Mixture of Bose and Fermi Superfluids**

, HUITAO SHEN, WEI ZHENG, Tsinghua Univ — We study Landau damping in Bose-Fermi superfluid mixture at finite temperature. We find that at low temperature, the Landau damping rate will be exponentially suppressed at both the BCS side and the BEC side of Fermi superfluid. The momentum dependence of the damping rate is obtained, and it is quite different from the BCS side to the BEC side. The relation between our result and the collective mode experiment in recently realized Bose-Fermi superfluid mixture is also discussed.

### **G1.00151 PHYSICS EDUCATION —**

### **G1.00152 The Physics of Quidditch Summer Camp: An Interdisciplinary Approach**

, DONNA HAMMER, TIM UHER, University of Maryland — The University of Maryland Physics Department has developed an innovative summer camp program that takes an interdisciplinary approach to engaging and teaching physics. The Physics of Quidditch Camp uniquely sits at the intersection of physics, sports, and literature, utilizing the real-life sport of quidditch adapted from the Harry Potter novels to stimulate critical thinking about real laws of physics and leaps of imagination, while actively engaging students in learning the sport and discussing the literature. Throughout the camp, middle school participants become immersed in fun physics experiments and exciting physical activities, which aim to build and enhance skills in problem-solving, analytical thinking, and teamwork. This camp has pioneered new ways of teaching physics to pre-college students, successfully engaged middle school students in learning physics, and grown a large demand for such activities.

### **G1.00153 Peer Grading in Astronomy Massive Open Online Course<sup>1</sup>**

, MARTIN FORMANEK, MATTHEW WENGER, CHRISTOPHER IMPEY, SANLYN BUXNER, University of Arizona — In this work we thoroughly investigate the peer grading process as it happened in the University of Arizona session based MOOC Astronomy: Exploring Time and Space offered during Spring 2015 through Coursera. Overall, 25400 learners from over 100 countries registered for this course. Of those, 14900 accessed at least one part of the course and 1332 users engaged in the peer grading. First of all we provide description of the peer graded assignments and we identify trends in behavior of people who participated in these exercises. E.g. time they spent on grading, number of assignments graded and patterns arising from comparing all three assignments. Furthermore, for the second assignment, we graded random sample of 300 essays by a group of trained undergraduate students and a group consisting of one of the course instructors together with graduate TAs and we compared results with grades from the peer grading. Specifically we look on Intraclass Correlation Coefficients for all three groups of graders to determine reliability of each group and correlations between final grades. Finally we assess factors influencing reliability of the peer graders participating in the MOOC based on the difference from our grades.

<sup>1</sup>This research was supported by Howard Hughes Medical Institute grant no. 415580

### **G1.00154 Roadrunner physics: using cartoons to challenge student preconceptions**

, RACHAEL HUXFORD, MATHEW RIDGE, JAMES OVERDUIN, JIM SELWAY, Towson University — The cartoon universe is governed by laws that differ radically from those in the real world, but also mirror some of our preconceptions of how the world "should" work. We all know that Wile E. Coyote will never be able to catch the Roadrunner with a fan attached to a sailboard, or an outboard motor submerged in a pail of water—but *why*, exactly? Can we attach some numbers to this knowledge? We have designed some classroom demonstrations accompanied by personal-response-type questions that use classic cartoon clips to challenge student thinking in introductory courses, prompting them to rediscover the truths of physics for themselves. We extend this idea to intermediate-level modern physics, showing that some phenomena in the cartoon universe can be reconciled with standard physics if the values of fundamental constants such as  $c$ ,  $G$  and  $h$  differ radically from those in the real world. Such an approach can both heighten student interest and deepen understanding in various physics topics.

### **G1.00155 The Hunt for Red October II: a demonstration for introductory electromagnetism**

, DANIEL ZILE, THOMAS SEBASTIAN, VIKTOR POLYAK, Towson University, ANJALEE RUTAH, Bryn Mawr School, JAMES OVERDUIN, Towson University — We have designed, constructed and tested a small-scale version of the silent submarine depicted in the 1990 Sean Connery thriller *The Hunt for Red October*. This vessel contains no moving parts. It uses onboard batteries and magnets to propel seawater salt ions out of the back of the boat, producing an equal and opposite forward thrust on the submarine thanks to Newton's third law. Such a craft could be very hard to detect by conventional means. Our objectives were to create a striking teaching demonstration for introductory electromagnetism courses and to determine why (to our knowledge) no navy has yet exploited such a seemingly revolutionary propulsion system for purposes of national defense. As teaching demonstrations, our prototypes are very successful at capturing student interest and convincing them of the reality and practical importance of electromagnetic fields. We have also identified a number of factors that may help to explain why a scaled-up model might not quite function as depicted in the film. We discuss several promising avenues for future student research.

### **G1.00156 Enhancing Student Success in Biology, Chemistry, and Physics by Transforming the Faculty Culture<sup>1</sup>**

, HOWARD JACKSON, LEIGH SMITH, KATHLEEN KOENIG, JILL BEYETTE, BRIAN KINKLE, ANNE VONDERHEIDE, University of Cincinnati — We present preliminary results of an effort to enhance undergraduate student success in the STEM disciplines. We explore a multistep approach that reflects recent literature and report initial results by each of the Departments of Biology, Chemistry, and Physics of implementing several change strategies. The central elements of our approach involve identified departmental Teaching and Learning Liaisons, a unique faculty development component by our teaching center, a vertical integration of leadership across department heads, the Dean, and the Provost, and the explicit acknowledgement that change happens locally. Teaching and Learning lunches across the departments have attracted an attendance of ~65% of the faculty. The use of Learning Assistants in classrooms has also increased sharply. Modest changes in the student success rates have been observed. These efforts and others at the decanal and provostal levels promise changes in student success.

<sup>1</sup>We acknowledge the financial support of the National Science Foundation through DUE 1544001 and 1431350.

**G1.00157 Students' Attitudes and Enrollment Trends in Physics and Engineering** , DELPHINE BANJONG, University of North Dakota — Science, Technology, Engineering, and Mathematics (STEM) fields are critical for meeting ever-increasing demands in the U.S. for STEM and related skills, and for ensuring the global competitiveness of the United States in technological advancement and scientific innovation. Nonetheless, few U.S. students consider a STEM degree after high school and fewer STEM students end up graduating with a STEM degree. In 2012, the United States ranked 35<sup>th</sup> in math and 27<sup>th</sup> in science out of 64 participating countries in the Program for International Student Assessment (PISA), sponsored by the Organization for Economic Cooperation and Development (OECD). Considering the significant role physics and engineering play in technological advancement, this work investigates the attitudes of students and recent enrollment trends in these important subject areas.

## **G1.00158 OUTREACH AND ENGAGING THE PUBLIC —**

**G1.00159 The World's Biggest Movie Theater: Promoting the Stars** , ARTHUR PALLONE, JACQUE DAY-PALLONE, Norwich University — A great celestial story is only as effective as the teller of the tale. With passion and knowledge at the helm, we must search for ways to pass on that enthusiasm to others while conveying sound science. At the core, our common link is an age-old awe of the sky. From the scientist to the elementary school student, we ask remarkably similar questions. What's out there? When will some object slam into the Earth? Are we alone? In our view as advocates for astronomy at the community level, the public will emerge to discover answers to their questions, if given the forum. It's our responsibility as astronomy advocates to help one another provide those forums. While some regions, perhaps through a school or by a turn of good fortune, offer public observatories with sophisticated telescopes, we also know that an observing event can take place in an open field or a parking lot, and be fully palpable as seen through a pair of binoculars, or by the naked eye. Based on our experience, we present an integrated approach—one that borrows elements from education, entertainment, advertising, and public relations—to help choose an event, hook and keep the public's attention while making them want more, and provide some tips for increasing media presence.

## **G1.00160 INTERNATIONAL ISSUES —**

**G1.00161 The African Synchrotron Light Source (AfLS)** , SEKAZI MTINGWA, Retired, AHMADOU WAGUE, Universite Cheikh Anta Diop, SIMON CONNELL, University of Johannesburg, SA, BRIAN MASARA, South African Institute of Physics (Zimbabwean), TSHEPO NTSOANE, Neasa, SA, LAWRENCE NORRIS, NSBP, USA, HERMAN WINICK, SLAC National Accelerator Laboratory, KENNETH EVANS-LUTTERODT, Brookhaven National Laboratory, TABBETHA DOBBINS, Rowan University, USA, TAREK HUSSEIN, Cairo University, Egypt, FEENE MARESHA, Ethiopian Academy of Sciences, Ethiopia, KRYSTLE MCLAUGHLIN, Lehigh University, PHILIP OLADIJO, Int. U. of Sci. & Tech. Botswana (Nigeria), ESNA DU PLESSIS, SASOL, SA, ROMAIN MURENZI, Executive Director of TWAS, Rwanda, KENNEDY REED, LLNL, USA, FRANCESCO SELTE, ESRF, Europe, SVERKER WERIN, MAX IV, Sweden, JONATHAN DORFAN, OIST, JAPAN, MOHAMMAD YOUSEF, Cairo University, Egypt — Africa is the only habitable continent without a synchrotron light source. An interim Steering Committee held a major conference on November 16-20, 2015 at the European Synchrotron Radiation Facility (ESRF) in Grenoble, France to bring together African scientists, policy makers, and stakeholders to discuss the possibility of a synchrotron light source in Africa. The use of light sources as a premier tool for research was highlighted for a broad range of disciplines. A Roadmap towards a synchrotron in Africa was discussed. Firm outcomes of the Conference were a set of Resolutions and a Roadmap document, with the election of a Steering Committee. ([www.africanlightsource.org](http://www.africanlightsource.org)).

## **G1.00162 HISTORY OF PHYSICS —**

**G1.00163 The Discovery of Electrography.** , LARISSA SAMUILOVA, Department of Mathematics, SUNYSuffolk, VLADIMIR SAMUILOV, Department of Materials Science and Engineering, SUNYSB — Prof. Jakob Narkiewicz-Jodko (1947–1905) major discoveries are: Electrography – the method of the visualization of corona discharge (corona discharge photography) from the bodies due to the application of high strength and high frequency electric fields [1-4], and the first observation of the propagation of the electromagnetic waves for information transfer over the distances [5,6]. They were made in his laboratory, located at his manor home Nadniemen in Eastern Europe. We describe these experiments and equipment used in the Lab for these discoveries. We also introduce a mathematical algorithm for the analysis of the electrography images. [1] Decrespe M. La vie et les oeuvres de M. de Narkiewicz-Jodko, member et collaborateur de l'Institut imperial de medecineexperimentale de Saint-Petersbourg, member of correspondent de la Societe de Medecine de Paris, etc./ Marius Decrespe.- Paris, Chamuel, 1896, 51p. [2] Annalen der Physik.- Leipzig, 1896. – Bd 293, 132 [3] Electrography// The Photographic news for amateur photographers.- 1896.- vol. 40, p.450 [4] Maack F. Elektrographie. Mit besonderer Berucksich-tigung der Versuche Narkiewicz-Jodko/ Ferdinand Maack// Wissenseschaltliche Zeitschrift... – 1898.- Bd 1, 1, 8-22; -1898.- Bd 1, 2/3, 89-99. [5] Séances de la societe francaise de physique/ Societe francaise de physique. – Paris, 1898, p. 77-79. [6] Present condition of wireless telegraphy// Consular reports: Commerce, manufacturers, etc. of their consular districts. Bureau of Foreign Commerce of United States.- Washington 1901, v.66. p. 44.

## **G1.00164 SUPERLATTICES, NANOSTRUCTURES, AND OTHER ARTIFICIALLY STRUCTURED MATERIALS —**

**G1.00165 Thermite Reaction to Produce Artificial Reefs** , ALEXANDRO TREVINO, KAREN MARTIROSYAN, RICHARD KLINE, University of Texas, Rio Grand Valley — The degradation of coral reefs is an ecological issue that has prompted new collaboration by different scientific communities that would assist in the regeneration of the reefs. Unfortunately, these processes can be inefficient and extremely expensive prompting a new scientific approach by using solid-state combustion synthesis to regenerate the reefs. In this report we aimed to consolidate a multi-composite material to produce artificial reefs by initiating thermite reaction based on aluminum and polytetrafluoroethylene (PTFE) with natural reefs. By Thermodynamic analysis and experimentation it was established that a range between .03-.07 number of moles of PTFE was sufficient to reach an adiabatic temperature of over 1900 K, a sustained reaction and a physically stable product was achieved. Reefs are primarily composed of carbonates but their exact chemical composition can vary. X-ray diffraction analysis was used to determine the chemical composition of the reef and revealed presence of oxides, carbonates, silicates. The dominant chemical compounds that were identified are, SiO<sub>2</sub> -17%, MgSiO<sub>3</sub>-14.5%, CaCO<sub>3</sub>- 11.4%, Ca(Si<sub>3</sub>O<sub>4</sub>). Using our thermite reaction we aimed to achieve optimal physical, chemical, and biological properties and maintain cost efficiency of the multi-composite material.

**G1.00166 Synthesis and Characterization of ZnS:Eu<sup>3+</sup> - CMC nanophosphors emitting white light over broad excitation range** , DILIP DE, Covenantuniversity, Ota, Ogun State, Nigeria, IKORYA AHMEN, Department of Physics, University of Agriculture, Makurdi, Benue State, Nigeria, VIENA BRUNO, Laboratoire de Chimie de la Matiere Condensee de Paris — In this paper we report for the first time the synthesis and characterization of nanophosphors of ZnS:Eu<sup>3+</sup> - embedded in sodium carboxymethyl cellulose matrix (CMC) that emits high quality white light over broad range of excitation. The nano-phosphors of cubic (zinc blende) structure were synthesized using precipitation technique with doping concentrations of Eu<sup>3+</sup> ions 1 mol% and 5 mol%. The crystal sizes were 2.56 nm and 2.91 nm respectively. Annealing at 300 °C in a sulfur-rich atmosphere altered the crystal size to 4.35 nm and 3.65 nm respectively and the band gap from 4.2 eV to 3.76 eV and 3.81 eV respectively. The as-synthesized samples gave pure orange-red emission when excited at wavelengths of 394 nm and 465 nm. After thermal annealing of the samples, a broad emission band in the blue-green region assigned to defect related states emerged or were enhanced. Also enhanced were the emission lines of Eu<sup>3+</sup> ions in the orange-red region. A combination of these two transitions gave white light of different shades (recorded on the CIE 1931 chromaticity diagram) from cool white through Day-light to warm white light, depending on Eu<sup>3+</sup> concentration and the excitation wavelengths (UV-330 to blue 465 nm), thus showing great potential applications of these nano-phosphors.

**G1.00167 Thermally Engineered Blue Photoluminescence of Porous Anodic Alumina Membranes for Promising Optical Biosensors** , SANG DON BU, SAM YEON CHO, Chonbuk National University, YONG CHAN CHOI, Chonbuk National University, Daegu Gyeongbuk Institute of Science & Technology, JIN WOO KIM, JIN KYU HAN, JIN HO KWAK, SUN A YANG, Chonbuk National University — Optical biosensors based on porous anodic alumina membranes (PAAMs) have shown to be an effective device because of their unique optical properties and biocompatibility. Among various optical properties, photoluminescence (PL) emission derived from PAAMs is one of the most suitable characteristics. However, the origin of PL from PAA is unclear and still in doubt. Therefore, it is essential for further potential practical applications to understand the origin of PL and PL variations. Here, we investigate the effects of post-annealing temperatures on the blue PL of amorphous PAAMs fabricated in oxalic acid. We find that the blue PL emission is strongly dependent on the thermal properties. A strong blue PL at a peak of ~460 nm is observed from the initial PAAM (not annealed PAAM) and this PL band can be divided into two Gaussian components at 458 ± 4 nm (P1 band) and 517 ± 7 nm (P2 band). As the temperature increases to 600 °C, the intensities of two PL bands gradually increase. During temperature increases from 600 to 700 °C, the P2 band increases but the P1 band decreases. The analyses of electron paramagnetic resonance, Fourier transform infrared spectroscopy, and ultraviolet-visible absorption spectroscopy show that the P1 and P2 bands originate from the unstable carboxylates and the stable carboxylates, respectively.

**G1.00168 Imaging TiO<sub>2</sub> nanoparticles on GaN nanowires with electrostatic force microscopy<sup>1</sup>** , TING XIE, ECE, University of Maryland, College Park, BAOMEI WEN, N5 sensors, Inc, GUANNAN LIU, ECE, University of Maryland, College Park, SHIQI GUO, ECE, The George Washington University, ABHISHEK MOTAYED, N5 sensors, Inc, THOMAS MURPHY, IREAP, University of Maryland, College Park, R.D. GOMEZ, ECE, University of Maryland, College Park — Gallium nitride (GaN) nanowires that are functionalized with metal-oxides nanoparticles have been explored extensively for gas sensing applications in the past few years. These sensors have several advantages over conventional schemes, including miniature size, low-power consumption and fast response and recovery times. The morphology of the oxide functionalization layer is critical to achieve faster response and recovery times, with the optimal size distribution of nanoparticles being in the range of 10 to 30 nm. However, it is challenging to characterize these nanoparticles on GaN nanowires using common techniques such as scanning electron microscopy, transmission electron microscopy, and x-ray diffraction. Here, we demonstrate electrostatic force microscopy in combination with atomic force microscopy as a non-destructive technique for morphological characterization of the dispersed TiO<sub>2</sub> nanoparticles on GaN nanowires. We also discuss the applicability of this method to other material systems with a proposed tip-surface capacitor model.

<sup>1</sup>This project was sponsored through N5 Sensors and the Maryland Industrial Partnerships (MIPS, 5418).

**G1.00169 Management of the von Roos operator.<sup>1</sup>** , MARTIN MOLINAR-TABARES, Organismo de Cuenca Noroeste, Comision Nacional del Agua, LAMBERTO CASTRO-ARCE, Departamento de Fisica, Matematicas e Ingenieria, Unidad Regional Sur, Universidad de Sonora, CARLOS FIGUEROA-NAVARRO, Departamento de Ingenieria Industrial, Unidad Regional Centro, Universidad de Sonora, JULIO CAMPOS-GARCIA, Departamento de Ciencias de la Salud, Unidad Cajeme, Universidad de Sonora — When an electron is inside a semiconductor medium its effective mass rises from the shielding of the crystalline structure. When we have a semiconductor with a constant concentration the effective mass has a fixed value, and in this case, it can be easy to solve the Schrodinger equation of the particle, but if the concentration varies spatially, the effective mass will no longer constant and the solution can be difficult to find. The general form of the kinetic energy operator for a particle with variable mass is proposed for von Roos, this operator is characterized by some parameters whose values are subjected to a restriction. From a numerical solution of the Schrodinger equation we analyze the energies of an electron with position-dependent effective mass working with some values of the parameter of the von Roos operator.

<sup>1</sup>We acknowledge the support of SNI CONACYT

**G1.00170 Oscillation modes and transmission into a Fibonacci slab.<sup>1</sup>** , LAMBERTO CASTRO-ARCE, Departamento de Fisica, Matematicas e Ingenieria, Unidad Regional Sur, Universidad de Sonora, MARTIN MOLINAR-TABARES, Organismo de Cuenca Noroeste, Comisin Nacional del Agua, JULIO CAMPOS-GARCIA, Departamento de Ciencias de la Salud, Unidad Cajeme, Universidad de Sonora, CARLOS FIGUEROA-NAVARRO, Departamento de Ingenieria Industrial, Unidad Regional Centro, Universidad de Sonora, LEONARDO ISASI-SIQUEIROS, Departamento de Fisica, Matematicas e Ingenieria, Unidad Regional Sur, Universidad de Sonora, BETSABE MANZANARES-MARTINEZ, Departamento de Fisica, Unidad Regional Centro, Universidad de Sonora — In our contribution we developed a study on the behavior of the transmission modes and a Pt / Zn slab of a Fibonacci array of longitudinal and transverse acoustic waves. We have worked with arrangements from n = 1 to 10 and has managed to find the energy bands and transmission, filling factor 0.4 observing the appearance of Pseudo-Gaps in the evolution of the study when the arrangement Fibonacci increases.

<sup>1</sup>We acknowledge the support of SNI CONACYT

**G1.00171 Shedding Light on the Formation of Gold Nanorods<sup>1</sup>** , ORLANDO LOPEZ, Brookhaven National Laboratory, DAMIEN HUDRY, Brown University, DMYTRO NYKYRANCHUK, Brookhaven National Laboratory — A significant interest in the study and synthesis of one-dimensional materials such as nanorods or nanowires is sparked by their potential application in electronics, photonics and biodetection. However, the synthesis of these low dimensional materials is not always reliable due to kinetic effects in symmetry breaking and high sensitivity to impurities. In this work we discuss the synthesis of gold nanorods and new ways to achieve symmetry breaking during the growth from seed solution, hence maximizing the yield of nanorods. We discuss the mechanism involved in symmetry breaking and general strategies to improve the nanorod morphology and synthetic yield. This work can serve as a starting point to design reproducible synthetic strategies for preparing high quality gold nanorods.

<sup>1</sup>This project was supported by the U.S. Department of Energy, Office of Science, under the Science Undergraduate Laboratory Internships Program and used resources of the C.F.N., which is a U.S. DOE Facility, at B.N.L., Contract No. DE-SC0012704

**G1.00172 Exciton Emission from Bare and Alq<sub>3</sub>/Gold Coated GaN Nanorods**, FATEMESADAT MOHAMMADI, University of Cincinnati, GERD KUHNERT, DETLEF HOMMEL, University of Bremen, Germany, HEIDRUN SCHMITZER, Xavier University, Cincinnati, HANS-PETER WAGNER, University of Cincinnati — We study the excitonic and impurity related emission in bare and aluminum quinoline (Alq<sub>3</sub>)/gold coated wurtzite GaN nanorods by temperature-dependent time-integrated (TI) and time-resolved (TR) photoluminescence (PL). The GaN nanorods were grown by molecular beam epitaxy. Alq<sub>3</sub> as well as Alq<sub>3</sub>/gold covered nanorods were synthesized by organic molecular beam deposition. In the near-band edge region a donor-bound-exciton (D<sup>0</sup>X) emission is observed at 3.473 eV. Another emission band at 3.275 eV reveals LO-phonon replica and is attributed to a donor-acceptor-pair (DAP) luminescence. TR PL traces at 20 K show a nearly biexponential decay for the D<sup>0</sup>X with lifetimes of approximately 180 and 800 ps for both bare and Alq<sub>3</sub> coated nanorods. In GaN nanorods which were coated with an Alq<sub>3</sub> film and subsequently with a 10 nm thick gold layer we observe a PL quenching of D<sup>0</sup>X and DAP band and the lifetimes of the D<sup>0</sup>X transition shorten. The quenching behaviour is partially attributed to the energy-transfer from free excitons and donor-bound-excitons to plasmon oscillations in the gold layer.

**G1.00173 Role of polymers and surfactants in synthesis of high quantum yield upconverting nanoparticles.**, KEVIN NEWCOMBE, BRIAN YUST, Univ of Texas Rio Grande Valley — Rare earth doped fluoride nanoparticles with a size of about 25 nm have been synthesized by either solvothermal or microwave assisted techniques. The role of differing biocompatible polymeric compounds to act as nucleation agents and surfactants, including polyethylene glycol, polyvinylpyrrolidone, and polyethylene oxide, in the final size, crystallinity, and optical properties is investigated in depth. These upconverting nanoparticles which can be excited in the near-infrared (NIR) are ideal for biomedical applications because of the low absorption of these excitation wavelengths by soft tissues in the body. Their fluorescence can be used for NIR imaging as well as non-invasive activation of drugs conjugated to the surface for cancer therapy. After optimizing the synthesis parameters, wide angle x-ray diffraction, FTIR, Raman, and Vis-NIR spectroscopy are used to characterize the samples. By varying the polymer added to the precursor solution, we can elucidate the primary mechanisms of interaction during the synthesis process and optimize for the best possible optical properties. Finally, the dependence of the fluorescence intensity on the biocompatible polymer type and concentration will also be investigated.

**G1.00174 Diagnostics of defects in AlGaIn/GaN high electron mobility transistor (HEMT) epi-layers via spectroscopic photo current-voltage (IV) measurements with variable-wavelength ultraviolet (UV) and visible light excitation.**, MIN P. KHANAL, BURCU OZDEN, VAHID MIRKHANI, KOSALA YAPABANDARA, MUHAMMAD SHEHZAD SULTAN, MINSEO PARK<sup>1</sup>, Dept. of Physics, Auburn University, LI SHEN, Dept. of Electrical and Computer Engineering, Auburn University — The reliability and performance of the nitride high electron mobility transistors (HEMTs) have been plagued by deleterious phenomena such as current collapse which is believed to be produced by electrically-active deep-level defects (or traps) that reside at the surface/interfaces and in the bulk of the AlGaIn/GaN HEMT layers. Therefore, identification of their physical/spectral locations and understanding the nature of defects is very important to improve the reliability of AlGaIn/GaN HEMTs. In this work, deep-level defects and traps located in the AlGaIn/GaN HEMT epi-layers were investigated by using spectroscopic photo IV measurements. An array of Schottky contacts was constructed on the HEMT layer produced by metal-organic chemical vapor deposition (MOCVD). The photo IV measurement was performed by collecting the photo current generated by the variable-wavelength UV/visible light illumination. It was successfully demonstrated that this technique can provide the information on the distribution of electrically-active defects along the in-depth direction and across the HEMT wafers. Therefore, it can be concluded that the spectroscopic measurements can be useful to assess the uniformity of defect distribution both along the in-depth direction and across the AlGaIn/GaN wafers.

<sup>1</sup>Corresponding author.

**G1.00175 Multifrequency scanning probe microscopy study of nanodiamond agglomerates<sup>1</sup>**, VASUDEVA ARAVIND, STEPHEN LIPPOLD, Clarion University, QIAN LI, EVGHENY STRELCOV, BARIS OKATAN, Oak Ridge National Laboratory, BENJAMIN LEGUM, Clarion University, SERGEI KALININ, Oak Ridge National Laboratory, CLARION UNIVERSITY TEAM, OAK RIDGE NATIONAL LABORATORY TEAM — Due to their rich surface chemistry and excellent mechanical properties and non-toxic nature, nanodiamond particles have found applications such as biomedicine, tribology and lubrication, targeted drug delivery systems, tissue scaffolds and surgical implants. Although single nanodiamond particles have diameters about 4-5nm, they tend to form agglomerates. While these agglomerates can be useful for some purposes, many applications of nanodiamonds require single particle, disaggregated nanodiamonds. This work is oriented towards studying forces and interactions that contribute to agglomeration in nanodiamonds. In this work, using multifrequency scanning probe microscopy techniques, we show that agglomerate sizes can vary between 50-100nm in raw nanodiamonds. Extremities of particles and Interfaces between agglomerates show dissipative forces with scanning probe microscope tip, indicating agglomerates could act as points of increased adhesion, thus reducing lubricating efficiency when nanodiamonds are used as lubricant additives.

<sup>1</sup>This research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

**G1.00176 Comparison of photoluminescence properties of HSA-protected and BSA-protected Au<sub>25</sub> nanoclusters**, MASATO TSUKAMOTO, HIDEYA KAWASAKI, TADASHI SAITOH, MITSURU INADA, Kansai Univ., KANSAI UNIV. COLLABORATION, KANSAI UNIV. COLLABORATION — Gold nanoclusters (NCs) have attracted great interest for a wide range of applications. In particular, red light-emitting Au<sub>25</sub> NCs have been prepared with various biological ligands. It has been shown that Au<sub>25</sub> NCs have Au<sub>13</sub>-core/6Au<sub>2</sub>(SR)<sub>3</sub>-semiring structure. The red luminescence thought to be originated from both core (670 nm) and semiring (625 nm). It is important to reveal a structure of Au<sub>25</sub> NCs to facilitate the progress of applications. However, the precise structure of Au<sub>25</sub> NCs has not been clarified. There is a possibility of obtaining structural information about Au<sub>25</sub> NCs to compare optical properties of the NCs that protected by slightly different molecules. Bovine and human serum albumin (BSA, HSA) are suitable one for this purpose. It has been suggested that rich tyrosine and cysteine residues in these molecules are important to produce the thiolate-protected Au NCs. If Au<sub>25</sub> NCs have core/shell structure, only the luminescence of the semiring will be affected by the difference of the albumin molecules. We carefully compared PL characteristics of BSA- and HSA- protected Au<sub>25</sub> NCs. As a result, there was no difference in the PL at 670 nm (core), while differences were observed in the PL at 625 nm (semiring). The results support that Au<sub>25</sub> NCs have core/semiring structure.

**G1.00177 Simulations of terahertz pulse emission from thin-film semiconductor structures**, ANDREY SEMICHAEVSKY, Lincoln University (PA) — The photo-Dember effect is the formation of transient electric dipoles due to the interaction of semiconductors with ultrashort optical pulses. Typically the optically-induced dipole moments vary on the ns- or ps- scales, leading to the emission of electromagnetic pulses with terahertz (THz) bandwidths. One of the applications of the photo-Dember effect is a photoconductive dipole antenna (PDA). This work presents a computational model of a PDA based on Maxwell's equations coupled to the Boltzmann transport equation. The latter is solved semiclassically for the doped GaAs using a continuum approach. The emphasis is on the accurate prediction of the emitted THz pulse shape and bandwidth, particularly when materials are doped with a rare-earth metal such as erbium or terbium that serve as carrier recombination centers. Field-dependent carrier mobility is determined from particle-based simulations. Some of the previous experimental results [1] are used as a basis for comparison with our model. [1] J. O'Hara, J.M.O. Zide, A.C. Gossard, A.J Taylor, R.D. Averitt, "Enhanced Terahertz Detection via ErAs:GaAs nanoisland superlattices", Applied Physics, 88, 251119, 2006.

**G1.00178 Nonlocal spin-confinement of electrons in graphene with proximity exchange interaction**, YEE SIN ANG, SHI-JUN LIANG, KELVIN J. A. OOI, Singapore University of Technology and Design, CHAO ZHANG, University of Wollongong, ZHONGSHUI MA, Peking University, LAY KEE ANG, Singapore University of Technology and Design — In graphene-magnetic-insulator hybrid structure such as graphene-Europium-oxide (EuO-G), proximity induced exchange interaction opens up a spin-dependent bandgap and spin splitting in the Dirac band. We study the bound state formation in a hetero-interface composed of EuO-G. We theoretically predict a remarkable nonlocal spin-confinement effect in EuO-G and show that spin-polarized quasi-1D electron interface state can be generated in a magnetic-field-free channel. Quasiparticle transport mediated by the interface state can be efficiently controlled by the channel width and electrostatic gating. Our results suggest a pathway to further reduce the dimensionality of graphene quasiparticles from 2D to 1D, thus offering an exciting graphene-based platform for the search of exotic 1D physics and spintronic applications.

**G1.00179 The electronic and transport properties of monolayer transition metal dichalcogenides: a complex band structure analysis<sup>1</sup>**, DOMINIK SZCZESNIAK, Qatar Energy and Environment Research Institute, Hamad bin Khalifa University, Qatar Foundation — Recently, monolayer transition metal dichalcogenides have attracted much attention due to their potential use in both nano- and opto-electronics. In such applications, the electronic and transport properties of group-VIB transition metal dichalcogenides ( $MX_2$ , where  $M=Mo, W$ ;  $X=S, Se, Te$ ) are particularly important. Herein, new insight into these properties is presented by studying the complex band structures (CBS's) of  $MX_2$  monolayers while accounting for spin-orbit coupling effects. By using the symmetry-based tight-binding model a nonlinear generalized eigenvalue problem for CBS's is obtained. An efficient method for solving such class of problems is presented and gives a complete set of physically relevant solutions. Next, these solutions are characterized and classified into propagating and evanescent states, where the latter states present not only monotonic but also oscillatory decay character. It is observed that some of the oscillatory evanescent states create characteristic complex loops at the direct band gaps, which describe the tunneling currents in the  $MX_2$  materials. The importance of CBS's and tunneling currents is demonstrated by the analysis of the quantum transport across  $MX_2$  monolayers within phase field matching theory.

<sup>1</sup>Present work has been prepared within the Qatar Energy and Environment Research Institute (QEERI) grand challenge ATHLOC project (project no. QEERI- GC-3008).

**G1.00180 Shot noise in quantum dots in presence of Fano and Dicke effects in Kondo regime<sup>1</sup>**, PEDRO ORELLANA, NATALIA CORTES, Universidad Tecnica Federico Santa Maria, VICTOR APEL, Universidad Catolica del Norte — The quantum dots allow studying systematically quantum-interference effects as Fano and Dicke effects due to the possibility of continuous tuning the relevant parameters governing the properties of these resonances, in equilibrium and nonequilibrium regimes. The condition for the Fano resonance is the existence of two scattering channels: a discrete level and a broad continuum band. On the other hand, the electronic version of the Dicke effect is analogous to the Dicke effect in optics, which takes place in the spontaneous emission of two closely-lying atoms radiating a photon into the same environment. In quantum dots this effect is due to quantum interference in the passage of an electron through two closely lying resonant states of the quantum dots coupled to common leads. In this work, we present a systematic investigation of the influence of the Dicke effect on shot-noise and Fano factor in a cross-shaped quantum dot array. The relevant quantities are obtained by the non-equilibrium Greens function technique. Our results show that at zero temperature, the electrical current, shot-noise and Fano factor exhibit characteristics of the Dicke effect.

<sup>1</sup>This work was partially supported by FONDECYT under grant 140571.

**G1.00181 Self assembly and optical properties of CdSe nanoplatelet superlattice**, YUNAN GAO, WILLIAM TISDALE, MIT, TISDALE LAB MIT TEAM — Colloidal CdSe nanoplatelets (NPs) are 1-D confined materials with atomic uniform thickness, and only have homogeneous broadening in energy level distributions and very narrow emission spectrum. Additionally, NPs have a giant oscillator strength that leads to a faster emission rate compared to quantum dots and rods. Due to these properties, NPs have shown promising potential applications in light-emitting diodes, colloidal lasers, and harvesting multiple exciton generation in photovoltaic cells. Self-assembly of superlattice has been studied broadly for many nano-particles, but not yet for CdSe NPs. We will show for the first time a selective control of CdSe NP superlattice self-assembly, i.e., self-assembled into columnar or lamellar superlattice. Moreover, we will present that the assembly morphology of superlattice has direct effects on their optical properties, like polarization, absorption efficiency and emission rate, etc., and also on their Forster energy transfer properties. The self-assembly is based on liquid interfacial self-assembly and transfer technique. The structure and properties of the superlattice are characterized by transmission electron microscopy, and time-, polarization- and space-resolved photo-luminescent micro-spectroscopy.

**G1.00182 Novel Application of Cluster Analysis to Transport Data in Single Molecule Break Junctions**, BEN WU<sup>1</sup>, JEFFREY IVIE<sup>2</sup>, TYLER JOHNSON<sup>3</sup>, ROLAND HIMMELHUBER<sup>4</sup>, OLIVER MONTI<sup>5</sup>, Univ of Arizona — Single molecule based devices represent the ultimate limit in device design, but uncovering the major factors that determine energy level alignment in single molecule junctions and their effect on the charge transport properties of single molecules is still a major challenge. Analysis of break junction data using a novel density based hierarchical clustering algorithm reveals the deep structure of the highly stochastic data that will help hypothesis-driven elucidation of some of the key parameters for quantum transport. The strength of this approach is its scale-invariance and the identification of nested structure that may be overlooked by standard data analysis techniques. The statistical relevance of identified clusters can be gauged using a density based validation index.

<sup>1</sup>Arnold and Mabel Beckman Foundation

<sup>2</sup>Dept. of Chemistry and Biochemistry

<sup>3</sup>Dept. of Chemistry and Biochemistry

<sup>4</sup>College of Optical Sciences

<sup>5</sup>Dept. of Chemistry& Biochemistry, Dept.of Physics

**G1.00183 The effect of oxidation on charge carrier motion in PbS quantum dot thin films studied with Kelvin Probe Microscopy<sup>1</sup>**, LAN PHUONG NGUYEN HOANG, PHEONA WILLIAMS, JASON MOSCATELLO, KATHERINE E. AIDALA, Mt Holyoke Coll, AIDALA GROUP TEAM — We developed a technique that uses scanning probe microscopy (SPM) to study the real-time injection and extraction of charge carriers in thin film devices. We investigate the effects of oxidation on thin films of Lead Sulfide (PbS) quantum dots with tetrabutyl-ammonium-iodide (TBAI) ligands in an inverted field effect transistor geometry with gold electrodes. By positioning the SPM tip at an individual location and using Kelvin Probe Force Microscopy (KPFM) to measure the potential over time, we can record how the charge carriers respond to changing the backgate voltage with grounded source and drain electrodes. We see relatively fast screening for negative backgate voltages because holes are quickly injected into the PbS film. The screening is slower for positive gate voltages, because some of these holes are trapped and therefore less mobile. We probe these trapped holes by applying different gate voltages and recording the change in potential at the surface. There are mixed reports about the effect of air exposure on thin films of PbS quantum dots, with initial exposure appearing to be beneficial to device characteristics. We study the change in current, mobility, and charge injection and extraction as measured by KPFM over hours and days of exposure to air.

<sup>1</sup>This work is supported by NSF grant DMR-0955348, and the Center for Hierarchical Manufacturing at the University of Massachusetts, Amherst (NSF CMMI-1025020).

**G1.00184 Electron Transport through Polyene Junctions in between Carbon Nanotubes: an Ab Initio Realization<sup>1</sup>**, YIING-REI CHEN, KAI-YU CHEN, Department of Physics, National Taiwan Normal University, KUN-PENG DOU, JUNG-SHEN TAI, Research Center for Applied Sciences, Academia Sinica, HSIN-HAN LEE, Department of Physics, National Taiwan Normal University, CHAO-CHENG KAUN, Research Center for Applied Sciences, Academia Sinica — With both *ab initio* and tight-binding model calculations, we study a system of polyene bridged armchair carbon nanotube electrodes, considering one-polyene and two-polyene cases, to address aspects of quantum transport through junctions with multiple conjugated molecules. The *ab initio* results of the two-polyene cases not only show the interference effect in transmission, but also the sensitive dependence of such effect on the combination of relative contact sites, which agrees nicely with the tight-binding model. Moreover, we show that the discrepancy mainly brought by *ab initio* relaxation provides an insight into the influence upon transmission spectra, from the junction's geometry, bonding and effective potential.

<sup>1</sup>This work was supported by the Ministry of Science and Technology of the Republic of China under Grant Nos. 99-2112-M-003-012-MY2 and 103-2622-E-002-031, and the National Center for Theoretical Sciences of Taiwan.

**G1.00185 Band alignment study on Al/SiO<sub>2</sub> and Cu/SiO<sub>2</sub> metal-oxide interface with the presence of point defect<sup>1</sup>**, JIANQIU HUANG<sup>2</sup>, ERIC TEA<sup>3</sup>, CELINE HIN<sup>4</sup>, Virginia Tech — Metal-Oxide interface has a wide use in electronic devices. Currently, technological development is aiming on the shrinkage of electronic devices' size. Based on the knowledge of electron tunneling effect, the reduction of dielectric thickness would cause an exponential increase on electron tunneling probability which contributes to current leakage. It might cause dielectric breakdown, which could make a severe and irreversible damage to the devices. Therefore, the main purpose of this study is to explore the possible factors that can lead to dielectric breakdown at metal-oxide interface. Density functional theory *ab initio* calculation has been applied to study the Al/SiO<sub>2</sub> and Cu/SiO<sub>2</sub> metal-oxide interface. Results on oxygen (di)vacancies at the interface will be presented and compared with the defect free model. The band alignment has been constructed to describe the variation of potential barrier height due to defect at interface. Results show the oxygen (di)vacancies at interface might trap electron and reduce potential barrier height. Moreover, the potential barrier height has a significant dependence on defects charge states.

<sup>1</sup>Supported by Air Force

<sup>2</sup>Ph.D student

<sup>3</sup>Post Doctoral

<sup>4</sup>Advisor

**G1.00186 Band alignment study on Al/SiO<sub>2</sub> and Cu/SiO<sub>2</sub> metal-oxide interface with the presence of H atom impurity and external electric field<sup>1</sup>**, JIANQIU HUANG<sup>2</sup>, ERIC TEA<sup>3</sup>, CELINE HIN<sup>4</sup>, Virginia Tech — Metal-Oxide interface has a wide use in electronic devices. Currently, technological development is aiming on the shrinkage of electronic devices' size. Based on the knowledge of electron tunneling effect, the reduction of dielectric thickness would cause an exponential increase on electron tunneling probability, which contributes to current leakage. It might cause dielectric breakdown, which could make a severe and irreversible damage to the devices. Therefore, the main purpose of this study is to explore the possible factors that could lead to dielectric breakdown at metal-oxide interface. Density functional theory *ab initio* calculation has been applied to study the Al/SiO<sub>2</sub> and Cu/SiO<sub>2</sub> metal-oxide interface. Previous study revealed the facts that oxygen (di)vacancies at interface might trap electron and vary potential barrier height. In this study, we introduced the H atom impurity at interface, and applied external electric field to the system. Charge density differences have been calculated to observe the charge alternation at the interface when impurity and external electric field existed. Band alignment revealed the potential barrier height variation due to the impurity and external electric field, which provided us how barrier height would respond to these two types of defects.

<sup>1</sup>Supported by Air Force

<sup>2</sup>Ph.D student

<sup>3</sup>Post Doctoral

<sup>4</sup>Advisor

**G1.00187 Single crystal complex oxide on flexible substrate.**, SAIDUR BAKAUL, CLAUDY SERRAO, OUKJAE LEE, SAYEEF SALAHUDDIN, University of California Berkeley — Flexible ferroelectrics are needed for various applications such as biocompatible energy harvesting and flexible memory. In this sector, most of the current research is focused on organic piezoelectric materials which have advantage of flexibility but suffers severely from poor energy conversion and generation efficiency. On the contrary, owing to very high electromechanical coupling factor (representing energy conversion efficiency) complex oxides are the best choices as energy harvesting and transduction elements, especially for transforming mechanical energies into electronic energy. Still their usage in energy harvesting is very limited mainly due to the stringent growth conditions of single crystals, high temperature needed for crystallization and lack of flexibility and stretchability. We have shown that single crystal Pb<sub>0.8</sub>Zr<sub>0.2</sub>TiO<sub>3</sub> can be epitaxially transferred on flexible plastic substrate. The transferred PZT shows 70 uC/cm<sup>2</sup> remnant polarization and dielectric constant over 100 even when it is bent. These results suggest the possibility of single crystal complex oxide devices on flexible platform.

**G1.00188 Charge reorganization in LaMnO<sub>3</sub>/LaNiO<sub>3</sub> superlattice interfaces**, FEDERICO IORI, ALEXANDRE GLOTER, Universite' Paris Sud - CNRS, UNRAVEL PROJECT TEAM, STEM GROUP TEAM — Functional properties of oxide heterostructure can recently be controlled and tuned through the electronic and structural mismatch at the interface. Artificial superlattices thin film can thus present complex magnetic structure at the interface different from their corresponding bulk building blocks. In this scenario when an antiferromagnetic bulk LMO and the paramagnetic bulk LNO are combined in thin film superlattices, LaMnO<sub>3</sub>/LaNiO<sub>3</sub>, strong exchange bias, new metal-insulator transition or antiferromagnetic order at the interface appear. In this work we study by *ab initio* Density Functional Theory how the induced magnetic moments in LNO films in LMO/LMO (111)-oriented can lead to charge transfer and reorganization at the interface among the Ni and Mn metal ions for different periodicities of the superlattices (3/3, 5/5, 7/7) and how it is possible to control them through atomic intermixing at the interface.

**G1.00189 Engineering SrTiO<sub>3</sub>/LaAlO<sub>3</sub> heterostructures thickness through a metallic capping layer electrodes**, FEDERICO IORI<sup>1</sup>, Universite Paris Sud - CNRS — The possibility to achieve conducting and superconducting properties at the interface between two bulk insulator oxides as SrTiO<sub>3</sub> (STO) and LaAlO<sub>3</sub> (LAO) in 2004 [1] has wide opened the route toward the discovery and control of broad functional emerging properties in different oxides heterostructures. Nonetheless the STO/LAO system still present not clarified questions concerning the possibility to control the presence of the 2DEG at the interface. In this work we present our theoretical results supported by experimental measurements concerning the possibility to tune the critical thickness of the LAO topmost layer through the deposition of a metallic capping layer at the surface. Our *ab initio* Density Functional Theory calculations show how different metallic contact can lead to a reduction of the LAO critical thickness of 4 u.c. still preserving the 2D electronic gas at the interface. [1] Otomo and Hwang, Nature 427, 423 (2004)

<sup>1</sup>UNRAVEL Marie Curie project

replacing MAR16-2015-009178.

**G1.00190 Growth and Study of Cuprate Thin Film Heterostructures Combining  $\text{La}_2\text{CuO}_{4+\delta}$  and  $\text{LaCuO}_{3-\delta}$** , RODRIGO MARMOL, FRANKLIN BURQUEST, NICHOLAS COX, BRITTANY NELSON-CHEESEMAN, University of St Thomas — Cuprate materials have shown promise as fuel cell cathode materials. Both the layered perovskite,  $\text{La}_2\text{CuO}_{4+\delta}$ , and its 3D perovskite counterpart,  $\text{LaCuO}_{3-\delta}$ , demonstrate the simultaneous electronic and ionic conduction necessary for fuel cell cathode materials. The layered perovskite allows for oxygen interstitial diffusion through the material. Meanwhile, the 3D perovskite readily creates oxygen vacancies, allowing for oxygen vacancy diffusion through the material. In this work, we investigate thin film heterostructures created from these two disparate materials to understand how the local oxygen diffusion phenomena affect the local structure and electrical transport of cuprates. The growth of these heterostructures is possible through the atomic monolayer control of Molecular Beam Epitaxy with in-situ monitoring via Reflective High Energy Electron Diffraction. The superlattice structure is characterized by x-ray reflectivity, and the crystal structure of the disparate phases is characterized by x-ray diffraction. A custom electrical transport system is used to characterize the electrical transport of the films. We compare these heterostructures with the single-phase films of  $\text{La}_2\text{CuO}_{4+\delta}$  and  $\text{LaCuO}_{3-\delta}$  in order to understand how this heterostructuring may modify the structure and electrical properties.

**G1.00191 Thermoelectric Properties of Barium Plumbate Doped by Alkaline Earth Oxides**, ANDREZA EUFRASIO, RUDRA BHATTA, IAN PEGG, BIPRODAS DUTTA, Vitreous State Laboratory. The Catholic University of America — Ceramic oxides are now being considered as a new class of thermoelectric materials because of their high stability at elevated temperatures. Such materials are especially suitable for use as prospective thermoelectric power generators because high temperatures are encountered in such operations. The present investigation uses barium plumbate ( $\text{BaPbO}_3$ ) as the starting material, the thermoelectric properties of which have been altered by judicious cation substitutions.  $\text{BaPbO}_3$  is known to exhibit metallic properties which may turn semiconducting as a result of compositional changes without precipitating a separate phase and/or altering the basic perovskite crystal structure. Perovskite structures are noted for their large interstitial spaces which can accommodate a large variety of “impurity” ions. As  $\text{BaPbO}_3$  has high electrical conductivity,  $\sigma = 2.43 \times 10^5 \Omega^{-1} \text{m}^{-1}$  at room temperature, its thermopower,  $S$ , is relatively low,  $23 \mu\text{V/K}$ , as expected. With a thermal conductivity,  $k$ , of  $4.83 \text{Wm}^{-1} \text{K}^{-1}$ , the figure of merit ( $ZT = S^2 \sigma T k^{-1}$ ) of  $\text{BaPbO}_3$  is only 0.01 at  $T = 300\text{K}$ . The objective of this investigation is to study the variation of thermoelectric properties of  $\text{BaPbO}_3$  as Ba and Pb ions are systematically substituted by alkaline earth ions.

**G1.00192 The way to enhance thermoelectric properties of  $\text{Bi}_2\text{O}_2\text{Q}$  (Q=S and Se) system by introducing chalcogen mixture net.**<sup>1</sup>, CHANGHOON LEE, JISOOK HONG, Pohang University of Science and Technology, WANG RO LEE, Chonbuk National University, DAE YEON KIM, 4Agency for Defense Development (ADD), JI HOON SHIM, Pohang University of Science and Technology — First principles density functional theory calculations were carried out for the series of bilayered semiconducting  $\text{Bi}_2\text{O}_2\text{Q}$  (Q=S, Se) and hypothetically constructed  $\text{Bi}_2\text{O}_2\text{S}_{0.5}\text{Se}_{0.5}$  compounds in which chalcogen square net of pure  $\text{Bi}_2\text{O}_2\text{Q}$  compound is replaced with having stripe type structure of chalcogen mixture net to explore their electronic structures, the change in their electronic structures under the chalcogen mixing, and the possibility for improving in their thermoelectric properties. By introducing chalcogen mixture net in pure  $\text{Bi}_2\text{O}_2\text{Q}$ , the band gap should be adjusted, and the indirect band gap in pure  $\text{Bi}_2\text{O}_2\text{Q}$  compound is changed to direct band gap. According to the analysis of calculated thermoelectric properties of  $\text{Bi}_2\text{O}_2\text{Q}$  and  $\text{Bi}_2\text{O}_2\text{S}_{0.5}\text{Se}_{0.5}$  compounds, thermoelectric properties are strongly enhanced in  $\text{Bi}_2\text{O}_2\text{S}_{0.5}\text{Se}_{0.5}$  compound. It seems to be due to the fact that the electrical conductivity is strongly enhanced by the decrease of dimensionality of its electronic structure and the broadening of sharpness of density of states near the Fermi level. Therefore, we believe that band modulation by introducing chalcogen mixture net in its pure compound  $\text{Bi}_2\text{O}_2\text{Q}$  compound gives a help to improve their thermoelectric properties.

<sup>1</sup>2013R1A1A2060341

**G1.00193 Tunneling of Heat: Potential-Barrier Analysis.**, DAVID SAROKA, KAMIL WALCZAK, Pace University — We examine quantum processes of heat (energy) transfer as carried by electrons tunneling via potential barriers of different shapes. As a starting point, we use analytical expressions for transmission functions related to rectangular and triangular potential barriers as well as point-like defects connecting two heat reservoirs (thermal baths). To calculate thermal conductance, we use Landauer formula for heat flux in its linear Taylor expansion with respect to temperature difference. Our results are discussed with respect to temperature, resonant states, specific parameters characterizing potential barrier (its height and width), and the effective mass of heat carriers. To get time-dependent heat fluxes reflected from and scattered on potential barriers, we use Gaussian-type wave-packet approach to tunneling of heat carried by electrons. Time-domain formulation of the scattering problem is performed by using the quantum mechanical concept of Gaussian wave packets.

**G1.00194 Inelastic Heat Transfer in Molecular Quantum Dots**, JOANNA DYRKACZ, KAMIL WALCZAK, Pace Univ — We examine electronic heat conduction via molecular complexes in the presence of local electron-phonon coupling effects. In off-resonance transport regime, even weak electron-phonon interactions lead to phonon-mediated changes of transport characteristics. In the nearly resonance conditions, the strong electron-phonon coupling reduces the height of the main conductance peak, generating additional satellites (phonon sidebands) in transport characteristics and shifting molecular energy spectrum via reorganization (polaron) energy. In the past, it was shown that inclusion of electron-phonon coupling effects into computational scheme reduces discrepancy between theoretical results and experimental data. The aim of this project is to study electron-phonon coupling effects on electronic heat transfer at molecular level. For that purpose, we use non-perturbative computational scheme based on inelastic version of Landauer formula, where the Green's functions technique combined with polaron transformation was used to calculate multi-channel transmission probability function, while accessibility of individual conduction channels is governed by Boltzmann statistics. Our analysis is based on the hypothesis that the dynamics created by electron-phonon interaction onto the molecular quantum dot asymmetrically connected to two thermal reservoirs will lead to thermal rectification effect. Our results will be discussed in a few aspects: electron-phonon coupling strength, phonon dispersion relationship, and heat fluxes generated by temperature difference as well as bias voltage.

**G1.00195 Electronic band gaps and transport properties in periodically alternating mono- and bi-layer graphene superlattices**, XIONG FAN, WENJUN HUANG, TIANXING MA, Beijing Normal University, LI-GANG WANG, Zhejiang University, HAI-QING LIN, Beijing Computational Science Research Center — We investigated electronic band structure and transport properties of periodically alternating mono- and bi-layer graphene superlattices (MBLG SLs). In such MBLG SLs, there exists the zero-averaged wave vector (zero- $\bar{k}$ ) gap, which is insensitive to the lattice constant, and this zero- $\bar{k}$  gap can be controlled via changing both the ratio of potentials' widths and the interlayer coupling coefficient of bilayer graphene. It is also found that there exist the extra Dirac points and their conditions are analytically presented. Lastly, it shows that the electronic transport properties and the energy gap ( $E_g$ ) of the first two bands in MBLG SLs are tunable by the interlayer coupling and the widths' ratio of the periodic mono- and bi-layer graphene.

**G1.00196 Exact solutions for 1D lattice models with topological complicated configuration<sup>1</sup>**, LEI FANG, DAVID SCHMELTZER, The City College of The City University of New York — In this work a transfer matrix method is developed to study 1D lattice models within the tight binding framework. Employing this method we show, from simple to difficult, the solutions of a semi-infinite wire, a finite open wire, a single closed ring and two coupled rings. We start by studying local properties of solutions in a homogeneous region. It is found that a calculation of the exponential of the transfer matrix is necessary for us to obtain the general form of wave functions in the entire homogenous region. Then by matching wave functions at boundaries or connecting junctions we can get equations that determine the spectrum. In this way we have solved the problem of two coupled rings (a topologically complicated configuration) and it is shown there can exist bound state in this system.

<sup>1</sup>This work was supported in part by the U.S. DOE Office of Basic Energy Sciences (Program Code: E304).

**G1.00197 Identifying radiation induced point defect in SiC nanowires: computational modeling.**, MING UU, University of Louisville — SiC nanowires (NWs) are expected to possess higher radiation tolerance compared to their crystalline counterpart due to their efficiency in eliminating point defects generated by the radiations. In this study, we will develop a computational modeling scheme to identify the radiation induced point defects in SiC NWs. A preliminary study on the hexagonal 2H-SiC NWs has demonstrated that the point defects on the surface of the SiC NWs only create local distortions and will not cause the destruction of the entire structure of the SiC NWs. It is also found that the local strain created by the antisite, the C-vacancy, and the Si-interstitial defects induces a few impurity states inside the energy gap, while defects such as the Si-vacancy and C-interstitial defects tend to produce a small tail at the top of the valence band. These observations suggest that the electronic properties of the SiC NWs will not be affected to any great extent by these types of point defects on the surface of the SiC NWs, and therefore the SiC NWs are expected to be tolerant or resistant responding to these types of radiation effect.

**G1.00198 Magnetotransport experiments in two-dimensional electron gases exposed to electromagnetic hybrid superlattices**, JAKOB SCHLUCK, STEFAN FASBENDER, STEPHAN WISSENBERG, THOMAS HEINZEL, Heinrich-Heine University Dusseldorf, KLAUS PIERZ, HANS-WERNER SCHUMACHER, PTB Braunschweig, DIMITRIS KAZAZIS, ULF GENNSER, CNRS-LPN Marcoussis — Hybrid lateral superlattices composed of a square array of antidots and a periodic one-dimensional magnetic modulation are prepared in Ga[Al]As heterostructures. The two-dimensional electron gases exposed to these superlattices are characterized by magnetotransport experiments in various magnetic field configurations. Commensurability resonances as a function of a parallel external magnetic field are observed even in the absence of closed orbits, and interpreted with the help of numerical simulations based on the semiclassical Kubo model. [1] In additional homogeneous perpendicular magnetic fields, quantum effects emerge, which can be attributed to the formation of closed quantized orbits.  
[1] J. Schluck et al., Phys. Rev. B 91, 195303 (2015)

**G1.00199 Electric field dependent Electoreflectance of GaAs/AlGaAs multiple quantum well Bragg structure at second quantum state**, MIM NAKARMI, Department of Physics, Brooklyn College and the Graduate Center of the CUNY, Brooklyn, NY 11210, USA, NARESH SHAKYA, Department of Applied Physics, NYU Tandon School of Engineering, Brooklyn, NY 11201, USA, VLADIMIR CHALDYSHEV, Ioffe Institute, 26 Polytekhnikeskaya, St. Petersburg 194021, Russia — Electoreflectance Spectroscopy was employed to study the effect of electric field on the excitonic transitions in a GaAs/AlGaAs multiple quantum well (MQW) Bragg structure. The sample used in this experiment consists of 60 periods of quantum well structures with GaAs well layer (~13 nm) and AlGaAs barrier layer (~94 nm), grown by molecular beam epitaxy on a semi-insulating GaAs substrate. The sample structure was designed to coincide the Bragg resonance peak with the  $x(e2-hh2)$  exciton transitions. We observed a significant enhancement of excitonic feature around the  $x(e2-hh2)$  exciton transition due to the double resonance along with the sharp features of  $x(e1-hh1)$  and  $x(e1-lh1)$  ground state exciton transitions by tuning the angle of incidence of the light. We will present the results on electric field dependent electoreflectance measurements of this structure and discuss the effect of electric field on the first and second energy states.

**G1.00200 "Flash" synthesis of "giant" Mn-doped CdS/ZnSe/ZnS nanocrystals with ZnSe layer as hole quantum-well**, RUILIN XU, JIAYU ZHANG, Advanced Photonics Center, Southeast University, Nanjing — Usually, exciton-Mn energy transfer in Mn-doped CdS/ZnS nanocrystals (NCs) can readily outcompete the exciton trapping by an order of magnitude. However, with the accumulation of non-radiative defects in the giant shell during the rapid growth of the thick shell (up to ~20 monolayers in no more than 10 minutes), the photoluminescence (PL) quantum yield of this kind of giant NCs is significantly reduced by the accumulation of non-radiative defects during the rapid growth of thick shell. That is because the exciton-Mn energy transfer in Mn-doped CdS/ZnS NCs is significantly inhibited by the hole trapping as the major competing process, resulting from the insufficient hole-confinement in CdS/ZnS NCs. Accordingly flash synthesis of giant Mn-doped CdS/ZnSe/ZnS NCs with ZnSe layer as hole quantum-well is developed to suppress the inhibition. Meanwhile  $Mn^{2+}$  PL peak changes profoundly from ~620 nm to ~540 nm after addition of ZnSe layer. Studies are under the way to explore the relevant mechanisms.

**G1.00201 Electron spin decoherence in silicon carbide nuclear spin bath**, LI-PING YANG, Beijing CSRC — In this paper, we study the electron spin decoherence of single defects in silicon carbide (SiC) nuclear spin bath. We find that, although the natural abundance of  $^{29}Si$  (4.7%) counter-intuitive result, is the suppression of heteronuclear-spin flip-flop process in finite magnetic field. Our results show that electron spin of defect centers in SiC are excellent candidates for solid state spin qubit in quantum information processing.

**G1.00202 Current conserving theory at the operator level**, JIANGTAO YUAN, YIN WANG, JIAN WANG, The university of Hongkong — The basic assumption of quantum transport in mesoscopic systems is that the total charge inside the scattering region is zero. This means that the potential deep inside reservoirs is effectively screened and therefore the electric field at interface of scattering region is zero. Thus the current conservation condition can be satisfied automatically which is an important condition in mesoscopic transport. So far the current conserving theory is well developed by considering the displacement current which is due to Coulomb interaction if we just focus on the average current. However, the frequency dependent shot noise does not satisfy the conservation condition since we do not consider the current conservation at the operator level. In this work, we formulate a generalized current conserving theory at the operator level using non-equilibrium Green's function theory which could be applied to both average current and frequency dependent shot noise. A displacement operator is derived for the first time so that the frequency dependent correlation of displacement currents could be investigated. Moreover, the equilibrium shot noise is investigated and a generalized fluctuation-dissipation relationship is presented.

**G1.00203 Photonic Surface-Bulk Waves in 1D All-Dielectric Metamaterials**, ANNE DELUA, DAVID KEENE, MAXIM DURACH, Georgia Southern University — It has been previously reported that it is impossible to satisfy the strong condition for the propagation of Dyakonov Surface Waves in 1D all-dielectric metamaterials. The strong condition requires that both evanescent and ordinary waves decay into the metamaterial. We show that the weak condition, when only ordinary waves decay, can be satisfied in 1D all-dielectric metamaterials, which gives rise to a new class of photonic resonances that combine evanescent extraordinary and non-evanescent ordinary waves in one excitation. By combining thin layers of such metamaterials with different dielectric and metal substrates one can excite resonances that are a hybrid between Fabry-Perot modes in the metamaterial layer and surface waves on the boundaries of this layer.

**G1.00204 Scattering on hyperbolic microspheres: From photonic nanojets to Poisson-Arago bright spots**, REED HODGES, CLEON DEAN, MAXIM DURACH, Georgia Southern University — We investigate optical properties of metal-dielectric metamaterial microspheres composed of subwavelength spherical shells of two different materials alternating in an onion-layer fashion. Recently such metamaterial spheres were considered as cavities and their whispering gallery modes were investigated. We focus on the scattering of external radiation by the meta-microspheres in this work. We show that different scenarios are produced by altering the metal fraction in the spheres: as the microsphere transitions from all-dielectric to hyperbolic to all-metal, the photonic nanojets transform into Poisson-Arago bright spots. A new phenomenon also emerges as the percentage of metal in the microsphere increases. “Hot spots” of optical fields intensity appear at the center of the sphere. Their intensity is much higher than that of the incident plane wave.

**G1.00205 Image magnification in transformation optics devices based on tapered waveguides**<sup>1</sup>, WILLIAM ZIMMERMAN, CHRISTOPHER JENSEN, VERA SMOLYANINOVA, Towson Univ, IGOR SMOLYANINOV, University of Maryland — Recent progress in metamaterial and transformation optics (TO) research gave rise to such fascinating devices as perfect lenses, invisibility cloaks, and numerous other unusual electromagnetic devices. However, the metamaterials have problems with low-loss broadband performance and complexity of fabrication, especially in the visible frequency range. Our TO devices allow us to circumvent these difficulties by using lithographically defined metal/dielectric waveguides to emulate metamaterial properties [1]. Adiabatic variations of the waveguide shape enable control of the effective refractive index experienced by light propagating inside the waveguide. The achieved image magnification is consistent with numerical simulations. We have studied wavelength and polarization dependent performance of the waveguides. Our experimental designs appear to be broadband, which has been verified in the 480-633 nm range. These novel optical devices considerably extend our ability to control light on sub-micrometer scales. [1]. V.N. Smolyaninova, et al., Phys. Rev. B 87, 075406 (2013)

<sup>1</sup>This research was supported by the NSF grant DMR-1104676

**G1.00206 OPTICAL SPECTRA OF A MULTILAYER STACK COMPOSED OF HIGH-TEMPERATURE SUPERCONDUCTOR AND DIELECTRIC**, SILVIA CORTES-LOPEZ, FELIPE PEREZ-RODRIGUEZ, Benemerita Universidad Autonoma de Puebla — Layered high-temperature superconductors behave as negative-refractive-index hyperbolic metamaterials, having effective permittivity components, parallel and perpendicular to the superconducting planes, with different infrared Josephson plasma frequencies [1]. Here, we theoretically study the reflectivity and transmissivity of a multilayer stack with alternating high-temperature superconductor and dielectric slabs. For TM electromagnetic waves, it was found that both reflectivity and transmissivity exhibit narrow photonic pass bands corresponding to two types of Fabry-Perot resonances, one occurring in the superconductor, whereas the other in the dielectric slab. For a stack of N unit cells, in each narrow photonic pass band there are N-1 transmissivity peaks, associated to the quantization of the Bloch phase within the stack. In contrast, when both types of Fabry-Perot resonances are close to each other, the infrared pass bands become wide and the N-1 strong peaks in the optical spectra are clearly-separated. In addition, new resonances are observed at the top and the bottom of the pass bands, and a photonic band just below the lower Josephson plasma frequency appears. A.L. Rakhmanov, et al, Phys. Rev. B 81, 075101 (2010).

**G1.00207 Microwave propagation in chiral metamaterials**, AIDA PRYBYLSKI, Norfolk State Univ, LUIS YON, Granby High School, Norfolk, VA, NATALIA NOGINOVA, Norfolk State Univ — Chiral hyperbolic metamaterials are predicted to show interesting properties associated with possible topological photonic states in these materials, which present new opportunities for light control and manipulation. As prototypes, we consider two metal-dielectric systems designed for microwave range: a twisted wires array, where chirality is associated with shape of metal inclusions, and a rotated layer system, with parallel wires in each layer, and direction of the wires orientation rotated from layer to layer. Systems with different content of metal and layer-to-layer distance were fabricated and studied in the free space propagation experiment. The results were discussed in terms of effective media consideration.

**G1.00208 Temperature-dependent thermal transport in holey silicon nanostructures investigated by impulsive stimulated thermal scattering**, RYAN DUNCAN, ALEJANDRO VEGA-FLICK, ALEXEI MAZNEV, Department of Chemistry, Massachusetts Institute of Technology, ZHENGMAO LU, LINGPING ZENG, JIAWEI ZHOU, JEAN-PHILIPPE PERAUD, EVELYN WANG, GANG CHEN, Department of Mechanical Engineering, Massachusetts Institute of Technology, KEITH NELSON, Department of Chemistry, Massachusetts Institute of Technology — Nanostructuring of semiconductor materials provides a promising means for the decoupling of their electronic and thermal conductivities, making such systems of great interest to the fields of thermoelectrics and microelectronics. Prior investigations indicated that Brillouin zone-folding and phononic band-gap formation may play a role in the diminished thermal conductivity observed in such structures, although it is unclear to what degree such effects manifest themselves over different temperature ranges. We investigate thermal transport properties as a function of temperature for a series of nanoporous silicon membranes using impulsive stimulated thermal scattering (ISTS)—a non-contact optical technique for measuring in-plane thermal transport. Measurements were carried out at temperatures ranging from 350 to 84 K on samples with pore diameters of 130 nm and pitch sizes ranging from 150 to 500 nm. Monte Carlo simulations for phonon transport were performed for comparison to experimental observations. We will discuss the experimental and computational results, and attempt to determine whether the experimental data are consistent with the diffuse boundary scattering model in which phononic crystal effects are absent.

**G1.00209 Counterintuitive behavior of simulated network’s conductance analogous to the Braess paradox**<sup>1</sup>, SÉBASTIEN TOUSSAINT, IMCN/NAPS, Université catholique de Louvain, Belgium, DEMETRIO LOGOTETA, MARCO PALA, IMEP-LAHC, Université Grenoble Alpes, France, VINCENT BAYOT, BENOIT HACKENS, IMCN/NAPS, Université catholique de Louvain, Belgium — Suppressing a channel from a two-terminal mesoscopic network defined in a two-dimensional electron system (2DES) can paradoxically increase its conductance. This counterintuitive behavior analogous to the Braess paradox is evidenced in [1] by simulating the networks conductance (G) when progressively depleting one of its channels with a biased local probe. By means of 3D self-consistent Poisson-Schrödinger simulations based on the NEGF formalism we investigate the occurrence circumstances of this transport anomaly under the influence of a scanning tip. By simulating the current density and local density of states within the network in the coherent and ballistic transport regime, we can follow the modification of the electron flow when the anomaly occurs. This allows to get insights about the role of a simulated disordered potential within the 2DES and permit to evaluate the tip influence on the 2DES potential landscape. Interference phenomena between different network paths can be modified by simulating G under a magnetic field orthogonal to the 2DES. Different geometries and network congestion are also discussed. [1] M. G. Pala et al., Phys. Rev. Lett. 108, 076802 (2012).

<sup>1</sup>S.T. acknowledges support from the Belgian FRS-FNRS (FRIA)

**G1.00210 SURFACES, INTERFACES AND THIN FILMS —**

**G1.00211 Evolution of the Adsorption Phases on (111) Terraces With Their Width<sup>1</sup>**, ALAIN PHARES, Villanova University, DAVID GRUMBINE, St. Vincent College — We study the evolution of the crystallization patterns, or phases, of monomer adsorption on (111) terraces, with the number  $M$  of atomic sites in the width of the terrace up to and including  $M = 8$ . Pairwise adsorbate-adsorbate first, second and third neighbor interactions, whether attractive or repulsive, are taken into account.

<sup>1</sup>This work is supported in part by the National Institute for Computational Sciences under grant number TG-CHE050014N.

**G1.00212 Studies of Surface morphology and Atomic Force Microscope-induced Surface Modifications in Calcium Manganese Oxide (CaMnO) Thin Films<sup>1</sup>**, ANTHONY JOHNSON, CACIE HART, ADEEL CHAUDHRY, BRIDGET LAWSON, NATALIE FERRONE, SAMUEL NEUBAUER, DAVID HOUSTON, RAJESWARI KOLAGANI, DAVID SCHAEFER, Towson University — CaMnO is a material of interest for applications as a catalyst for renewable energy applications. Our recent work on epitaxial thin films of this material has shown that films with a tensile lattice mismatch strain exhibit structural and electrical properties that indicate oxygen deficiency. We are studying the influence of strain and oxygen stoichiometry variations on surface morphology as revealed by atomic force microscopy. Our previous work in epitaxial thin films of the hole doped manganite nanoscale has demonstrated surface modifications induced by a voltage-biased AFM tip. Such surface modifications have been shown to be associated with changes in cation and oxygen stoichiometry. We will report results of similar studies on strained CaMnO thin films; relevant for understanding the surface mobility of oxygen vacancies.

<sup>1</sup>We acknowledge support from the Towson Office of University Undergraduate Research, Fisher Endowment Grant and Undergraduate Research Grant from the Fisher College of Science and Mathematics, and Seed Funding grant from the School of Emerging technologies

**G1.00213 Glow-Discharge Production of Oxygen from the Martian Atmosphere**, CALEB HUGHES, RONALD OUTLAW, None — One of the most crucial aspects of any mission to Mars is a continual supply of oxygen for astronaut respiration on site. The most popular approach to this problem favors in-situ oxygen production on Mars, utilizing the  $\text{CO}_2$  Martian atmosphere. However, this requires a large energy budget. NASA's current plans for Mars include sending a system called MOXIE, which produces oxygen through solid oxide electrolysis at high temperatures. An alternative approach utilizes the 6 Torr Martian atmosphere to provide a continual source of oxygen by breaking down the molecule into CO and O using a glow-discharge. After dissociation, a thin film Ag membrane uniquely permeates the atomic oxygen which then recombines to  $\text{O}_2$  on the downstream side, where it is subsequently stored. By taking advantage of recent advances in thin film technology to reduce the thickness of the film to many orders of magnitude less than used in the initial study, a corresponding increase in  $\text{O}_2$  flux can be realized. The Ag thin film requires the support of a porous ceramic substructure. With this system, it is shown that this method produces a viable energy efficient alternative to MOXIE.

**G1.00214 Electronic Phase Exhibits Attraction Between Like Net Charges**, THOMAS MANZ, New Mexico State Univ — A new electronic phase transition was observed in thin plastic films metallized with gold, optionally with an additional layer of aluminum metallization. This phase transition occurred only when the dielectric layers of two metallized films faced each other. When charged to high voltage magnitudes and then grounded, an electronic phase transition occurred during the discharge step that led to a strong attraction between the paired metallized films, even though the films carried like net charges. The resulting electronic phase (and its attractive force) persisted for several days with no apparent decay at ambient temperatures (c. 25 C). After rotating the films along an axis not parallel to the films, the magnetic field due to rotational motion of the charge carriers relative to the thin films persisted for seconds before dissipation. This demonstrates free current lifetimes lasting seconds. Computations and experiments were performed that show the underlying mechanism for the attraction of like net charges is scattering of electromagnetic waves by an electric field cusp at the charged interfaces. Scattering theory calculations reveal this scattering should be most prevalent in the infrared and microwave regions. This has potential applications for shielding electronic circuits from electromagnetic noise at these wavelengths.

**G1.00215 Resistivity Effects of Cation Ordering in Highly-Doped  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  Epitaxial Thin Films**, FRANKLIN BURQUEST, School of Engineering, University of St. Thomas, St. Paul, MN 55105, RODRIGO MARMOL, University of Saint Thomas, NICHOLAS COX, BRITTANY NELSON-CHEESEMAN, School of Engineering, University of St. Thomas, St. Paul, MN 55105 — Highly-doped  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  (LSCO) films ( $0.5 \leq x \leq 1.0$ ) are promising for many applications due to their electronic, ionic, and phonon transport. In this study, we investigate the effect of "electrostatic strain" on the electrical transport of LSCO thin films with large doping ( $x=0.5, 0.75, \text{ and } 1.0$ ). This "electrostatic strain" is applied by ordering differently charged A-site cations ( $\text{La}^{3+}$  vs.  $\text{Sr}^{2+}$ ) into charged A-O layers within the crystal structure. This causes internal polar electrostatic forces, which have been shown to cause stretching of the apical oxygen bond in analogous epitaxial nickelate films. Thin film samples are grown concurrently to minimize extraneous effects on film structure and properties. Atomic force microscopy and x-ray reflectivity demonstrate that the films are single crystalline, epitaxial, and smooth. X-ray diffraction is used to measure the c-axis of the films as a function of doping and dopant cation ordering. Electrical transport data of the ordered samples is compared with transport data of conventional disordered cation samples. Preliminary data indicates significant differences in resistivity at both 300K and 10K between the cation-ordered and cation-disordered samples. This work indicates that dopant cation ordering within the layered cuprates could significantly modify the conduction mechanisms at play in these materials.

**G1.00216 Effects of Cd Interlayer on CdS/CdTe Thin Film Photovoltaics**, DAVID RIVELLA, LUIS CERQUEIRA, M. ALPER SAHINER, Seton Hall University — CdS/CdTe thin films are well known for their photovoltaic effects. However, it is also known that there are various factors that limit the output of the photovoltaic cells. In these particular thin films, a limiting factor is the interaction of CdS and the CdTe layers. By adding a Cd layer between CdS and CdTe, a buffer zone was created. Therefore, the interaction between the aforementioned layers was changed. In this study, the buffer zone was added to the photovoltaic cells, while the ratio of Cd to Te in the CdTe layer was varied, in order to observe the effects of the buffer in regards to the diffusion of Te in traditional CdTe/CdS photovoltaics. The samples were created on ITO coated glass using pulsed laser deposition. This created uniform samples with an approximate thickness of 0.75 microns. In order to test the effect of the Cd buffer layer, the CdTe layers were deposited with varying ratios of Cd to Te. XRD analysis confirmed that the deposited Cd and Te formed crystalline CdTe. The active carrier concentrations were then determined using Hall Effect measurements. The photovoltaic properties were measured using Keithley source meter set-up. The effect of structural modifications on the active carrier concentrations and photovoltaic properties will be discussed.

**G1.00217 Exploration of Al-Doped ZnO in Photovoltaic Thin Films**, CHRISTOPHER CICCARIANO, M. ALPER SAHINER, Seton Hall University — The electrical properties of Al doped ZnO-based thin films represent a potential advancement in the push for increasing solar cell efficiency. Doping with Aluminum will theoretically decrease resistivity of the film and therefore achieve this potential as a viable option in the P-N junction phase of photovoltaic cells. The n-type semi-conductive characteristics of the ZnO layer will theoretically be optimized with the addition of Aluminum carriers. In this study, Aluminum doping concentrations ranging from 1-3% by mass were produced, analyzed, and compared. Films were developed onto ITO coated glass using the Pulsed Laser Deposition technique. Target thickness was 250 nm and ellipsometry measurements showed uniformity and accuracy in this regard. Active dopant concentrations were determined using Hall Effect measurements. Efficiency measurements showed possible applications of this doped compound, with upwards of 7% efficiency measured, using a Keithley 2602 SourceMeter set-up. XRD scans showed highly crystalline structures, with effective Al intertwining of the hexagonal wurtzite ZnO molecular structure. This alone indicates a promising future of collaboration between these two materials.

**G1.00218 Electrical Properties Analysis of Copper doped CdTe/CdS Deposited Thin Films on ITO Coated Glass Substrates**, DARREN LESINSKI, JAMES FLAHERTY, M. ALPER SAHINER, Seton Hall University — CdTe proves to be a viable source for renewable energy in the form of photovoltaic conversion. While CdTe/CdS naturally provide interesting results adding dopants to the cell can yield higher conversion efficiencies. Copper, famous for its electrical properties, can be used as a dopant in the CdTe layer. In conjunction with its dopant characteristics Copper also improves cell performance by acting as a low resistant and high current back contact. All thin films were synthesized using pulsed laser deposition onto ITO coated glass substrates. The CdS layer across all cells has an approximate thickness of 1500 Angstroms. The following CdTe layer has an approximate thickness of 5500 Angstroms. This created the base cell that was then doped. Cu, typically deposited using sublimation or vapor deposition, was done by PLD as well. Two of the three base cells were treated with Cu using the same deposition parameters. The third cell also received a CdCl treatment on top of the Cu layer to understand the effect when the oxygen layer is deferred. Ellipsometer measurements were used to confirm layer thickness. XRD analysis was used to confirm the presence of Cu and the crystal structure of the thin films. A Hall Effect Measurement system was used to measure active charge carrier concentration introduced by dopant. Also, a Keithley sourcemeter was utilized to determine photovoltaic properties. Notable results discussed will be the effects of Copper dopant on the electrical properties of CdS/CdTe based solar cells.

**G1.00219 Synthesis and Characterization of Varying Concentrations of Ag-doped ZnO Thin Films**, JUSTIN HACHLICA, PATRICK WADIE-IBRAHIM, M. ALPER SAHINER, Seton Hall Univ — Silver doped ZnO is a promising compound for photovoltaic solar cell use. Doping this compound with varying amounts of silver will theoretically make this type of thin film more efficient by reducing the overall resistance and increasing the voltage and current output. The extent of this promise is being tested experimentally, by analysis of both the electrical and the surface roughness properties of the cells. Ag-doped Zinc Oxide is deposited by method of Pulsed Laser Deposition (PLD) onto Indium Tin Oxide (ITO) coated Glass. Annealing effects were also observed by varying the temperature at which the annealing occurred after synthesis of the sample. Thickness is confirmed by use of Ellipsometry. X-Ray Diffraction (XRD) measurements confirmed a ZnO crystal structure on the thin films. The active dopant carrier concentrations were determined using a Hall Effect Measuring System. Finally, the photovoltaic properties of the film are recorded by using a Keithley Source Meter. The structural characterization and electrical results of the effect of Ag doping on ZnO will then be discussed.

**G1.00220 Tetrahedral cluster and pseudo molecule: New approaches to Calculate Absolute Surface Energy of Zinc Blende (111)/(-1-1-1) Surface<sup>1</sup>**, YIOU ZHANG, JINGZHAO ZHANG, KINFAT TSE, LUN WONG, CHUNGKAI CHAN, BEI DENG, JUNYI ZHU, Chinese Univ of Hong Kong — Determining accurate absolute surface energies for polar surfaces of semiconductors has been a great challenge in decades. Here, we propose pseudo-hydrogen passivation to calculate them, using density functional theory approaches. By calculating the energy contribution from pseudo-hydrogen using either a pseudo molecule method or a tetrahedral cluster method, we obtained (111)/(-1-1-1) surfaces energies of Si, GaP, GaAs, and ZnS with high self-consistency. Our findings may greatly enhance the basic understandings of different surfaces and lead to novel strategies in the crystal growth.

<sup>1</sup>We would like to thank Su-huai Wei for helpful discussions. Computing resources were provided by the High Performance Cluster Computing Centre, Hong Kong Baptist University. This work was supported by the start-up funding and direct grant with the Project

**G1.00221 Surface studies of gallium nitride quantum dots grown using droplet epitaxy on bulk, native substrates**, CHRISTINA JONES, SUNYEOL JEON, RACHEL GOLDMAN, Univ of Michigan - Ann Arbor, YIZHAK YACOBY, Hebrew University, ROY CLARKE, Univ of Michigan - Ann Arbor — Gallium nitride (GaN) and its applications in light-emitting diodes play an integral part in efficient, solid-state lighting, as evidenced by its recognition in the 2014 Nobel prize in physics. In order to push this technology towards higher efficiency and reliability and lower cost, we must understand device growth on bulk GaN substrates, which have lower defect densities and strain than template GaN substrates grown on sapphire. In this work, we present our findings on the surface properties of GaN quantum dots (QDs) grown on commercial bulk GaN. QDs are grown using the droplet epitaxy method and analyzed using a surface X-ray diffraction technique called Coherent Bragg Rod Analysis (COBRA), which uses phase retrieval to reconstruct atomic positions near the substrate surface. While several QD growth conditions in our study produce dense QDs, COBRA reveals that only low nitridation temperatures result in GaN QDs that are coherent with the bulk GaN substrate. Results are supported with atomic force microscopy and high-resolution transmission electron microscopy.

**G1.00222 Noncontact Atomic Force Microscopy Study of Surface Structural Transitions and Charge Distribution Modulations on SrTiO<sub>3</sub>(100)**, OMUR DAGDEVIREN, GEORG SIMON, KE ZOU, CHARLES AHN, FRED WALKER, ERIC ALTMAN, UDO SCHWARZ, Yale University — The surface structures of SrTiO<sub>3</sub>(100) single crystals were examined as a function of annealing time and temperature in either oxygen or ultra-high vacuum (UHV) using noncontact atomic force microscopy (NC-AFM), Auger electron spectroscopy (AES), and low-energy electron diffraction (LEED). Samples were subsequently analyzed for the effect the modulation of their charge distribution had on their surface potential. It was found that the evolution of the surface roughness, termination, and reconstruction depends crucially on the preparation scheme. For example, transitions from (1x1) termination to an intermediate c(4x2) reconstruction to ultimately a (sqrt(13) x sqrt(13))-R33.7 surface were observed for annealing in oxygen. In UHV, the inverse transition occurred and was accompanied by an increase in surface Sr while the surface oxygen content decreased. Complementary NC-AFM measurements showed a non-monotonic trend for surface roughness with annealing temperature, which is explained by electrostatic modulations of the surface potential caused by increasing oxygen depletion. This is further corroborated by experiments in which the apparent roughness tracked in NC-AFM could be correlated with changes in the surface charge distribution.

**G1.00223 Diffusion of Copper through Ti overlayer<sup>1</sup>**, BRITT LONG, A. MENCHACA, A. R. CHOURASIA, Texas AM University-Commerce — The Cu/Ti interface has been characterized by x-ray photoelectron spectroscopy and resistivity measurements. Thin films of titanium were deposited on copper substrates by e-beam method. The thickness of the Ti film was kept at 50 Å. The interface was annealed at temperatures of 100, 200, 300 and 400C. The Ti 2p and Cu 2p regions were analyzed by XPS. The diffusivity of copper through titanium has been investigated. The resistivity measurements were done by the four probe method. The correlation between the resistivity and the surface composition has been evaluated.

<sup>1</sup>Work supported by Organized Research, TAMU-Commerce

**G1.00224 Fabrication and structural characterization of highly ordered titania nanotube arrays**, HONGTAO SHI, Department of Physics and Astronomy, Sonoma State University, Rohnert Park, CA 94928, ROSITA ORDONEZ, Department of Physics and Astronomy, Sonoma State University — Titanium (Ti) dioxide nanotubes have drawn much attention in the past decade due to the fact that titania is an extremely versatile material with a variety of technological applications. Anodizing Ti in different electrolytes has proved to be quite successful so far in creating the nanotubes, however, their degree of order is still not nearly as good as nanoporous anodic alumina. In this work, we first deposit a thin layer of aluminum (Al) onto electropolished Ti substrates, using thermal evaporation. Such an Al layer is then anodized in 0.3 M oxalic acid, forming an ordered nanoporous alumina mask on top of Ti. Afterwards, the anodization of Ti is accomplished at 20 V in solutions containing 1 M NaH<sub>2</sub>PO<sub>4</sub> and 0.5% HF or H<sub>2</sub>SO<sub>4</sub>, which results in the creation of ordered titania nanotube arrays. The inner pore diameter of the nanotubes can be tuned from ~50 nm to ~75 nm, depending on the anodization voltage applied to Al or Ti. X-ray diffractometry shows the as-grown titania nanotubes are amorphous. Samples annealed at different temperatures in ambient atmosphere will be also reported.

**G1.00225 High-Performance Simulations of the Diffusion Characteristics of a Pentacene Derivative on Gold Surfaces**, RYAN MILLER, AMANDA LARSON, KARSTEN POHL, Univ of New Hampshire — Pentacene serves as a backbone for several molecules that provide attractive qualities for organic photovoltaic devices. One of these pentacene derivatives is 5,6,7-trithiapentacene-13-one (TTPO), which is unique in that it achieves its lowest energy configuration on Au(1 1 1) surfaces with the thiol group angled down towards the surface, allowing many molecules to pack closely together and form molecular nanowires. However, TTPO diffuses on flat surfaces, making it difficult for the self-assembly process to be initiated. With the help of the low-energy sites in surface defects and Au(7 8 8) step edges, TTPO molecules can be anchored in place on surfaces, allowing for chain formation to begin. By using high-performance Density Functional Theory based molecular dynamics calculations, the molecules can be shown to stay localized to these bonding sites and serve as a basis for chain formation. In addition, by simulating various temperatures with a Nose-Hoover thermostat, we can analyze how temperature affects anchoring ability and diffusion properties.

**G1.00226 Resistance of superhydrophobic and oleophobic surfaces to varied temperature applications on 316L SS**, HAMZA SHAMS, DHA Suffa University (DSU), Pakistan, KANZA BASIT, SAJID SALEEM, National University of Sciences and Technology (NUST), Pakistan, BILAL A. SIDDIQUI, DHA Suffa University (DSU), Pakistan — 316L SS also called Marine Stainless Steel is an important material for structural and marine applications. When superhydrophobic and oleophobic coatings are applied on 316L SS it shows significant resistance to wear and corrosion. This paper aims to validate the coatings manufacturer's information on optimal temperature range and test the viability of coating against multiple oil based cleaning agents. 316L SS was coated with multiple superhydrophobic and oleophobic coatings and observed under SEM for validity of adhesion and thickness and then scanned under FFM to validate the tribological information. The samples were then dipped into multiple cleaning agents maintained at the range of operating temperatures specified by the manufacturer. Coating was observed for deterioration over a fixed time intervals through SEM and FFM. A comparison was drawn to validate the most critical cleaning agent and the most critical temperature at which the coating fails to leave the base substrate exposed to the environment.

**G1.00227 XPS and AFM Investigation of Ti-CuO Interface**, DARIUS DURANT, RITESH BHAKTA, A. R. CHOURASIA, Texas AM University-Commerce — The techniques of x-ray photoelectron spectroscopy and atomic force microscopy have been employed to study the Ti/CuO interface. Thin films of titanium were deposited on CuO at room temperature by e-beam method. The thickness of the titanium film was varied between 3 Å and 10 Å. The titanium 2p, oxygen 1s and copper 2p regions were investigated by XPS. The spectral data show the reduction of CuO to elemental copper. Titanium is observed to get oxidized to TiO<sub>2</sub>. The thickness of TiO<sub>2</sub> depended upon the initial thickness of the titanium overlayer. The reaction is observed to continue until the titanium overlayer is 7 Å thick. Beyond this thickness unreacted titanium is observed. The AFM study shows nonuniformity of the TiO<sub>2</sub> film on copper. The study provides a means of preparing TiO<sub>2</sub> of nano-dimensions.

**G1.00228 Neutron scattering study of the freezing of water near a cupric oxide surface<sup>1</sup>**, J. TORRES, Z. N. BUCK, F. Z. ZHANG, T. CHEN, R. A. WINHOLTZ, H. KAISER, H. B. MA, H. TAUB, U. Mo., M. TYAGI, NIST — Oscillating heat pipes (OHP) offer promising two-phase heat transfer for a variety of applications, including cooling of electronic devices.<sup>2</sup> Recently, it has been shown that a hydrophilic CuO coating on either the evaporator or condenser sections of a flat-plate OHP can significantly enhance its thermal performance.<sup>3</sup> This finding has motivated us to assess the strength of the CuO/H<sub>2</sub>O interaction by investigating the freezing behavior of H<sub>2</sub>O in proximity to a CuO surface. Using the High-Flux Backscattering Spectrometer at NIST, we have measured the intensity of neutrons scattered elastically from a well-hydrated sample of CuO-coated Cu foils that mimic the oxide surfaces in a flat-plate OHP. We observe abrupt freezing of bulk-like H<sub>2</sub>O above the CuO surface at 270 K followed by continuous freezing of the interfacial H<sub>2</sub>O down to 265 K. This freezing behavior is qualitatively similar to that found for water near a zwitterionic single-supported bilayer lipid membrane.<sup>3</sup> Further studies are planned to compare the diffusion coefficients of the interfacial water for the coated and uncoated OHPs.<sup>2</sup> F. Z. Zhang *et al.*, submitted to J. Heat Transfer. <sup>3</sup>M. Bai *et al.*, Europhys. Lett. **98**, 48006 (2012); Miskowiec *et al.*, Europhys. Lett. **107**, 28008 (2014).

<sup>1</sup>Supported by NSF Grant Nos. DMR-0944772 and DGE-1069091.

**G1.00229 The effect of ultraviolet irradiation on data retention characteristics of resistive random access memory.**, KENTARO KINOSHITA, KOUHEI KIMURA, KOUTOKU OHMI, SATORU KISHIDA, Tottori University — It is getting more and more serious to generate soft-errors by cosmic radiation, with increasing the density of memory devices. Therefore, the irradiation resistance of resistance random access memory (ReRAM) to cosmic radiation has to be elucidated for practical use. In this paper, we investigated the data retention characteristics against ultraviolet irradiation to ReRAM with Pt/NiO/ITO structure. Soft-errors were confirmed to be caused by ultraviolet irradiation in both low and high resistance states. The analysis of irradiation frequency dependence of data retention characteristics suggested that electronic excitation by the irradiation caused the errors. Based on a statistically estimated soft-error rate, the errors were suggested to be caused by aggregation and dispersion of oxygen vacancies due to the generation of electron-hole pairs and valence change by the ultraviolet irradiation.

**G1.00230 Effects of Post-Deposition Annealing on the Properties of Calcium Manganese Oxide Thin Films<sup>1</sup>**, NATALIE FERRONE, ADEEL CHAUDHRY, CACIE HART, BRIDGET LAWSON, DAVID HOUSTON, SAMUEL NEUBAUER, ANTHONY JOHNSON, DAVID SCHAEFER, RAJESWARI KOLAGANI, Towson University — We will present our results on the effects of post-deposition annealing on the structural and electrical properties of CaMnO<sub>3-d</sub> thin films grown by Pulsed Laser deposition. The thin films are epitaxially grown on (100) LaAlO<sub>3</sub> which has larger in-plane lattice parameters than that of bulk CaMnO<sub>3</sub>, which leads to bi-axial tensile strain in the thin films. Results from our laboratory show that bi-axial tensile strain leads to low resistivity in thinner films, the resistivity increasing with increasing thickness. These results are suggestive of a coupling between strain and oxygen stoichiometry in the thin films. We have investigated the effects of post-deposition annealing in various gas ambients towards the goal of understanding the effects of relaxation and oxygen stoichiometric changes. We will present a comparison of the structural and electrical properties of as-grown and post-annealed films over a range of thicknesses.

<sup>1</sup>Support from Towson University Office of Undergraduate Research, Fisher Endowment Grant & Undergraduate Research Grant from the Fisher College of Science & Mathematics, Seed Funding grant from the School of Emerging technologies, & NSF grant ECCS 112856

## G1.00231 ATOMIC, MOLECULAR AND OPTICAL (AMO) PHYSICS —

**G1.00232 Second quantization of propagation of light through Rb vapor**, ZHIHAO XIAO, ROBERT LANNING, Department of Physics & Astronomy, Louisiana State University, MI ZHANG, IRINA NOVIKOVA, EUGENIY MIKHAILOV, Department of Physics, College of William & Mary, JONATHAN DOWLING, Department of Physics & Astronomy, Louisiana State University — We model the propagation of squeezed light, in Laguerre-Gaussian spatial modes, through a non-linear medium such as Rb vapor. We examine the changes in both quantum state and spatial modes. We simulate the injection into a Rb vapor cell a linearly polarized laser beam to create squeezed vacuum state of light linearly polarized in the perpendicular direction. We fully quantize the optical field's propagation which is originally based on semi-classical calculation. The Rb atomic structure is simplified to a three-level system. We reveal the mechanism that how squeezed state of light is generated in this process and compare the theory with our experiment. We further investigate the impact on squeezing due to the change of parameters and produce schemes which improve the squeezing in the desired spatial modes.

**G1.00233 Modelling Spatial Modes of Squeezed Vacuum**, R. NICHOLAS LANNING, ZHIHAO XIAO, Louisiana State University, MI ZHANG, IRINA NOVIKOVA, EUGENIY E. MIKHAILOV, College of William and Mary, JONATHAN P. DOWLING, Louisiana State University — We develop a fully quantum model to describe the spatial mode properties of squeezed light generated as a strong laser beam propagates through a Rb vapor cell. Our results show that a Gaussian pump beam can generate a collection of higher order Laguerre-Gaussian squeezed vacuum modes, each carrying a particular squeeze parameter and squeeze angle. We show that a proper sorting of modes could lead to improved noise suppression and thus make this method of squeezed light generation very useful for precision metrology.

**G1.00234 Ground state configurations in two-mode quantum Rabi models<sup>1</sup>**, SUREN CHILINGARYAN, B. M. RODRÍGUEZ-LARA, Instituto Nacional de Astrofísica, Óptica y Electrónica — We study two models describing a single two-level system coupled to two boson field modes in either a parallel or orthogonal configuration. Both models may be feasible for experimental realization through Raman adiabatic driving in cavity QED. We study their ground state configurations; that is, we find the quantum precursors of the corresponding semi-classical phase transitions. We found that the ground state configurations of both models present the same critical coupling as the quantum Rabi model. Around this critical coupling, the ground state goes from the so-called normal configuration with no excitation, the qubit in the ground state and the fields in the quantum vacuum state, to a ground state with excitations, the qubit in a superposition of ground and excited state, while the fields are not in the vacuum anymore, for the first model. The second model shows a more complex ground state configuration landscape where we find the normal configuration mentioned above, two single-mode configurations, where just one of the fields and the qubit are excited, and a dual-mode configuration, where both fields and the qubit are excited.

<sup>1</sup>S A Chilingaryan acknowledges financial support from CONACYT

**G1.00235 Quantum Phase Slip Localization on the Percolation Cluster Backbone<sup>1</sup>**, NOAH BRAY-ALI, Joint Quantum Institute, University of Maryland, College Park and National Institute of Standards and Technology, Gaithersburg, MD 20899 — Quantum phase slips proliferate at the superfluid-to-Mott insulator transition of interacting lattice bosons with commensurate filling in one dimension. The backbone of the incipient infinite cluster at percolation threshold is topologically one-dimensional but localizes quantum phase slips. We calculate the quantum depletion of the condensate fraction on the percolation cluster for weak interactions. Finally we estimate the critical interaction strength where quantum phase slips delocalize using a strong-disorder renormalization group approach applied to the percolation backbone.

<sup>1</sup>Support provided by National Research Council Post-Doctoral Research Associateship

**G1.00236 Quantum-coherence driven self-organized criticality and non-equilibrium light localization.**, PANKAJ JHA, KOSMAS TSAKMAKIDIS, YUAN WANG, XIANG ZHANG, Univ of California - Berkeley — In its 28 years since its introduction in 1987, self-organized criticality (SOC) has had a major impact across a broad range of seemingly dissimilar fields of science. However, until now, it has primarily been applied to classical systems, and it remains a fundamental open question whether the theory also finds a place in complex systems driven by quantum coherence (QC). Here, on the basis of a many-body quantum-field theory and corroborating Maxwell-Bloch-Langevin computations, we report on the first example of fractal SOC driven, in the nano-world, by quantum coherence. We show that a quantum-coherently controlled active nano-plasmonic heterostructure allows, in the regime where the light speed is very close to zero, for the phase-synchronization in space of a continuous ensemble of nano-optical oscillators, giving rise to a fundamentally new kind of non-equilibrium light localization. We observe all hallmarks of SOC in this quantum many-body photonic nano-system of interacting heavy bosons, and we identify two critical points, one signifying the onset of spontaneous spatial self-organization, followed in time by another one that signifies the onset of activity. Our analysis reveals a quantum-coherence driven self-organized double-critical property in photonics and a new type of robust light localization, far out of thermodynamic and optical equilibria, with a broad range of potential applications in nano-optics and condensed-matter photonics.

**G1.00237 Anomalous diffusion of light in complex media**, ROXANA REZVANI NARAGHI, CREOL and Department of Physics, University of Central Florida, MARIELENA BURDGE, ARISTIDE DOGARIU, CREOL, University of Central Florida — Light propagation in random materials is often modeled by a diffusion approximation to the radiation transfer equation. This approach inherently ignores interference effects and describes only the energy propagation. When the interaction is strong, however, the scattering events become correlated and wave interferences can cause the diffusion to be slow down. One result of this process is the appearance of localized modes, whereby the energy inside the material is confined to small spatial regions due to constructive interferences. This anomalous, sub-diffusive character of energy propagation could be justified within the scaling theory of localization where the optical diffusion coefficient is size dependent. Moreover, when the concentration of scatterers increases, the near-field interactions between scatterers placed in close proximity of each lead to a new transport regime. In these conditions, the energy spread is not only diffusive but it also evolves through evanescent coupling between individual scatterers. Based on measurements of photon path-length distributions, we report the observation of such distinct regimes of energy transport.

**G1.00238 Topological photonics: an observation of Landau levels for optical photons<sup>1</sup>**, NATHAN SCHINE, ALBERT RYOU, ARIEL SOMMER, JONATHAN SIMON, Univ of Chicago — We present the first experimental realization of a bulk magnetic field for optical photons. By using a non-planar ring resonator, we induce an image rotation on each round trip through the resonator. This results in a Coriolis/Lorentz force and a centrifugal anticonfining force, the latter of which is cancelled by mirror curvature. Using a digital micromirror device to control both amplitude and phase, we inject arbitrary optical modes into our resonator. Spatial- and energy- resolved spectroscopy tracks photonic eigenstates as residual trapping is reduced, and we observe photonic Landau levels as the eigenstates become degenerate. We show that there is a conical geometry of the resulting manifold for photon dynamics and present a measurement of the local density of states that is consistent with Landau levels on a cone. While our work already demonstrates an integer quantum Hall material composed of photons, we have ensured compatibility with strong photon-photon interactions, which will allow quantum optical studies of entanglement and correlation in manybody systems including fractional quantum Hall fluids.

<sup>1</sup>This work was supported by DOE, DARPA, and AFOSR.

**G1.00239 Topological  $Z_2$  Gapless Photonic Crystals**, BIYE XIE, ZIDAN WANG, The University of Hong Kong — Topological properties of electronic materials with gapless band structure such as Topological Semimetals (TSMs) and Topological Metals (TMs) have drew lots of attention to both theoretical and experimental physicists recently. Although theoretical prediction of TSMs and TMs have been done well, experimental study of them is quite difficult to perform due to the fact that it is very difficult to control and design certain electronic materials. However, since the topological properties stem from the geometric feature, we can study them in Photonic Crystals (PhCs) which are much easy to be controlled and designed. Here we study 2-dimension PhCs consisting of gyrotropic materials with hexagonal structure. In the Brillouin corner, the dispersion relation has gapless points which are similar to Dirac Cones in electronic materials. We firstly derive the effective Hamiltonian of this system and show that if certain perturbation is added to this effective Hamiltonian, this system belongs to All class according to Altland and Zirbauer topological classification and is described by a  $Z_2$  topological charge. Finally we also propose a way to detect this  $Z_2$  topological charge using momentum space Aharonov-Bohm interferometer which is firstly proposed by L.Duca and T.Li, etc.

**G1.00240 Real-time emission spectrum from a hybrid atom-optomechanical cavity**, IMRAN MIRZA, Department of Physics, University of Michigan, Ann Arbor, USA — Hybrid quantum systems are promising candidates for opening new avenues for quantum technologies [G. Kurizki et. al, PNAS, 112 (13), 3866-3873 (2015)]. Hybrid atom-optomechanical (HAOM) systems set an intriguing example in this context. From the perspective of practical utilizations of these HAOM systems in future quantum devices, it is crucial to fully understand the excitation dynamics as well as the spectral features of these systems. In this poster, I'll present my calculations of single-photon time-dependent (TD) spectrum emitted by such a HAOM system in a strong atom-cavity as well as strong cavity-mechanics (strong-strong) coupling regime ["Real-time emission spectrum from a hybrid atom-optomechanical cavity", Imran M. Mirza, J. Opt. Soc. Am. B, 32 (8), 1604-1614 (2015)]. In order to make the system more realistic the effects of dissipation through the mechanical oscillator, optical cavity and spontaneous emission from the two-level emitter are also incorporated. The TD spectrum reveals some novel features that are not possible to observe otherwise. For instance, time order in which different side bands appears which explains different photon-phonon interactions responsible for the production of distinct spectral resonances. .

**G1.00241 Cooling a nanomechanical resonator using spin-dependent transport and noise interference in Andreev reflections**, PASCAL STADLER, WOLFGANG BELZIG, GIANLUCA RASTELLI, University of Constance — Nanoelectromechanical systems promise to manipulate mechanical motion in the quantum regime using electron transport. For such a goal, a necessary condition is the ability of cooling the resonator into or near to its quantum ground state. A still open challenge in this field is the achievement of active cooling using purely electron transport in, for instance, suspended carbon nanotube quantum dots. We consider the quantum transport in a carbon nanotube quantum dot suspended between two electric nanocontacts. Due to the interaction between electrons and flexural mechanical modes, the electron transport results in inelastic vibration-assisted tunneling processes. These give rise to a mechanical damping and to a steady nonequilibrium phonon occupation of the resonator. We discuss these effects for two different coherent transport regimes: (i) spin-polarized current between two ferromagnets [1,2] and (ii) subgap Andreev current between a superconductor and normal metal [3].  
[1] P. Stadler, W. Belzig, and G. Rastelli, Phys. Rev. Lett. 113, 047201 (2014)  
[2] P. Stadler, W. Belzig, and G. Rastelli, Phys. Rev. B 91, 085432 (2015)  
[3] P. Stadler, W. Belzig, and G. Rastelli, arXiv:1511.04858 (submitted)

**G1.00242 Transient Loschmidt Echo and Orthogonality Catastrophe in highly excited Quantum Ising Spin Chains**, MARCO SCHIRO, Institut de Physique Theorique, Universite Paris Saclay, CNRS, CEA, CARLA LUPO, Politecnico di Torino, Corso Duca degli Abruzzi, 24, 10129 Torino Italy and Universite Paris Sud Paris XI, 15 Rue Georges Clemenceau, 91400 Orsay — We study the response to sudden local perturbations of highly excited Quantum Ising Spin Chains. The key quantity encoding this response is the overlap between time-dependent wave functions, which we write as a transient Loschmidt echo. We compute the Echo perturbatively in the case of a weak local quench and study its asymptotics at long times, which contains crucial information about the structure of the highly excited non-equilibrium environment induced by the quench. Our results reveal that the Echo decays exponentially, rather than power law as in the low-energy Orthogonality Catastrophe, a further example of quench-induced decoherence. The emerging decoherence scale is set by the strenght of the local potential and the bulk excitation energy. In addition, the transient evolution features aging behavior at the Ising quantum critical point.

**G1.00243 Minimally entangled typical thermal states versus matrix product purifications for the simulation of equilibrium states and time evolution**, MORITZ BINDER, THOMAS BARTHEL, Duke Univ — We compare matrix product purifications and minimally entangled typical thermal states (METTS) for the simulation of equilibrium states and finite-temperature response functions of strongly correlated quantum many-body systems. For METTS, we highlight the interplay of statistical and DMRG truncation errors, discuss the use of self-averaging effects, and describe schemes for the computation of response functions. We assess the computation costs and accuracies of the two methods for critical and gapped spin chains and the Bose-Hubbard model. For the same computation cost, purifications yield more accurate results than METTS except for temperatures well below the systems energy gap. (Phys. Rev. B 92, 125119 (2015))

**G1.00244 Investigation of the coupling of the momentum distribution of a BEC with its collective of modes<sup>1</sup>**, EMANUEL HENN, PEDRO TAVARES, AMILSON FRITSCH, FRANKLIN VIVANCO, GUSTAVO TELLES, VANDERLEI BAGNATO, Physics Institute of São Carlos - University of São Paulo — In our group we have a strong research line on quantum turbulence and the general investigation of Bose-Einstein condensates (BEC) subjected to oscillatory excitations. Inside this research line we investigate first the behavior of the normal modes of the BEC under this excitation and observe a non-linear behavior in the amplitude of the quadrupolar mode. Also, inside this same procedure of investigation we study the momentum distribution of a BEC to understand if it is possible to extract Kolmogorov like excitation spectra which would point to a turbulent state of matter. The condensate is perturbed, and we let it evolve in-trap after which we perform standard time-of-flight absorption imaging. The momentum distribution is extracted and analyzed as a function of the in-trap free evolution time for a 2D projected cloud. We show that the momentum distribution has its features varying periodically with the same frequency as the quadrupolar mode displayed by the atomic gas hinting at a strong coupling of both. The main consequence of that one cannot be assertive about the quantitative features of the extract spectrum of momentum and we can only rely on its qualitative features.

<sup>1</sup>Financial Support: FAPESP, CNPq

**G1.00245 One-dimensional Bose-Einstein condensation of photons in a microtube**, ALEX KRUCHKOV, École Polytechnique Fédérale de Lausanne (EPFL) — This study introduces a quasiequilibrium one-dimensional Bose-Einstein condensation of photons trapped in a microscopical waveguide. Light modes with a cut-off frequency ("photon's mass") interact through different processes of absorption, re-emission, and scattering on molecules of dye. In this work I consider conditions for the one-dimensional condensation of light and the role of photon-photon interactions in the system. The computational technique in use is the Matsubara's Green's functions formalism modified for the quasiequilibrium system under study.

**G1.00246 Spontaneous Exciton Condensate in Transition Metal Dichalcogenides electron-hole bilayer System<sup>1</sup>**, BISHWAJIT DEBNATH, YAFIS BARLAS, DARSHANA WICKRAMARATNE, MAHESH NEUPANE, ROGER LAKE, University of California Riverside — Spontaneous Bose-Einstein Exciton condensation (BEC) in spatially separated graphene layers has received intense theoretical and experimental attention, due to its promise for low-dissipation electronic devices. We have investigated BN-separated monolayers of transition metal dichalcogenides (TMDs) to explore the possibility of achieving exciton superfluidity in this class of 2D materials. The top and bottom monolayers can consist of either same TMD (homo-bilayer) or a combination of different TMDs (hetero-bilayer). The particle density in each monolayer is tuned by independent gate biasing. In TMDs, the almost equivalent particle-hole symmetry is an assisting factor towards achieving condensation. The calculated exciton binding energies are found to be as large as 50 – 250 meV, which is a result of the large effective masses in the TMDs. For BN thicknesses of around 3nm, the interaction strength is large and no longer in the weak coupling regime. Therefore, to calculate the excitonic gap, we use a modified Eliashberg formalism in which the phonon-mediated interaction is replaced with the inter-layer screened coulomb interaction between TMD bilayers.

<sup>1</sup>This work was supported in part by FAME, one of six centers of STARnet, a Semiconductor Research Corporation program sponsored by MARCO and DARPA and NSF EFRI-2DARE 143395

**G1.00247 Josephson Effect in Trapped Spin-orbit Coupled Bose-Einstein Condensation**, WAI HO TANG, The Univ of Hong Kong — Spin-orbit coupling (SOC) has given rise to many novel states of matter including topological insulators and superconductors. Recent experimental realization of SOC in neutral cold atom systems have opened a new avenue to study its effects in Bose-Einstein condensate. In this study, we discuss the Josephson-like mode in the spin-orbit coupled condensate, and study its decoherence due to thermal effect. We discuss experimental implications of our results.

**G1.00248 Entanglement like properties in Spin-Orbit Coupled Ultra Cold Atom and violation of Bell like Inequality**, SANKALPA GHOSH, RAHUL KUMAR, Physics Department, Indian Institute of Technology, Delhi, India — We show that the general quantum state of synthetically spin-orbit coupled ultra cold bosonic atom whose condensate was experimentally created recently (Y. J. Lin *et al.*, Nature, **471**, 83, (2011)), shows entanglement between motional degrees of freedom (momentum) and internal degrees of freedom (hyperfine spin). We demonstrate the violation of Bell-like inequality (CHSH) for such states that provides a unique opportunity to verify fundamental principle like quantum non-contextuality for commuting observables which are not spatially separated. We analyze in detail the Rabi oscillation executed by such atom-laser system and how that influences quantities like entanglement entropy, violation of Bell like Inequality etc. We also discuss the implication of our result in testing the quantum non-contextuality and Bell's Inequality violation by macroscopic quantum object like Bose-Einstein Condensate of ultra cold atoms.

**G1.00249 Measurement of optical nonlinearity of highly dispersive medium using optical heterodyne detection technique**, ARUP BHOWMICK, Senior Research Fellow, ASHOK MOHAPATRA, Reader-F — We discuss the optical heterodyne detection technique to study the absorption and dispersion of a probe beam propagating through a medium with a narrow resonance. The technique has been demonstrated for Rydberg Electro-magnetically induced transparency (EIT) in rubidium thermal vapor and the optical non-linearity of a probe beam with variable intensity is studied. A quantitative comparison of the experimental result with a suitable theoretical model is presented. The limitations and the working regime of the technique are discussed.

**G1.00250 Pair condensation of a spin-imbalanced two-dimensional Fermi gas**, DEBAYAN MITRA, PETER BROWN, STANIMIR KONDOV, PETER SCHAUSS, WASEEM BAKR, Princeton University — Strongly interacting Fermi gases of ultracold atoms are a clean and tunable platform for exploring high critical temperature superfluidity. This is particularly interesting because the physics of these gases has a close connection to superconductivity in strongly correlated materials. Early experiments in 3D gases have shed light on the crossover from BCS superfluidity to Bose-Einstein condensation of molecules and on the fate of superfluidity in spin-imbalanced gases. Here we study a strongly-interacting spin-imbalanced Fermi gas in two dimensions, where the low dimensionality enhances correlations and phase fluctuations in the gas. We observe pair condensation in the imbalanced gas and map out the temperature-polarization phase diagram for a range of interactions strengths. At low temperatures, we observe phase separation between the superfluid and the normal gas over a wide range of imbalance. The measurement of the phase diagram of strongly interacting fermions in two dimensions opens the door for a detailed investigation of exotic phases enhanced in two dimensions and in optical lattices like the elusive FFLO phase.

**G1.00251 Supersolidity in the one-dimensional Bose-Hubbard Model**, B. TANATAR, B. HETENYI, BILKENT UNIVERSITY — We show how a variational Monte Carlo method can be constructed based on the Baeriswyl wavefunction to calculate the ground-state properties of one-dimensional Bose-Hubbard model. The phase diagram obtained is in excellent agreement with previous quantum Monte Carlo results. We also investigate the sensitivity of the system to a boundary twist, and find that it is sizeable even for integer fillings. To understand the nature of the phase we use a single-particle and a many-particle localization quantity and find that at integer fillings the system exhibits many-particle localization, at the same time, single particles as a result of bosonic exchange, can delocalize over the entire lattice. Away from integer fillings, where the system is known to be superfluid, delocalization is found at both the single-particle and many-particle level. We interpret these results as a signature of supersolidity in the Bose-Hubbard model at integer filling.

**G1.00252 A spinor boson AB chain**, GREIS JULIETH CRUZ REYES, Universidad Santo Tomas, ROBERTO FRANCO, JERESON SILVA VALENCIA, Universidad Nacional de Colombia, UNIVERSIDAD SANTO TOMAS COLLABORATION, UNIVERSIDAD NACIONAL DE COLOMBIA COLLABORATION — Recent research is focused on superlattices arising from optical lattices, which allow a tunable environment. Experimentally bosons present transitions from superfluid to Mott insulator by changing the energy offset in the unit cell [Nat. Commun. 5:5735 (2014)]. Many studies displayed that ground state of spinless boson systems on superlattices present superfluid, Mott insulator and an additional CDW phase created by the energy shift between the sites into the unit cell [Phys. Rev. A 83, 053621 (2011)]. The first confinement methods were magnetic traps, which freezes the spin; with optical lattices the grade of freedom of spin plays an important role. We consider bosons with spin  $S=1$  on a superlattice made by two sites with energy offset per unit cell (AB chain). The Hamiltonian that describes the system is the Bose-Hubbard model with the superlattice potential (W) and the exchange interaction (V) parameters. This model supports CDW, Mott insulator and superfluid phases. For W near to U, with  $V=0$ , Mott phase disappears, but for V increasing, a new CDW appears due to the spin interaction, while the half-integer CDW decrease. These results are widely different from spinless boson, where the CDW phases are stables.

**G1.00253 Bose-Hubbard Model on Penrose Tiling Lattice**, JOHNSON CHAN, The Univ of Hong Kong, DIMITRIOS GALANAKIS, None — The standard Bose-Hubbard model has provided a paradigmatic example to explore the quantum phases in a strongly interacting boson system. However, studies so far have considered lattice models with the conventional lattice symmetry (square, triangular, honeycomb etc. in two dimensions), and very few studies in the case of a quasi-crystal. Experimentally, quasi-crystal optical lattices have been realized in the experiments and this provides a very timely opportunity to investigate the possible quantum states of a Bose-Hubbard model in a quasi-crystal. In our work, we performed the first Quantum Monte Carlo of Bose-Hubbard model on a Penrose tiling lattice at finite temperature. We compute the phase diagram and investigate the behavior of phase transitions by looking at several observables, including momentum distribution, distribution of condensate fraction and density distributions. Our work can be checked in future experiments.

**G1.00254 Photoelectric devices with quantum coherence**, SU SHANHE, Beijing CSRC — A photoelectric device consisting of a three-level system contacted with two fermionic baths and a photon bath is built. Making the Born-Markov approximation, the equation of motion for the density operator in a Lindblad-like form is derived. We obtain the coherence and the efficiency of the system under the steady-state condition. Results show that quantum coherence can enhance the photoelectric conversion efficiency. The efficiency at maximum power can be larger than the CA efficiency bound with the existence of coherence.

**G1.00255 Spectral singularity in composite systems and simulation of laser resonant chamber**<sup>1</sup>, XIZHENG ZHANG, Beijing CSRC — A non-Hermitian system with spectral singularity (SS) exhibits fascinating phenomena which never appear in a Hermitian system. We investigate the existence of SS for a composite system which is consisted of two separated scattering centers A and B embedded in a one-dimensional free space, one of which is non-Hermitian at last. We show that the composite system has a SS at  $k_c$  if the reflection amplitudes  $r^A(k_c)$  and  $r^B(k_c)$  of two scattering centers satisfy the condition  $r_R^A(k_c) r_L^B(k_c) e^{i2k_c(x_B - x_A)} = 1$ , based on the theorem proposed by Ali (PRL 102, 220402 (2009)). Multi-scattering-centers generalization of the theorem is also obtained. As an application, we construct a simple system to simulate the resonant chamber for generating laser light.

<sup>1</sup>Spectral singularity in composite systems and simulation of laser resonant chamber

**G1.00256 Dark state in a nonlinear optomechanical system with quadratic coupling<sup>1</sup>**, YUE-XIN HUANG, XIANG-FA ZHOU, GUANG-CAN GUO, YONG-SHENG ZHANG, Univ of Sci & Tech of China — We consider a hybrid system consisting of a cavity optomechanical device with nonlinear quadratic radiation pressure coupled to an atomic ensemble. By considering the collective excitation, we show that this system supports nontrivial, nonlinear dark states. The coupling strength can be tuned via the lasers that ensure the population transfer adiabatically between the mechanical modes and the collective atomic excitations in a controlled way. In addition, we show how to detect the dark-state resonance by calculating the single-photon spectrum of the output fields and the transmission of the probe beam based on two-phonon optomechanically induced transparency. Possible application and extension of the dark states are also discussed.

<sup>1</sup>Supported by the National Fundamental Research Program of China (Grants No. 2011CB921200 and No. 2011CBA00200), the Strategic Priority Research Program of the Chinese Academy of Sciences (Grant No. XDB01030200), and NSFC (Grants No. 61275122 and 11474266)

**G1.00257 Bose gas with generalized dispersion relation plus an energy gap<sup>1</sup>**, M. A. SOLIS, Instituto de Fisica, UNAM, J. G. MARTINEZ, J. GARCIA, Facultad de Ciencias, UNAM — We report the critical temperature, the condensed fraction, the internal energy and the specific heat for a  $d$ -dimensional Bose gas with a generalized dispersion relation plus an energy gap, i.e.,  $\varepsilon = \varepsilon_0$  for  $k = 0$  and  $\varepsilon = \varepsilon_0 + \Delta + c_s k^s$ , for  $k > 0$ , where  $\hbar k$  is the particle momentum,  $\varepsilon_0$  the lowest particle energy,  $c_s$  a constant with dimension of energy multiplied by a length to the power  $s > 0$ . When  $\Delta > 0$ , a Bose-Einstein critical temperature  $T_c \neq 0$  exists for any  $d/s \geq 0$  at which the internal energy shows a peak and the specific heat shows a jump. The critical temperature and the specific heat jump increase as functions of the gap but they decrease as functions of  $d/s$ . Thermodynamic properties are  $\varepsilon_0$  independent since this is just a reference energy. For  $\Delta = 0$  we recover the results reported in Ref. [1].  
V. C. Aguilera-Navarro, M. de Llano y M. A. Solís, Eur. J. Phys. **20**, 177 (1999).

<sup>1</sup>We acknowledge partial support from grants PAPIIT IN111613 and CONACyT 221030

**G1.00258 Derivation and Inter-relationship of Planck time, the Hubble constant, and Cosmic Microwave Background Radiation from the Neutron and the Quantum Properties of Hydrogen**, D. W. CHAKERES, Department of Radiology, The Ohio State University, Columbus, OH, 43210, R. VENTO, Retired, S. S. MOSES, J. B. SAUZA, V. M. ANDRIANARIJAONA, Department of Physics, Pacific Union College, Angwin, CA, 94508 — Planck time,  $t_P$ , is presently the only fundamental constant that unites the physical domains of  $c$ ,  $\hbar$ , and  $G$ , and is therefore a globally defined normalized time constant. This study shows a method to derive  $t_P$ ,  $H_0$ ,  $G$ , and the Cosmic Microwave Background Radiation (CMBR) peak spectral radiance from the frequency equivalents of the neutron and the quantum properties of hydrogen such as Rydberg's constant, Bohr radius, electron mass and electron charge. All of the derivations are within the experimental ranges, including errors. Moreover, these results exceed what is experimentally possible because the natural unit data are of high precision. The constants are evaluated within a combined classic integer and harmonic fraction, power law relationship. The logarithmic base of the annihilation frequency of the neutron, approximately  $2.27 \cdot 10^{23}$  Hz, scales the independent axis to an integer and partial harmonic fraction system. The dependent axis is scaled by the properties of hydrogen. On the line that defines Planck time squared,  $t_P^2$ , there exist unique points directly related to  $H_0$ , and the CMBR. Therefore these three fundamental cosmic constants are mathematically and conceptually closely inter-related, and each derivable from the others.

**G1.00259 Strong Field QED Simulation of Laser-Plasma Interaction Using BUMBLEBEE.**, XIAOLIN JIN, YUNXIAN TIAN, TAO HUANG, WENLONG CHEN, BIN LI, University of Electronic Science and Technology of China — Next generation laser intensity could reach  $10^{24}$  W/cm<sup>2</sup>, making strong field quantum electrodynamics (QED) effects in laser-plasma interaction a promising research field. The model of photon and pair production in strong field QED is implemented into our 1D3V particle-in-cell (PIC) code BUMBLEBEE with Monte Carlo (MC) algorithm. We apply the kirk and bell model to simulate the photon and pair production, where photon is produced through bremsstrahlung process and the pair is produced through the Bethe-Heitler process. There are two stages in the QED pair production process. Firstly, the intense laser interacts with a relativistic electron or positron to produce the photon. Secondly, the photon interacts with the same laser field to produce the  $e^+e^-$  pair. The QED process is coupled to laser-plasma interaction processes before pushing the particles at each step. Using this code, the evolutions of the particles in ultrahigh intensity laser ( $\sim 10^{23}$ W/cm<sup>2</sup>) interaction with aluminum foil target are observed. Four different initial plasma profiles are considered in the simulations.

**G1.00260 A Control Based System of Mechanical Loss Measurement for High Quality Factor Oscillators**, LOUIS LOUIS GITELMAN, American University, NICOLAS SMITH, California Institute of Technology, ISAAC JAFAR, Columbia University, GREGORY HARRY, JONATHAN NEWPORT, American University, MATT ABERNATHY, California Institute of Technology, LIGO COLLABORATION — In this poster we will present the control system being developed to measure the quality factor of optics used in the Advanced LIGO gravitational wave detectors to predict thermal noise levels. It works by locking the phase between the optic's exciter and normal mode to  $\pi/2$  and locking the optics's amplitude allowing one to equate the energy output of the exciter to the mechanical loss of the optic. To do this the amplitude of the normal mode is detected using a birefringence meter and lockin amplifier, which is then fed back to an electrostatic exciter to control the mode's amplitude and phase with a PID controller written on a python script. The poster will discuss the components and assembly of this system and the theoretical control structure behind it. It will also discuss the speed, accuracy and general feasibility of this method of quality factor measurement relative to other methods, and steps to improve and develop this method of quality factor measurement and the possible applications for LIGO and in general.

**G1.00261 ABSTRACT WITHDRAWN** —

**G1.00262 Abnormal Dispersion of Optical Modes in a non-Hermitian system: Feasibility and Applications**, JING CHEN, RUIPENG GUO, LITING WU, School of Physics, Nankai University, Tianjin 300071, China — We analyze the dispersions of optical eigen-modes in a non-Hermitian system. We show that abnormal dispersion of optical modes can be realized by using the concept of optical parity-time symmetry. Physical significance of these effects is discussed. The feasibility in realizing these abnormal dispersions in passive systems and the connection with damped polaritons in various photonic and phononic systems are discussed. This investigation can find many attractive applications in manipulating the dynamic of coupled optical waves, if the parasite tradeoff of loss effect can be relieved by proper gain effects.

**G1.00263 Optical tweezers theory near a flat surface: a perturbative method<sup>1</sup>**, HENRIK FLYVBJERG, RAFAEL S. DUTRA, Department of Micro- and Nanotechnology, Technical University of Denmark, PAOLO A. MAIA NETO, H. MOYSES NUSSENZVEIG, Institute of Physics, Universidade Federal do Rio de Janeiro — We propose a perturbative calculation of the optical force exercised by a focused laser beam on a microsphere of arbitrary radius that is localized near a flat glass surface in a standard optical tweezers setup. Starting from the Mie-Debye representation for the electric field of a Gaussian laser beam, focused by an objective of high numerical aperture, we derive a recursive series that represents the multiple reflections that describe the reverberation of laser light between the microsphere and the glass slide. We present numerical results for the axial component of the optical force and the axial trap stiffness. Numerical results for a configuration typical in biological applications a microsphere of 0.5  $\mu$ m radius at a distance around 0.25  $\mu$ m from the surface show a 37% [1] Viana N B, Rocha M S, Mesquita O N, et al. (2007) Towards absolute calibration of optical tweezers. Phys Rev E 75:021914-114. [2] Dutra R S, Viana N B, Maia Neto P A, et al. (2014) Absolute calibration of forces in optical tweezers. Phys Rev A 90:013825-113.

<sup>1</sup>Rafael S. Dutra thanks the Brazilian "Science without Borders" program for a postdoctoral scholarship.

**G1.00264 Hard X-ray Pump, X-ray Probe Spectroscopy of Single Crystals.<sup>1</sup>**, AARON LOETHER, MATT DECAMP, Univ of Delaware, DONALD WALKO, Argonne National Lab — Recent advancements in intense x-ray pulses have made it possible to perform hard x-ray pump probe spectroscopy. Inspired by optical pump probe, we've built a retroreflector for use with synchrotron based x-rays, using Germanium crystals at Bragg condition in place of mirrors, to control relative timing of x-ray pulses and perform time resolved measurements. Testing of multiple versions of the retroreflector was done both experimentally and via simulation; the comparison allows us to show efficiencies achievable theoretically and realistically. A proof of concept time resolved diffraction experiment on a Germanium 111 crystal was performed utilizing high intensity broadband x-ray pulses and the resulting heating and propagated strains were measured by low intensity monochromatic x-ray pulses.

<sup>1</sup>This work was supported from the DOE-EPSCoR Grant No. DE-FG02-11ER46816. Use of the 178 Advanced Photon Source was supported by the U. S. Department of Energy, Office of Science, 179 Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357

**G1.00265 Observations of the high vibrational levels of the  $B''B^1\Sigma_u^+$  state of  $H_2$** , ROBERT EKEY, University of Mount Union, ALEXANDER CHARTRAND, Bryn Mawr College, WENQI DUAN, University of Iowa, ELIZABETH MCCORMACK, Bryn Mawr College — Double-resonance laser spectroscopy via the  $EF^1\Sigma_g^+, v' = 6, J' = 0 - 2$  state was used to probe the high vibrational levels of the  $B''B^1\Sigma_u^+$  state of molecular hydrogen. Resonantly-enhanced multiphoton ionization spectra were recorded by detecting ion production as a function of energy using a time of flight mass spectrometer. New measurements of energies for the  $v = 51 - 66$  levels for the  $B''B^1\Sigma_u^+$  state are reported, which, taken with previous results, span the  $v = 46 - 69$  vibrational levels. Results for energy levels are compared to theoretical calculations [L. Wolniewicz, T. Orlikowski, and G. Staszewska, J. Mol. Spec. 238, 118 (2006)]. The average difference between the 84 measured energies and calculated energies is  $-3.8 \text{ cm}^{-1}$  with a standard deviation of  $5.3 \text{ cm}^{-1}$ . This level of agreement showcases the success of the theoretical calculations in accounting for the strong rovibronic mixing of the  $^1\Sigma_u^+$  and  $^1\Pi_u^+$  states.

**G1.00266 ABSTRACT WITHDRAWN —**

**G1.00267 QUANTUM INFORMATION, CONCEPTS AND COMPUTATION —**

**G1.00268 Geometric Decompositions of Bell Polytopes with Practical Applications**, PETER BIERHORST, National Institute of Standard and Technology, Boulder, CO — In the well-studied (2,2,2) Bell experiment consisting of two parties, two measurement settings per party, and two possible outcomes per setting, it is known that if the experiment obeys no-signaling constraints, then the set of admissible experimental probability distributions is fully characterized as the convex hull of 24 distributions: 8 Popescu-Rohrlich (PR) boxes and 16 local deterministic distributions. Here, we refine this result to show that in the (2,2,2) case, any nonlocal nonsignaling distribution can always be uniquely expressed as a convex combination of exactly one PR box and (up to) eight local deterministic distributions. In this representation each PR box will always occur only with a fixed set of eight local deterministic distributions with which it is affiliated. This decomposition has multiple applications: we demonstrate an analytical proof that the minimum detection efficiency for which nonlocality can be observed is  $2/3$  even for theories constrained only by the no-signaling principle, and we develop new algorithms that speed the calculation of important statistical functions of Bell test data. Finally, we enumerate the vertices of the no-signaling polytope for the (2, n, 2) "chained Bell" scenario and find that similar decomposition results are possible in this general case. Here, our results allow us to prove the optimality of a bound, derived in (Barrett et al., PRL, 2006) on the proportion of local theories in a local/nonlocal mixture that can be inferred from the experimental violation of a chained Bell inequality.

**G1.00269 Implementing entangling gates via quantum walks through branching graphs.**, DMITRY SOLENOV, THOMAS CAVIN, Department of Physics, Saint Louis University, St. Louis, MO 63103 — Efficient quantum gates are essential to quantum computing. It was found recently that quantum walks can enhance performance of quantum gates. We investigate how the propagation of a complicated, branching system can be solved analytically by first mapping it to linear chain. We found that certain types of systems, including systems of  $n$  qubits, can be algorithmically mapped to a system of disjoint linear chains. In particular, we found a solution for the 3 qubit system that performs either a trivial return walk or a return walk with a phase of  $\pi$  introduced.

**G1.00270 Error Threshold for the 4.6.12 Topological Color Code**, COLIN TROUT, Georgia Inst of Tech, SHOTA NAGAYAMA COLLABORATION<sup>1</sup> — Topological color codes are interesting candidates for fault-tolerant quantum computation. Relative to surface codes, color codes have a larger set of transversal gates, which reduces the resources required for state distillation to achieve universal quantum computation. Here we study a family of color codes defined by the 4.6.12 semi-regular lattice. We adapt a minimum weight perfect matching decoder to report an error threshold for the 4.6.12 topological color code under the circuit-based error model.

<sup>1</sup>Keio University



**G1.00277 The Quantum-Classical Boundary for Optical Interferometric Measurements** , PATRICK M. BIRCHALL, JONATHAN C. F. MATTHEWS, HUGO CABLE, Centre for Quantum Photonics, University of Bristol — We study the fundamental precision limits for measurements of optical phase when loss of probe light dominates the decoherence, and a limited number of photons are passed through the sample. It has long-been argued that non-classical states can be used to achieve an important advantage in precision in measurements of this sort, where it is not possible to use high-power laser light. As well as being of fundamental interest for understanding the ultimate physical limits for precision measurement, there are practical applications to measurements of delicate or photosensitive samples. Here we compare optimal measurement strategies using classical and non-classical probe states, where the number of passes through the unknown phase can be freely controlled. We find that the increase in precision that can be achieved using non-classical techniques is in fact small. Our results narrow the potential applications of measurements using non-classical states to cases where there is greater quantum advantage due to practical constraints on the measurements involved.

## **G1.00278 ABSTRACT WITHDRAWN —**

**G1.00279 Experimental realization of optimal control with robustness to coupling errors** , FEIHAO ZHANG, GUILU LONG, Tsinghua Univ — Optimal control theory is applied in quantum information processing for its ability to find objective evolution in complex quantum system. The negative factors, like the coupling to the environment, will impede the ideal evolution and increase their effect over time. In this work, we introduce a new method for finding objective propagator with robustness to coupling errors. The bath disturbance is analyzed by the time scale decomposition of spin dynamics. And the optimization is based on a gradient algorithm. We will give the experimental comparison between this robust optimal control method and the original one in spin system. Results show the advantage of this method in a noisy environment.

**G1.00280 Nonlinear Effects in Coupled Microtoroidal Optical Microcavities** , XIAOFEI LIU, GUI LU LONG, Tsinghua Univ, QUANTUM INFORMATION GROUP IN DEPARTMENT OF PHYSICS, THU TEAM — Nonlinear effect plays an important role in modern physics. Thanks to the great improvement of the fabrication technology, the quality factor of microcavities can reach more than 100 million. This gives rise to many amazing phenomena. Recently, a new kind of nonlinear effect, optomechanics, which involves the interaction between the photon and phonon, has made important progress both in experiment and theory. Here, we will study the nonlinear effect in coupled microcavities, and three-way electromagnetic induced transparency and so on.

**G1.00281 First-principles hyperfine tensors for electrons and holes in silicon and GaAs** , PERICLES PHILIPPOPOULOS, McGill University, STEFANO CHESI, Beijing Computational Science Research Center, WILLIAM COISH, McGill University — Knowing (and controlling) hyperfine interactions in silicon and III-V semiconductor nanostructures is important for quantum information processing with electron and nuclear spin states. We have performed density-functional theory (DFT) calculations that fully account for spin structure of the Bloch states (in contrast with approaches that rely on the density alone). Using this method, we confirm the known value for the contact hyperfine coupling in the conduction band of silicon, but find a significant deviation in the value for the conduction band of GaAs relative to the accepted value, estimated in ref. [1]. Moreover, this method can be used to calculate the full hyperfine tensor for the valence band, where spin-orbit effects may be strong, precluding methods that determine hyperfine couplings from the density alone. This general method can be applied to a broad class of materials with strong combined spin-orbit and hyperfine interactions. [1] D. Paget, G. Lampel, B. Sapoval, and V. I. Safarov Phys. Rev. B 15, 5780 (1977)

**G1.00282 Hyperfine interaction mediated electric-dipole spin resonance: The role of the frequency modulation<sup>1</sup>** , RUI LI, Beijing Computational Science Research Center — The electron spin in semiconductor quantum dot can be coherently controlled by an external electric field, an effect called electric-dipole spin resonance (EDSR). There are several mechanisms underlie the EDSR, among which there is a hyperfine mechanism, where the spin-electric coupling is mediated by the electron-nucleus hyperfine interaction. Here, we investigate the influence of the frequency modulation (FM) to the driving electric field on the spin-flip efficiency. Our results reveal that FM plays an important role in the hyperfine mechanism. Without FM, the electric field almost cannot flip the electron spin, the spin-flip probability is only about 20%. While under the FM, the spin-flip probability can be improved approximately to 70%. Especially, we find there is a lower bound on the modulation amplitude, which is related to the width of the hyperfine field fluctuation of the nuclear spins.

<sup>1</sup>This work is supported by National Natural Science Foundation of China Grant No. 11404020 and Postdoctoral Science Foundation of China Grant No. 2014M560039

**G1.00283 Entangled Terahertz photon pair emitting diode with a HgTe quantum dot** , LI-KUN SHI, Beijing CSRC, KAI CHANG, SKLSM, Institute of Semiconductors, Chinese Academy of Sciences, P. R. China, CHANG-PU SUN, Beijing Computational Science Research Center, Beijing 100094, China — We propose an experimentally feasible scheme for generating entangled terahertz photons in topological insulator quantum dots (TIQDs). We demonstrate theoretically that in TIQDs with disorders and irregular shapes: 1) the fine structure splitting, which is the obstacle to produce entangled photons in conventional semiconductor quantum dots, is inherently absent for one-dimensional massless excitons due to the time-reversal symmetry; 2) the selection rules obey winding number conservation instead of the conventional angular momentum conservation between edge states with a linear dispersion. With these two advantages, the entanglement of the emitted photons during the cascade in our scheme is robust against unavoidable disorders and morphology fluctuations of the TIQD.

**G1.00284 Measure of the Quantum Speedup in Closed and Open systems<sup>1</sup>** , ZHEN-YU XU, College of Physics, Optoelectronics and Energy, Soochow University, Suzhou 215006, China — We construct a general measure for detecting the quantum speedup in both closed and open systems. This speed measure is based on the changing rate of the position of quantum states on a manifold with appropriate monotone Riemannian metrics. Any increase in speed is a clear signature of real dynamical speedup. To clarify the mechanisms of quantum speedup, we first introduce the concept of longitudinal and transverse types of speedup, and then apply the proposed measure to several typical closed and open quantum systems, illustrating that entanglement and the memory effect of the environment together can become resources for longitudinally or transversely accelerating dynamical evolution under certain conditions. Remarkably, a direct measurement of such speedup is feasible without the need for a tomographic reconstruction of the density matrix, which greatly enhances the feasibility of practical experimental tests.

<sup>1</sup>This work was supported by the National Natural Science Foundation of China (Grant No. 11204196)

**G1.00285 Has Macroscopic Superposition in Superconducting Qubits Really Been Demonstrated?** , ALAN M. KADIN, Princeton Junction, NJ, STEVEN B. KAPLAN, Estes Park, CO — Quantum computing depends on many qubits coupled via quantum entanglement, where each qubit must be a simultaneous superposition of two quantum states of different energies, rather than one state or the other as in classical bits. It is widely believed that observations of energy quantization and Rabi oscillations in macroscopic superconducting circuits prove that these are proper qubits with quantum superposition. But is this really the only interpretation? We propose a novel paradigm for macroscopic quantum systems, in which energies are quantized (with photon-mediated transitions), but the quantized states are realistic objects without superposition. For example, a circuit could make a transition from one quantized value of flux to another, but would never have both at the same time. We further suggest a superconducting circuit that can put this proposal to a test [1]. Without quantum superposition, most of the potential benefit of quantum computing would be lost. [1] A.M. Kadin and S.B. Kaplan (2014), "Superconducting Quantum Computing Without Entanglement?", <http://arxiv.org/abs/1408.5410>.

**G1.00286 A local realistic model of quantum information systems explaining the four Bell states** , JEFFREY BOYD, Retired — Can quantum computers and other information systems (like cryptography) be explained by local realism? The overwhelming consensus is NO. Thirty years of Bell test experiments proved Einstein, Podolsky and Rosen (EPR) wrong. Unknown to most physicists a new form of local realism has arisen, drastically different than EPR. The Theory of Elementary Waves (TEW) proposes that two entangled particles are both following the same elementary bi-ray. The same Bell test experiments that invalidate EPR, validate TEW. What is an elementary bi-ray? In TEW waves and particles usually travel in opposite directions. In entanglement experiments the picture is more complex. A bi-ray consists of two coaxial elementary rays, moving in opposite directions. Such bi-rays can explain all four Bell states on the basis of this peculiar form of local realism. Bell theory would classify TEW as nonlocal, even though it is local and realistic. The word nonlocal needs to be discarded, since elementary bi-ray is a more accurate and fertile descriptor of the same phenomena. TEW explains entanglement swapping heralding entanglement between distant spinning electrons in NV cavities, or trapped ions. The question is: So what? Would anything in quantum information science change if TEW were true? We think not.

**G1.00287 Quantum Dualism: Hypermind?** , R. JONES, Emporia State University — Today the consensus view is that thought and mind is a combination of processes like memory, generalization, comparison, deduction, organization, analogy, etc. performed by classical computational machinery. (R. Jones, Trans. Kansas Acad. Sci., vol. 109, 3/4, 2006) But I believe quantum mechanics is a more plausible dualist theory of reality. (R. Jones, Bull. Am. Phys. Soc., vol. 5, 2011) In a quantum computer the processing (thinking) takes place either in computers in Everett's many worlds or else in the many dimensional Hilbert space. (Depending upon your interpretation of QM.) If our brains were quantum computers then there might be a world of mind which is distinct from the physical world that our bodies occupy. (4 space) This is much like the spirit-body dualism of Descartes and others. My own view is that thought and mind are classical phenomena (see [www.robert-w-jones.com](http://www.robert-w-jones.com), philosopher, theory of thought and mind) but it would be interesting to run an artificial intelligence like my A.S.A. H. on a quantum computer. Might this produce, for the first time, a hypermind in its own universe?

**G1.00288  $P \neq NP$  Millenium-Problem(MP) TRIVIAL Physics Proof Via NATURAL TRUMPS Artificial-"Intelligence" Via: Euclid Geometry, Plato Forms, Aristotle Square-of-Opposition, Menger Dimension-Theory Connections!!! NO Computational-Complexity(CC)/ANYthing!!! Geometry!!!** , LONDON CLAY, KARL MENDER, GIAN-CARLO ROTA, ALEXANDRIA EUCLID, EDWARD SIEGEL, FUZZYICS —  $P \neq NP$  MP proof is by computer-"science"/SEANCE(!!!)(CS) computational-"intelligence" lingo jargonial-obfuscation(JO) NATURAL-Intelligence(NI) DISambiguation! CS  $P=(?)=NP$  MEANS (Deterministic)•(PC)=(?)=(Non-D)•(PC) i.e.  $D \bullet (P)=(?)=N \bullet (P)$ . For inclusion(equality) vs. exclusion(inequality) irrelevant (P) simply cancels!!! (Equally any/all other CCs IF both sides identical). Crucial question left:  $(D)=(?)=(ND)$ , i.e.  $D=(?)=N$ . Algorithmics[Sipser[Intro. Thy.Comp.('97)-p.49;Fig.1.15!!!]]: Deterministic (D) serial VS. Non-deterministic (N) NON-serial, branch fork forms triangles, its vertices a plane. Menger Dimension-Theory: Dimensionality: D serial is  $\dim(D)=1$ (definition), VS. N non-serial is  $\dim(N)=[2(\text{branching;fork;triangle;plane})+E(\text{probabilistic})]>2(>>>)\neq 1!$  Hence by (Euclid[~300 BCE]) simple geometry,  $\dim(D)=1 \neq \dim(N)>2$ , Left-to-Right INclusion VS. Right-to-Left EXclusion. Thus TRIVIALY  $P \neq NP$ !!! QED FIN, i.e.  $D \neq N$  by ~300 BCE GEOMETRY, just "a tad" before CS CC JO!!! Harder proofs, but still amenable to NI analysis, are any combinations with DISsimilar CCs, especially LHS combining D with low CC and/or RHS combining N with different CCs: EXP and/or LOG! MUCH HARDER but still amenable to CC NI are: CROSS-MIXTURES:  $P=(?)=N \bullet \text{LOG}$ ,  $\text{EXP}=(?)=N \bullet P$ ,  $\text{EXP}=(?)=N \bullet \text{LOG}$ ,...

**G1.00289 A Practical Experiment to Obtain Either Which-Way or Interference Photon Distributions at a Distance Using Delayed Choice and Without Correlating Measurement Results on Entangled Photons** , DOUGLAS SNYDER, None — For a pair of entangled signal-idler photons, one may "lose" the idler photon (that provides which-way information to the entangled signal photon) in many other photons with similar characteristics to the idler photon before the signal photon is detected, thereby losing the which-way information supplied to the signal photon and eliminating the entanglement. The experiment allows for a delayed choice on the idler photons (whether or not to lose the idler photon before the signal photon is detected) to determine the distribution of distant signal photons (either overall which-way or overall interference) without making correlations between signal and idler photon detections. When the idler photon is lost, it is lost in an optical microcavity filled with photons in the same mode as the idler photon. The experiment could provide the basis for a useful quantum communications device. It might be possible to use a micropost coated with a material such as Vantablack in place of the optical microcavity.

**G1.00290 Quantum Entanglement in a two-atom two photon system** , SAMINA MASOOD, University of Houston Clear Lake — We study the quantum entanglement in a two atom and two photon system and show that the quantum entanglement can be used in quantum computation to develop more efficient systems.

**G1.00291 Quantum Knowledge Diagrams-2, Principles and Application** , DOUGLAS SNYDER, None — The principles behind quantum knowledge can be extracted from the specific empirical implementations so that pictorial elements can be developed representing fundamental concepts of quantum knowledge. With these elements, one can represent quantum knowledge principles underlying specific empirical implementations more simply and in a way that allows for a more direct comparison of quantum knowledge principles underlying various specific empirical implementations. These representations are quantum knowledge diagrams. Basic diagram elements include: 1) a which-way process; 2) a non-which-way process (showing interference); 3) availability of the which-way or non which-way information to the environment, generally through detection, or lack of such availability; 4) particles; 5) entanglement, or lack thereof, of 2 or more particles; 6) delayed choice. Quantum knowledge principles underlying specific empirical implementations are developed and diagrammed.

**G1.00292 MATTER AT EXTREME CONDITIONS** —

**G1.00293 New impact sensitivity test of liquid explosives.** <sup>1</sup>, ANDREI TIUTIAEV, Samara state technical university, VALERI TREBUNSKIY, Retired — The sensitivity of liquid explosive in the presence of gas bubbles increases many times as compared with the liquid without gas bubbles. Local hot spot in this case formed as a result of compression and heating of the gas inside the bubbles. If we consider that in the liquid as a result of convection, wave motion, shock, etc. gas bubbles are easily generated, the need to develop a method for determining sensitivity of liquid explosives to impact and a detailed study of the ignition explosives with bubbles is obvious. On a mathematical model of a single steam bubbles in the fluid theoretically considered the process of initiating explosive liquid systems to impact. For the experimental investigation, the well-known K-44 -II with the metal cap were used. Instead of the metal cap in the standard method in this paper there was polyurethane foam cylindrical container with LHE, which is easily deforms by impact. A large number of tests with different liquid explosives were made. It was found that the test LHE to impact with polyurethane foam to a large extent reflect the real mechanical sensitivity due to the small loss of impact energy on the deformation of the metal cap, as well as the best differentiation LHE sensitivity due to the higher resolution method.

<sup>1</sup>Results obtained in the samara state technical university

**G1.00294 Ultrafast laser diagnostics for understanding hot spot initiation in energetic materials**, IAN KOHL, DARCIE FARROW, SEAN KEARNEY, ROBERT KNEPPER, JEFFREY KAY, Sandia Natl Labs — Ultrafast laser diagnostics have opened new pathways for investigation of shock physics and initiation of energetic materials. Recent work (Bolme LANL/Armstrong LLNL) has demonstrated that short laser pulses can be utilized for direct laser drive and coupled with imaging, spectroscopic, and interferometric tools for studies of dynamic shock loading on picosecond time scales. At Sandia, we are developing diagnostic platforms which extend this earlier work by combining Ultrafast Shock Interferometry (USI) (Armstrong LLNL) and femtosecond transient absorption spectroscopy for tabletop measurement of Hugoniot/Equation-of-state data and characterization of shock structure in heterogeneous materials with micron spatial resolution while probing shock-induced changes in the electronic structure, which have been proposed to drive rapid chemical changes behind the shock front. We will describe the details of our measurement systems, as well as recent progress toward new laser-diagnostic data on inert/explosive thin-film samples.

**G1.00295 High Pressure Structures and Equations of State of HIO<sub>3</sub> and HI<sub>3</sub>O<sub>8</sub>**<sup>1</sup>, JOSEPH ZAUG, ELISSAIO STAVROU, Lawrence Livermore National Laboratory, BRIAN LITTLE, Air Force Research Laboratory - RWM, SORIN BASTEA, JONATHAN CROWHURST, Lawrence Livermore National Laboratory — Knowledge of high-pressure thermodynamic properties of iodine containing oxides and acids is important toward improving the accuracy of semi-empirical predictions of extreme condition explosive and combustive chemistry of iodine containing formulations. Here we report on the synthesis of explosive chemical products HIO<sub>3</sub> and HI<sub>3</sub>O<sub>8</sub> and on the structures and isotropic equations of state up to 35 and 45 GPa respectively. EOS model parameters are provided including parametrized exponential-6 interatomic potential values used to conduct thermochemical calculations of iodine containing reactants.

<sup>1</sup>This work was performed under the auspices of the U.S. Department of Energy jointly by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344

**G1.00296 Anomalous bond length behavior and a new solid phase of bromine under pressure**, MIN WU, Zhejiang University of Technology, JOHN TSE, YUANMING PAN, University of Saskatchewan — The behavior of diatomic molecular solids under pressure have attracted great interests and been extensively studied. Under ambient pressure, the structure of bromine is known to be a molecular phase (phase I). With increasing pressure, it transforms into an incommensurate phase (phase V) before eventually to a monoatomic phase (phase II). However, between phases I and V, the interatomic distance was found to first increase with pressure and then decrease abruptly. This anomalous bond length behavior is accompanied by the splitting of the Raman bands. These phenomena have not been resolved. Here we suggest a new solid phase that explains the Raman spectra. Furthermore, the anomalous bond length behavior is found to be the result of subtle second neighbor intermolecular interactions and is an intrinsic property of bromine in molecular phases.

**G1.00297 Propagation of light in a Dense Medium.**, SAMINA MASOOD, University of Houston Clear Lake, IRAM SALEEM, University of Houston — Propagation of light is studied in a very dense system. Renormalization scheme of QED is used to understand the propagation of light in a hot and dense medium. We consider a medium of a very large chemical potential with relatively small temperature. The generalized results of vacuum polarization of photon in a hot and dense medium is used to study the behavior of light in such a system. Our hypothetical system corresponds to a heat bath of electrons at an equilibrium temperature and the density of electrons is larger as compared to the temperature of the medium. Such type of systems have previously been identified as classical systems because the chemical potential is large enough to dominate temperature.

**G1.00298 High Pressure synchrotron XRD and Raman studies of Ho<sub>0.5</sub>Y<sub>1.5</sub>Ti<sub>2</sub>O<sub>7</sub>.**<sup>1</sup>, MELANIE WHITE, RAVHI KUMAR, JASON BAKER, BRIAN LIGHT, Univ of Nevada - Las Vegas — Pyrochlore oxides are of interest for their spin-frustrated systems and their proposed use in high-level nuclear waste management. We sought to examine the structural stability of these materials under extreme conditions in order to help determine their viability for applications. A compression and decompression study of Ho<sub>0.5</sub>Y<sub>1.5</sub>Ti<sub>2</sub>O<sub>7</sub> was done in approximately 5 GPa intervals to above 55 GPa with both synchrotron powder x-ray diffraction at the Argonne National Laboratory Advanced Photon Source, and Raman spectroscopy at the University of Nevada - Las Vegas High Pressure Science and Engineering Center (HiPSEC). In both studies, pressurization of sample was achieved using a symmetric-style diamond anvil cell (DAC). The results are compared with the high pressure behavior of other rare earth titanates. A reversible phase transition is observed between 45 and 49 GPa in both studies. The x-ray diffraction patterns are analyzed in order to identify the crystal structure of the new phase. Vibrational modes are assigned to the Raman spectra and tracked as a function of pressure. Our poster will discuss the results in detail.

<sup>1</sup>This research was sponsored by the NNSA under the SSAA program through the DOE Cooperative Agreement DE-NA0001982. Portions of this study were performed at HPCAT (Sector 16) Advanced Photon Source (APS), Argonne National Laboratory.

**G1.00299 PHYSICS OF CLIMATE —**

**G1.00300 A new model of the electron temperature in the topside ionosphere** , ZAHRA PANAH ESTARKHI<sup>1</sup>, ALI BAKHSHAYESHI<sup>2</sup>, Islamic Azad University of Mashhad — hra Panahi Estarkhi, Ali Bakhshayeshi *Young Researchers and Elite club, Mashhad Branch, Islamic Azad University, Mashhad, Iran Department of physics, Mashhad Branch, Islamic Azad University, Mashhad, Iran* -abstract- By using empirical models of electron density in the ionosphere, height equations as a function of electron density from  $\alpha$ -Chapman, Epstein and exponential functions have been achieved. Plotting the achieved height equations, the one derived from Epstein function has been known as the best fit for height. Locating height derived from Epstein function in an empirical function for electron temperature, a new empirical model for electron temperature as a function of electron density has been achieved and applied to obtain directly the electron temperature for every electron density in the topside ionosphere. Latitudinal and seasonal variations for Te have been plotted in the heights above hmF2 to 1000km to compare the new Te model with the previous empirical model and the measured data from the ISIS database. The results are compared and the possible reasons for difference and similarities are also discussed.

<sup>1</sup>Phd student

<sup>2</sup>Physics teacher at Islamic Azad University of Mashhad

**G1.00301 Algorithms for ice halo detection in all-sky images**<sup>1</sup> , MICHELLE KING, MORTON GREENSLIT, SYLKE BOYD, University of Minnesota - Morris — The effect of cirrus clouds on the radiation budget of the atmosphere depends not only on optical depth and frequency of occurrence, but also on the composition of the clouds. Ice halo phenomena signal the presence of hexagonal crystal habits. Long-term observations on frequency, duration, and type of halo appearances can give ground-based insight into the behavior of cirrus composition. We are capturing images of the entire sky at 30 second intervals using an all-sky camera. We have created a program that analyzes these images for the presence of halos. The algorithm removes the lens distortion, excludes low-level clouds from further analysis, measures the radial RGB color channel intensity, and uses this radial intensity to assess for ice halo presence. We will present our algorithms for image analysis, including removing the lens distortion and low-level clouds, as well as the algorithm to assign a halo probability. We will also present our observation results for the year 2015.

<sup>1</sup>Supported by HHMI and UROP

**G1.00302 Construction of a low-cost LIDAR for cirrus cloud observations**<sup>1</sup> , BRITTNEY FERRIAN, KEVIN J BOYD, SYLKE BOYD, University of Minnesota - Morris — Our physical understanding of the Earth's climate is critically linked to our quantitative understanding of cloud coverage and behavior. In particular, cirrus clouds are pivotal players in the radiation balance of the Earth. We have taken a route to capture the characteristics of cirrus clouds using an all-sky camera, and analyzing halo phenomena. That gives us a 2d distribution of the cloud. Neither altitude nor optical thickness can be determined from photographs alone. We are interested in combining altitude and thickness information with the brightness information gathered in images. That requires that the Lidar measures are taken at the time at which a halo photograph is taken. A simple LIDAR instrument with cheap and readily available components is being constructed for this purpose. We will present the layout of the instrument design, challenges in construction and weather-proofing and preliminary measurement results.

<sup>1</sup>supported by HHMI and UROP

**G1.00303 Measurement of Water Vapor in the Lower Troposphere Using LIDAR** , FRANCIS MENSAH<sup>1</sup>, Virginia Union University, Richmond, VA, PETER INSTIFUL<sup>2</sup>, Prairie View A & M University, Houston, TX, ARTHUR THORPE<sup>3</sup>, Howard University — Water vapor is an important atmospheric variable which plays a key role in air quality, global warming, and climate change. It is known as a highly variable atmospheric constituent. Moreover, water vapor remains one of the most poorly characterized meteorological parameters. For example, water vapor measurements have proven to be difficult below 500 m in the lower troposphere. The overlap which exists between the incident laser beam and the receiver FOV is a factor affecting the lidar observation in the near field range. Because of its particular importance in tropospheric processes and the extraordinary ability of Raman Lidar through the SOLEX system to sense accurately its high temporal and spatial structure in the atmosphere, we present here some particular details about the use of Raman Lidar SOLEX system to measure water vapor at lower atmosphere at several fixed ranges. A comparison is made between data obtained from the laser system and the ones obtained from calibrated temperature and relative humidity's sensors at the same location.

<sup>1</sup>Department of Natural and Physical Sciences

<sup>2</sup>Department of Chemistry and Physics

<sup>3</sup>Department of Physics and Astronomy

**G1.00304 Effect of Seasonal Variation of Anomalous Condition on Radio Propagation in Nigeria** , ISRAEL EMMANUEL, BABATUNDE ADEYEMI, EMMANUEL OGOLO, ADEKUNLE ADEDIJI, Federal University of Technology Akure Nigeria — Daily variation of effective earth radius factor and seasonal variation of refractivity gradients from surface to around 1000 m above ground level in the tropospheric layer are presented based on observation from the meteorological data obtain from ECMWF database. Thirty four years (1979 -2014) of data from surface and profile of Era Interim of the temperature and relative humidity are used to determine the surface anomalous propagation over some selected location I Nigeria. Estimation of anomalous propagation are observed for onset and peak of rainy and dry seasons. The occurrence of anomalous strongly depends on the local time and synoptic weather conditions which have an appreciable on the refractivity vertical profile, especially the seasonal north – south movement of inter tropical Convergence Zone (ITCD) which provide wet and dry seasonal variations of anomalous were also determined. Spatial distribution of refractivity gradient for both wet and dry seasons are also obtained. The highest occurrence of duct were noticed in the night and morning (00:00 UTC and 06:00UTC) across the country though it was low in the northern part of the country, while low or no occurrence of duct were observed in the afternoon and evening (12:00 UTC and 18:00 UTC). Also percentage occurrence of duct were also high and low during the wet and dry seasons respectively.

**G1.00305 INSTRUMENTATION AND MEASUREMENTS —**

### **G1.00306 Charge Content In Nanometer Rings from Atomic Force Microscope (AFM) Traces<sup>1</sup>**

, F. ZYPMAN, Yeshiva University, S. EPPPELL, Case Western Reserve University, M. FEINSTEIN, Y. FRIED, D. LAZAREV, C. METZGER, Yeshiva University — The last few years have seen a growing interest in identifying charge content in small structures such as graphene ribbons and aromatic borings. More generally it is believed that charge content in proteins holds the key to the ultimate understanding of biological self-assembly. Here we describe a model system, a charged ring inside liquid probed by an AFM tip, and show how the charge content and the relative size of the ring with respect to the tip affect the measured force. More importantly, we explain how to measure the charge from the AFM experimental data [1]. The process involves the modeling of the dynamics of the tip-cantilever sensor under the influence of the charged sample, but also of ambient hydrodynamic forces, electrostatic interactions that appear due to charge induction in the tip and electrolytic screening. Of particular relevance is the possibility of our approach to treat analytically the size of ions. This is relevant when the tip-sample distance becomes sub-nanometric, and the more common description via Poisson-Boltzmann equation breaks down. [1] Mehlman and F.R. Zypman, Scanning Probe Microscope Force Reconstruction Algorithm via Time-Domain Analysis of Cantilever Bending Motion, J. Adv. Microsc. Res. 9, 268-274 (2014).

<sup>1</sup>Funding for this research "Instrument Development: Charge Sensing In Fluids With Nanometer Precision" is provided by Chemical Measurement & Imaging, National Science Foundation, Grant number 1508085.

### **G1.00307 Analyzing qPlus sensor assemblies for optimized simultaneous scanning tunneling and non-contact atomic force microscopy operation using finite element method**

, OMUR DAGDEVIREN, UDO SCHWARZ, Yale University — Scanning tunneling microscopy (STM) and non-contact atomic force microscopy (NC-AFM) are powerful methods that can not only visualize a surface's atomic structure, but also probe its electronic and chemical properties with picoampere, piconewton, and picometer resolution. Quartz tuning forks in qPlus configuration that have a metallic probe tip attached to the end of the free prong have gained considerable popularity in recent years for simultaneous high-resolution STM/NC-AFM experiments. Due to the small size of the tuning forks and the complexity of the sensor architecture, it is, however, not intuitive to judge how variations in the execution of the individual assembly steps affect the completed sensor's performance. In this presentation, we analyze the influence of each assembly step on the sensor's final performance using finite element method. The results show that when the tunneling current is collected using a separate wire, the exact realization of this wire connection has major effect on the sensor's performance. In addition, we show how other design choices such as the exact amount of epoxy used at key interfaces affects parameters such as spring constant,  $Q$ -factor, and resonance frequency.

### **G1.00308 Angle-Resolved Light-Matter Interaction in Anisotropic Layered Black Phosphorus**

, SHENGXI HUANG, XI LING, MIT, EDDWI HASDEO, Tohoku University, LIANGBO LIANG, RPI, ORNL, WILLIAM PARKIN, UPenn, YUKI TATSUMI, AHMAD NUGRAHA, Tohoku University, ALEXANDER PURETZKY, ORNL, PAUL DAS, UPenn, BOBBY SUMPTER, DAVID GEOHEGAN, ORNL, JING KONG, MIT, RIICHIRO SAITO, Tohoku University, MARIJA DRNDIC, UPenn, VINCENT MEUNIER, RPI, MILDRED DRESSELHAUS, MIT — Orthorhombic black phosphorus (BP) and other layered materials, such as gallium telluride and tin selenide, stand out among two-dimensional (2D) materials owing to their anisotropic in-plane structure. This anisotropy adds a new dimension to the properties of 2D materials and stimulates the development of angle-resolved photonics and electronics. However, understanding the effect of anisotropy has remained unsatisfactory to-date, as shown by a number of inconsistencies in the recent literature. We use angle-resolved absorption and Raman spectroscopies to investigate the role of anisotropy on the electron-photon and electron-phonon interactions in BP. We highlight, both experimentally and theoretically, a non-trivial dependence between anisotropies and flake thickness, photon and phonon energies. We show that the anisotropic optical absorption is a reliable and simple way to identify the crystalline orientation of BP, which cannot be determined from Raman spectroscopy without the explicit consideration of excitation wavelength and flake thickness.

### **G1.00309 Open-Source Programming for Automated Generation of Graphene Raman Spectral Maps<sup>1</sup>**

, P. VENDOLA, M. BLADES, W. PIERRE, S. JEDLICKA, S.V. ROTKIN, Lehigh University — Raman microscopy is a useful tool for studying the structural characteristics of graphene deposited onto substrates. However, extracting useful information from the Raman spectra requires data processing and 2D map generation. An existing home-built confocal Raman microscope was optimized for graphene samples and programmed to automatically generate Raman spectral maps across a specified area. In particular, an open source data collection scheme was generated to allow the efficient collection and analysis of the Raman spectral data for future use.

<sup>1</sup>NSF ECCS-1509786

### **G1.00310 Effects of magnetic field and pressure in magnetoelastic stress reconfigurable thin film resonators for magnetic field sensing**

, PETER FINKEL, MARGO STARUCH, Naval Research Laboratory — The magnetic response of microdevices is significantly enhanced at structural resonance allowing for improved sensitivity and signal-to-noise ratio. The magnetic field resolution of these devices can be further improved when operating in vacuum due to an increase in mechanical quality factor. In this work, free-standing CoFe thin film doubly clamped stress reconfigurable resonators were investigated as a function of magnetic field and pressure. A large uniaxial anisotropy resulting from residual uniaxial tensile stress was revealed from magnetic hysteresis loops with the easy magnetization axis aligned along the length of the beams. The quality factor of the driven resonator beams under vacuum is increased by 30 times which is expected to lead to improved signal to noise ratio, combined with a predicted reduction in the intrinsic magnetic noise by a factor of 6 potentially reaching as low as  $\sim 25$  pT/ $\sqrt{\text{Hz}}$  at 1 Torr. Stress reconfigurable sensors operating under vacuum could thus further improve the limit of detection and advance development of magnetic field sensing technology.

### **G1.00311 Fabrication and performance analysis of a simple, cost-effective copper oxide / zinc oxide semiconductors composite for gas sensing**

, RAFAEL VELAZQUEZ, MANUEL RIVERA, ERIC LI, PETER FENG, University of Puerto Rico — We report on our studies of composite zinc oxide semiconductor (COS) nanoparticles as sensing materials for the development of high-performance gas sensors. The average diameter of the nanoparticles is 40 nm. The basic electrical properties of sensing materials have been measured. The morphologic surface and crystalline structures of COS are characterized by using scanning electron microscopy (SEM) and Raman scattering spectroscopy, respectively. By using synthesized COS of CuO-ZnO materials, prototypic highly sensitive gas sensors have been designed, fabricated and tested. Important stability and repeatability features have been obtained. The sensitivities of the COS based sensors to methane and hydrogen gases as a function of time and the gas concentrations have been determined. Various sensing parameters including the sensitivity, response time, recovery time, and thermal effect on the gas sensor performance have also been investigated in order to reveal the sensing ability. Analyses of experimental data indicate that the obtained response and recovery are almost 10 times faster than conventional sensors constructed solely from one material.

**G1.00312 Microfabrication of Arrays of Superconducting Transition Edge Sensors for CMB Measurements**, CHRYSTIAN POSADA, JUNJIA DING, AMY BENDER, TRUPTI KHAIRE, Argonne National Laboratory, SERGI LENDINEZ, Universitat de Barcelona, SAMUEL CIOCYS, University of California, Berkeley, GENSHENG WANG, VOLODYMYR YEFREMENKO, Argonne National Laboratory, STEVE PADIN, JOHN CARLSTROM, University of Chicago, CLARENCE CHANG, VALENTINE NOVOSAD, Argonne National Laboratory, SPT3G COLLABORATION<sup>1</sup> — The cosmic microwave background (CMB) provides a unique window for exploring fundamental physics. Increasing the sensitivity of CMB experiments requires fabricating focal planes with orders of magnitude more detectors than current instruments. This work presents the procedures used at Argonne National Laboratory for the fabrication of large arrays of dual-polarized multichroic detectors for CMB measurements. The detectors are composed of a broad-band sinuous antenna coupled to a Nb microstrip transmission line. In-line filters define the spectral response, allowing for individual measurement of three band-passes (95 GHz, 150GHz and 220 GHz). A Ti /Au termination resistor is used to couple the mm-wave signal to Ti/Au transition edge sensor (TES) bolometers. There are six bolometers per pixel, for a total of 16,140 detectors in the CMB receiver being fabricated. The monolithic microfabrication of the detector arrays will be presented and discussed in detail.

<sup>1</sup>The SPT3G collaboration is developing the third-generation camera for CMB measurements with the South Pole Telescope. Additional information can be found in the following link: <https://pole.uchicago.edu/spt/>

**G1.00313 Measurement of the low energy spectral contribution in coincidence with valence band (VB) energy levels of Ag(100) using VB-VB coincidence spectroscopy**<sup>1</sup>, R.W. GLADEN, P.V. JOGLEKAR, Z.H. LIM, K. SHASTRY, Univ of Texas, Arlington, S.L. HULBERT, Brookhaven National Laboratory, A.H. WEISS, Univ of Texas at Arlington — A set of coincidence measurements were obtained for the study and measurement of the electron contribution arising from the inter-valence band (VB) transitions along with the inelastically scattered VB electron contribution. These Auger-unrelated contributions arise in the Auger spectrum (Ag 4p VVV) obtained using Auger Photoelectron Coincidence Spectroscopy (APECS). The measured Auger-unrelated contribution can be eliminated from Auger spectrum to obtain the spectrum related to Auger. In our VB-VB coincidence measurement, a photon beam of energy 180eV was used to probe the Ag(100) sample. The coincidence spectrum was obtained using two Cylindrical Mirror Analyzers (CMA's). The scan CMA measured the low energy electron contribution in the energy range 0-70eV in coincidence with VB electrons measured by the fixed CMA. In this talk, we present the data obtained for VB-VB coincidence at the valence band energy of 171eV along with the coincidence measurements in the energy range of 4p core and valence band.

<sup>1</sup>NSF DMR 0907679, NSF Award Number: 1213727. Use of the National Synchrotron Light Source, Brookhaven National Laboratory, was supported by the U.S. DOE, Office of Science, Office of Basic Energy Sciences, under Contract No. DEAC02-98CH10886

**G1.00314 Simulation-based Extraction of Key Material Parameters from Atomic Force Microscopy**<sup>1</sup>, HUSEEN ALSAFI, GRAY PENNINGTON, Towson Univ — Models for the atomic force microscopy (AFM) tip and sample interaction contain numerous material parameters that are often poorly known. This is especially true when dealing with novel material systems or when imaging samples that are exposed to complicated interactions with the local environment. In this work we use Monte Carlo methods to extract sample material parameters from the experimental AFM analysis of a test sample. The parameterized theoretical model that we use is based on the Virtual Environment for Dynamic AFM (VEDA) [1]. The extracted material parameters are then compared with the accepted values for our test sample. Using this procedure, we suggest a method that can be used to successfully determine unknown material properties in novel and complicated material systems.

<sup>1</sup>We acknowledge Fisher Endowment Grant support from the Jess and Mildred Fisher College of Science and Mathematics, Towson University.

**G1.00315 Modeling of the energy resolution of a 1 meter and a 3 meter time of flight positron annihilation induced Auger electron spectrometers.**<sup>1</sup>, A FAIRCHILD, V CHIRAYATH, R GLADEN, A MCDONALD, Z LIM, M CHRYSLER, A KOYMEN, A WEISS, Univ of Texas, Arlington — Simion 8.1® simulations were used to determine the energy resolution of a 1 meter long Time of Flight Positron annihilation induced Auger Electron Spectrometer (TOF-PAES). The spectrometer consists of: 1. a magnetic gradient section used to parallelize the electrons leaving the sample along the beam axis, 2. an electric field free time of flight tube and 3. a detection section with a set of ExB plates that deflect electrons exiting the TOF tube into a Micro-Channel Plate (MCP). Simulations of the time of flight distribution of electrons emitted according to a known secondary electron emission distribution, for various sample biases, were compared to experimental energy calibration peaks and found to be in excellent agreement. The TOF spectra at the highest sample bias was used to determine the timing resolution function describing the timing spread due to the electronics. Simulations were then performed to calculate the energy resolution at various electron energies in order to deconvolute the combined influence of the magnetic field parallelizer, the timing resolution, and the voltage gradient at the ExB plates. The energy resolution of the 1m TOF-PAES was compared to a newly constructed 3 meter long system. The results were used to optimize the geometry and the potentials of the ExB plates for obtaining the best energy resolution.

<sup>1</sup>This work was supported by NSF grant NSF grant No. DMR 1508719 and DMR 1338130

**G1.00316 Spectra of electrons emitted as a result of the sticking and annihilation of low energy positrons to the surfaces of graphene and highly oriented pyrolytic graphite (HOPG)**<sup>1</sup>, M CHRYSLER, V CHIRAYATH, A MCDONALD, Z LIM, K SHASTRY, R GLADEN, A FAIRCHILD, A KOYMEN, A WEISS, University of Texas at Arlington — Positron annihilation induced Auger electron spectroscopy (PAES) was used to study the positron induced low energy electron spectra from HOPG and a sample composed of 6-8 layers of graphene grown on polycrystalline copper. A low energy (~2eV) beam of positrons was used to implant positrons into a surface localized state on the graphene and HOPG samples. Measurements of the energy spectra of the positron induced electrons obtained using a TOF spectrometer indicate the presence of an annihilation induced KLL C Auger peak (at ~263 eV) along with a narrow low energy secondary peak due to an Auger mediated positron sticking (AMPS) process. A broad spectral feature was also observed below ~15 eV which we believe may be due to a VVV C Auger transition not previously observed. The energy dependence of the integrated intensity of the AMPS peak was measured for a series of incident positron kinetic energies ranging from ~1.5 eV up to 11 eV from which the binding energy of the surface localized positron state on graphene and HOPG was estimated. The implication of our results regarding the applicability of AMPS and PAES to the study of graphene surfaces and interfaces will be discussed.

<sup>1</sup>This work was supported by NSF grant No. DMR 1508719 and DMR 1338130

**G1.00317 Scanning SQUID microscopy in a cryogen-free refrigerator**, BRIAN T. SCHAEFER, DAVID LOW, LASSP/Department of Physics, Cornell University, Ithaca, New York, USA, GUENEVERE E. D. K. PRAWIROATMODJO, Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark, J. KEVIN NANGOI, JIHOON KIM, KATJA C. NOWACK, LASSP/Department of Physics, Cornell University, Ithaca, New York, USA — With helium prices rising and supply becoming increasingly uncertain, it has become attractive to use dry cryostats with cryocoolers rather than liquid helium to reach low temperatures. However, a cryocooler introduces vibrations at the sample stage, making scanning probe experiments more challenging. Here, we report our progress on a superconducting quantum interference device (SQUID) microscope implemented for the first time in a compact, cryogen-free 5 K system. Our microscope is designed to reach submicron spatial resolution and a flux sensitivity of approximately  $1 \mu\Phi_0/\sqrt{\text{Hz}}$ , where  $\Phi_0$  is the magnetic flux quantum. To enable height feedback while approaching and scanning samples, we mount the SQUID on a quartz tuning fork. Our system promises to meet the capabilities of similar systems implemented in helium cryostats.

**G1.00318 Refocusing and high field generation of terahertz radiation in two-color laser filamentation**<sup>1</sup>, YUNGGUN YOO, DONGHOON KUK, KI-YONG KIM, Univ of Maryland-College Park — We have demonstrated strong terahertz (THz) field generation by using femtosecond two-color laser mixing in air. In this experiment, we have tested THz energy scaling and refocusing by varying the lens focal length from 200 mm to 1 m. We find that the output THz energy greatly enhances with increasing focal length (or plasma filament length), which is consistent with previous reports. In addition, contrary to our previous concern that long filamentation may yield more THz energy but unfavorably increase the focused spot size, both short and long filamentation provide small spot sizes (35–50 microns in FWHM). This implies that the peak field 8 MV/cm, previously achieved with a 200 mm focal length, can be greatly enhanced with long filamentation and tight refocusing. In addition, for real-time THz beam profiling, an uncooled microbolometer camera is used with lock-in detection, providing enhanced signal-to-noise ratios at a broad range of THz (1–40 THz) frequencies.

<sup>1</sup>Work supported by DOE, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. 014216-001

**G1.00319 Generation of scalable terahertz radiation from cylindrically focused laser pulses in air**<sup>1</sup>, DONGHOON KUK, YUNGGUN YOO, ERIC ROSENTHAL, NIHAL JHAJJ, HOWARD MILCHBERG, KI-YONG KIM, Univ of Maryland-College Park — We have demonstrated scalable terahertz (THz) generation via cylindrical focusing of two-color laser pulses in air. In this experiment, we have used a terawatt (TW) laser system which can deliver >50 mJ, 800 nm, 50 fs pulses at a 10 Hz repetition rate. A 800 nm pulse passing through a nonlinear crystal (BBO) generates its second harmonic pulse (400 nm). Both pulses pass through a cylindrical lens and are focused together to generate a 2-dimensional plasma sheet in air. This yields two diverging THz lobes, characterized by an uncooled microbolometer. This observed radiation angle and pattern is explained by the optical-Cherenkov radiation theory. The diverging THz radiation is re-focused to yield strong THz field strengths (>20 MV/cm) at the focus. At laser energy of 40 mJ, cylindrical focusing provides THz energy of >30 microjoules, far exceeding the output produced by spherical focusing. This shows that cylindrical focusing can effectively minimize ionization-induced defocusing, previously observed in spherical focusing, and can allow scalable THz generation with relatively high laser energies (>20 mJ).

<sup>1</sup>Work supported by DOE, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. 014216-001

**G1.00320 Interaction of high density, thin, gas jets with ultrashort laser pulses at 1 kHz repetition rates**<sup>1</sup>, YAN TAY, DONGHOON KUK, HOWARD MILCHBERG, KI-YONG KIM, Univ of Maryland-College Park — We have investigated the interaction of thin (50–150 microns), high-density ( $10^{19}$ – $10^{21}$  cm<sup>-3</sup>) gas jets with 30 fs, >5 mJ, 800 nm laser pulses at a 1 kHz repetition rate. Capillary tubes with various diameters (50–500 microns) are used to produce dense gas jets in continuous flow at high backing pressure (~1000 psi) and cryogenic temperature (130 K). The gas/plasma density profiles are characterized by optical interferometry, and Rayleigh/Mie scattering is measured to characterize coexisting atomic clusters. Our result shows a peak plasma density of  $10^{21}$  cm<sup>-3</sup> near the nozzle orifice, approaching the critical plasma density at 800 nm laser wavelength. This high density plasma efficiently produces X-rays and terahertz radiation, as well as energetic electrons and ions at high-repetition-rates (kHz), without generating unwanted debris as in solid targets.

<sup>1</sup>Work supported by DOE, Fusion Energy Sciences under Award No. DE-SC0010706

**G1.00321 Ultrasmall Angle X-ray Scattering (USAXS) and Wide Angle X-ray Scattering (WAXS) Studies on the Complex Metal Hydride NaAlH<sub>4</sub>**, TABBETHA DOBBINS, CHRISTOPHER BENNETT<sup>1</sup>, JAMES TORRES, Rowan University, Dept. of Physics & Astronomy, JAN ILAVSKY, Argonne National Laboratory, Advanced Photon Source — This research seeks to understand the role of ScCl<sub>3</sub>, ZrCl<sub>4</sub>, and VCl<sub>3</sub> catalysts in NaAlH<sub>4</sub>. We have examined these hydrides at multiple length scales using an X-ray scattering instrument which is capable of measuring scattering wave vector, Q, of 0.0001 Å<sup>-1</sup> to 6.0 Å<sup>-1</sup>. The ultrasmall angle X-ray scattering (USAXS) instrument sector 9ID-D of the Advanced Photon Source (APS) simultaneously collects using USAXS, SAXS, and WAXS detectors. Studies were performed during in-situ heating up to 170°C (just below the H desorption temperature for uncatalyzed NaAlH<sub>4</sub>). Results showed that NaAlH<sub>4</sub> has a surface fractal (highly porous) morphology. Isothermal studies performed at 30°C, 65°C, 100°C, 135°C, and 170°C reveals changes at low Q (Q~0.001 Å<sup>-1</sup> to 0.01 Å<sup>-1</sup>) associated with highly interconnected intraparticle porosity which is suitably described by a power-law slope for a Gaussian polymer chain structure of p~2. At high scattering wave vector, Q~0.03 Å<sup>-1</sup>, the presence of a pore population which obeys Porod scattering and appears to have a size at 21 nm is present. These fine pores increase in their population density as temperature is elevated. The WAXS data reveals thermal expansion to occur, but no solid state phase transformation to the product phase.

<sup>1</sup>currently at NASA-Goddard

**G1.00322 Adaptive measurement of spin decoherence time  $T_2$** , YIHAO ZHANG, WEN YANG, Beijing Computational Science Research Center — Spin decoherence time  $T_2$  is an important parameter in quantum mechanics. In order to estimate it accurately and efficiently, we propose a scheme for spin decoherence time  $T_2$  estimation of a single spin using adaptive measurement. While the ordinary scheme of measuring  $T_2$  yield an estimate precision scales with mean-square error  $\sim 1/\sqrt{N}$  (N is the number of measurements). We present some simulated measurement which shows that the adaptive scheme, that is, the time between measurements was depended on the prior measurement results, will give a better scaling than MSE.

**G1.00323 Single-shot ultrafast interferometric imaging**<sup>1</sup>, DAIWEI ZHU, DONGHOON KUK, KI-YONG KIM, Univ of Maryland-College Park — We have developed a new interferometric method capable of capturing 2-dimensional, time-varying phase and amplitude profiles in a single shot. Most single-shot interferometry provides one-dimensional spatial information as demonstrated in detecting laser-produced transients, phase transition, and plasma generation. By contrast, our new method can provide 2-dimensional spatial information at multiple time delays in a single shot. In this scheme, we analyze the limits of spatial and temporal resolution and have tested the working principle with a computer simulation. This new diagnostic holds a great potential in study ultrafast phenomena occurring on sub-picosecond time scales.

<sup>1</sup>Work supported by NSF under Award No. 1351455.

**G1.00324 Elastic scattering of Electrons and Positrons by Cadmium Atom\*)** , B. C. SAHA, Department of Physics, Florida AM University, Tallahassee, FL-32307., A. K. F. HAQUE, Department of Physics, University of Rajshahi, Rajshahi-6205, Bangladesh, M. I. HOSSAIN, Department of Physics, Florida AM University, Tallahassee, FL-32307., M. A. UDDIN, M. A. R. PATOARY, Department of Physics, University of Rajshahi, Rajshahi-6205, Bangladesh, M. MAAZA, Council for Scientific and Industrial Research, PO Box-395, Pretoria 0001, South Africa, A. K. BASAK, Department of Physics, University of Rajshahi, Rajshahi-6205, Bangladesh — The differential, integrated elastic, total and momentum transfer cross sections with Sherman functions for the elastic scattering of electrons and positrons by cadmium atom have been calculated. These calculations are done within the framework of complex electron/positron-atom optical potential and relativistic Dirac partial wave analysis at energies 6.4 to 1000 eV for both electrons and positrons impact. Our results are compared with available experimental and other theoretical cross section values. Details of our findings will be presented at the conference. \*) BCSaha is thankful to NNSA for partial support.

**G1.00325 Low energy  $C^{6+} + H_2$  scattering: Molecular Close-Coupling Treatment\*)** \pard\pard<sup>1</sup> , BIDHAN SAHA, Department of Physics, Florida AM University, Tallahassee, FL-32307. — h —abstract—\pard Collisions of multiply charged ions with molecules are very common in astrophysical plasmas[1]. The ion-molecule calculations are rather more complicated than their atomic counter part. For multi charged ions in X-ray ionized astronomical environments the charge exchange provides a recombination mechanism. To understand this detailed information on the collision cross sections is essential. In highly charged ion-molecule problem the Coulomb term plays an important role; using a pseudo-diatomic technique the colliding system can be approximated by a model potential for the ionic core of  $H_2$  with encouraging results [2-5]. Freezing the target,  $H_2$  can easily be treated as an atom with appropriate ionization potential (Ip). Our results show good agreement with available experimental findings.\pard[1] B. C. Saha, Atomic Structure and Collision process, Narosa Pub. House (2011).2] B. C. Saha et. al., Phys Rev A 44, R1, (1991).3] B C Saha et. al., J. Mol. Structure 487, 11, (1999).4] A. Kumar et al Phys Rev A 59, 1273, (1999).5] B. C. Saha Phys Rev A 56, 2909, (1997).\-/abstract-\

<sup>1</sup>Partially Support by NNSA

## G1.00326 GENERAL PHYSICS —

**G1.00327 Absolute Summ** , ALFRED PHILLIPS JR., Source Institute — Summ means the entirety of the multiverse. It seems clear, from the inflation theories of A. Guth and others, that the creation of many universes is plausible. We argue that Absolute cosmological ideas, not unlike those of I. Newton, may be consistent with dynamic multiverse creations. As suggested in W. Heisenberg's uncertainty principle, and with the Anthropic Principle defended by S. Hawking, et al, human consciousness, buttressed by findings of neuroscience, may have to be considered in our models. Predictability, as A. Einstein realized with Invariants and General Relativity, may be required for new ideas to be part of physics. We present here a two postulate model geared to an Absolute Summ. The seedbed of this work is part of Akhnaton's philosophy (see S. Freud, Moses and Monotheism). Most important, however, is that the structure of human consciousness, manifest in Kenya's Rift Valley 200,000 years ago as Homo sapiens, who were the culmination of the six million year co-creation process of Hominins and Nature in Africa, allows us to do the physics that we do. .

**G1.00328 Analysis about the force of electrons revolve around the nucleus** , HAN YONGQUAN, 15611860790 — 1, Let's compare the difference of two algorithms: the electrostatic force between protons and electrons,  $F_1 = ke^2 / r^2$ ,  $r$  is the radius of the electron around the nucleus movement – within  $10^{-10}$  meters; Electronic movement speed is close to the light- about  $10^7$  meters per second, the size of the centripetal force  $F_2 = v^2 m / r$ .  $F_1$  should be approximately equal to  $F_2$ , calculate the ratio of  $F_1$  and  $F_2$ ,  $F_2 / F_1 = (v^2 m / r) (ke^2 / r^2) / = (10^7 * 10^7 * 0.91 * 10^{-30} / r) / (9 * 10^9 * 1.6 * 10^{-19} * 1.6 * 10^{-19} / r^2) = 4 \times 10^3$ . The calculation shows that not only the electrostatic force and other force. 2, The radius of the electron orbiting around the nucleus named  $r$ ,  $F = Ke^2 / r^2 = 9 \times 10^9 \times 1.6 \times 10^{-19} / r^2 = v^2 m / r$ ,  $r = 2.5 \times 10^{-14}$  meters, namely that the radius of hydrogen atom is about  $2.5 \times 10^{-14}$  meters, that is different with the observed result ( $10^{-10}$  meters). Electrons revolve around the nucleus may faster than  $10^7$  m/s, can almost reach  $10^8$  meters per second, if the electronic moves by  $10^8$  meters per second, hydrogen atom radius is approximately  $2.5 \times 10^{-16}$  meters, has converged in the interior of the nucleus, it is not possible. Use density to instead of electricity, can solve this problem. Author: hanyongquan TEL: 15611860790

**G1.00329 Nuclear Structure of the Noble Gas** , NAKYEONG SEONG, life and light institute — Modern physics usually pictures the nuclear structure as about sphere and treats various detailed situation as perturbative, which may be obscured. In addition, the explanation why <sup>235</sup>U undergoes nuclear fission and <sup>238</sup>U does not is too difficult and unclear for the people to understand. However, in this paper, we introduce a new approach on the nuclear structure of the noble gas, which simultaneously can explain several phenomena that is obscurely elucidated by modern physics. We consider a 1:1 ratio between protons and neutrons and need the concept of the symmetry of the nuclear structure, because the electron's shell of the noble gas is fully occupied. From these, we can predict the number of neutrons of each noble gas exactly

**G1.00330 Negative Casimir entropies** , YANG LI, KIMBALL MILTON, Univ of Oklahoma — In the last decade, various results on the entropy related to the Casimir interactions between two bodies have been obtained and the striking feature that negative values of Casimir entropy frequently appear. The origin of this effect lies in many factors, such as the dissipation of the materials, the geometry of the configuration and so on. We recently investigated the entropies of one body systems. Although the self-free energy of one body systems are always divergent, the self-entropy could be finite in many cases. These phenomenon may throw more light on thermal dynamical behavior of quantum field systems.

## G1.00331 ABSTRACT WITHDRAWN —

**G1.00332 Number relativity** , PHILIP SHIN<sup>1</sup>, None — Number relativity 1. Every equation of the relativity is just the way to understand through to solve one question of the math problem. We just add the hypothesis into the number. 2. Sequence of number is the machine physics for software(computer) as the number order is program equation as calculator. 3. When zero is denominator, it is not existing as it is doing something by nothing. So nothing means time as we put zero denominator into time.

<sup>1</sup>My personal physics imagine.

**G1.00333 Kelvin Absolute Temperature Scale Identified as Length Scale and Related to de Broglie Thermal Wavelength.** , SIAVASH SOHRAB, Northwestern University — Thermodynamic equilibrium between matter and radiation leads to de Broglie wavelength  $\lambda_{d\beta} = h/m_{\beta}v_{r\beta}$  and frequency  $\nu_{d\beta} = k/m_{\beta}v_{r\beta}$  of matter waves and stochastic definitions of Planck  $h = h_k = m_k < \lambda_{rk} > c$  and Boltzmann  $k = k_k = m_k < \nu_{rk} > c$  constants,  $\lambda_{rk}\nu_{rk} = c$ , that respectively relate to spatial ( $\lambda$ ) and temporal ( $\nu$ ) aspects of vacuum fluctuations. Photon mass  $m_k = \sqrt{hk/c^3}$ ,  $amu = \sqrt{hkc} = 1/N^o$ , and universal gas constant  $R^o = N^o k = \sqrt{k/hc}$  result in internal  $U_k = Nh\nu_{rk} = Nm_k c^2 = 3Nm_k v_{mpk}^2 = 3NkT$  and potential  $pV = uN\hat{v}/3 = N\hat{u}/3 = NkT$  energy of photon gas in *Casimir vacuum* such that  $H = TS = 4NkT$ . Therefore, Kelvin absolute thermodynamic temperature scale [degree K] is identified as length scale [meter] and related to most probable wavelength and de Broglie thermal wavelength as  $T_{\beta} = \lambda_{mp\beta} = \lambda_{d\beta}/3$ . Parallel to Wien displacement law obtained from Planck distribution, the displacement law  $\lambda_w S T = c_2/\sqrt{3}$  is obtained from Maxwell–Boltzmann distribution of speed of “photon clusters”. The propagation speeds of sound waves in ideal gas versus light waves in photon gas are described in terms of  $v_{r\beta}$  in harmony with perceptions of Huygens. Newton formula for speed of long waves in canals  $\sqrt{p/\rho}$  is modified to  $\sqrt{gh} = \sqrt{\gamma p/\rho}$  in accordance with adiabatic theory of Laplace.

**G1.00334 Time Dilation And Changes Of Material Properties Of An Atom (Body) In Speed Of Near Light Speed Based On The ”Substantial Motion”;** Theory of Iranian Philosopher, Mulla Sadra , HASSAN GHOLIBEIGIAN<sup>1</sup>, No Company Provided, KAZEM GHOLIBEIGIAN<sup>2</sup>, None — Iranian Philosopher, Sadr-ol-Moteallehin (1571-1640) said in his famous book, Asfar: "the Universe moves in its entity... and time is its fourth dimension, and time is magnitude of the motion (momentum) of the matter in its entity". In other words, time for each atom is momentum of its involved fundamental particles, [APS March Meeting 2015, abstract V1.023]. When an atom (body) moves in speed of near light speed, speed of its involved fundamental particles become slow, and consequently the magnitude of its momentum (time) will decrease. On the other hands, when the spin and orbital angular momentum of an atom changed, it means that its properties, mass, strength of its electromagnetic field and its interaction with momentum changed. As a result, each atom (body) which moves in light speed, lower or faster than that, will get a new identity and vice versa. The special relativity can be the special form of this theory. In this way, black holes will be lighter than their involved masses at rest (a paradox with general relativity). Dark matter/energy may be created at first in B.B (Convection Bang) [AGU Fall Meeting 2015, abstract ID: 58425], in more than light speed, so, if we speed protons to more than light speed (in LHC), we may see dark mater/energy in new space-time.

<sup>1</sup>AmirKabir University of Technology

<sup>2</sup>Student, Technische Universitt Wien (TU WIEN)

**G1.00335 Exploring Baryons for Dark Matter** , SHANTILAL GORADIA, Retired — There is on-going research for the detection of WIMPs based on a speculative idea of supersymmetry, which attempts to unify the fundamental forces of nature, including gravity. The detection of WIMPs is expected to find a solution to the issue of dark matter. We continue to hold and support our view of the millennium that gravity is not a fundamental force of Nature. We are therefore exploring baryons as the particles to address the issue of dark matter. We poster present our analyses to support our proposal.

**G1.00336 Siegel[JMMM 7,312('78)] FIRST EXPERIMENTAL DISCOVERY of Giant-Magnetoresistance Decade Pre “Fert” and “Gruenberg”;** [’88 – ‘78] = 10-Years = One-Decade Sounds, for Nuclear-Power Naïve “Panacea” for Global-Warming/Climate-Chan , MASTERACE HOFFMANN, EDWARD SIEGEL, failure-PREVENTION-associates (fPa) — Siegel[JMMM 7,312('78); Monju (12/'95) LMFBR PRE-DICTION!!!] following: Wigner[JAP 17,857('46)]-(Alvin)Weinberg(ANL/ORNL/ANS)-(Sidney)Siegel(ANL/ORNL/ANS)-Seitz-Overhauser-Rollnick-Pollard-Lofaro-Markey-Pringle[Nuclear-Power;From Physics to Politics('79)] FIRST EXPERIMENTAL DISCOVERY [Siegel<<<“Fert”-“Gruenberg”:2007-Physics-Nobel/2006:-Wolf/Japan-prizes:['88 – '78]=10-years =1-decade precedence!!!] of granular giant-magnetoresistance(GMR) [Google: “EDWARD SIEGEL GIANT-MAGNETORESISTANCE ICMO 1977 FLICKER”]; [Google: “Ana Mayo If LEAKS ‘Could’ KILL”]; in austenitic/FCC Ni/Fe-based (so MIScaled))”super” alloy-182/82 transition-welds GENERIC ENDEMIC EXTANT detrimental (SYNONYMS): Wigner’s-disease/Ostwald-ripening/spinodal-decompositio/OVERAgeing/EMBRITTLEMENT/THERMAL-leading-to-mechanical (TLTM)-INstability/“sensitization” in: nuclear-reactors/spent-fuel dry-casks/refineries/jet/missile/rocket-engines/... SOUNDS A DIRE WARNING FOR NAIVE Hansen-Sommerville-Holdren-DOE-NRC-OSTP-WNA-NEI-AIP-APS-... calls/media-hype/P.R./spin-doctoring for carbon-“free” nuclear-power as a SUPPOSED “panacea” for climate-change/global-warming: “TRUST BUT VERIFY!!!” ; a VERY LOUD CAVEAT EMPTOR!!!

**G1.00337 History of “NANO”-Scale VERY EARLY Solid-State (and Liquid-State) Physics/Chemistry/Metallurgy/ Ceramics; Interstitial-Alloys Carbides/Nitrides/Borides/... Powders and Cermets, Rock Shocks, ...** , COLIN MAIDEN, EDWARD SIEGEL, failure-PREVENTION-associates (fPa) / Thermalloy-Technology(TAT) / TATL — History of “NANO”: Siegel-Matsubara-Vest-Gregson[Mtls. Sci. and Eng. 8, 6, 323('71); Physica Status Solidi (a)11,45('72)] VERY EARLY carbides/nitrides/borides powders/cermets solid-state physics/chemistry/metallurgy/ ceramics FIRST-EVER EXPERIMENTAL NANO-physics/chemistry[1968 ->Physica Status Solidi (a)11,45('72); and EARLY NANO-“physics”/NANO-“chemistry” THEORY(after: Kubo('62)-Matsubara('60s-'70s)-Fulde ('65); [ref.: Sugano[Microcluster-Physics, Springer('82; '98)] Siegel [('70-'73) —>Statphys-13, The Technion, Haifa(1977)-C. Kuper and I, Reiss editors, in Annals Israel Academy of Sciences, volume 2(1978); International Conference on Lattice-Dynamics, Paris('77)-M. Balkanski editor, Flammarion('78); International Conference on Magnetic Alloys and Oxides(“ICMAO”), The Technion, Haifa('77)-A. Hirsh and G. Barnea editors, in Journal of Magnetism and Magnetic Materials (JMMM 7, 312) (1978){where Siegel FIRST EXPERIMENTAL DISCOVERY of granular-giant-magnetoresistance(GMR)[JMMM 7, 312('78)] and FIRST THEORETICAL PREDICTION of colossal-magnetoresistance(CMR)[JMMM 7, 338('78)]}; Semiconductors and Insulators 5: 39,47,62('79)=THREE-contiguous-papers!!!; Scripta Metallurgica 13, 913('79)], AIP Shock-Physics Meetings: Chicago('11); Seattle('13); Tampa('15); ...

**G1.00338 Implications of the general constraints for single-qubit quantum process tomography<sup>1</sup>** , RAMESH BHANDARI, Laboratory for Physical Sciences, NICHOLAS PETERS, Oak Ridge National Laboratory — We revisit the general constraints of single qubit quantum process tomography and derive simplified forms in the Pauli basis. These forms give insight into the structure of the process matrix, which we examine in light of several examples. Specifically, we study some qubit leakage error models and show how different error models are manifest in the process matrix.

<sup>1</sup>NAP’s research sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U. S. Department of Energy.

**G1.00339 Optical determination of MoSe<sub>2</sub> layer number**, XIAN ZHANG, JAMES HONE, Columbia University, COLUMBIA TEAM — We mechanically exfoliate mono- and few-layers of molybdenum diselenide. The exact number of layers is determined by atomic force microscopy, high-resolution Raman spectroscopy, and photoluminescence. We have quantitatively summarized the relation between Raman A<sub>1g</sub> mode positions and the layer numbers, from both 532nm wavelength and 633nm wavelength Raman lasers. The spectrum analysis is based on 1-4 layer MoSe<sub>2</sub> flakes. These observations provide useful information for the future opto-electronic devices based on these materials.

**G1.00340 Flexible low-power RF nanoelectronics in the GHz regime using CVD MoS<sub>2</sub>**, MARUTHI YOGESH, University of Texas at Austin — Two-dimensional (2D) materials have attracted substantial interest for flexible nanoelectronics due to the overall device mechanical flexibility and thickness scalability for high mechanical performance and low operating power. In this work, we demonstrate the first MoS<sub>2</sub> RF transistors on flexible substrates based on CVD-grown monolayers, featuring record GHz cutoff frequency (5.6 GHz) and saturation velocity (~1.8106 cm/s), which is significantly superior to contemporary organic and metal oxide thin-film transistors. Furthermore, multicycle three-point bending results demonstrated the electrical robustness of our flexible MoS<sub>2</sub> transistors after 10,000 cycles of mechanical bending. Additionally, basic RF communication circuit blocks such as amplifier, mixer and wireless AM receiver have been demonstrated. These collective results indicate that MoS<sub>2</sub> is an ideal advanced semiconducting material for low-power, RF devices for large-area flexible nanoelectronics and smart nanosystems owing to its unique combination of large bandgap, high saturation velocity and high mechanical strength.

**G1.00341 Experimental Greenberger-Horne-Zeilinger type six-photon quantum nonlocality**, CHAO ZHANG, YUN-FENG HUANG, ZHAO WANG, BI-HENG LIU, CHUAN-FENG LI, GUANG-CAN GUO, Univ of Sci & Tech of China, KEY LABORATORY OF QUANTUM INFORMATION TEAM — Quantum nonlocality gives us deeper insight into quantum physics. In addition, quantum nonlocality has been further recognized as an essential resource for device-independent quantum information processing in recent years. Most experiments of nonlocality are performed using a photonic system. However, until now, photonic experiments of nonlocality have involved at most four photons. Here, for the first time, we experimentally demonstrate the six-photon quantum nonlocality in an all-versus-nothing manner based on a high-fidelity (88.4%) six-photon Greenberger-Horne-Zeilinger (GHZ) state. Our experiment pushes multi-photon nonlocality studies forward to the six-photon region and might provide a larger photonic system for device-independent quantum information protocols.

**G1.00342 Theoretical studies of graphene nanoribbon quantum dot qubits<sup>1</sup>**, CHIH-CHIEH CHEN, Department of Physics, Zhejiang University, YIA-CHUNG CHANG, Research Center for Applied Sciences, Academic Sinica — Graphene nanoribbon quantum dot qubits have been proposed as promising candidates for quantum computing applications to overcome the spin-decoherence problems associated with typical semiconductor (e.g., GaAs) quantum dot qubits. We perform theoretical studies of the electronic structures of graphene nanoribbon quantum dots by solving the Dirac equation with appropriate boundary conditions. We then evaluate the exchange splitting based on an unrestricted Hartree-Fock method for the Dirac particles. The electronic wave function and long-range exchange coupling due to the Klein tunneling and the Coulomb interaction are calculated for various gate configurations. It is found that the exchange coupling between qubits can be significantly enhanced by the Klein tunneling effect. The implications of our results for practical qubit construction and operation are discussed.

<sup>1</sup>This work was supported in part by the Ministry of Science and Technology, Taiwan, under Contract No. MOST 104-2112-M-001-009-MY2.

**G1.00343 InAs Quantum Dots embedded in GaAs: Properties from Basic Electrical Measurements**, AZZOUZ SELLAI, Sultan Qaboos University, Physics Department, P.O. Box 36, ABDELMADJID MESLI, IM2NP, UMR 6242 CNRS, Aix-Marseille University, Av. Normandie-Niemen, 13397 Marseille Cedex 20 — C-V and I-V data from a GaAs Schottky diode in which InAs quantum dots (QDs) were embedded are analyzed. The capacitance due to QDs is fitted with an analytical equation that takes into account Gaussian broadening of sub-band levels and contribution of the wetting layer. The voltage range over which the excess capacitance extends is used to estimate the number of charges contained in the QDs. The energy levels of electrons, entirely confined in the QDs, are computed based on a model in which InAs dots are considered of conical shapes and where the effective mass is taken as both position- and energy-dependent. To reconcile the computed energy values with those from the C-V fits, one has to consider a confinement potential other than the potential due to the GaAs/InAs band discontinuity. I-V data could be analyzed using a model that combines field and thermionic emission processes with two distinct behaviors depending on the temperature and bias. Deviations occur at temperatures above 200 K and voltages above 0.4 V. In comparison with the structure with only the wetting layer, the structure with QDs exhibits an excess current in the low-bias forward regime, an indication of contributions from tunneling electrons.

**G1.00344 Effect of the In by Bi substitution in the Sm<sub>2</sub>InTaO<sub>7</sub> system for the photocatalytic splitting of water**, PABLO DE LA MORA, MELISSA MENDEZ GALVAN, Facultad de Ciencias, GUSTAVO TAVIZON, Facultad de Quimica, Universidad Nacional Autonoma de Mexico, JUAN RAMIREZ DE ARELLANO, Tecnologico de Monterrey, Campus Ciudad de Mexico — Tantalum oxide-based photocatalysts with octahedrally coordinated d<sup>10</sup> configuration, represent promising semiconductor systems to develop photocatalysts with visible-light response in the photochemical splitting of water. Several Indium oxide-based compounds have shown acceptable activity in water photolysis. Recently, the pyrochlore Sm<sub>2</sub>InTaO<sub>7</sub> (a 4f-d<sup>10</sup>-d<sup>0</sup> system) was reported as a visible-light photocatalyst for water splitting. In the present work, by solid state reaction, we have obtained and structurally characterized compounds of the Sm<sub>2</sub>In<sub>1-x</sub>Bi<sub>x</sub>TaO<sub>7</sub> system. In these systems we have found that the optical band gap value depends on the Bi content; this value is 2.7, 2.52 and 2.1eV for x=0, 0.15 and 0.30 respectively. The specific surface area values we have found are typical of solid state reaction products, 0.5-1.2 m<sup>2</sup>/g. To understand the effect of the In substitution by Bi, the compounds were studied with first principles calculations using the WIEN2k package and the gap was evaluated using the mBJ potential

**G1.00345 Motion of Ferrofluid Droplets Under Oscillating Magnetic Field<sup>1</sup>**, YU GU, HUIYANANGEL CHOW, KARL MORRIS, Saint Joseph's University — Ferrofluids are stable, colloidal suspensions of single-domain ferromagnetic particles of nanometer size. Because of their good sealing properties and ease of actuation, ferrofluids are ideal for applications in Lab-On-Chip, or micro-total analysis systems (μTAS). In particular, because of their changing viscosity and surface properties under magnetic fields, as well as previously reported nonlinear behavior in bulk volumes, understanding the periodic movement of ferrofluid droplets for applications in pumping, valving and switching is important. We characterize the movement of ferrofluid droplets with volumes from 80 nL to 200 nL under oscillating magnetic fields in the frequency range 1Hz to 100Hz. Oil-based ferrofluid droplets are placed in circular cross-sectional capillaries and motion is recorded using a high-speed camera, then distilled using computer-assisted image analysis. Kinematics variables such as the position and velocity of the droplets' centers of mass are observed. Nonlinear behaviors in droplet shape and travel distance per cycle of actuation are also presented.

<sup>1</sup>This work was supported by the Research Corporation for Science Advancement

**G1.00346 Electronic Transport and Spatial/Temporal Photocurrent in Monolayer Molybdenum Disulfide Grown by CVD.** , ZHENGFENG YANG, Univ of Illinois - Urbana, ROBERTO GRASSI, University of Minnesota, MARCUS FREITAG, IBM Thomas J. Watson Research Center, YI-HSIEN LEE, National Tsing Hua University, TONY LOW, University of Minnesota, WENJUAN ZHU, Univ of Illinois - Urbana — We systematically investigate the electronic transport in transistors/Hall-bar devices and spatial/temporal photocurrent in photodetectors based on monolayer MoS<sub>2</sub> grown by CVD. We found that the maximum photocurrent occurs when laser spot is close to the metal/MoS<sub>2</sub> contact and is tunable by the applied drain voltage, which can be explained by the modulation of the local electric field at the Schottky barrier, consistent with predictions from our quantum transport simulation. We observed that the maximum photocurrent at drain contact is much larger than the one at source contact, and the DC currents show rectifying behavior. These phenomena can be explained by the different Schottky barrier heights at the two contacts. By measuring Hall-bar device at various temperatures from 100K to 400K, the extracted barrier height at drain contact is about 50mV larger than the one at source contact, consistent with the photocurrent and DC current observations. Photocurrent was measured at various powers and a photoresponsivity of 3.07 mA/W was extracted at low powers. When the power increases above 20uW, the photocurrent starts to saturate. Temporal response of the photocurrent is also dependent on the laser power. These studies of photocurrents and electronic transport in CVD MoS<sub>2</sub> highlight the importance of the contacts in the electronic/optoelectronic devices and reveal the physical mechanism of the photocurrent/electronic transport in these devices.

**G1.00347 Modelling large-particle diffusion in porous media as anisotropic continuous-time random walk** , SHAHAR AMITAI, RAPHAEL BLUMENFELD, Imperial College London — We test the fidelity of modelling diffusion of finite-size particles in porous media by continuous-time random walk (CTRW), where the step-size and waiting-time distributions of the former,  $P_l$  and  $P_t$ , are used as input to the latter. As the particle size is increased, the diffusion undergoes a transition from normal to anomalous. We find that, based only on  $P_l$  and  $P_t$ , CTRW does not predict correctly this transition. We show that the discrepancy is due to the change in effective connectivity (topology) of the porous media with increasing particle size. We propose a method to capture this within the CTRW model by adding anisotropy. This adjustment yields good agreement with the simulated diffusion process, making it possible to use CTRW, with all its advantages, to model diffusion of any finite size particle in confined geometries.

**G1.00348 Deformation in Thin Glassy Polymer Films from Surface towards Interior** , MITHUN CHOWDHURY<sup>1</sup>, Princeton University, JOHANN P. DE SILVA, GRAHAM L.W. CROSS, Trinity College Dublin — Polymer thin glassy films occupy an important place in last two decades of condensed matter research, concerning its surprising surface mobility and spatially dependent structural relaxation. However, ranges of cleverly designed indirect measurements on confined polymer glassy films already probed its mechanical properties; it is still a challenging task to directly probe such small confined volume through conventional mechanical testing. We have designed confined layer compression testing with a precisely designed and aligned flat probe during nanoindentation, which was further accompanied with atomic force microscopy. Due to natural confinement from the surrounding material, we show that a state of 'uniaxial strain' is created beneath the probe under small axial strains. By this methodology we are able to directly probe uniaxial flows under both anelastic and plastic conditions while doing controlled creep studies at different positions in the film starting from surface towards interior. Depending on the extent of deformation, we found ranges of effects, such as densification, anelastic yield, and plastic yield. Enhanced creep rate upon deformation supports the idea of 'deformation induced mobility'.

<sup>1</sup>Work performed at Trinity College Dublin

**G1.00349 Many-Body Localization in Simulation of Fermionic Systems** , ADRIAN CHAPMAN, AKIMASA MIYAKE, Univ of New Mexico — In the widely-known setting of Anderson localization, noninteracting particles in a disordered potential remain confined to their initial positions, even in the infinite-time limit. Many-body localization (MBL) is the extension of this phenomenon to the regime in which the particles are weakly interacting. Recent results have demonstrated examples of many-body localized systems whose evolution may be approximately simulated classically as a result of this confinement to within a logarithmic light cone. Here we attempt to turn the question on its head and ask whether MBL could be used as a means of simulating quantum computations that na?vely appear difficult. We focus on one-dimensional fermionic systems, which admit techniques for classical simulation in the noninteracting case but are universal for quantum computation upon the introduction of interactions. I will describe some recent progress in this direction as well as discuss possible future endeavours.

**G1.00350 Graphene-hBN-Graphene Photodetector with Low Dark Current** , RUYUE ZHANG, School of Physics, Nankai University, ZHIBO LIU, Teda Applied Physics Institute, Nankai University — Graphene is a highly promising material for high speed, broadband, and high responsivity photo detection. However, the only 2.3% absorption of incident infrared-to-visible lights in graphene significantly limits their potential for applications. What is more, most of them are based on field effect transistor structures containing mechanically exfoliated graphene with high dark current, not suitable for practical large-scale device applications. We are aimed to study the photo response of pure monolayer graphene prepared by chemical vapor deposition and fabricate high efficient photodetectors by varying its structure. We performed the transfer of CVD-grown graphene by PMMA, studied the dark and photo I-V characteristics and the photosensitivity properties of pure monolayer graphene. A graphene-hBN-graphene structure of photodetector was designed, in which a boron nitride layer was sandwiched between two CVD graphene layers. Low dark current compared with the pure monolayer graphene photodetector was easily obtained for 532 nm incident lights due to the dielectric properties of boron nitride. And because of the low dark current, photocurrents can be easily distinguished from the background. High responsivity was obtained because incident light act on two layers of graphene simultaneously. The new structure graphene photodetector shows a great promise for a wide variety of application fields.

**G1.00351 Supporting Kibble-Zurek Mechanism in Quantum Ising Model through a Trapped Ion.** , CHANGKANG HU, JINMING CUI, YUNFENG HUANG, ZHAO WANG, DONGYANG CAO, JIAN WANG, WEIMIN LV, YONG LU, University of Science and Technology of China, LE LUO, Indiana University-Purdue University Indianapolis, ADOLFO CAMPO, University of Massachusetts Boston, YONGJIAN HAN, CHUANFENG LI, GUANGCAN GUO, University of Science and Technology of China — The Kibble-Zurek mechanism is the paradigm to account for the non adiabatic dynamics of a system across a phase transition. Its study in the quantum regime is hindered by the requisite of ground state cooling. We report the experimental quantum simulation of critical dynamics in the transverse-field Ising model by a set of Landau-Zener crossings in pseudo-momentum space, that can be probed with high accuracy using a single trapped ion. Our results support the Kibble-Zurek mechanism in the quantum regime and advance the quantum simulation of critical systems far-away from equilibrium.

**G1.00352 Extremely Large Magnetoresistance in Bi<sub>0.96</sub>Sb<sub>0.04</sub>** , SUDESH SUDESH, PAWAN KUMAR, SATYABRATA PATNAIK, School of Physical Sciences, Jawaharlal Nehru University, New Delhi-110067, India — Recent experimental evidence for Weyl fermions in topological semimetals has attracted considerable attention. These materials are three-dimensional analogue of graphene. The present work is motivated by the recent prediction of Weyl semi-metallic phase in Bi<sub>1-x</sub>Sb<sub>x</sub> alloys. In this paper we present the electronic transport properties studied under high applied magnetic fields in Bi<sub>0.96</sub>Sb<sub>0.04</sub> alloys. The sample exhibits extremely high magneto-resistance; MR(5 K, 8 T) = 9.810<sup>4</sup> %. This value is comparable to the MR observed in recently discovered other members of these emergent materials. Most importantly, this composition shows large MR at room temperature, MR (300 K, 8 T) = 435%, which is almost twice to that observed in Dirac semimetal Cd<sub>3</sub>As<sub>2</sub> (= 200 % at 14.5 T) and Weyl semimetal NbP (= 250% at 9 T). We also discuss single crystal growth techniques as well as Hall and Shubnikov de Haas (SdH) oscillation data. **References** [1] S. Singh et.al, *arxiv:1512.00863v2* (2015). [2] C. Shekhar et.al, *Nat. Phys.* **11** 645–650 (2015). [3] Z. Wang et.al, *Phys. Rev. B* **88** 125427 (2013).

<sup>1</sup>We acknowledge the DIST-FIST supported low temperature-high magnetic field facility at JNU and AIRF, JNU for the access of experimental facilities to carry out this study. Sudesh and P. Kumar thank UGC, (Government of India) for financial support

**G1.00353 Observation of Superconductivity by Sr Intercalation in Topological Insulator Bi<sub>2</sub>Se<sub>3</sub>**, SHRUTI SHRUTI, VISHAL MAURYA, PRAKRITI NEHA, SUDESH SUDESH, SATYABRATA PATNAIK, Jawahar Lal Nehru University, New Delhi, India — Bi<sub>2</sub>Se<sub>3</sub> is a well-known 3D topological insulator. Here we show that Sr intercalation into the van der Waals gaps of Bi<sub>2</sub>Se<sub>3</sub> induces superconductivity with a maximum  $T_c$  of 2.9 K. The single crystals of Sr<sub>x</sub>Bi<sub>2</sub>Se<sub>3</sub> for  $x = 0$  to 0.2 were prepared by self-flux method. The optimally doped sample Sr<sub>0.1</sub>Bi<sub>2</sub>Se<sub>3</sub> shows a large superconducting shielding fraction of 93% with  $T_{c-onset}$  of 2.94 K. Using transport measurement, the anisotropy in Sr<sub>0.1</sub>Bi<sub>2</sub>Se<sub>3</sub> is found to be  $\Gamma = 1.5$  with an upper critical field  $H_{c2}(0)$  equal to 2.1 T for magnetic field applied along the  $ab$  plane of the sample. Along  $ab$  plane of the sample, the lower critical field  $H_{c1,ab}(0)$  is estimated to be 0.39 ± 0.02 mT. Hall and Seebeck measurements show electronic carrier concentration of  $n = 1.85 \times 10^{19} \text{ cm}^{-3}$  at 10 K. Such low carrier concentration indicates the possibility of unconventional pairing state.

**G1.00354 Effect of a vibrating side wall on convective heat transfer in an enclosure with varying bottom wall temperature distribution**, SAEID RAHEIMPOUR ANGENEH, MURAT K. AKTAS, TOBB ETU — This study mainly focuses on the thermal convection in a rectangular enclosure in the presence of streaming motion while temperature profile of bottom wall is sinusoidal. The effect of wall displacement amplitude and the bottom wall temperature profile on convective heat transfer in the enclosure are determined with the help of a parametric study. By vibrating side wall of the enclosure, oscillating flow is actuated. The top wall of the enclosure is kept at initial temperature and isothermal while the side walls are adiabatic. In order to predict the oscillatory and time averaged mean flow fields, fully compressible form of the Navier – Stokes equations are considered. Simulation of the convective transport in the enclosure is obtained by a control-volume method based, explicit computational scheme is used. The aim of this study is to provide interpretation of the flow and thermal transport physics. The influence of nonzero mean vibrational flow on the thermal convection from a surface with sinusoidal temperature distribution has never been investigated before. Conclusions may lead up to design of new heat removal applications.

**G1.00355 Maximum hydrogen production from genetically modified microalgae biomass<sup>1</sup>**, JOSE VARGAS, Florida State University, VANESSA KAVA, Universidade Federal do Paran, JUAN ORDONEZ, Florida State University — A transient mathematical model for managing microalgae derived H<sub>2</sub> production as a source of renewable energy is developed for a well stirred photobioreactor, PBR. The model allows for the determination of microalgae and H<sub>2</sub> mass fractions produced by the PBR in time. A Michaelis-Menten expression is proposed for modeling the rate of H<sub>2</sub> production, which introduces an expression to calculate the resulting effect on H<sub>2</sub> production rate after genetically modifying the microalgae. The indirect biophotolysis process was used. Therefore, an opportunity was found to optimize the aerobic to anaerobic stages time ratio of the cycle for maximum H<sub>2</sub> production rate, i.e., the process rhythm. A system thermodynamic optimization is conducted with the model equations to find accurately the optimal system operating rhythm for maximum H<sub>2</sub> production rate, and how wild and genetically modified species compare to each other. The maxima found are sharp, showing up to a ~60% variation in hydrogen production rate within 2 days around the optimal rhythm, which highlights the importance of system operation in such condition. Therefore, the model is expected to be useful for design, control and optimization of H<sub>2</sub> production.

<sup>1</sup>Brazilian National Council of Scientific and Technological Development, CNPq (project 482336/2012-9)

**G1.00356 Upper and Lower Concurrence Bounds of Entanglement Swapping of Two Bell-Diagonal States**, BRIAN KIRBY, SIDDHARTHA SANTRA, VLADIMIR MALINOVSKY, MICHAEL BRODSKY, U.S. Army Research Laboratory — Entanglement swapping is one of the basic operations of a quantum network. While the swapping is easily understood for fully entangled states, it is less well understood for partially mixed states. A particularly important class of mixed states which we will consider are the Bell-diagonal states, comprising a mixture of the pure Bell states. Bell-diagonal states are versatile as they can range from completely mixed to completely pure and from zero to perfect entanglement. Also Bell-diagonal states have well defined entanglement measures, such as concurrence. Therefore, an understanding of entanglement swapping with Bell-diagonal states is essential to quantum information processing and the realization of quantum networks. Here we rigorously treat the result of swapping of two, generally different, partially mixed, Bell-diagonal states and present numerical bounds on the its concurrence. In addition, we give an analytical solution for the concurrence of the state resulting from the swapping of two identical rank-two Bell-diagonal states in terms of the concurrence of the input states. Our results provide a simple method for analyzing the performance of quantum networks which utilize entanglement swapping of Bell-diagonal states.

**G1.00357 Degradation mechanism of a low band gap polymer PTB7 by oxidation**, SOOHYUNG PARK, JUNKYEONG JEONG, Yonsei University, HYUNBOK LEE, Kangwon National University, YEONJIN YI, Yonsei University — Recently, the PCE of OPVs is at the 10% mark by using donor materials having a low band gap, such as poly(4,8-bis[(2-ethylhexyl)oxy]benzo[1,2-b:4,5-b']dithiophene-2,6-diyl-alt-3-fluoro-2-[(2-ethylhexyl)carbonyl]thieno[3,4-b]thiophene-4,6-diyl) (PTB7) and its analogues. In spite of the significant PCE improvement, the lifetime issue still remains open problem. To solve these technical limitations fundamentally, the degradation mechanism should be understood. It can be revealed by investigating the electronic structures of polymers with controlled exposure of oxygen, moisture and light. In this study, ultraviolet, X-ray and inverse photoelectron spectroscopy measurements were performed with step-by-step exposure of controlled oxygen, moisture and light to investigate the degradation mechanism of each polymer film. Theoretical calculations using density functional theory (DFT) were also performed to understand detailed degradation process. From the experimental results, we demonstrate that push-pull polymers are more sensitive to environmental conditions, compared with non-push-pull (conventional) polymers such as poly(3-hexylthiophene-2,5-diyl) (P3HT). In addition, we show high photo-oxidation of PTB7 is originated from the structural reason.

**G1.00358 Large and high-quality single-crystal growth of cuprate superconductor Bi-2223 using the traveling-solvent floating-zone (TSFZ) method<sup>1</sup>**, SHINTARO ADACHI, TOMOHIRO USUI, KENTA KOSUGI, NAE SASAKI, Hirosaki University, KENTARO SATO, MASAKI FUJITA, Tohoku University, KAZUYOSHI YAMADA, KEK, Japan, TAKENORI FUJII, University of Tokyo, TAKAO WATANABE, Hirosaki University — In high superconducting transition temperature (high- $T_c$ ) cuprates, it is empirically known that  $T_c$  increases on increasing the number of CuO<sub>2</sub> planes in a unit cell  $n$  from 1 to 3. Bi-family cuprates are ideal for investigating the microscopic mechanism involved. However, it is difficult to grow tri-layered Bi-2223, probably owing to its narrow crystallization field. Here, we report improved crystal growth of this compound using the TSFZ method under conditions slightly different from those in an earlier report [J. Cryst. Growth 223, 175 (2001)]. A Bi-rich feed-rod composition of Bi<sub>2.2</sub>Sr<sub>1.9</sub>Ca<sub>2</sub>Cu<sub>3</sub>O<sub>y</sub> and a slightly oxygen-reduced atmosphere (mixed gas flow of O<sub>2</sub> (10%) and Ar (90%)) were adopted for the crystal growth. In addition, to increase the supersaturation of the melts, we applied a large temperature gradient along the solid-liquid interface by shielding a high-angle light beam using Al foil around the quartz tube. In this way, we succeeded in preparing large ( $2 \times 2 \times 0.05 \text{ mm}^3$ ) and high-quality (almost 100% pure) Bi-2223 single crystals.

<sup>1</sup>Hirosaki University Grant for Exploratory Research by Young Scientists and Newly-appointed Scientists

**G1.00359 Excitonic Lasing in Solution-Processed Subwavelength Nanosphere Assemblies.**<sup>1</sup>, KANNATASSEN APPAVOO, CFN, Brookhaven National Laboratory, XIAOZE LIU, VINOD MENON, Dept. of Physics, City College of New York, MATTHEW SFEIR, CFN, Brookhaven National Laboratory — Lasing in solution-processed nanomaterials has gained significant interest because of the potential for low-cost integrated photonic devices. Still, a key challenge is designing low-threshold lasing devices based on a comprehensive understanding of the system's spectral and temporal dynamics. Here we show low-threshold random lasing in sub-wavelength thin films of coupled, highly crystalline zinc oxide nanospheres, with an overall thickness on the order of  $\lambda/4$ . The cavity-free geometry consists of 35nm zinc oxide nanospheres that collectively localize the in-plane emissive light fields while minimizing scattering losses, resulting in excitonic lasing with fluence thresholds at least an order of magnitude lower than previous UV-blue random and quantum-dot lasers. Fluence-dependent effects, as quantified by sub-picosecond transient spectroscopy, highlight the role of phonon-mediated processes in excitonic lasing. Sub-picosecond evolution of distinct lasing modes, together with 3D electromagnetic simulations, indicate a random lasing process - in violation of the commonly cited criteria of strong scattering from individual nanostructures. These results show that coupled nanostructures with high crystallinity can function as building blocks for high-performance optoelectronics.

<sup>1</sup>Research is carried out at the Center for Functional Nanomaterials, Brookhaven National Laboratory, which is supported by the U.S.DOE (DE-AC02-98CH10886). This work is supported by the National Science Foundation through Grant No. DMR 1410249.

**G1.00360 Non-saturating magnetoresistance of  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$  thin films in pulsed magnetic fields up to 60T.**<sup>1</sup>, WEI NIU, MING GAO, XUEFENG WANG, Nanjing University — The mixed-valence manganite  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$  (LSMO) is an interesting material for spintronics due to its intrinsic magnetoresistance properties. In this work, high quality LSMO films with atomic terraces are epitaxially grown on  $\text{SrTiO}_3$  (100) substrates by laser molecular beam epitaxy. The magnetoresistance of LSMO thin films has been measured in pulsed magnetic fields up to 60T over a wide temperature range. Unsaturated magnetoresistances and resistance relaxation of LSMO thin films have been found at different temperatures. Unlike polycrystalline manganites, a linear increase with fields of the magnetoconductance at low temperature which is attributed to the spin-dependent tunneling via grain boundaries. However, the unsaturation magnetoresistances of our LSMO thin films at different temperature show two kinds of trends: quadratic at low temperature; quasi-linear at high temperature. We attribute the unsaturation behavior to the scattering of domain walls.

<sup>1</sup>National Laboratory of Solid State Microstructures, Collaborative Innovation Center of Advanced Microstructures, and School of Electronic Science and Engineering, Nanjing University, Nanjing 210093, China

**G1.00361 Superconductive density-of-states (DOS) depletion effect manifested in interlayer magnetotransport of overdoped Bi-2212**<sup>1</sup>, TOMOHIRO USUI, SHINTARO ADACHI, YUKI TERAMOTO, Hirosaki Univ., ITSUHIRO KAKEYA, Kyoto Univ., AKIHIRO KONDO, KOICHI KINDO, ISSP, Univ. of Tokyo, SHOJIRO KIMURA, Tohoku Univ., TAKAO WATANABE, Hirosaki Univ. — To determine the mechanism of high superconducting transition temperature (high- $T_c$ ) superconductivity, we must understand the relationship between the pseudogap (PG) and superconductivity. For this purpose, we measure the out-of-plane resistivity  $\rho_c(T, H)$  of an overdoped  $\text{Bi}_{1.6}\text{Pb}_{0.4}\text{Sr}_2\text{CaCu}_{1.96}\text{Fe}_{0.04}\text{O}_{8+\delta}$  (Bi-2212) single crystal under pulsed magnetic fields up to 60 T. Above  $T_c$ , magnetoconductivity (MC) is due to two positive components: one component rapidly increases with increasing fields but saturates at higher fields, and the other component gradually increases as  $H^2$ . The former decreases with increasing temperature and vanishes around the onset temperature of superconductive fluctuation  $T_{scf}$ . Thus, it is attributed to the superconductive DOS depletion effect. The latter is present both below and above  $T_{scf}$ . Thus, it is attributed to the PG effect. Subsequent analysis below  $T_c$  shows that the peak structure for  $\rho_c(T, H)$  is primarily due to the superconductive DOS depletion effect. This result supports the scenario that the PG results in high- $T_c$  superconductivity.

<sup>1</sup>Hirosaki University Grant for Exploratory Research by Young Scientists and Newly-appointed Scientists

**G1.00362 First-principles path-integral molecular dynamics study of diffusion process of hydrogen in face-centered cubic metals**, HAJIME KIMIZUKA, SHIGENOBU OGATA, Department of Mechanical Science and Bioengineering, Osaka University — We investigated the H diffusivity in face-centered cubic Pd and Al by performing path-integral molecular dynamics (PIMD) modeling in the framework of density functional theory (DFT); in our calculations, we took nuclear quantum effects into consideration. The DFT results showed that the H-migration barriers ( $E_m$ ) in Pd and Al exhibited similar values (approximately 0.16 eV), while the H atoms were stable at octahedral (O) sites for Pd and at tetrahedral (T) sites for Al. The PIMD-based free-energy profiles for H migration between the O-site and T-site were evaluated using the thermodynamic integration of the centroid forces at 150-600 K. We confirmed that the quantum effects significantly affected the  $E_m$  and the difference between the energies of the H atom at the O-site and the T-site ( $E_{O-T}$ ); The  $E_m$  and  $E_{O-T}$  values in Pd at 300 K *increased* by 32% and 98%, respectively, relative to the classical limit. On the other hand, the  $E_m$  and  $E_{T-O}$  (i.e.,  $-E_{O-T}$ ) values in Al at 300 K *decreased* by 3% and 41%, respectively. This suggested that the quantum nature of H nuclei was essential for understanding the H-diffusion kinetics in these metals even above ambient temperature.

**G1.00363 Nanoscale Properties and Stability Simulations of Alkali Activated Cement Phases from First Principle Calculations**, ONGUN OZCELIK, CLAIRE WHITE, Princeton University — Using first principle density functional calculations, we present the nanoscale properties of interactions, local bonds, charge distributions, mechanical properties and strength of alkali activated cement phases which are the most promising alternative to the ordinary Portland cement with a much lower cost to the environment. We present results on the stability and long term durability of various alkali activated cement structures, effects of external alkali agents on their properties and ways of utilizing them for further applications. We compare the calculated properties of alkali activated cement with those of ordinary Portland cement and contribute to the formation of long term durability data of these phases. Comparison with X-ray and neutron scattering experiment results are also provided via pair distribution functions extracted from simulation results.

**G1.00364 Investigation Into the Utilization of 3D Printing in Laser Cooling Experiments**, ERIC HAZLETT, Carleton College — With the advancement of 3D printing new opportunities are abound in many different fields, but with the balance between the precisions of atomic physics experiments and the material properties of current 3D printers the benefit of 3D printing technology needs to be investigated. We report on the progress of two investigations of 3D printing of benefit to atomic physics experiments: laser feedback module and the other being an optical chopper. The first investigation looks into creation of a 3D printed laser diode feedback module. This 3D printed module would allow for the quick realization of an external cavity diode laser that would have an adjustable cavity distance. We will report on the first tests of this system, by looking at Rb spectroscopy and mode-hop free tuning range as well as possibilities of using these lasers for MOT generation. We will also discuss our investigation into a 3D-printed optical chopper that utilizes an Arduino and a computer hard drive motor. By implementing an additional Arduino we create a low cost way to quickly measure laser beam waists

**G1.00365 Entanglement fidelity for elastic electron-electron scattering in a strongly coupled semiclassical plasmas under the influence of electric field**, BABATUNDE FALAYE, Ave Santa Barbara 145, Col Planetario Lindavista, Mexico D.F., C. P. 07730-CR -07051 — This study presents the effects of electric field, AB-flux field and uniform magnetic field directed along  $z$ -axis on electron-electron scattering encircled by a strongly coupled semiclassical plasmas. The all-inclusive effects result into a strongly repulsive system while the localizations of quantum levels change and the eigenvalues increase. We have employ perturbation formalism in our calculations. The condition  $|E_{nm}^{(0)}| \gg |E_{nm}^{(1)}| > |E_{nm}^{(2)}| > |E_{nm}^{(3)}| > \dots > |E_{nm}^{(n)}|$  holds. We find that, the combined effect of the fields is stronger than solitary effect and consequently, there is a substantial shift in the bound state energy of the system. We also find that to perpetuate a low-energy elastic electron-electron scattering in a strongly semiclassical plasmas, a strong electric field and a weak magnetic field are required where AB-flux field can be used as a regulator. The entanglement fidelity in the scattering process is also examined. We have used partial wave analysis to derive the entanglement fidelity. We find that for a low electric field intensity, the entanglement fidelity varies with projectile energy.

**G1.00366 “Multifractals in Transmission of Off-line & On-line E-Voting Systems”**<sup>1</sup>, WH- MAKSOED<sup>2</sup>, Prodi of Physics UI, Depok 16424- INDONESIA — An e-voting systems is a voting system in which the election data is recorded, stored & processed primarily as digital information. Those are 2 type of e-voting systems: off-line & on-line systems[Alaguvel & Gnanavel, 2013]. “Using transfer matrix method & multifractal theory, we studied the transmission properties of 1D generalized Fibonacci structures GF(m,n) in which m & n different intervals are integer according to a substitution rule[Yuannong Zhang, *et.al*:Multifractal properties of 1D quasi-period Photonic Crystal”. “Transmission spectra of 1D fractal multilayer structures are found to exhibit self-similar properties” says Zhukovsky & Lavrinenko in “Spectral self-similarity in fractal 1D photonic structures”, Photonics & Nanostructures, 2005 whereas Jacob Trevino, *et.al* studies ‘structural properties, photonic density of state & bandedge modes of Vogel spiral arrays of dielectric cylinders in air’.\_

<sup>1</sup>Acknowledgment to HE. Mr. AUGUST PARENGKUAN if accepts 1995-2005 Invoicing & Fulfillments to “KOMPAS” cq the Prodi of Physics ITB

<sup>2</sup>intended to devotes the SPIE Smain Femamm:”Texture classification approach based on 2D MULTIFRACTAL Analysis” coincides with Lusang Mining,Ltd & A.Ivanovich Mikoyan

**G1.00367 Comparison of clinical and paraclinical findings among patient with Kawasaki disease in Bandar abbas Koodakan Hospital in 2011-14**, DAVOOD BORJALI, None — Title: Comparison of clinical and paraclinical findings among patient with Kawasaki disease in Bandar abbas Koodakan Hospital in 2011-14 Kawasaki disease(KD) is a kind of vasculitis diagnosed by clinical manifestation and it caused acquired heart disease in children because of coronary arteries involvement. Method: patient divided to three group of American Japanese and incomplete and also study in two group according to fever days and then clinical features and laboratory data were checked. Result: A total of 150 patients were enrolled during the study period. number of patients with incomplete Kawasaki disease was 128 american group was 28 and Japanese was 4 patients, the most prevalent symptom was scaling of extremities(61bladder most seen in group with fever more than five days. Keyword: Kawasaki , epidemiology , criteria

**G1.00368 “OPTICAL CATALYTIC NANOMOTORS”**<sup>1</sup>, GLORY ROSARY-OYONG,SE<sup>2</sup>, Kompas-TV, Jl. Palmerah Selatan 1, Jakarta 10270- INDONESIA — D. Kagan, *et.al*, 2009:” a motion-based chemical sensing involving fuel-driven nanomotors is demonstrated. The new protocol relies on the use of an optical microscope for tracking charge in the speed of nanowire motors in the presence of target analyte”. Synthetic nanomotors are propelled by catalytic decomposition of .. they do not require external electric, magnetic or optical fields as energy..<pubs.acs.org/cen/science/83/i08/8308sci1.html>. Accompanying Fig 2.6( a ) of optical micrograph of a partial monolayer of silica microbeads [J.Gibbs, 2011 ] retrieves WF Paxton:”rods were characterized by transmission electron & dark-field optical microscopy.” & LF Valadares:”dimer due to the limited resolution of optical microscopy, however the result..’.

<sup>1</sup>Acknowledged to HE. Mr. Prof. SEDIONO M.P. TJONDRONEGORO

<sup>2</sup>Of Tanda Kehormatan Bintang GERILYA n:6801/v/1992:” ..atas jasa-jasanya yang luar biasa dengan menunjukkan keberanian,kebijaksanaan & kesetiaan..” to HerMajesty Miss Glory Rosary-OYONG,SE

**G1.00369 Probing voltage induced bond rupture in a molecular junction**<sup>1</sup>, HAIXING LI, Department of Applied Physics and Applied Mathematics, Columbia University, TIMOTHY SU, NATHANIEL KIM, Department of Chemistry, Columbia University, PIERRE DARANCET, Argonne National Laboratory Center for Nanoscale Materials, JAMES LEIGHTON, MICHAEL STEIGERWALD, COLIN NUCKOLLS, Department of Chemistry, Columbia University, LATHA VENKATARAMAN, Department of Applied Physics and Applied Mathematics, Columbia University — We use scanning tunneling microscope break junction to study electric field breakdown at the single molecule level. We investigate breakdown phenomena in atomic chains composed of Si—Si, Si—O, Si—C, Ge—Ge and C—C bonds that are commonly found in the low- $\kappa$  dielectric material. We see different bond rupture behaviors in a range of molecular backbones, and use the results from a statistically large number of measurements to determine which bond breaks. We find that Si—Si and Ge—Ge bonds rupture above a 1V bias. We also find that the Si—C bond is more robust than Si—O or Si—Si bond at above 1V. Finally, we illustrate how an additional conductance pathway in parallel to the Si—Si bond changes bond rupture behavior under an electric field. We carry out ab initio calculations on these systems and demonstrate that the mechanism for bond rupture under electric field involves “heating” of the molecule through electron-vibrational mode coupling.

<sup>1</sup>Haixing Li is supported by Semiconductor Research Corporation and New York CAIST program. We thank the NSF for the support of these studies under grant no. CHE-1404922.

**G1.00370 On the magnetic structure and band gap of the double perovskite Ba<sub>2</sub>CuOsO<sub>6</sub>: Density functional analysis**<sup>1</sup>, CHANGHOON LEE, JISOOK HONG, JI HOON SHIM, Pohang University of Science and Technology, MYUNG-HWAN WHANGBO, North Carolina State University — The ordered double-perovskite Ba<sub>2</sub>CuOsO<sub>6</sub>, consisting of 3d and 5d transition-metal magnetic ions (Cu<sup>2+</sup> and Os<sup>6+</sup>, respectively), is a magnetic insulator. It obeys the Curie-Weiss law with  $\theta = -13.3$  K. We evaluated the spin exchange interactions of Ba<sub>2</sub>CuOsO<sub>6</sub> by performing energy-mapping analysis based on DFT+U calculations and determined the band gap of Ba<sub>2</sub>CuOsO<sub>6</sub> by DFT+U and DFT+U+SOC calculations. The antiferromagnetic ordering of Ba<sub>2</sub>CuOsO<sub>6</sub> is due largely to the spin exchange interactions between Cu<sup>2+</sup> ions, which are enhanced by the empty eg orbitals of the intervening Os<sup>6+</sup> ions. Both electron correlation and spin-orbit coupling are necessary to open a band gap for Ba<sub>2</sub>CuOsO<sub>6</sub>.

<sup>1</sup>2013R1A1A2060341

**G1.00371 Local nature of impurity induced spin-orbit torques** , SERGEY NIKOLAEV, SPINTEC, Grenoble, France, ALAN KALITSOV, MINT Center, University of Alabama, AL, USA, MAIRBEC CHSHIEV, SPINTEC, Grenoble, France, OLEG MRYASOV, MINT Center, University of Alabama, AL, USA — Spin-orbit torques are of a great interest due to their potential applications for spin electronics. Generally, it originates from strong spin orbit coupling of heavy 4d/5d elements and its mechanism is usually attributed either to the Spin Hall effect or Rashba spin-orbit coupling. We have developed a quantum-mechanical approach based on the non-equilibrium Green's function formalism and tight binding Hamiltonian model to study spin-orbit torques and extended our theory for the case of extrinsic spin-orbit coupling induced by impurities. For the sake of simplicity, we consider a magnetic material on a two dimensional lattice with a single non-magnetic impurity. However, our model can be easily extended for three dimensional layered heterostructures. Based on our calculations, we present the detailed analysis of the origin of local spin-orbit torques and persistent charge currents around the impurity, that give rise to spin-orbit torques even in equilibrium and explain the existence of anisotropy.

**G1.00372 An Experimental and Modeled Comparison of Diffraction in Imaging Systems** , SPENCER KETCHUM, WILBERT SLOWMAN, MEGAN PACIARONI, Fort Lewis College — The resolution limit of imaging systems is always ultimately limited by diffraction. However, diffraction is often neglected in the analysis and design of both front and back illumination imaging systems in favor of the simpler ray tracing model. In many systems, paraxial optics provides a reasonable model for the design of systems with high resolution. This is certainly true for the majority of front-illuminated imaging systems; however, in back illuminated (shadowgraphic) imaging systems resolution is very strongly affected by diffraction. In this paper, we present a detailed experimental comparison of imaging resolution differences between front and back illuminated imaging systems for non-scattering and scattering environments. Additionally, modeling results of both systems are compared with the experimental results and classical optical theory. Preliminary results and calculations show that physical optics creates a stronger effect on resolution in back illuminated systems in either scattering or non-scattering environments.

**G1.00373 Emergent Magnetism in Mesoporous Materials<sup>1</sup>** , SHER ALAM, CHEP, and Collaborative Research with KEK, Japan, AJAYAN VINU, University of Queensland — We discuss the emergence of magnetism in Mesoporous Materials. We have obtained experimental results showing a variety of magnetic behaviors arising, by using different types of mesoporous or nanoporous templates. Since the templates allow different magnetic properties to arise naturally we have dubbed this as dynamic templating method. Our procedure and realization incidentally demonstrates the idea of Nanoarchitectonics proposed by Aono, as a MANA concept. Which, simply means to allow different nano-blocks to interact to obtain a certain desired structure and properties.

<sup>1</sup>Emergent Magnetism in Mesoporous Materials

**G1.00374 “Heavy-water Lattice and Heavy-Quark”<sup>1</sup>** , WH- MAKSOED,SSI<sup>2</sup>, Prodi of Physics UI, Depok 16424- INDONESIA — Refer to Birgitt Roettger-Roessler: **“Feelings at the Margins”**, 2014 retrieved the Vienna, 2006 UNIDO Research Programme: Combating Marginalization and Poverty through Industrial Development/COMPID. Also from Vienna, on Feb 18-22, 1963 reported Technical Report Series 20 about **“Heavy Water Lattice”** . Failed to relates scale-invariant properties of public-Debt growth to convergence in perturbation theory, sought JH Field: **“Convergence & Gauge Dependence Properties:..”**. Furthers, in GP Lepage: **“On the Viabilities of Lattice Perturbation Theory”**, 1992 stated: “in terms of physical quantities, like the heavy-quark potential, greatly enhanced the predictive power of lattice perturbation theory”.

<sup>1</sup>acknowledgements to HE. Mr. H. TUK SETYOHADI, Jl. Sriwijaya Raya 3, South-Jakarta, INDONESIA

<sup>2</sup>Ownership of Pasirtomo, northEast Jasinga Gold ore & PT. DAYA SADHANA BHAKTI devotes to Her Majesty Miss Dyah Adhi Wulandari/TRISAKTI University- Jakarta, INDONESIA

**G1.00375 Enhanced charge transport in highly conducting PEDOT-PSS films after acid treatment** , V. AKSHAYA SHIVA, RAVI BHATIA, REGHU MENON, Indian Inst of Science — The high electrical conductivity, good stability, high strength, flexibility and good transparency of poly(3,4-ethylenedioxythiophene)-poly(styrenesulfonate) (PEDOT-PSS), make it useful for many applications including polymeric anodes for organic photovoltaics, light-emitting diodes, flexible electrodes, supercapacitors, electrochromic devices, field-effect transistors and antistatic-coatings. However, the electrical conductivity of PEDOT-PSS has to be increased significantly for replacement of indium tin oxide (ITO) as the transparent electrode in optoelectronic devices. The as prepared (pristine) PEDOT-PSS film prepared from the PEDOT-PSS aqueous solution usually has conductivity below  $1\text{Scm}^{-1}$ , remarkably lower than ITO. Significant conductivity enhancement has been observed on transparent and conductive PEDOT-PSS films after a treatment with inorganic acids. Our study investigates the charge transport in pristine and  $\text{H}_2\text{SO}_4$ ,  $\text{HNO}_3$ ,  $\text{HCl}$  treated PEDOT-PSS films. We have treated the films with various concentrations of acids to probe the effect of the acid treatment on the conduction mechanism. The study includes the measurement of dc and electric field dependent conductivity of films in the temperature range of 4.2K-300K. We have also performed magneto-resistance measurements in the range of 0-5T. An enhancement by a factor of  $\sim 10^3$  has been observed in the room temperature conductivity. The detailed magneto-transport studies explain the various mechanisms for the conductivity enhancement observed.

**G1.00376 Rouse–Bueche Theory and The Calculation of The Monomeric Friction Coefficient in a Filled System.** , LUCA MARTINETTI, CHRISTOPHER MACOSKO, FRANK BATES, Univ of Minnesota - Twin Cities — According to flexible chain theories of viscoelasticity, all relaxation and retardation times of a polymer melt (hence, any dynamic property such as the diffusion coefficient) depend on the monomeric friction coefficient,  $\zeta_0$ , i.e. the average drag force per monomer per unit velocity encountered by a Gaussian submolecule moving through its free-draining surroundings. Direct experimental access to  $\zeta_0$  relies on the availability of a suitable polymer dynamics model. Thus far, no method has been suggested that is applicable to filled systems, such as filled rubbers or microphase-segregated A–B–A thermoplastic elastomers at temperatures where one of the blocks is glassy. Building upon the procedure proposed by Ferry for entangled and unfilled polymer melts, the Rouse–Bueche theory is applied to an undiluted triblock copolymer to extract  $\zeta_0$  from the linear viscoelastic behavior in the rubber-glass transition region, and to estimate the size of Gaussian submolecules. At iso-free volume conditions, the so-obtained matrix monomeric friction factor is consistent with the corresponding value for the homopolymer melt. In addition, the characteristic Rouse dimensions are in good agreement with independent estimates based on the Kratky–Porod worm-like chain model. These results seem to validate the proposed approach for estimating  $\zeta_0$  in a filled system. Although preliminary tested on a thermoplastic elastomer of the A–B–A type, the method may be extended and applied to filled homopolymers as well.

**G1.00377 Collective organization in aerotactic motion** , MARCO G. MAZZA, Max Planck Institute for Dynamics and Self-Organization — Some bacteria exhibit interesting behavior in the presence of an oxygen concentration. They perform an aerotactic motion along the gradient until they reach their optimal oxygen concentration. But they often organize collectively by forming dense regions, called bands, that travel towards the oxygen source. We have developed a model of swimmers with stochastic interaction rules moving in proximity of an air bubble. We perform molecular dynamics simulations and also solve advection-diffusion equations that reproduce the aerotactic behavior of mono-flagellated, facultative anaerobic bacteria. If the oxygen concentration in the system sinks locally below a threshold value, the formation of a migrating aerotactic band toward the bubble can be observed.

**G1.00378 Estimating topological properties of weighted networks from limited information<sup>1</sup>**, ANDREA GABRIELLI, Istituto dei Sistemi Complessi (ISC) - Consiglio Nazionale delle Ricerche (CNR), GIULIO CIMINI, IMT - Institute of Advanced Studies (Lucca, Italy), DIEGO GARLASCHELLI, Lorentz Institute, Leiden University (NL), ANGELO SQUARTINI, IMT - Institute of Advanced Studies (Lucca, Italy) — A typical problem met when studying complex systems is the limited information available on their topology, which hinders our understanding of their structural and dynamical properties. A paramount example is provided by financial networks, whose data are privacy protected. Yet, the estimation of systemic risk strongly depends on the detailed structure of the interbank network. The resulting challenge is that of using aggregate information to statistically reconstruct a network and correctly predict its higher-order properties. Standard approaches either generate unrealistically dense networks, or fail to reproduce the observed topology by assigning homogeneous link weights. Here we develop a reconstruction method, based on statistical mechanics concepts, that exploits the empirical link density in a highly non-trivial way. Technically, our approach consists in the preliminary estimation of node degrees from empirical node strengths and link density, followed by a maximum-entropy inference based on a combination of empirical strengths and estimated degrees. Our method is successfully tested on the international trade network and the interbank money market, and represents a valuable tool for gaining insights on privacy-protected or partially accessible systems.

<sup>1</sup>Acknowledgement to "Growthcom" ICT - EC project (Grant no: 611272) and "Crisislab" Italian Project

**G1.00379 ABSTRACT MOVED TO F43.013 —**

**Tuesday, March 15, 2016 1:00PM - 2:30PM —**

**Session G2 APS: Graduate School Fair Reception** Graduate School Fair Space/Exhibit Hall EF - Crystal Bailey, APS

**1:00PM G2.00001 Graduate School Reception** — Considering graduate school? Come by and meet with representatives from physics departments in a casual, low-key environment to learn about their programs and research opportunities. Don't miss out on this chance to learn more about grad school and to plan your next steps. Light refreshments will be provided.

**Tuesday, March 15, 2016 2:30PM - 5:30PM —**

**Session H1 DCMP: Hidden Order in URu<sub>2</sub>Si<sub>2</sub> Revealed by Advanced Spectroscopies** Ballroom I  
- John Mydosh, Kamerlingh Onnes Laboratorium and Instituut-Lorentz Universit

**2:30PM H1.00001 Chirality density wave of the "hidden order" phase in URu<sub>2</sub>Si<sub>2</sub><sup>1</sup>**, GIRSH BLUMBERG, Rutgers University — Many novel electronic ground states have been found to emerge from the hybridization between localized *d*- or *f*-electron states and conduction electron states in correlated electron materials. The heavy fermion compound URu<sub>2</sub>Si<sub>2</sub> exhibits the coexistence of two such ground states: so-called "hidden order" (HO) below T<sub>HO</sub> = 17.5 K and superconductivity below T<sub>c</sub> = 1.5 K. Despite 30 years of research the symmetry of the order parameter associated with HO phase below 17.5 K has remained ambiguous.

Here we report results of polarization resolved Raman spectroscopy study aimed to specify the symmetry of the low energy excitations above and below the HO transition. These excitations involve transitions between interacting heavy uranium *5f* orbitals, responsible for the broken symmetry in the HO phase. From the symmetry analysis of the collective mode, we determine that the HO parameter breaks local vertical and diagonal reflection symmetries at the uranium sites, resulting in crystal field states with distinct chiral properties, which order to a commensurate *chirality density wave* ground state [1]. We further explore the competition between the HO phase and large moment antiferromagnetic (LMAFM) phase [2], and the connection between the HO chirality density wave and the unconventional superconductivity which has recently been proposed to be of a chiral *d*-wave type [3].

1. H.H. Kung, R.E. Baumbach, E.D. Bauer, V.K. Thorsmølle, W.L. Zhang, K. Haule, J.A. Mydosh, and G. Blumberg. Chirality density wave of the 'hidden order' phase in URu<sub>2</sub>Si<sub>2</sub>. *Science*, **347**, 1339 (2015).
2. K. Haule and G. Kotliar. Complex Landau-Ginzburg theory of the hidden order in URu<sub>2</sub>Si<sub>2</sub>. *Eur. Phys. Lett.* **89**, 57006 (2010).
3. T. Yamashita et al. Colossal thermomagnetic response in the exotic superconductor URu<sub>2</sub>Si<sub>2</sub>. *Nature Phys.* **11**, 17 (2014).

<sup>1</sup>Work was performed in collaboration with H.-H. Kung, R. Baumbach, E. Bauer, K. Haule, M. B. Maple, and J. Mydosh. Research at Rutgers was supported by DOE BES Award DE-SC0005463 and by NSF under Awards NSF DMR-1104884.

**3:06PM H1.00002 Magneto-optical measurements as tests for time-reversal symmetry breaking in the hidden order and superconducting phases of URu<sub>2</sub>Si<sub>2</sub><sup>1</sup>**, AHARON KAPITULNIK<sup>2</sup>, Stanford University — It is now experimentally well established that the superconducting (SC) phase of URu<sub>2</sub>Si<sub>2</sub> with T<sub>c</sub> = 1.5 K emerges from the hidden order (HO) phase with T<sub>HO</sub> = 17.5 K. Thus, it is of great interest to discern the different symmetries of both phases. In particular, recent theoretical proposals for time-reversal symmetry breaking (TRSB) order parameters of either phases pose the question of whether the HO one drives the SC one, or TRSB appears in the SC phase independently. In this talk we report high resolution polar Kerr effect (PKE) measurements as a function of temperature for several high-quality single crystals of URu<sub>2</sub>Si<sub>2</sub>. We find an onset of PKE below the superconducting transition that is consistent with a TRS-breaking order parameter. This effect appears to be independent of an additional, possibly extrinsic, PKE generated in the hidden order phase, and contains structure below T<sub>c</sub> suggestive of additional physics within the superconducting state.

<sup>1</sup>Work supported by DOE.

<sup>2</sup>Work done in collaboration with E. R. Schemm, R. E. Baumbach, P. H. Tobash, F. Ronning, and E. D. Bauer.

**3:42PM H1.00003 Colossal thermomagnetic response in chiral *d*-wave superconductor URu<sub>2</sub>Si<sub>2</sub><sup>1</sup>**, YUJI MATSUDA, Department of Physics, Kyoto University, Kyoto, Japan — The heavy-fermion compound URu<sub>2</sub>Si<sub>2</sub> exhibits unconventional superconductivity at T<sub>c</sub> = 1.45 K deep inside the so-called hidden order phase. An intriguing aspect is that this system has been suggested to be a candidate of a chiral *d*-wave superconductor [1], and possible Weyl-type topological superconducting states have been discussed recently. Here we report on the observation of a highly unusual Nernst signal due to the superconducting fluctuations above T<sub>c</sub>. The Nernst coefficient is anomalously enhanced (by a factor of ~ 10<sup>6</sup>) as compared with the theoretically expected value of the Gaussian fluctuations. This colossal Nernst effect intimately reflects the highly unusual superconducting state of URu<sub>2</sub>Si<sub>2</sub>. The results invoke possible chiral or Berry-phase fluctuations associated with the broken time-reversal symmetry of the superconducting order parameter [2]. [1]Y. Kasahara et al. *Phys. Rev. Lett.* **99**, 116402 (2007). [2]T. Yamashita et al. *Nature Phys.* **11**, 17 (2015).

<sup>1</sup>In collaboration with T. Yamashita, Y. Shimoyama, H. Sumiyoshi (Kyoto), S. Fujimoto (Osaka), T. Shibauchi (Tokyo), Y. Haga (JAEA), T. D. Matsuda (TMU), Y. Onuki (Ryukyus), A. Levchenko (Wisconsin-Madison).

**4:18PM H1.00004 Evidence for preservation of crystallographic four-fold rotational symmetry in hidden order of  $\text{URu}_2\text{Si}_2$** <sup>1</sup>, HIROSHI AMITSUKA, Graduate School of Science, Hokkaido University — Recent experimental studies have suggested that the four-fold rotational symmetry around the tetragonal *c* axis is broken in the hidden-ordered state of  $\text{URu}_2\text{Si}_2$  below 17.5 K [1-5]. Those experimental findings give strong constraints on the theoretical arguments, and have provoked discussions on the electric/magnetic “nematic” ordering. However, the detected signals that suggest the broken symmetry are extremely weak in magnitude, and thus it is very important to test the reproducibility of the observations. Among the reported experiments, the orthorhombic distortion detected by X-ray diffraction is particularly important, because it may prove the broken rotational symmetry to be a thermodynamic phenomenon. We have performed synchrotron X-ray backscattering measurements of a high-quality single crystal with  $\text{RRR} > 350$  with the highest spatial resolution ever achieved. We will present the most reliable evidence for the preservation of crystallographic four-fold rotational symmetry in the hidden-order state. We will also present the tests for reproducibility of magnetic torque measurements, and discuss the intrinsic nature of  $\text{URu}_2\text{Si}_2$ . [1] R. Okazaki et al., Science 331, 439 (2011). [2] S. Tonegawa et al., Phys. Rev. Lett. 109, 036401 (2012). [3] S. Kambe et al., Phys. Rev. Lett. 110, 246406 (2013). [4] S. Tonegawa et al., Nat. Commun. 5, 4188 (2014). [5] S. C. Riggs et al., Nat. Commun. 6, 6425 (2015).

<sup>1</sup>This work was supported by JSPS KAKENHI Grant Number 25400346 and 15K05885 (J-Physics).

**4:54PM H1.00005 The Optical Phase Diagram of  $\text{URu}_2\text{Si}_2$ : Effects of Anisotropy, Charge Coherence and Fermi Surface Gapping**, RICARDO LOBO, ESPCI PSL, CNRS, UPMC —  $\text{URu}_2\text{Si}_2$  is a heavy fermion with a Kondo temperature of 370 K. Hybridization between heavy *f* electrons with conduction electrons creates a crossover to a Kondo liquid state having coherent transport properties below 70 K. At 17.5 K, a second-order mean-field transition creates an electronically ordered state, which clear origin remains unknown. The formation of an unconventional superconducting phase below 1.5 K completes the thermal phase diagram. The charged nature of this phase diagram, makes it a fertile ground for optical investigations. Here I discuss the optical properties of the hidden order, the Kondo coherent and the Kondo phases. On the *ab*-plane, an incoherent conductor exists at room temperature. Upon crossing into the Kondo coherent state, a sharp Drude peak develops and narrows quickly upon further cooling. Along the *c*-axis the Drude peak is present at all temperatures and is mostly insensitive to the formation of the coherent Kondo state. When entering the hidden order phase, a 6.5 meV gap opens. It follows a mean-field temperature dependence in the *ab*-plane but remains constant along the *c*-axis where it fills-up rather than close. In parallel, phonons are very sensitive to the Kondo coherence and couple strongly to the electronic continuum. The optical properties of  $\text{URu}_2\text{Si}_2$  shows a strongly anisotropic behavior between the *ab*-plane and the *c*-axis.

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**  
**Session H2 DCMP DMP GMAG: Emergent Topological Phenomena in Pyrochlore Iridates II**  
 Ballroom II - Zhi-Xun Shen, Stanford Univ

**2:30PM H2.00001 Metal-insulator transitions of bulk and domain-wall states in pyrochlore iridates.**, KENTARO UEDA, RIKEN CEMS — A family of pyrochlore iridates  $R_2\text{Ir}_2\text{O}_7$  offers an ideal platform to explore intriguing phases such as topological Mott insulator and Weyl semimetal [1]. Here we report transport and spectroscopic studies on the metal-insulator transition (MIT) induced by the modulations of effective electron correlation and magnetic structures, which is finely tuned by external pressure, chemical substitutions ( $R = \text{Nd}_{1-x}\text{Pr}_x$  and  $\text{Sm}_y\text{Nd}_{1-y}$ ), and magnetic field. A reentrant insulator-metal-insulator transition is observed near the paramagnetic insulator-metal phase boundary reminiscent of a first-order Mott transition for  $R = \text{Sm}_y\text{Nd}_{1-y}$  compounds ( $y \sim 0.8$ ). The metallic states on the magnetic domain walls (DWs), which are observed for  $R = \text{Nd}$  in real space [2] as well as in transport properties [3], is simultaneously turned into the insulating one. These findings imply that the DW electronic state is intimately linked to the bulk states. For the mixed  $R = \text{Nd}_{1-x}\text{Pr}_x$  compounds, the divergent behavior of resistivity with antiferromagnetic order is significantly suppressed by applying a magnetic field along [001] direction [4]. It is attributed to the phase transition from the antiferromagnetic insulating state to the novel Weyl (semi-)metal state accompanied by the change of magnetic structure. The present study combined with experiment and theory suggests that there are abundant exotic phases with physical parameters such as electron correlation and Ir-5*d* magnetic order pattern. Work performed in collaboration with J. Fujioka, B.-J. Yang, C. Terakura, N. Nagaosa, Y. Tokura (University of Tokyo, RIKEN CEMS), J. Shiogai, A. Tsukazaki, S. Nakamura, S. Awaji (Tohoku University). <sup>1</sup>This work was supported by JSPS FIRST Program and Grant-in-Aid for Scientific Research (Grants No. 80609488 and No. 24224009). [1] W. Witczak-Krempa, G. Chen, Y. B. Kim, and L. Balents, Annu. Rev. Condens. Matter Phys. 5, 57 (2014). [2] Eric Yue Ma, Yong-Tao Cui, Kentaro Ueda, Shujie Tang, Kai Chen, Nobumichi Tamura, Phillip M. Wu, Jun Fujioka, Yoshinori Tokura, and Zhi-Xun Shen, Science 350, 538 (2015). [3] K. Ueda, J. Fujioka, Y. Takahashi, T. Suzuki, S. Ishiwata, Y. Taguchi, M. Kawasaki, and Y. Tokura, Phys. Rev. B 89, 075127 (2014). [4] K. Ueda, J. Fujioka, B.-J. Yang, J. Shiogai, A. Tsukazaki, S. Nakamura, S. Awaji, N. Nagaosa, and Y. Tokura, Phys. Rev. Lett. 115, 056402 (2015).

**3:06PM H2.00002 Mobile metallic domain walls in an all-in-all-out magnetic insulator**<sup>1</sup>, ERIC YUE MA, Stanford Univ — Magnetic domain walls are boundaries between regions with different configurations of the same magnetic order. In a magnetic insulator where the magnetic order is tied to its bulk insulating property, it has been postulated that electrical properties are drastically different along the domain walls, where the order is inevitably disturbed. Here we report the discovery of highly conductive magnetic domain walls in a magnetic insulator  $\text{Nd}_2\text{Ir}_2\text{O}_7$ , which has an unusual all-in-all-out magnetic order, via transport and spatially resolved microwave impedance microscopy. The domain walls have a virtually temperature-independent sheet resistance (averaged over mesoscopic distances) of  $\sim 1$  kilohm per square, show smooth morphology with no preferred orientation, are free from pinning by disorders, and have strong thermal and magnetic field responses that agree with expectations for all-in-all-out magnetic order.

<sup>1</sup>This work is supported by funding from NSF, Moore Foundation, JSPS, NSFC and DOE

**3:42PM H2.00003 Topological Domain-Wall Metals in Pyrochlore Iridates**, YOUHEI YAMAJI, Quantum-Phase Electronics Center, The University of Tokyo — Emergent quantum phases [1-3] of pyrochlore iridium oxides  $R_2\text{Ir}_2\text{O}_7$  (*R*: rare-earth elements) have attracted a broad interest. Previous theoretical studies have predicted Weyl semimetals in non-collinear magnetic phases, called the all-in-all-out (AIAO) orders in  $\text{Y}_2\text{Ir}_2\text{O}_7$  [1]. The Weyl electrons are, however, easily annihilated in a pair [4]. Recently, we have predicted that magnetic domain walls in the AIAO phase of the pyrochlore iridium oxides host two-dimensional metallic states characterized by a zero-dimensional class A Chern number [5], even after the pair-annihilation of the Weyl electrons. By employing a symmetry adapted effective hamiltonian, we also predict a helical transport emerging from a spontaneous symmetry breaking at the magnetic domain wall as well as a subsequent metal-insulator transition [6]. [1] X. Wan, A. M. Turner, A. Vishwanath, and S. Y. Savrasov, Phys. Rev. B 83, 205101 (2011). [2] E.-G. Moon, C. Xu, Y. B. Kim, and L. Balents, Phys. Rev. Lett. 111, 206401 (2013). [3] I. F. Herbut and L. Janssen, Phys. Rev. Lett. 113, 106401 (2014). [4] K. Ueda, et al., Phys. Rev. Lett. 109, 136402 (2012). [5] Y. Yamaji and M. Imada, Phys. Rev. X 4, 021035 (2014). [6] Y. Yamaji and M. Imada, arXiv:1507.04153.

**4:18PM H2.00004 Exotic topological states near a quantum metal-insulator transition in pyrochlore iridates<sup>1</sup>**, ZHAOMING TIAN, huazhong University of Science and Technology — Pyrochlore iridates have attracted great interest as prime candidates that may host topologically nontrivial states, spin ice ordering and quantum spin liquid states, in particular through the interplay between different degrees of freedom, such as local moments and mobile electrons. Based on our extensive study using our high quality single crystals, we will discuss such examples, i.e. chiral spin liquid in a quadratic band touching state, Weyl semimetallic state and chiral domain wall transport nearby a quantum insulator-semimetal transition in pyrochlore iridates. References: [1] D. E. MacLaughlin et al Phys. Rev. B 92,054432 (2015) [2] Y. Machida et al, Nature 463 210 (2010) [3] T. Kondo et al, unpublished. [4] Z. Tian et al unpublished. [5] A. Sushkov et al. arXiv1507.01038 (2015) [6] Y. Yamaji et al, arXiv 1507.04153v1 (2015)

<sup>1</sup>This work is based on the collaboration with Nakatsuji Satoru, Kohama Yoshimitsu, Tomita Takahiro, Kindo Koichi, Jun J. Ishikawa, Balents Leon, Ishizuka Hiroaki, Timothy H. Hsieh. ZM. Tian was supported by JSPS Postdoctoral Fellowship (No.P1402)

**4:54PM H2.00005 Interplay of magnetic and electronic states in pyrochlore iridates**, LEON BALENTS, Kavli Institute for Theoretical Physics, UCSB — The pyrochlore iridates are a series of compounds undergoing antiferromagnetic ordering and metal-insulator transitions. They are of interest because they combine electron correlation effects and the potential for non-trivial band topology. We will discuss the theoretical picture of these materials, from electronic structure to magnetism and phase transitions, and how they may be controlled through applied fields and temperature. Comparison will be made between theory and recent experiments.

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**

**Session H3 DCMP GQI: Charge Noise Mitigation in Multiple Quantum Dot Qubits** Ballroom III - Thaddeus Ladd, Hrl Laboratories

**2:30PM H3.00001 Reduced sensitivity to charge noise in semiconductor spin qubits via symmetric operation**, MATTHEW REED, HRL Laboratories, LLC — Gated semiconductor quantum dots controlled with the exchange interaction are attractive candidates for quantum information processing because of their long coherence time and electrical controllability. Exchange is conventionally modulated by detuning the chemical potentials of neighboring dots over a fixed tunnel barrier, an approach whose precision is limited by charge noise. In this talk we demonstrate a "symmetric" mode of operation which substantially reduces the sensitivity of exchange operations to gate fluctuations. The method involves biasing a double-dot symmetrically between the charge-state anti-crossings, where the derivative of the exchange energy with respect to gate voltages is minimized. Exchange remains highly tunable by adjusting the tunnel coupling. We propose a metric, insensitivity, to quantify the techniques improvement and find that it increases by at least a factor of five between operating regimes. We also demonstrate a substantial increase in the number of Rabi fringes observed.

**3:06PM H3.00002 Symmetric operation and nuclear notch filtering in GaAs double quantum dots<sup>1</sup>**, FERDINAND KUEMMETH, Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen — Spin qubits based on few-electron semiconducting quantum dots are promising candidates for quantum computation, due to their potential for miniaturization, scalability and fault tolerance. In this talk I will present recent results on how to mitigate electrical and nuclear noise in GaAs singlet-triplet qubits.

The traditional way of implementing exchange rotations in singlet-triplet qubits involves detuning the qubit away from the symmetric (1,1) charge configuration, thereby temporarily hybridizing with the (0,2) charge state. Due to the large dipole coupling the resulting qubit oscillation suffers from detuning noise, motivating operation at sweet spots [1] or in the multi-electron regime [2]. Alternatively, exchange rotations can be implemented by symmetrically lowering the middle barrier. This method yields less relative exchange noise, significantly enhanced free induction decay times, and quality factors comparable to those reported in silicon quantum dot devices using similar techniques [3].

In order to decouple the singlet-triplet qubit from nuclear spin fluctuations, we investigate Carr-Purcell-Meiboom-Gill (CPMG) sequences in more detail. At high magnetic fields we find that qubit dephasing is limited by narrow-band high-frequency noise arising from Larmor precession of <sup>69</sup>Ga, <sup>71</sup>Ga, <sup>75</sup>As nuclear spins, similar to what has been observed at intermediate magnetic field [4]. By aligning the notches of the CPMG filter function with differences of the discrete nuclear Larmor frequencies we demonstrate a qubit coherence time of 0.87 ms, i.e. more than five orders of magnitude longer than the duration of a  $\pi$  exchange gate in the same device.

[1] O. E. Dial et al. Physical Review Letters 110, 146804 (2013). [2] A. P. Higginbotham et al, Phys Rev Lett 112, 026801 (2014). [3] M. D. Reed et al, arXiv:1508.01223 (2015). [4] H. Bluhm et al. Nature Physics 7, 109 (2011).

<sup>1</sup>Support through IARPA-MQCO, Army Research Office, and the Danish National Research Foundation is acknowledged.

**3:42PM H3.00003 Optimizing fidelities of quantum dot hybrid qubits<sup>1</sup>**, SUSAN COPPERSMITH, University of Wisconsin-Madison — The quantum dot hybrid qubit, which can be viewed as a hybrid between a spin and charge qubit, has an attractive combination of speed and fabrication simplicity. The initial experiments implementing this qubit yielded process fidelities of  $\sim 88\%$  [1] and  $\sim 93\%$  [2] for pulsed-gating and ac-gating, respectively. We present experimental evidence that these fidelities were limited by charge noise, and we present theoretical and experimental evidence that the sensitivity of qubit operations to charge noise can be reduced substantially by appropriate adjustment of the tunnel couplings. Our work indicates that, with suitable optimization, this qubit can achieve gate fidelities of well over 99%. [1] D. Kim et al., *Nature* **511**, 70 (2014). [2] D. Kim, et al., *npj Quant. Inf.* **1**, 15004 (2015).

<sup>1</sup>This work was supported in part by ARO (W911NF-12-0607), NSF (PHY-1104660), and ONR (N00014-15-1-0029).

**4:18PM H3.00004 Double sweet-spot operation of the resonant exchange qubit in three-electron quantum dots<sup>1</sup>**, GUIDO BURKARD, University of Konstanz, Germany — The resonant exchange (RX) qubit is a promising variant of the exchange-only spin qubit in a triple quantum dot which responds to a narrow-band resonant frequency. But the advantage of a permanently applied exchange splitting for spin control generally entails an increased susceptibility to charge noise. We have investigated the influence of electrical charge noise on a resonant exchange (RX) qubit by taking into account uncorrelated noise in each quantum dot, giving rise to two independent noisy bias parameters  $\varepsilon$  and  $\Delta$  [1]. Calculating the energy splitting of the two qubit states as a function of these two bias detuning parameters, we have identified sweet spots, where the qubit is least susceptible to noise. Our investigation shows that the sweet spots exist within the low-bias regime, in which the bias detuning parameters have the same magnitude as the hopping parameters between the dots. By calculating and comparing the charge dephasing rates at the various operating points of the RX qubit, we identify a new favorable operating regime for the RX qubit in the case of weak noise, based on these double sweet spots. In contrast, spin noise can be mitigated using exchange-based dynamical decoupling sequences that have been optimized using two different strategies, Uhrig dynamical decoupling (UDD) and optimized filter function dynamical decoupling (OFDD) [2]. Finally, we give a brief outlook towards the possibility of long-distance coupling between resonant exchange qubits mediated by a microwave cavity [3].

[1] M. Russ and G. Burkard, Phys. Rev. B **91**, 235411 (2015).

[2] N. Rohling and G. Burkard, arXiv:1510.04098.

[3] M. Russ and G. Burkard, Phys. Rev. B (accepted) [arXiv:1508.07122].

<sup>1</sup>Supported by DFG through SFB 767 and ARO through grant No. W911NF-15-1-0149.

**4:54PM H3.00005 Feedback-tuned, noise resilient gates for encoded spin qubits**, HENDRIK BLUHM, RWTH Aachen University — Spin 1/2 particles form native two level systems and thus lend themselves as a natural qubit implementation. However, encoding a single qubit in several spins entails benefits, such as reducing the resources necessary for qubit control and protection from certain decoherence channels. While several varieties of such encoded spin qubits have been implemented, accurate control remains challenging, and leakage out of the subspace of valid qubit states is a potential issue. Optimal performance typically requires large pulse amplitudes for fast control, which is prone to systematic errors and prohibits standard control approaches based on Rabi flopping. Furthermore, the exchange interaction typically used to electrically manipulate encoded spin qubits is inherently sensitive to charge noise. I will discuss all-electrical, high-fidelity single qubit operations for a spin qubit encoded in two electrons in a GaAs double quantum dot. Starting from a set of numerically optimized control pulses<sup>1</sup>, we employ an iterative tuning procedure based on measured error syndromes to remove systematic errors. Randomized benchmarking yields an average gate fidelity exceeding 98 % and a leakage rate into invalid states of 0.2 %. These gates exhibit a certain degree of resilience to both slow charge and nuclear spin fluctuations due to dynamical correction analogous to a spin echo. Furthermore, the numerical optimization minimizes the impact of fast charge noise. Both types of noise make relevant contributions to gate errors. The general approach is also adaptable to other qubit encodings and exchange based two-qubit gates<sup>2</sup>.

<sup>1</sup>Pascal Cerfontaine, Tim Botzem, David P. DiVincenzo, and Hendrik Bluhm, Phys. Rev. Lett. **113**, 150501 (2014)

<sup>2</sup>Sebastian Mehl, Hendrik Bluhm, and David P. DiVincenzo, Phys. Rev. B **90**, 045404 (2014)

## Tuesday, March 15, 2016 2:30PM - 5:30PM –

Session H4 DPOLY: Dillon Medal Symposium Ballroom IV - Darrin Pochan, University of Delaware

**2:30PM H4.00001 John H. Dillon Medal: Tapered Block Copolymers: Tuning Self-Assembly and Properties by Manipulating Monomer Segment Distributions**, THOMAS EPPS, Univ of Delaware — The self-assembly of block copolymers (BCPs) presents unique opportunities to design materials with attractive chemical and mechanical properties based on the ability of BCPs to form periodic structures with nanoscale domain spacings. One area of recent progress in our group focuses on the behavior of tapered BCPs in which the segment distribution at the interface between blocks is synthetically varied to tune morphology, domain density profiles, thermal transitions as well as mechanical and transport properties. Two application targets for these materials are lithium-ion conducting membranes for batteries and nanostructured thin films for nanotemplates and barrier membranes. In the first target area, we found that the taper volume fraction and composition allow us to manipulate the self-assembly of salt-doped BCPs in a well-defined manner that permits optimization of morphology and ion-content. Additionally, we found that the tapered interfaces influence the glass-transition behavior of the ion-conducting block leading to significant changes in lithium-ion transport (ion conductivity). In the second target area, we found the taper content alters the rate of self-assembly as well as the rate of island/hole formation (and ultimate island/hole size) upon thermal annealing. Additionally, using reflectivity techniques, we probed the domain density profiles as a function of taper composition and linked these profiles to changes in domain spacing and glass transition temperature. Overall, these studies show the versatility of tapering to provide a unique handle for simultaneously optimizing multiple materials properties.

**3:06PM H4.00002 Dodecagonal Quasicrystal Phase in a Diblock Copolymer Melt<sup>1</sup>**, FRANK BATES, TIMOTHY GILLARD, University of Minnesota, SANGWOO LEE, RPI — Recent experiments with low molecular weight asymmetric poly(isoprene-*b*-lactide) (PI-PLA) diblock copolymers have established an equilibrium Frank-Kasper  $\sigma$ -phase at compositions between 18 and 22 percent by volume PLA, which transforms to a BCC phase followed by disordering with increasing temperature. This presentation will describe synchrotron small-angle x-ray scattering and dynamic mechanical spectroscopy experiments conducted following rapid temperature quenches from the disordered state to temperatures associated with the  $\sigma$ -phase. We document the development of a long-lived dodecagonal quasicrystalline (DQC) phase that transforms with time into the associated quasicrystal approximate  $\sigma$ -phase at a rate that is highly temperature dependent. Remarkably, the DQC does not form from either the  $\sigma$ -phase or BCC state. These finding will be discussed in the context of an apparent spontaneous structural transition that occurs when the disordered melt is supercooled below a threshold temperature coincident with the BCC to  $\sigma$ -phase order-order transition temperature.

<sup>1</sup>Support provided by the National Science Foundation (1104368)

**3:18PM H4.00003 A Cool Way to Form High-Conductivity Two-Dimensional Polymers Using Ice**, MOON JEONG PARK, Pohang University of Science and Technology — Ice surfaces are used as removable hard templates to form two-dimensional polyaniline (PANI) nanosheets. Distinctly high current flows of 5.5 mA at 1 V and a high electrical conductivity of 35 S/cm were obtained for the PANI nanosheets, which marked a significant improvement from the literature values on other PANIs reported over the past decades. These improved electrical properties of ice-templated PANI nanosheets were attributed to the long-range ordered edge-on p-stacking of the quinoid ring, ascribed to the ice surface-assisted vertical growth of PANI. The unprecedented advantages of the ice-templated PANI nanosheets are two-fold. First, the PANI nanosheet can be easily transferred onto various types of substrates via float off from the ice surfaces. Second, PANI can be patterned into any shape using predetermined masks, and this is expected to facilitate the eventual convenient and inexpensive application of conducting polymers in versatile electronic device forms.

**3:30PM H4.00004 Molecular transport into and out of ionic-liquid filled block copolymer vesicles in water** , TIMOTHY LODGE, LETITIA YAO, SOONYONG SO, University of Minnesota — We have developed a method to prepare stable, size-controlled block copolymer vesicles that contain ionic liquid in the interior, but that are dispersed in water. Such nanoemulsions are of interest as nanoreactors, because the mass transfer and cost limitations of ionic liquids are circumvented. However, a crucial question is whether target molecules (*e.g.*, reagents and products) can enter and leave the vesicles, respectively, on a useful time scale (*i.e.*, seconds or shorter). In this talk we will briefly describe methods to prepare such vesicles with narrow size distributions, using poly(styrene)-*block*-poly(ethylene oxide) and poly(butadiene)-*block*-poly(ethylene oxide) copolymers of various compositions. We will then present results of pulsed-field gradient NMR measurements of probe diffusion that yield independent measurements of the entry and escape rates for selected small molecules, as a function of membrane thickness and temperature.

**3:42PM H4.00005 Influencing the structure of block copolymer micelles with small molecule additives** , MEGAN ROBERTSON, AVANTIKA SINGH, TYLER COOKSEY, University of Houston, BRYCE KIDD, RACHELE PIEMONTE, Virginia Tech, SHU WANG, KIM MAI LE, University of Houston, LOUIS MADSEN, Virginia Tech — Amphiphilic block copolymer micelles in water are under broad exploration for drug delivery applications due to their high loading capacity and targeted drug delivery. We aim to understand the kinetic and thermodynamic processes that underlie the self-assembly of diblock copolymer micelle systems. The present work focuses on diblock copolymers containing poly(ethylene oxide) (a hydrophilic polymer) and polycaprolactone (a hydrophobic polymer), which spontaneously self-assemble into spherical micelles in water. Addition of a common good solvent (a co-solvent) for both of the constituting blocks, such as tetrahydrofuran (THF), reduces the interfacial tension at the core-corona interface. We are currently investigating the effect of this phenomenon on the micelle structural properties, using small-angle scattering and nuclear magnetic resonance. We have characterized the hydrodynamic radius, core radius, corona thickness, aggregation number, degree of swelling of the micelle core with the co-solvent, and unimer (free chain) concentration, as a function of the co-solvent concentration. Fundamental knowledge from these studies will inform design of drug delivery systems by allowing us to tailor micelle properties for optimal cargo loading.

**3:54PM H4.00006 Computationally Guided Design of Polymer Electrolytes for Battery Applications** , ZHEN-GANG WANG, MICHAEL WEBB, BRETT SAVOIE, THOMAS MILLER, California Institute of Technology — We develop an efficient computational framework for guiding the design of polymer electrolytes for Li battery applications. Short-times molecular dynamics (MD) simulations are employed to identify key structural and dynamic features in the solvation and motion of Li ions, such as the structure of the solvation shells, the spatial distribution of solvation sites, and the polymer segmental mobility. Comparative studies on six polyester-based polymers and polyethylene oxide (PEO) yield good agreement with experimental data on the ion conductivities, and reveal significant differences in the ion diffusion mechanism between PEO and the polyesters. The molecular insights from the MD simulations are used to build a chemically specific coarse-grained model in the spirit of the dynamic bond percolation model of Druger, Ratner and Nitzan. We apply this coarse-grained model to characterize Li ion diffusion in several existing and yet-to-be synthesized polyethers that differ by oxygen content and backbone stiffness. Good agreement is obtained between the predictions of the coarse-grained model and long-timescale atomistic MD simulations, thus providing validation of the model. Our study predicts higher Li ion diffusivity in poly(trimethylene oxide-*alt*-ethylene oxide) than in PEO. These results demonstrate the potential of this computational framework for rapid screening of new polymer electrolytes based on ion diffusivity.

**4:06PM H4.00007 Theory and Simulations of Tapered Diblock Polymers<sup>1</sup>** , LISA M. HALL, YOUNGMI SEO, JONATHAN R. BROWN, The Ohio State University — We study tapered block polymers, AB diblock polymers with a gradient region inserted between the pure A and B blocks such that composition smoothly transitions from A to B (or B to A in the case of inverse tapers). Phase diagrams were created using self consistent field theory (SCFT), and coarse-grained molecular dynamics (MD) simulations were used to study polymer conformations and diffusion, including diffusion of monomer-sized penetrants preferentially dissolved in one of the phases. As has been observed experimentally, we find that tapering makes the A and B blocks more miscible, decreasing domain spacing and shifting the order to disorder transition to lower temperatures. We predict a widening of the bicontinuous double gyroid region of the phase diagram for moderate length normal tapers versus diblocks, suggesting taper length can be used as a control parameter to obtain network phases even at high molecular weight, as may be desirable in transport applications. Additionally, in some inverse tapered systems, SCFT predicts phases not present in the standard AB diblock phase diagram, and MD simulations show how the chains fold back and forth across the interface. In these inverse tapered polymers, as segregation strength is increased, the competing effects of folding and stretching produces lamellae that have domain spacing nearly independent of temperature. We also find that diffusion of penetrants in normal tapers is significantly faster than that in inverse tapers, which is likely related to their unusual conformations.

<sup>1</sup>This material is based upon work supported by DOE Grant SC0014209.

**4:18PM H4.00008 High-Tg Polynorbornene-Based Block and Random Copolymers for Butanol Pervaporation Membranes** , RICHARD A. REGISTER, DONG-GYUN KIM, Princeton University, TAMAMI TAKIGAWA, TOMOMASA KASHINO, OLEKSANDR BURTOVYY, ANDREW BELL, Promerus LLC — Vinyl addition polymers of substituted norbornene (NB) monomers possess desirably high glass transition temperatures (T<sub>g</sub>); however, until very recently, the lack of an applicable living polymerization chemistry has precluded the synthesis of such polymers with controlled architecture, or copolymers with controlled sequence distribution. We have recently synthesized block and random copolymers of NB monomers bearing hydroxyhexafluoroisopropyl and n-butyl substituents (HFANB and BuNB) via living vinyl addition polymerization with Pd-based catalysts. Both series of polymers were cast into the selective skin layers of thin film composite (TFC) membranes, and these organophilic membranes investigated for the isolation of n-butanol from dilute aqueous solution (model fermentation broth) via pervaporation. The block copolymers show well-defined microphase-separated morphologies, both in bulk and as the selective skin layers on TFC membranes, while the random copolymers are homogeneous. Both block and random vinyl addition copolymers are effective as n-butanol pervaporation membranes, with the block copolymers showing a better flux-selectivity balance. While polyHFANB has much higher permeability and n-butanol selectivity than polyBuNB, incorporating BuNB units into the polymer (in either a block or random sequence) limits the swelling of the polyHFANB and thereby improves the n-butanol pervaporation selectivity.

**4:30PM H4.00009 Glassy Structural Trapping in Soft Multi-Face Colloids** , RODNEY PRIESTLEY, Princeton University — Nanoparticles with soft, heterogeneously patterned surfaces often exhibit unique, multi-functional behaviors in response to environmental stimuli. The soft, polymeric nature of the particle surface, moreover, allows for the tailoring of both surface architecture and chemical composition towards particular applications. We have recently demonstrated that Precipitation-Induced Self Assembly (PISA) can be used to form soft Janus colloids as well as multi-faceted colloids in a scalable approach in which many colloidal characteristics can be controlled independently. Here, we present evidence not only of kinetic trapping in the formation of rapidly precipitated, multi-surface polymer particles; but also delineate the role of polymer vitrification in the determination of multi-faceted particle structures.

**4:42PM H4.00010 Effect of Protein Supercharging on Interaction with Polyelectrolytes**, BRADLEY OLSEN, ALLIE OBERMEYER, CAROLYN MILLS, XUEHUI DONG, MIT — Complexation of proteins with polyelectrolytes can lead to a liquid-liquid phase separation to generate a viscous complex coacervate phase rich in protein and polyelectrolyte. However, many proteins do not readily coacervate at conditions near neutral pH and physiological ionic strength. Here, protein supercharging is used to systematically explore the effect of protein charge on the complex coacervation with polycations. Four model proteins were chemically modified to generate a panel of proteins with varying surface charge, with both the average charge and charge distribution quantified by mass spectrometry. Proteins phase separated with the qP4VP and qPDMAEMA polycations when the ratio of negatively charged residues to positively charged residues was greater than 1.1-1.2. Efficient partitioning of the protein into the coacervate phase required larger charge ratio (1.5-2.0). The model proteins were also encapsulated in complex coacervate core micelles. Dynamic light scattering was used to assess the formation of micelles with PEOGMA-*b*-qP4VP and revealed micellar hydrodynamic radii of approximately 25-30 nm. Small angle neutron scattering and transmission electron microscopy were used to confirm the formation of spherical micelles.

**4:54PM H4.00011 Self-assembly of Open-Shell-containing Block Polymer Thin Films**, BRYAN BOUDOURIS, LIZBETH ROSTRO, ADITYA BARADWAJ, JENNIFER LASTER, Purdue University — Radical polymers, where a stable open-shell group is present on each repeat unit of a non-conjugated macromolecular backbone, are emerging as promising materials in organic electronic and magnetic applications. As such, designing molecular motifs that allow for the self-assembly of these open-shell species into nanostructured domains could be beneficial in a host of next-generation flexible electronic applications. In addition, the relatively flexible nature of their macromolecular backbone and ability to conduct charge in the amorphous state offer distinct advantages regarding their self-assembly relative to block polymers based on conjugated semiconducting polymers. Here, we demonstrate the controlled synthesis and self-assembly of diblock copolymers containing radical polymer moieties. In fact, we show that A-B diblock copolymers, where the A moiety contains nitroxide radical functionalities and the B moiety is a closed-shell, low glass transition temperature polymer, self-assemble into ordered structures with domain spacing values that are consistent with common coil-coil diblock copolymers ( $d = 30$  nm). In this way, we present a means by which to readily generate electronically-active macromolecules that self-assemble into nanostructured thin films with controlled morphologies over long ranges.

**5:06PM H4.00012 Direct Immersion Annealing of Block Copolymer Thin Films**, ALAMGIR KARIM<sup>1</sup>, University of Akron — We demonstrate ordering of thin block copolymer (BCP) films via direct immersion annealing (DIA) at enhanced rate leading to stable morphologies. The BCP films are immersed in carefully selected mixtures of good and marginal solvents that can impart enhanced polymer mobility, while inhibiting film dissolution. DIA is compatible with roll-to-roll assembly manufacturing and has distinct advantages over conventional thermal annealing and batch processing solvent-vapor annealing methods. We identify three solvent composition-dependent BCP film ordering regimes in DIA for the weakly interacting polystyrene-poly(methyl methacrylate) (PS-PMMA) system: rapid short range order, optimal long-range order, and a film instability regime. Kinetic studies in the “optimal long-range order” processing regime as a function of temperature indicate a significant reduction of activation energy for BCP grain growth compared to oven annealing at conventional temperatures. An attractive feature of DIA is its robustness to ordering other BCP (e.g. PS-P2VP) and PS-PMMA systems exhibiting spherical, lamellar and cylindrical ordering. Inclusion of nanoparticles in these films at high concentrations and fast ordering kinetics study with neutron reflectivity and SANS will be discussed.

<sup>1</sup>This is (late) Contributed Talk Abstract for Dillon Medal Symposium at DPOLY - discussed with DPOLY Chair Dvora Perahia

**5:18PM H4.00013 Functional Thin Films from Aligned Block Copolymers and Blends**, BRYAN VOGT, ZHE QIANG, KEVIN CAVICCHI, Univ of Akron — Block copolymer (BCP) self-assembly provides a simple, cost effective route to fabricating nanoscale patterns. Here we describe how we can modulate the alignment/orientation of BCP films using a modified solvent vapor annealing (SVA) method where the BCP is covered with an elastomer during SVA and controlled deswelling of the elastomer macroscopically produces a shear force that aligns the BCP domains. By proper selection of the BCP or BCP + functional precursors, functional nanopatterns can be obtained. Thin films of cylindrical forming polystyrene-block-polydimethylsiloxane (PS-*b*-PDMS) are shear aligned. High temperature calcination converts the PDMS to silica and removes the PS to yield the silica nanolines. The spacing of these features is effectively halved by the use of bilayer films. Sequential shear-alignment of two distinct layers can generate arbitrary line based nanostructured features such as a rhombic array, but the size of the features is defined by the BCP. Oligomeric phenolic resin can effectively modulate the size and morphology of amphiphilic BCPs even at high loadings ( $\geq 70$  wt

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**  
**Session H5 GMAG DMP: Frustrated Magnetism: Spin Liquids in 2D** 301 - Arun Paramekanti, University of Toronto

**2:30PM H5.00001 Paired states of Chern-Simons fermions in quantum spin models**, ANDREW ALLOCCA, Univ of Maryland-College Park, TIGRAN SEDRAKYAN, Fine Theoretical Physics Institute, Univ of Minnesota and Physics Frontier Center, Joint Quantum Institute, Univ of Maryland, VICTOR GALITSKI, Univ of Maryland-College Park — We consider exotic states constructed from the two-dimensional quantum spin-1/2 XY model on the square and hexagonal lattices. By applying a Chern-Simons transformation we represent the quantum spin model as a system of spinless fermions interacting via attached fluxes. The interaction is then decoupled in the Cooper and excitonic channels giving possible unconventional states of Chern-Simons fermions. We examine the mean field properties of these states and their relations to the original spin model.

**2:42PM H5.00002 Symmetry fractionalization of visons in Z<sub>2</sub> spin liquids**, YANG QI, Perimeter Institute for Theoretical Physics, MENG CHENG, Station Q, Microsoft Research, CHEN FANG, Massachusetts Institute of Technology — In this work we study symmetry fractionalization of vison excitations in topological Z<sub>2</sub> spin liquids. We show that in the presence of the full SO(3) spin-rotational symmetry and if there is an odd number of spin- $\frac{1}{2}$  per unit cell, the symmetry fractionalization of visons is completely fixed. On the other hand, visons can have different classes of symmetry fractionalization if the spin-rotational symmetry is reduced. As a concrete example, we show that visons in the Balents-Fisher-Girvin Z<sub>2</sub> spin liquid have crystal symmetry fractionalization classes which are not allowed in SO(3) symmetric spin liquids, due to the reduced spin-rotational symmetry.

**2:54PM H5.00003 Haldane-Hubbard Mott Insulator: From Tetrahedral Spin Crystal to Chiral Spin Liquid**, CIARAN HICKEY, University of Toronto, LUKASZ CINICIO, Perimeter Institute for Theoretical Physics, ZLATKO PAPIC, University of Leeds, ARUN PARAMAKANTI, University of Toronto — Motivated by recent experimental realizations of artificial gauge fields in ultracold atoms, we study the honeycomb lattice Haldane-Hubbard Mott insulator of spin-1/2 fermions using exact diagonalization and density matrix renormalization group methods. We show that this model exhibits various chiral magnetic orders including a wide regime of triple-Q tetrahedral order. Incorporating third-neighbor hopping frustrates and ultimately melts this tetrahedral spin crystal. From analyzing low energy spectra, many-body Chern numbers, entanglement spectra, and modular matrices, we identify the molten state as a chiral spin liquid with gapped semion excitations.

**3:06PM H5.00004 Unification of bosonic and fermionic  $Z_2$  spin liquids on a rectangular lattice**, SHUBHAYU CHATTERJEE, JULIA STEINBERG, SUBIR SACHDEV, Harvard University — Recent theories [1] have postulated the presence of a fractionalized Fermi liquid ( $FL^*$ ) in the pseudogap metal phase of cuprates. The  $FL^*$  phase can be described as a spin liquid co-existing with fermionic charge carrying quasiparticles. Underdoped cuprates also show a variety of competing orders, including nematic order which reduce the  $C_4$  symmetry of the square lattice to  $C_2$ . Motivated by this, we classify mean-field bosonic spin liquids on a rectangular lattice using projective symmetry groups (PSG) [2], and find equivalent descriptions in terms of fermionic partons [3]. In particular, we find a fermionic spin liquid ansatz corresponding to a bosonic  $Z_2$  spin liquid with favorable mean field energy [4]. The fermionic ansatz might be useful to investigate the transition from a  $FL^*$  to a fermi liquid. [1]. Density-wave instabilities of fractionalized Fermi liquids: D. Chowdhury and S. Sachdev, PRB 90, 245136 (2014) [2] Quantum orders and symmetric spin liquids: XG Wen, PRB 65 (16), 165113 (2002) [3] Unification of bosonic and fermionic theories of spin liquids on the kagome lattice: Y-M. Lu, G. Y. Cho, A. Vishwanath, arXiv:1403.0575 [4] Large-N expansion for frustrated quantum antiferromagnets: N. Read and S. Sachdev, PRL 66, 1773 (1991)

**3:18PM H5.00005 Coupled wire construction of chiral spin liquids<sup>1</sup>**, RONNY THOMALE, Univ of Wuerzburg, TOBIAS MENG, TU Dresden, TITUS NEUPERT, PCTS, Princeton University, MARTIN GREITER, Univ of Wuerzburg — We develop a coupled wire construction of chiral spin liquids. The starting point are individual wires of electrons in the Mott regime that are subject to a Zeeman field and Rashba spin-orbit coupling. Suitable spin-flip couplings between the wires yield an Abelian chiral spin liquid state which supports spinon excitations above a bulk gap, and chiral edge states. The approach generalizes to non-Abelian chiral spin liquids at level k with parafermionic edge states.

<sup>1</sup>RT is supported by the European Research Council through ERC-StG-336012-TOPOLECTRICS. MG and RT are supported by DFG-SFB 1170.

**3:30PM H5.00006 Variational Monte Carlo study of chiral spin liquid in quantum antiferromagnet on the triangular lattice**, WENJUN HU, Rice University, SHOUSHU GONG, Florida State University, DONNA SHENG, California State University, Northridge, DONNA SHENG TEAM — We investigate the Heisenberg model with chiral coupling on the triangular lattice by using Gutzwiller projected fermionic states and the variational Monte Carlo technique. As the chiral coupling grows, a gapped spin liquid with non-trivial magnetic fluxes and nonzero chiral order is stabilized. Furthermore, we calculate the topological Chern number and the degeneracy of the ground state, both of which lead us to identify this flux state as the chiral spin liquid with  $C = 1/2$  fractionalized Chern number. Finally, we add spatial anisotropy in the model to study the effects for the chiral order.

**3:42PM H5.00007 Valence-bond-solid domain walls in a 2D quantum magnet<sup>1</sup>**, HUI SHAO, Beijing Computational Science Research Center, WENAN GUO, Beijing Normal University, ANDERS SANDVIK, Boston University — sing quantum Monte Carlo simulations, we study properties of domain walls in a square-lattice  $S=1/2$  Heisenberg model with additional interactions which can drive the system from an antiferromagnetic (AFM) ground state to a valence-bond solid (VBS). We study the finite-size scaling of the domain-wall energy at the putative "deconfined" critical AFM-VBS point, which gives access to the critical exponent governing the domain-wall width. This length-scale diverges faster than the correlation length and also is related to the scale of spinon deconfinement. Our results show additional evidence of deconfined quantum criticality and are compatible with critical exponents extracted from finite-size scaling of other quantities.

<sup>1</sup>NSFC Grant No. 11175018, NSF Grant No. DMR-1410126

**3:54PM H5.00008 Field-induced magnetization jumps and quantum criticality in the 2D J-Q model<sup>1</sup>**, ADAM IAIZZI, ANDERS SANDVIK, Boston Univ — The J-Q model is a 'designer hamiltonian' formed by adding a four spin 'Q' term to the standard antiferromagnetic  $S = 1/2$  Heisenberg model. The Q term drives a quantum phase transition to a valence-bond solid (VBS) state: a non-magnetic state with a pattern of local singlets which breaks lattice symmetries. The elementary excitations of the VBS are triplons, i.e. gapped  $S=1$  quasiparticles. There is considerable interest in the quantum phase transition between the Néel and VBS states as an example of deconfined quantum criticality. Near the phase boundary, triplons deconfine into pairs of bosonic spin-1/2 excitations known as spinons. Using exact diagonalization and the stochastic series expansion quantum monte carlo method, we study the 2D J-Q model in the presence of an external magnetic field. We use the field to force a nonzero density of magnetic excitations at  $T=0$  and look for signatures of Bose-Einstein condensation of spinons. At higher magnetic fields, there is a jump in the induced magnetization caused by the onset of an effective attractive interaction between magnons on a ferromagnetic background. We characterize the first order quantum phase transition and determine the minimum value of the coupling ratio  $q \equiv Q/J$  required to produce this jump.

<sup>1</sup>Funded by NSF DMR-1410126

**4:06PM H5.00009 Chiral phase of a simple two-dimensional spin-1 quantum magnet<sup>1</sup>**, OLEG STARYKH, University of Utah, ZHENTAO WANG, Rice University, CRISTIAN D. BATISTA, T-Division and CNLS, Los Alamos National Laboratory — We investigate the evolution of the ground state of a simple spin-1 antiferromagnet with easy-axis single-ion anisotropy  $D(S^z)^2$ , with  $D < 0$ , on a two-dimensional triangular lattice. The ground state changes from a quantum paramagnet one, at sufficiently large  $|D|$ , to a magnetically ordered  $120^\circ$  one at small  $D \sim 0$ . Besides breaking the continuous  $U(1)$  symmetry of global spin rotations along the  $z$ -axis, this non-collinear ordering also breaks the discrete  $Z_2$  chiral symmetry, which raises the possibility of an intermediate chiral spin liquid state, spontaneously breaking spatial inversion and mirror symmetries. We show that this interesting novel state indeed appears as a result of the condensation of bound  $\langle S_n^+ S_m^- - S_n^- S_m^+ \rangle$  pairs. The resulting Ising-like nematic state supports a regular pattern of spin currents on the bonds of the triangular lattice. It represents quantum analogue of the classical chiral spin liquid proposed by Villain in 1977.

<sup>1</sup>Supported by NSF DMR-1507054

**4:18PM H5.00010 Critical scaling corrections in 2D dimerized antiferromagnets<sup>1</sup>**, NUSEN MA, Boston University, Sun Yat-sen University, HUI SHAO, Beijing Computational Science Center, Boston University, DAO-XIN YAO, Sun Yat-sen University, ANDERS SANDVIK, Boston University — 2D dimerized antiferromagnets can be driven through a quantum-critical point by tuning the ratio  $g = J_2/J_1$  between inter- and intra-dimer couplings. It has been shown [1] that the systems fall into two classes, depending on whether or not a certain bond-inversion symmetry is present in the dimer pattern. The two classes should have the same leading critical exponents but different exponents controlling the scaling corrections. We here investigate the scaling corrections using quantum Monte Carlo simulations for several different dimerization patterns. We will discuss systematic methods to extract the scaling corrections in the thermodynamic limit.

[1]L. Fritz, R. L. Doretto, S. Wessel, S. Wenzel, S. Burdin, and M. Vojta, Phys. Rev. B 83, 174416 (2011).

<sup>1</sup>Supported by NSF DMR-1410126, NSFC-11574404 11275279, and NBRPC-2012CB821400

**4:30PM H5.00011 Novel spin liquid with a gapped Fermi surface in the kagome Kondo-lattice model**, GIA-WEI CHERN, University of Virginia, ZHENTAO WANG, Rice University, KIPTON BARROS, Los Alamos National Laboratory — Geometrical frustration in the Kagome lattice is well known as a source of many exotic phases. Here we study the under-screened Kondo-lattice model (KLM) on the kagome lattice at large electron-spin coupling, a regime in which perturbative approaches such as RKKY are invalid. We employ a recently developed linear-scaling, dynamical sampling method to study the KLM on large kagome lattices. At low temperatures, our simulations uncover an intriguing classical spin liquid phase with short-range correlations. Surprisingly, when  $T \rightarrow 0$  a wide gap in the electronic spectrum can appear at any filling fraction between 0.5 to 0.63. We characterize this new spin liquid and discuss the origin of spontaneous gap formation.

**4:42PM H5.00012 A tensor product state approach to spin-1/2 square J1-J2 antiferromagnetic Heisenberg model: evidence for deconfined quantum criticality**<sup>1</sup>, LING WANG, Beijing Computational Science Research Center, ZHENG-CHENG GU, Perimeter Institute, FRANK VERSTRAËTE, University of Vienna, XIANG-GANG WEN, Massachusetts Institute of Technology — We study this model using the cluster update algorithm for tensor product states (TPSs). We find that the ground state energies at finite sizes and in the thermodynamic limit are in good agreement with the exact diagonalization study. At the largest bond dimension available  $D = 9$  and through finite size scaling of the magnetization order near the transition point, we accurately determine the critical point  $J_2^{c1} = 0.53(1)J_1$  and the critical exponents  $\beta = 0.50(4)$ . In the intermediate region we find a paramagnetic ground state without any static valence bond solid (VBS) order, supported by an exponentially decaying spin-spin correlation while a power law decaying dimer-dimer correlation. By fitting a universal scaling function for the spin-spin correlation we find the critical exponents  $\nu = 0.68(3)$  and  $\eta_s = 0.34(6)$ , which is very close to the observed critical exponents for deconfined quantum critical point (DQCP) in other systems. Thus our numerical results strongly suggest a Landau forbidden phase transition from Neel order to VBS order at  $J_2^{c1} = 0.53(1)J_1$ .

<sup>1</sup>This project is supported by the EU Strep project QUEVADIS, the ERC grant QUERG, and the FWF SFB grants FoQuS and ViCoM; and the Institute for Quantum Information and Matter

**4:54PM H5.00013 Magnetic fluctuations and dynamics in the vicinity of quantum spin liquids: Cluster dynamical mean-field study of the Kitaev model**, JUNKI YOSHITAKE, Dept. of Appl. Phys., Univ. of Tokyo, JOJI NASU, Dept. of Phys., Tokyo Inst. Tech., YUKITOSHI MOTOME, Dept. of Appl. Phys., Univ. of Tokyo — The quantum spin liquid, which does not show any long-range ordering down to the lowest temperature, has attracted broad interest as a new quantum state of matter. Since the ground state of the Kitaev model was shown to be a quantum spin liquid in two dimensions [1], there has been an explosion in both theoretical and experimental studies. Nevertheless, dynamical properties at finite temperatures remain a challenge, despite the relevance to analysis of recent experiments for Ir and Ru compounds. In this contribution, we address this problem by using the cluster dynamical mean-field approximation, which we newly develop on the basis of the Majorana fermion representation. Using the continuous-time quantum Monte Carlo method for the impurity solver, we calculate the magnetic susceptibility, dynamical spin structure factor, and relaxation time in the nuclear magnetic resonance. We find that these quantities show peculiar temperature dependences in the paramagnetic state when approaching the quantum spin liquid by decreasing temperature, which reflects the fractionalization of quantum spins. We will discuss the results while changing the anisotropy and sign (ferro/antiferro) of the exchange interactions, in comparison with experiments. [1] A. Kitaev, Ann. Phys. **321**, 2 (2006).

**5:06PM H5.00014 Protection against a spin gap in two-dimensional insulating antiferromagnets with a Chern-Simons term**, IMAM MAKHFUDZ, PIERRE PUJOL, LPT-IRSAMC and Univ. Paul Sabatier Toulouse France — We propose a mechanism for the protection against spin gapped states in doped antiferromagnets. It requires the presence of a Chern-Simons term that can be generated by a coupling between spin and an insulator. We first demonstrate that in the presence of this term the vortex loop excitations of the spin sector behave as anyons with fractional statistics. To generate such a term, the fermions should have a massive Dirac spectrum coupled to the emergent spin field of the spin sector. The Dirac spectrum can be realized by a planar spin configuration arising as the lowest-energy configuration of a square lattice antiferromagnet Hamiltonian involving a Dzyaloshinskii-Moriya interaction. The mass is provided by a combination of dimerization and staggered chemical potential. We finally show that for realistic parameters, anyonic vortex loop condensation will likely never occur and thus the spin gapped state is prevented. We also propose real magnetic materials for an experimental verification of our theory. Reference: Imam Makhfudz and Pierre Pujol, Phys. Rev. B **92**, 144507 (2015).

**5:18PM H5.00015 Interaction-driven fractional quantum Hall state of hard-core bosons on kagome lattice at one-third filling**<sup>1</sup>, D. N. SHENG, California State University, Northridge, S. S. GONG, National High Magnetic Field Lab, W. ZHU, California State University, Northridge — There has been a growing interest in realizing topologically nontrivial states of matter in band insulators, where a quantum Hall effect can appear as an intrinsic property of the band structure. While the on-going progress is under way with a number of directions, the possibility of realizing novel interaction-generated topological phases, without the requirement of a nontrivial invariant encoded in single-particle wavefunction or band structure, can significantly extend the class of topological materials and is thus of great importance. Here, we show an interaction-driven topological phase emerging in an extended Bose-Hubbard model on kagome lattice, where the non-interacting band structure is topological trivial with zero Berry curvature in the Brillouin zone. By means of an unbiased state-of-the-art density-matrix renormalization group technique, we identify that the groundstate in a broad parameter region is equivalent to a bosonic fractional quantum Hall Laughlin state, based on the characterization of universal properties including groundstate degeneracy, edge excitations and anyonic quasiparticle statistics. Our work paves a way of finding interaction induced topological phase at the phase boundary of conventionally ordered solid phases.

<sup>1</sup>This research is supported by the DOE grants No. DE-FG02-06ER46305, and the NSF grant No. DMR-1408560

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**

**Session H6 GMAG DMP: Perpendicular Anisotropy Multi-layers and Hard Magnets** 302 - Mazin  
Almaqablah, Western Digital Corporation

**2:30PM H6.00001 Electric-field-induced modification in Dzyaloshinskii-Moriya interaction of Co monolayer on Pt(111)**, KOHJI NAKAMURA, TORU AKIYAMA, TOMONORI ITO, Mie University, TERUO ONO, Kyoto University, MICHAEL WEINERT, University of Wisconsin - Milwaukee — Magnetism induced by an external electric field ( $E$ -field) has received much attention as a potential approach for controlling magnetism at the nano-scale with the promise of ultra-low energy power consumption. Here, the  $E$ -field-induced modification of the Dzyaloshinskii-Moriya interaction (DMI) for a prototypical transition-metal thin layer of a Co monolayer on Pt(111) is investigated by first-principles calculations by using the full-potential linearized augmented plane wave method that treats spin-spiral structures in an  $E$ -field. With inclusion of the spin-orbit coupling (SOC) by the second variational method for commensurate spin-spiral structures, the DMI constants were estimated from an asymmetric contribution in the total energy with respect to the spin-spiral wavevector. The results predicted that the DMI is modified by the  $E$ -field, but the change is found to be small compared to that in the exchange interaction (a symmetric contribution in the total energy) by a factor of ten.

**2:42PM H6.00002 Random Field effects in perpendicular-anisotropy multilayer films** , JIAN XU, University of Chicago, DANIEL SILEVITCH, THOMAS ROSENBAUM, California Institute of Technology — With the application of a magnetic field transverse to the magnetic easy axis, randomly-distributed 3D collections of dipole-coupled Ising spins form a realization of the Random-Field Ising Model. Tuning the strength of the site-specific random field, and hence the disorder, via the applied transverse field regulates the domain reversal energetics and hence the macroscopic hysteresis loop. We extend this approach to two dimensions, using sputtered Perpendicular Magnetic Anisotropy (PMA) Co/Pt multilayer thin films. We characterize the coercive fields and hysteresis loops at a series of temperatures and transverse fields.

**2:54PM H6.00003 Polarization dependent soft x-ray spectro-microscopy of local spin structures**<sup>1</sup> , MACCALLUM ROBERTSON, Center for X-Ray Optics, LBNL, CHRISTOPHER AGOSTINO , National Center for Electron Microscopy, LBNL, MI-YOUNG IM, Center for X-Ray Optics, LBNL, SERGIO MONTOYA , ERIC FULLERTON , Center for Magnetic Recording Research, UCSD, PETER FISCHER, Materials Sciences Division, LBNL — Quantitative information about element-specific contributions to local magnetic spin and orbital moments is readily available by XMCD spectroscopy and images of magnetic domain patterns with a few tens of nanometer spatial resolution. We show that the x-ray spectroscopic analysis of x-ray microscopy images provides quantitative information about local spin structures. We have investigated two prototypical multilayered PMA film systems prepared by sputtering, specifically (Co 0.3 nm/Pt 0.5 nm)<sub>x30</sub> and (Fe 0.7nm/Gd 0.4nm)<sub>x100</sub> systems. A spectroscopic sequence of full-field magnetic transmission soft x-ray microscopy (MTXM) images covering about 8mm field-of-views with a spatial resolution of about 20nm were recorded across the Co and Fe L edges, resp. To modulate the magnetic contrast, two sets of images were obtained with left and right circular polarization. Standard XMCD spectroscopy analysis procedures were applied to retrieve the local spectroscopic behavior. We observe a decrease of the L3/L2 ratio when approaching the domain walls, indicating a non-uniform spin configuration along the vertical profile of a domain, which we will discuss in view of both systems' magnetic anisotropies.

<sup>1</sup>U.S. DOE under Contract No. DE-AC02-05-CH11231

**3:06PM H6.00004 Nanoparticulate CoPt Thin Films**<sup>1</sup> , YASAMAN BAREKATAIN, GEORGE HADJIPANAYIS, Department of Physics and Astronomy, University of Delaware, MAGNETICS BLAB TEAM — Equiatomic FePt and CoPt alloys are very attractive for application in high density recording media because of the high magnetocrystalline anisotropy K of their **fct** (L1<sub>0</sub>) structure with values exceeding 2MJ/m<sup>3</sup>. The aim of this study is to fabricate a nanoparticulate CoPt film consisting of CoPt nanoparticles embedded in a matrix. To obtain this we have used co-sputtering of CoPt with different materials M= BN, C, Cu and SiO<sub>2</sub>. Our first experiments were done on CoPt films with thickness of 200 nm. The as-sputtered films had the **fcc** structure and a coercivity of 150 Oe. Annealing at 700 °C for 30 min led to an increase in coercivity to 4 kOe. Optimization studies are under way to find the optimum sputtering conditions to obtain a fully ordered tetragonal structure with the highest value of coercivity which can then be used in the nanoparticulate composites. Work supported by DOE BES- FG02-04ERU4612

<sup>1</sup>DOE DE-FG02-04ERU4612

**3:18PM H6.00005 Microscopic evidence of strain-mediated magnetoelectric coupling in Co/Pt multilayers/PMN-PT(011) heterostructures** , YING SUN, Tsinghua University, WENBO WANG, WEIDA WU, Rutgers University, XIAOLI ZHENG, JIANWANG CAI, Institute of Physics, Chinese Academy of Sciences, YONGGANG ZHAO, Tsinghua University, MING LIU, Xian Jiaotong University — A promising way to control magnetization(M) via an electric field(E-field) is using magnetoelectric(ME) effect in FM/FE heterostructures. We use magnetic(electric) force microscopy(M(e)FM) to study the strain-mediated E-field modulation of M in (Co/Pt)<sub>n</sub> with perpendicular magnetic anisotropy(PMA) or in-plane anisotropy on PMN-PT(011) substrates. MFM were performed on (Co/Pt)<sub>n</sub> with an DC E-field applied to PMN-PT. In MeFM, we superimpose an AC modulation on a DC one and utilize lock-in technique to detect weak ME effect. For (Co/Pt)<sub>n</sub> with PMA, MFM images show stripe domains with no obvious changes at varied DC E-fields. However, MeFM shows interesting structures and the image contrast reverses sign at opposite strain slopes of the PMN-PT substrate. For sample with in-plane anisotropy, both MFM and MeFM images show dipole-like domains. Interestingly, the MeFM image contrast reverses sign at opposite strain slopes of the substrate. The sign reversal of MeFM contrast indicates that features revealed by MeFM are intrinsic local ME effect. Our MeFM data are consistent with the ferromagnetic resonance results showing that strain-induced anisotropy change will cause part of M switching to the in-plane direction. Possible scenarios will be discussed.

**3:30PM H6.00006 Effect of perpendicular magnetic anisotropy and Dzyaloshinskii-Moriya interaction on the enhancement of domain wall creep velocity in Pt/Co thin films by piezoelectric strain**<sup>1</sup> , PHILIPPA M. SHEPLEY, GAVIN BURNELL, THOMAS A. MOORE, University of Leeds — We investigate piezoelectric strain control of domain wall creep motion in perpendicularly magnetized Pt/Co thin films. Domain wall (DW) motion has potential applications in data storage and spintronics, where the use of voltages rather than magnetic fields to control magnetization reversal could reduce power consumption. Materials with perpendicular magnetic anisotropy (PMA) are of particular interest due to their narrow domain walls and potential for efficient current-induced DW motion. Sputtered Ta/Pt/Co(t)/X films (t=0.78-1.0nm, X= Pt, Ir/Pt or Ir) on thin glass substrates were bonded to biaxial piezoelectric transducers, to which 150V was applied to produce a tensile out-of-plane strain of 9x10<sup>-4</sup>. This reduced the PMA by 10kJ/m<sup>3</sup> and increased the DW creep velocity by up to 90%. DW energy can be calculated from the PMA and the Dzyaloshinskii-Moriya interaction (DMI) field. DW creep measurements of DMI field found no change with strain. The change in DW velocity with strain is linear with the change in DW energy for Pt/Co DWs with a mixed Bloch-Neel structure. Pt/Co/Pt films with higher DW velocity changes were found to have purely Bloch DWs. We conclude that the velocity of Bloch DWs is more sensitive to strain-induced changes than that of Bloch-Neel DWs.

<sup>1</sup>funded by EPSRC

**3:42PM H6.00007 Thermal Stability of Magnetic States in Circular Thin-Film Nanomagnets with Large Perpendicular Magnetic Anisotropy<sup>1</sup>**, GABRIEL CHAVES-O'FLYNN, New York Univ NYU — The scaling of the energy barrier to magnetization reversal in thin-film nanomagnets with perpendicular magnetization as a function of their lateral size is of great interest and importance for high-density magnetic random access memory devices. Experimental studies of such elements show either a quadratic or linear dependence of the energy barrier<sup>2,3</sup> on element diameter. I will discuss a theoretical model we developed to determine the micromagnetic configurations that set the energy barrier for thermally activated reversal of a thin disk with perpendicular magnetic anisotropy as a function of disk diameter<sup>4</sup>. We find a critical length in the problem that is set by the exchange and effective perpendicular magnetic anisotropy energies, with the latter including the size dependence of the demagnetization energy. For diameters smaller than this critical length, the reversal occurs by nearly coherent magnetization rotation and the energy barrier scales with the square of the diameter normalized to the critical length (for fixed film thickness), while for larger diameters, the transition state has a domain wall, and the energy barrier depends linearly on the normalized diameter. Simple analytic expressions are derived for these two limiting cases and verified using full micromagnetic simulations with the string method. Further, the effect of an applied field is considered and shown to lead to a plateau in the energy barrier versus diameter dependence at large diameters. Based on these findings I discuss the prospects and material challenges in the scaling of magnetic memory devices based on thin films with strong perpendicular magnetic anisotropy.

<sup>1</sup>In collaboration with G. Wolf, J. Z. Sun and A. D. Kent. Supported by NSF-DMR-1309202 and in part by Spin Transfer Technologies Inc. and the Nanoelectronics Research Initiative through the Institute for Nanoelectronics Discovery and Exploration.

<sup>2</sup>J. Z. Sun *et al.*, Phys. Rev. B **8**, 104426 (2013).

<sup>3</sup>H. Sato *et al.*, Appl. Phys. Lett. **105**, 062403 (2014)

<sup>4</sup>G. D. Chaves-O'Flynn, G. Wolf, J. Z. Sun and A. D. Kent, Phys. Rev. Applied **4**, 024010 (2015).

**4:18PM H6.00008 Large electric-field control of perpendicular magnetic anisotropy in strained [Co/Ni] / PZT heterostructures**, DANIEL GOPMAN, CINDI DENNIS, P. J. CHEN, NIST - Natl Inst of Stds & Tech, YURY IUNIN, Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow Region, Russia, ROBERT SHULL, NIST - Natl Inst of Stds & Tech — We present a piezoelectric/ferromagnetic heterostructure with PMA - a Co/Ni multilayer sputtered directly onto a Pb(Zr,Ti)O<sub>3</sub> (PZT) substrate. Chemical-mechanical polishing was used to reduce the roughness of PZT plates to below 2 nm *rms*, enabling optimal magnetoelectric coupling via the direct interface between PZT and sputtered Co/Ni films with large PMA ( $K_{\text{eff}} = (95 \pm 9 \text{ kJ/m}^3)$ ). We grew the following layer stack: Ta(3)/Pt(2)/[Co(0.15)/Ni(0.6)]<sub>x4</sub>/Co(0.15)/Pt(2)/Ta(3); numbers in parentheses indicate thicknesses in nm. Applied electric fields up to  $\pm 2 \text{ MV/m}$  to the PZT generated 0.05% in-plane compression in the Co/Ni multilayer, enabling a large electric-field reduction of the PMA ( $\Delta K_{\text{eff}} \geq 10^3 \text{ J/m}^3$ ) and of the coercive field (35%). Our results demonstrate that: (i) heterostructures combining PZT and [Co/Ni] exhibit larger PMA ( $K_{\text{eff}} \sim 10^5 \text{ J/m}^3$ ) than previous magnetoelectric heterostructures based on Co/Pt and CoFeB, enabling thermally stable hybrid magnetoelectric/spintronic devices only tens of nm in diameter and (ii) electric-field control of the PMA is promising for more energy efficient switching of spintronic devices.

**4:30PM H6.00009 Properties of easy-plane/ perpendicular magnetic anisotropy bilayers with varied interlayer exchange coupling<sup>1</sup>**, LORENZO FALLARINO<sup>2</sup>, VOLKER SLUKA, Department of Physics, New York University, New York, NY 10003, USA., BARTEK KARDASZ, MUSTAFA PINARBASI, Spin-Transfer Technologies Inc., Freemont, CA 94538, USA., ANDREW D. KENT, Department of Physics, New York University, New York, NY 10003, USA. — We explore the possibility of an easy-cone ground state in coupled easy plane/easy axis magnetic bilayers. The samples consist of a Co/Ni multilayer with perpendicular magnetic anisotropy and a CoFe layer with easy-plane anisotropy separated by a variable thickness Ru layer. Using ferromagnetic resonance spectroscopy, we characterize the magnetic behavior of the coupled thin films for different Ru thicknesses by determining the resonance fields for both the acoustic and optical FMR modes. In particular, we observe a gap in the resonance field opening up between the two modes in angular-dependent FMR, which is direct evidence for the presence of interlayer coupling. Quantitative comparisons with a theoretical model indicate that by varying the Ru thickness the coupling strength can be tuned continuously from ferromagnetic to the anti-ferromagnetic. These results are consistent with a canted magnetic ground state in zero field, a state of interest for applications in spin-torque devices, such as current tunable spin-torque oscillators.

<sup>1</sup>Supported by NSF-DMR1309202 and Spin-Transfer Technologies Inc.

<sup>2</sup>Second affiliation: CIC nanoGUNE, 20018 Donostia-San Sebastian, Basque Country, Spain.

**4:42PM H6.00010 Giant magnetic anisotropy of Co, Ru, and Os adatoms on MgO (001) surface.**, HONGBO WANG, XUEDONG OU, FENGREN FAN, ZHENGWEI LI, HUA WU, Fudan Univ — Large magnetic anisotropy energy (MAE) is desirable and critical for nanoscale magnetic devices. Here, using ligand-field level diagrams and density functional calculations, we well explain the very recent discovery [I. G. Rau *et al.*, Science **344**, 988 (2014)] that individual Co adatom on MgO (001) surface has a large MAE of more than 60 meV. More importantly, we predict that a giant MAE up to 110 meV could be realized for Ru adatoms on MgO (001), and even more for the Os adatoms (208 meV). This is a joint effect of the special ligand field, orbital multiplet, and significant spin-orbit interaction, in the intermediate-spin state of the Ru or Os adatoms on top of the surface oxygens. The giant MAE could provide a route to atomic scale memory.

**4:54PM H6.00011 ABSTRACT WITHDRAWN —**

**5:06PM H6.00012 Perpendicular Magnetic Anisotropy of Tb/Fe and Gd/Fe Multilayers Studied with Torque Magnetometer**, ATAUR CHOWDHURY, Physics Department, UAF — Perpendicular magnetic anisotropy (PMA) of multilayers critically depend on the magnetic and structural ordering of the interface. To study the effect of interface on PMA, Tb/Fe and Gd/Fe multilayers with varying Fe (0.8-9.0 nm) and Gd (0.5-2.8 nm) or Tb (0.3-6.3 nm) layer thicknesses were fabricated by planar magnetron sputtering. The magnetometer results of spin orientation clearly reveals that samples with Gd or Tb layer thickness of more than 1.2 nm display no PMA, regardless of the Fe layer thickness. Tb/Fe and Gd/Fe multilayers with thin (<1.2 nm) Tb or Gd layers display large PMA, but no PMA is observed when the Fe layer thickness is increased to 4.0 nm and higher. The bulk magnetization and anisotropy energy constant of the samples are found to increase with increasing Fe layer thickness. Torque measurement also reveals that there are two distinctly different axes of spin alignment at different energy. Tb/Fe and Gd/Fe multilayers with similar composition reveal similar magnetic and structural characteristics, and it may imply that single-ion-anisotropy of rare-earth element, which is quite large for Tb ions and very small for Gd ions, may not be the dominating cause of PMA in Tb/Fe and Gd/Fe multilayers. A detailed explanation of the results will be provided based on exchange interaction at the interface.

**5:18PM H6.00013 Stripe glasses in ferromagnetic thin films**, ALESSANDRO PRINCIPI, MIKHAIL KATSNELSON, Institute for Molecules and Materials, Radboud University — Domain walls in magnetic multilayered systems can exhibit a very complex and fascinating behavior. The magnetization of thin films of hard magnetic materials is in general perpendicular to the thin-film plane, but its direction changes periodically, forming an alternating spin-up and spin-down stripe pattern. The latter is stabilized by the competition between the ferromagnetic coupling and dipole-dipole interactions, and disappears when a moderate in-plane magnetic field is applied. It has been suggested that such a behavior may be understood in terms of a self-induced stripe glassiness. In this paper we show that such a scenario is compatible with the experimental findings. The strong out-of-plane magnetic anisotropy of the film is found to be beneficial for the formation of both the stripe-ordered and glassy phases. At zero magnetic field the system can form a glass only in a narrow interval of fairly large temperatures. An in-plane magnetic field, however, shifts the glass transition towards lower temperatures, therefore enabling it at or below room temperature. In good qualitative agreement with the experimental findings, we show that a moderate in-plane magnetic field of the order of 30 mT can lead to the formation of defects in the stripe pattern.

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**

**Session H7 DMP FIAP: Dopants and Defects in Semiconductors: Spin Related Transport** 303

- Lourdes Salamanca-Riba, University of Maryland

**2:30PM H7.00001 Anomalous organic magnetoresistance from competing carrier-spin-dependent interactions with localized electronic and nuclear spins**, MICHAEL E. FLATT, University of Iowa

— Transport of carriers through disordered electronic energy landscapes occurs via hopping or tunneling through various sites, and can enhance the effects of carrier spin dynamics on the transport. When incoherent hopping preserves the spin orientation of carriers, the magnetic-field-dependent correlations between pairs of spins influence the charge conductivity of the material. Examples of these phenomena have been identified in hopping transport in organic semiconductors and colloidal quantum dots, as well as tunneling through oxide barriers in complex oxide devices, among other materials. The resulting room-temperature magnetic field effects on the conductivity or electroluminescence require external fields of only a few millitesla. These magnetic field effects can be dramatically modified by changes in the local spin environment. Recent theoretical and experimental work has identified a regime for low-field magnetoresistance in organic semiconductors in which the spin-relaxing effects of localized nuclear spins and electronic spins interfere<sup>1</sup>. The regime is studied experimentally by the controlled addition of localized electronic spins, through the addition of a stable free radical (galvinoxyl) to a material (MEH-PPV) that exhibits substantial room-temperature magnetoresistance (initially suppressed by the doping, as the localized electronic spin mixes one of the two spins whose correlation controls the transport. At intermediate doping, when one spin is fully decohered but the other is not, there is a regime where the magnetoresistance is insensitive to the doping level. For much greater doping concentrations the magnetoresistance is fully suppressed as both spins that control the charge conductivity of the material are mixed. The behavior is described within a theoretical model describing the effect of carrier spin dynamics on the current. Generalizations to amorphous and other disordered crystalline semiconductors will also be described. This work was supported by DOE and an ARO MURI and was done in collaboration with N. J. Harmon, K. Sahin-Tiras, Y. Wang and M. Wohlgenannt.

**3:06PM H7.00002 Near-infrared induced charge dynamics of the nitrogen vacancy center in diamond**, DAVID A. HOPPER, RICHARD R. GROTE, ANNEMARIE L. EXARHOS, LEE C. BASSETT, University of Pennsylvania

— The nitrogen-vacancy (NV) center in diamond is a key functional element in emerging quantum technologies such as nodes in quantum information processing and nanoscale sensors for condensed matter physics and biology. Recent efforts to optimize the NV's functionality lead to the discovery of photoinduced charge-state switching between the negative (NV<sup>-</sup>) and neutral (NV<sup>0</sup>) states which holds great potential to enhance the fidelity of spin readout. While the charge state dynamics under visible illumination have been studied, the effect of infrared light remains unexplored. Here, we use a tunable, pulsed infrared source to illuminate NV centers under various spin and optical states. Precise time-domain control of visible, microwave, and infrared pulses together with single-shot charge readout allows for the direct probing of spin and charge dynamics induced by the infrared light. This new understanding is relevant for the development of advanced protocols to leverage the NV's complete spin, charge, and optical dynamics for quantum control and sensing applications.

**3:18PM H7.00003 Formation and Annealing Behaviors of Qubit Centers in 4H-SiC from First Principles**, MINGWEN ZHAO, Shandong University, XIAOPENG WANG, Tulane University, HONGXIA BU, Shandong University, HONGYU ZHANG, East China University of Science and Technology, XIUJIE HE, AIZHU WANG, Shandong University, MINGWEN ZHAO'S LAB IN SHANDONG UNIVERSITY

TEAM — Inspired by finding that the nitrogen-vacancy center in diamond is a qubit candidate, similar defects in silicon carbide have drawn considerable interest. However, the generation and annealing behaviors of these defects remain unclear. Using first-principles calculations, we describe the equilibrium concentrations and annealing mechanisms based on the diffusion of silicon vacancies. The formation energies and energy barriers along different migration paths, which are responsible for the formation rates, stability, and concentrations of these defects, are investigated. The effects on these processes of charge states, annealing temperature, and crystal orientation are also discussed. These theoretical results are expected to be useful in achieving controllable generation of these defects in experiments.

**3:30PM H7.00004 First principle investigation of isolated vacancy in (111) diamond surface<sup>1</sup>**, WENHAO HU, MICHAEL FLATTÉ, Department of Physics and Astronomy, University of Iowa

— As the simplest intrinsic defect, isolated vacancy has been studied intensively theoretically and experimentally in diamond's bulk phase. Nevertheless, its correspondence in surface phase still lacks people's attention. Nitrogen vacancy center has become the most ideal candidates for solid states computing due to its long coherence time at room temperature. Resembling NV center, the isolated vacancy on surface exhibits a similar ambient potential and the same 3-fold rotational symmetry due to the asymmetry of surface, which implies a similar character in them. In our work, the isolated vacancy in clean and hydrogen terminated (111) surface of diamond are investigated from first principle perspective. Full potential LAPW method implemented in WIEN2K is exploited under GGA approximation. To evaluate the surface effect, the defect depth from topmost layer to fifth subsurface are considered with different slab thickness. By checking the spin density distribution and electronic structure, the hydrogen vacancy in H-terminated surface exhibit a spin- $\frac{1}{2}$  center with a 0/-1 transition level located in the middle of band gap. The -1/-2 transition level of carbon vacancy in the subsurface approaches the 0/-1 transition level implying the potential stability of spin-1 center.

<sup>1</sup>The work was supported by an AFOSR MURI.

**3:42PM H7.00005 Coherence studies on silicon vacancies in SiC generated via proton irradiation**, PETER BRERETON, DON PUENT, US Naval Academy, EVAN GLASER, SAM CARTER, US Navy Research Laboratory

— Single spins in defects in wide bandgap semiconductors are the canonical platform for scalable quantum technologies in the solid state. The silicon vacancy (VSi) in silicon carbide has very recently been shown to exhibit similar spin coherence to the diamond nitrogen vacancy center but in a material that has a mature technological base for fabrication and is an order of magnitude cheaper. Additionally, SiC has several polytypes, allowing the engineering of the spin behavior of the silicon vacancy. In this work, we generate ensembles of VSi via proton irradiation of 4H-SiC. We then measure the spin lifetimes and coherence times of ensembles of defect spins via optically detected magnetic resonance and Hahn pulse techniques. We show that the spin coherence time is strongly dependent on distance from the proton damage layer, therefore setting important parameters for the fabrication of long-lifetime single defect devices.

**3:54PM H7.00006 Magnetoresistance Phenomena in a Variety of Amorphous Semiconductors and Insulators<sup>1</sup>**, MICHAEL MUTCH, DAVID WESTLEY, PATRICK LENAHAAN, Pennsylvania State University, SEMICONDUCTOR SPECTROSCOPY LAB AT PENN STATE UNIVERSITY TEAM — We report on near zero-field magnetoresistance (MR) phenomena in a variety of amorphous semiconductors and insulators. We utilize electrically detected magnetic resonance (EDMR) measurements at multiple fields and frequencies to complement MR measurements. EDMR, the electrically detected analog of electron paramagnetic resonance (EPR), provides both information about the chemical nature and energy levels of point defects involved. Semiconductors in this study include a-BC:H, a-C:H, diamond-like carbon (DLC), and a-Si:H. Insulators include a-SiN:H, a-SiOC:H, a-SiCN:H. In hydrogenated amorphous systems, near featureless EPR and EDMR spectra are often difficult to analyze. We utilize multiple field and frequency EDMR results including ultra-low field/frequency ( $\nu = 85$  MHz,  $B = 3$  mT) EDMR measurements to provide insight into defect chemistry in these systems. We have also made EDMR and MR conditions over a wide range of metal/semiconductor heterojunction and metal/insulator/semiconductor biasing conditions. By comparing variable bias measurements with band diagrams, we gain an elementary understanding of defect energy levels. We believe our results will be of significant importance for understanding defect mediated spin-dependent transport in these systems.

<sup>1</sup>The authors would like to thanks Dr. Sean King of Intel Corporation for the provision of samples.

**4:06PM H7.00007 Exploration of Defects in 4H-SiC MOSFETs via Spin Dependent Charge Pumping**, MARK ANDERS, PATRICK LENAHAAN, Pennsylvania State Univ, AIVARS LELIS, U.S. Army Research Laboratory — 4H-SiC MOSFETs have great promise for use in high temperature and high voltage applications. Unfortunately, defects at the SiC/SiO<sub>2</sub> interface reduce the performance of these devices. Previously, our group utilized electrically detected magnetic resonance (EDMR) detected via spin dependent recombination (SDR) to identify such SiC/SiO<sub>2</sub> interface defects utilizing the bipolar amplification (BAE) biasing scheme; we observed SiC silicon vacancies, E-prime centers, and hydrogen complexed E-prime centers. All of these defects must have levels around the middle of the SiC band gap because they are effective recombination centers. We expanded our studies to include EDMR detection via spin dependent charge pumping (SDCP) at low field, X band, and K band, allowing EDMR exploration of nearly the entire 4H-SiC band gap. Perhaps the most important finding of the (nearly) full band gap measurements is the absence of the carbon dangling bond spectrum in the SDCP. Additionally, in nMOSFETs, we observe an SDCP EDMR spectrum dominated by a silicon vacancy, whereas in pMOSFETs, we also observe a strong, nearly isotropic single line spectrum with  $g = 2.00244$  and  $2.00248$  when the c-axis is nearly parallel and perpendicular to the magnetic field, respectively. The results suggest that silicon vacancy centers dominate nMOSFET interfaces whereas additional defects clearly play important roles in pMOSFETs.

**4:18PM H7.00008 Double electron-electron resonance measurements of diamond to determine  $T_2$  dependence on concentration of paramagnetic impurities<sup>1</sup>**, VIKTOR STEPANOV, SUSUMU TAKAHASHI, University of Southern California — A nitrogen-vacancy (NV) center in diamond is a promising candidate for investigation of fundamental sciences and applications to a nanoscale magnetic field sensing device because of unique properties of a NV center in diamond including capability to detect optically detected magnetic resonance (ODMR) signals from a single NV and initialize its spin state. Fundamental studies and applications of NV centers rely on coherent control of the NV centers that is limited by decoherence time ( $T_2$ ) and, as often observed,  $T_2$  is limited by paramagnetic impurity contents in diamond crystals. In this work, we will investigate  $T_2$  dependence on concentration of nitrogen impurities in type-Ib and type-IIa diamond crystals. For precise determination of the nitrogen concentration, we employ a home-built high-frequency electron spin resonance spectrometer which enables broadband double electron-electron resonance spectroscopy with high spectral resolution. [1,2]

[1] F. H. Cho, V. Stepanov and S. Takahashi, Rev. Sci. Instrum. **85**, 075110 (2014).

[2] F. H. Cho, V. Stepanov, C. Abeywardana and S. Takahashi, Methods Enzymol. **563**, **95** (2015).

<sup>1</sup>This work is supported by the National Science Foundation (DMR-1508661) and the Searle scholars program.

**4:30PM H7.00009 Electrical detection and imaging of individual phosphorus and silicon-dangling bonds states at the crystalline silicon to silicon dioxide interface**, KAPILDEB AMBAL, Univ of Utah, PHILIPP RAHE, University of Nottingham, ADAM PAYNE, Univ of Utah, JAMES SLINKMAN, RFSoI Technology Development, IBM Microelectronics, CLAYTON C WILLIAMS, CHRISTOPH BOEHME, Univ of Utah — Nuclear spins of phosphorus [P] donor atoms in crystalline silicon are promising qubit candidates, but utilizing these systems for scalable quantum devices will require the ability to probe individual donors on atomic length scales and address these systems by application of well-controlled electric fields<sup>1</sup>. In this talk we focus on identifying individual P donor and P<sub>b</sub> (dangling bond) states by measuring electric current through a crystalline silicon (100) - SiO<sub>2</sub> interface, observing charge flow through individual pairs of P donors and highly localized ( $\text{\AA}$ -range) silicon dangling bond states. The experiments were conducted with neutral P donor states using a low-temperature ( $T = 4.3\text{K}$ ) ultra-high vacuum scanning probe microscope with a quartz tuning fork sensor that allows simultaneous AFM and local current measurements in complete darkness. This so called conduction-atomic force microscopy experiment<sup>2</sup> yields images of the dangling bond states coupled to individual phosphorus donors. I-V responses on these isolated highly localized charge percolation paths further support the hypothesis that individual P-donor - P<sub>b</sub> states are being addressed, and that spin-states may be probed using spin-dependent charge-carrier recombination current between <sup>31</sup>P and the interface defects. [1] B. E. Kane, Nature **393**, 133 (1998); [2] S. Kremmer et al., Surf. Interface Anal. **33**, 168 (2002).

**4:42PM H7.00010 ESR Experiments on a Single Donor Electron in Isotopically Enriched Silicon<sup>1</sup>**, LISA TRACY, DWIGHT LUHMAN, STEPHEN CARR, JOHN BORCHARDT, NATHANIEL BISHOP, GREGORY TEN EYCK, TAMMY PLUYM, JOEL WENDT, WAYNE WITZEL, ROBIN BLUME-KOHOUT, ERIK NIELSEN, MICHAEL LILLY, MALCOLM CARROLL, Sandia National Labs — In this talk we will discuss electron spin resonance experiments in single donor silicon qubit devices fabricated at Sandia National Labs. A self-aligned device structure consisting of a polysilicon gate SET located adjacent to the donor is used for donor electron spin readout. Using a cryogenic HEMT amplifier next to the silicon device, we demonstrate spin readout at 100 kHz bandwidth and Rabi oscillations with 0.96 visibility. Electron spin resonance measurements on these devices show a linewidth of 30 kHz and coherence times  $T_2^* = 10$  us and  $T_2 = 0.3$  ms. We also discuss estimates of the fidelity of our donor electron spin qubit measurements using gate set tomography. This work was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. DOE Office of Basic Energy Sciences user facility. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a Lockheed-Martin Company, for the U. S. Department of Energy under Contract No. DE-AC04-94AL85000.

<sup>1</sup>ESR Experiments on a Single Donor Electron in Isotopically Enriched Silicon

**4:54PM H7.00011 Nanoscale thermal imaging using a scanning spin probe.** , ABDELGHANI LARAOUI, HALLEY AYCOCK-RIZZO, Department of Physics, CUNY-City College of New York, YANG GAO, ELISA RIEDO, CUNY-Advanced Research Science Center, Department of Physics, Georgia Institute of Technology, CARLOS MERILES, Department of Physics, CUNY-City College of New York — We use a 30-nm diamond-nanocrystal-hosted nitrogen-vacancy (NV) center attached to the apex of a silicon tip as a local temperature sensor. First, we apply an electrical current to heat up the tip to a predefined operating temperature and rely on the NV to monitor the small thermal changes the tip experiences as it is brought into contact with surfaces of varying thermal conductivity. With the aid of a combined AFM/confocal setup, we image engineered microstructures with nanoscale resolution, and attain excellent agreement between the thermal conductivity and topographic maps [1]. Given the small mass of the NV-hosting diamond nanoparticle, our technique shows a fast time response of order hundred microseconds, limited by the heat dissipation time of the tip. In a second approach, we heat nanostructured gold deposited on glass substrate by injecting a direct current. By monitoring the frequency shift of NV spin transitions upon scanning the AFM tip we reconstruct nanometer-resolved temperature maps. Our technique promises multiple applications ranging from the investigation of phonon dynamics in nanostructures to the characterization of heterogeneous phase transitions in various solid-state systems. [1] A. Laraoui, et al., Nat. Commun, in press.

**5:06PM H7.00012 Optimizing the Growth of (111) Diamond for Diamond Based Magnetometry<sup>1</sup>** , ERIC KAMP, PATRICK GODWIN, NITIN SAMARTH, Pennsylvania State University, DAVID SNYDER, Pennsylvania State University Applied Research Laboratory, CHARLES DE LAS CASAS, DAVID D. AWSCHALOM, Institute for Molecular Engineering, University of Chicago — Magnetometers based on nitrogen vacancy (NV) ensembles have recently achieved sub-picotesla sensitivities [Phys. Rev. X 5, 041001(2015)], putting the technique on par with SQUID and MFM magnetometry. Typically these sensors use (100) oriented diamond with NV centers forming along all four (111) crystal orientations. This allows for vector magnetometry, but is a hindrance to the absolute sensitivity. Diamond grown on (111) oriented substrates through microwave plasma enhanced chemical vapor deposition (MP-CVD) provides a promising route in this context since such films can exhibit preferential orientation greater than 99% [Appl. Phys. Lett. 104, 102407(2014)]. An important challenge though is to achieve sufficiently high NV center densities required for enhancing the sensitivity of an NV ensemble magnetometer. We report systematic studies of the MP-CVD growth and characterization of (111) oriented diamond, where we vary growth temperature, methane concentration, and nitrogen doping. For each film we study the Nitrogen to NV ratio, the  $NV^-$  to  $NV^0$  ratio, and alignment percentage to minimize sources of decoherence and ensure preferential alignment. From these measurements we determine the optimal growth parameters for high sensitivity, NV center ensemble scalar magnetometry.

<sup>1</sup>Funded by NSF-DMR

**5:18PM H7.00013 First principles identification of divacancy configurations in 4H- and 6H-SiC** , ADAM GALI, Wigner Research Centre for Physics, Hungarian Academy of Sciences, VIKTOR IVÁDY, Linköping University, KRISZTIÁN SZÁSZ, Wigner Research Centre for Physics, Hungarian Academy of Sciences, IGOR. A. ABRIKOSOV, ERIK JANZÉN, Linköping University — Based on the combination of ab initio simulations and group theory considerations it was proposed earlier that the high spin divacancy defect in silicon carbide (SiC) with similar electronic structure as the NV center in diamond could be utilized as a solid state quantum bit [1]. Recent demonstrations have shown coherent manipulation of divacancy and related defect spins in 4H- [2], 6H- and 3C-SiC [3]. In hexagonal SiC polytypes, point defects can exist in numerous different configurations. Associating potentially interesting photoluminescence (PL) centers with their microscopic configurations is of great importance as quantum information applications often require single defect control. In our study, we carry out large-scale first principles calculation to identify the aforementioned divacancy related point defects. By resolving accuracy issues of ab initio supercell techniques, we were able to obtain convergent PL energies, zero-field-splitting, and hyperfine parameters. Our results confirm previous assignment of the divacancy related PL1-PL4 PL lines in 4H-SiC to their microscopic structure, provide the identification of QL1-QL6 PL lines in 6H-SiC, as well as propose defect configurations for the unknown PL5-PL6 centers in 4H-SiC that yields strong signal at room temperature. [1] A. Gali et al., Mater. Sci. Forum 645-648, 395 (2010). [2] W. F. Koehl et al., Nature 479, 84 (2011). [3] A. L. Falk et al., Nature Commun. 4, 1819 (2013).

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**  
**Session H8 DCMP: Superconductivity: CDW's and Chalcogenides 304 -**

**2:30PM H8.00001 Universality of commensurate 4a-period charge density modulations throughout the cuprate pseudogap regime** , ANDREJ MESAROS, LASSP, Department of Physics, Cornell University, KAZUHIRO FUJITA, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, MOHAMMAD HAMIDIAN, Department of Physics, Harvard University, HIROSHI EISAKI, Institute of Advanced Industrial Science and Technology, Tsukuba, SHIN-ICHI UCHIDA, Department of Physics, University of Tokyo, J.C. DAVIS, MICHAEL J. LAWLER, EUN-AH KIM, LASSP, Department of Physics, Cornell University — Theories for the hole-doped Mott insulator, representing underdoped cuprates, are based upon the strong real space ( $r$ -space) interactions, and have long predicted a modulation of charge that is commensurate with the underlying lattice. Such a charge density modulation (CDM) state is unrelated to any momentum space ( $k$ -space) features such as the nesting of regions on a Fermi surface. Experimentally, with increasing hole density, the reported wavevector  $Q$  of the CDM diminishes continuously with increasing hole-density as if driven by  $k$ -space phenomena. Using a novel technique based upon phase-sensitive electronic structure visualization, we demonstrate that the cuprate CDM actually exhibits a commensurate 4a-period throughout the entire underdoped region of the  $Bi_2Sr_2CaCu_2O_8$  phase diagram. Our technique is designed for extracting  $Q$  from inhomogeneous, short-ranged CDM, as the ones observed in experiments. Thus, a strong-interaction  $r$ -space perspective appears to be relevant to achieving a predictive theory for the cuprate pseudogap regime.

**2:42PM H8.00002 Photoemission spectra of charge density wave states in cuprates** , WEI-LIN TU, Dept. of Physics, National Taiwan University, PENG-JEN CHEN, TING-KUO LEE, Institute of Physics, Academia Sinica — Angle-resolved photoemission spectroscopy (ARPES) experiments have reported many exotic properties of cuprates, such as Fermi arc at normal state, two gaps at superconducting state and particle-hole asymmetry at the antinodal direction[1]. On the other hand, a number of inhomogeneous states or so-called charge density waves (CDW) states have also been discovered in cuprates by many experimental groups. The relation between these CDW states and ARPES spectra is unclear. With the help of Gutzwiller projected mean-field theory[2], we can reproduce the quasiparticle spectra in momentum space. The spectra show strong correspondence to the experimental data with afore-mentioned exotic features in it. \pard1. I. Vishik et al, PNAS 109, 18332-18337(2012).. Wei-Lin Tu and Ting-Kuo Lee, arXiv: 1505.07728(2015).

**2:54PM H8.00003 Anisotropic Fermi surface reconstruction in the cuprate superconductor  $\text{YBa}_2\text{Cu}_3\text{O}_y$** , NICOLAS DOIRON-LEYRAUD, OLIVIER CYR-CHOINIERE, SVEN BADOUX, BASTIEN MICHON, AREZOO AFSHAR, ALEXANDRE OUELLET, LOUIS TAILLEFER, University of Sherbrooke, RUIXING LIANG, DOUG BONN, WALTER HARDY, University of British Columbia — Recent X-ray scattering experiments on underdoped  $\text{YBa}_2\text{Cu}_3\text{O}_y$  have revealed a transition from two-dimensional short-range charge-density wave modulations to a state of three-dimensional long-range charge order as a function of magnetic field [1]. Transport experiments have shown that the Fermi surface reconstruction (FSR) occurs at that transition [2]. To examine the symmetry of this FSR we have measured the thermopower of high-quality single crystals of  $\text{YBa}_2\text{Cu}_3\text{O}_y$  with dopings  $p = 0.11$  and  $0.12$  as a function of magnetic field up to  $45$  T. At low temperatures we observe a clear anisotropy of the Seebeck coefficient between the  $a$  and  $b$  axes, strong evidence of a uniaxial stripe-like FSR. The onset of this  $a$ - $b$  anisotropy as a function of magnetic field and temperature correlates well with other transport, thermodynamic, and diffraction measurements, defining a high-magnetic field and low-temperature long-range quasi-1D charge-ordered state. [1] S. Gerber et al., Science aac6257 (2015). [2] G. Grissonanche et al., arXiv:1508.05486.

**3:06PM H8.00004 Correlation strength and  $T_c$ : quantum oscillations in  $\text{YBa}_2\text{Cu}_4\text{O}_8$  under hydrostatic pressure**, C. PUTZKE, L. MALONE, University of Bristol, S. BADOUX, B. VIGNOLLE, D. VIGNOLLES, W. TABIS, LNCMI-Toulouse, P. WALMSLEY, M. BIRD, N.E. HUSSEY, University of Bristol, C. PROUST, LNCMI-Toulouse, A. CARRINGTON, University of Bristol — The unusual normal state electronic structure of the cuprates is widely believed to be at the heart of understanding high-temperature superconductivity in these materials. Recent quantum oscillation measurements in  $\text{YBa}_2\text{Cu}_3\text{O}_{7-d}$  (Y123) have found a strong increase in the quasiparticle effective mass close to two separate critical points in the temperature-doping phase diagram [1]. Here we present a study of quantum oscillations in the double chain cuprate superconductor  $\text{YBa}_2\text{Cu}_4\text{O}_8$  (Y124). Instead of varying the doping by changing  $d$  (in Y123) we study the evolution of the quantum oscillations under hydrostatic pressure. Pressure increases  $T_c$  by around  $0.6\text{K/kbar}$ , primarily, it is thought, by increasing charge transfer between the chains and planes. Unlike in Y123, where the increase in  $T_c$  close to optimal doping is accompanied by a strong increase in quasiparticle mass, in Y124 we find that the mass decreases. Our results suggest that the mechanism that leads to the mass enhancement in the cuprates (most likely the emergence of a competing charge density wave instability) does not directly lead to an enhancement of the superconducting critical temperature. References [1]: B.J. Ramshaw et al. Science 348, 6232 (2014)

**3:18PM H8.00005 Spin-fermion model with overlapping hot spots and charge modulation in cuprates.**, PAVEL A. VOLKOV, Ruhr-Universitt Bochum, KONSTANTIN B. EFETOV, Ruhr-Universitt Bochum; National University of Science and Technology "MISIS", Moscow — We study particle-hole instabilities in the framework of the spin-fermion model. In contrast to previous studies, we assume that adjacent hot spots can overlap due to a shallow dispersion of the electron spectrum in the antinodal region and take the effects of a remnant Coulomb interaction into account. We demonstrate that at sufficiently small values  $|\varepsilon(\pi, 0) - E_F| < \Gamma$ , where  $\Gamma$  is a characteristic energy of the fermion-fermion interaction due to the paramagnons, the leading particle-hole instability is a d-form factor Fermi surface deformation rather than the charge modulation along the Brillouin zone diagonals. At lower temperatures, we find that the deformed Fermi surface is further unstable to formation of a d-form factor charge density wave (CDW) with a wave vector along one of the Brillouin zone axes. These findings can explain the robustness of this order in hole-doped cuprates. The approximations made are justified by a small parameter that allows one an Eliashberg-like treatment. Comparison with experiments suggests that in many cuprate compounds the prerequisites for the proposed scenario are indeed fulfilled and the results obtained may explain important features of the charge modulations observed recently.

**3:30PM H8.00006 X-ray diffraction study of charge density wave fluctuations in  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  under uniaxial pressure**, THOMAS CROFT, CHRISTOPHER LESTER, University of Bristol, ALESSANDRO BOMBARDI, BENJAMIN MOSER, Diamond Light Source, STEPHEN HAYDEN, University of Bristol — Charge density wave (CDW) order now appears to be a universal feature of the cuprate phase diagram.  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  (LSCO) is a canonical example with a simple crystal structure and  $T_{\text{CDW}} \sim 80$  K. In other 214-cuprates (LBCO, Eu/Nd-LSCO), the onset of CDW order is closely associated with a transition from a low-temperature orthorhombic (LTO) to a low-temperature tetragonal (LTT) phase. Despite lack of long range LTT order in LSCO, several experiments detect the presence of local LTT regions. These may arise from LTO domain boundaries that support the LTT structure and also serve as the origin of the CDW. Here we report X-ray diffraction measurements on LSCO ( $x = 0.13$ ) under applied uniaxial strain. The experiment utilized a piezo-based device allowing the sample to be detwinned *in-situ*. In the absence of applied strain, a transition to the LTO phase is observed at  $\sim 230$  K. LTT type peaks are also observed at this temperature and CDW order is seen to set in  $< 100$  K. On application of compressive strain, the amplitude and onset temperature of LTT and CDW phases are largely unaffected after removing domain boundaries suggesting these phases originate from a fluctuating state within the bulk and are not simply localized around boundary regions.

**3:42PM H8.00007 Seebeck coefficient of underdoped LSCO in high magnetic fields : Fermi-surface reconstruction by charge-density-wave order**, SVEN BADOUX, AREZOO AFSHAR, BASTIEN MICHON, ALEXANDRE OUELLET, SIMON FORTIER, NICOLAS DOIRON-LEYRAUD, LOUIS TAILLEFER, University of Sherbrooke, Sherbrooke, Canada, DAVID LEBOEUF, LNCMI, Grenoble, France, THOMAS CROFT, STEPHEN HAYDEN, University of Bristol, Bristol, UK, HIDENORI TAKAGI, University of Tokyo, Tokyo, Japan, KAZUYOSHI YAMADA, Tohoku University, Sendai, Japan, DAVID GRAF, NHMFL, Tallahassee, USA — The Seebeck coefficient  $S$  of the hole-doped cuprate  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  (LSCO) was measured in magnetic fields large enough to suppress superconductivity, for a range of Sr concentrations  $x$  in the underdoped regime. For  $x = 0.12, 0.125$  and  $0.13$ ,  $S/T$  is seen to drop upon cooling and become negative at low temperature. The same behavior is observed in the Hall coefficient  $R_H(T)$ . In analogy with other hole-doped cuprates at similar hole concentrations [1-4], the sign change in  $S$  and  $R_H$  shows that the Fermi surface of LSCO undergoes a reconstruction caused by the onset of charge-density-wave modulations. Such modulations have indeed been detected in LSCO by X-ray diffraction in precisely the same doping range [5].

- [1] D. LeBoeuf et al., Nature 450, 533 (2007).
- [2] D. LeBoeuf et al., Phys. Rev. B 83, 054506 (2011).
- [3] F. Laliberte et al., Nat. Commun. 2, 432 (2011).
- [4] N. Doiron-Leyraud et al., Phys. Rev. X 3, 021019 (2013).
- [5] T. Croft et al., Phys. Rev. B 89, 224513 (2014).

**3:54PM H8.00008 Doping dependence of the charge-density-wave order in  $\text{HgBa}_2\text{CuO}_{4+\delta}$** , BIQIONG YU, School of Physics and Astronomy, University of Minnesota — Following the original discovery of short-range charge-density-wave (CDW) order in the orthorhombic double-layer cuprate  $\text{YBa}_2\text{Cu}_3\text{O}_{6+\delta}$  (YBCO) below optimal doping, resonant X-ray scattering measurements have revealed that the simple tetragonal single-layer compound  $\text{HgBa}_2\text{CuO}_{4+\delta}$  (Hg1201;  $T_c = 71$  K) exhibits short-range CDW order as well [1]. Here we report on the doping dependence of the CDW order in Hg1201 and contrast our results with the extensive data available for YBCO [2]. Work done in collaboration with: W. Tabis, G. Yu, M.J. Veit, N. Barišić, M.K. Chan, C.J. Dorow, X. Zhao, M. Greven (University of Minnesota); M. Bluschke, E. Weschke (BESSY, Berlin); T. Kolodziej, I. Bialo, A. Kozłowski (AGH, Krakow); M. Hepting, H. Gretarsson, M. Le Tacon, M. Minola, B. Keimer (MPI, Stuttgart); Ronny Sutarto (CLS, Saskatoon); Y. Li (PKU, Beijing); L. Braicovich, G. Dellea, G. Ghiringhelli (CNR-SPIN, Milano); A. Kreyssig, M. Ramazanoglu, A.I. Goldman (Iowa State University and Ames Lab); T. Schmitt (PSI, Switzerland). [1] W. Tabis et al., Nature Comm. 5, 5875 (2014), [2] R. Comin and A. Damascelli, arXiv:1509.03313.

<sup>1</sup>We acknowledge the support from US Department of Energy, Office of Basic Energy Sciences

**4:06PM H8.00009 Nematicity in Stripe Ordered Cuprates Probed via Resonant X-Ray Scattering**, CHRISTOPHER MCMAHON, ANDREW ACHKAR, University of Waterloo, MARTIN ZWIEBLER, Leibniz Institute for Solid State Materials Research IFW Dresden, FEIZHOU HE, RONNY SUTARTO, Canadian Light Source, ISIAH DJANTO, ZHIHAO HAO, MICHEL GINGRAS, University of Waterloo, MARKUS HUCKER, GENDA GU, Brookhaven National Laboratory, ALEXANDRE REVCOLEVSKI, Synthese, Propriétés et Modélisation des Matériaux (SP2M), HARRY ZHANG, None, YOUNG-JUNE KIM, University of Toronto, JOCHEN GECK, Leibniz Institute for Solid State Materials Research IFW Dresden, DAVID HAWTHORN, University of Waterloo — In underdoped cuprate superconductors, a rich competition occurs between superconductivity and charge density wave (CDW) order. Under debate, however, is whether rotational symmetry breaking (nematicity) also plays a central role - whether it occurs intrinsically and generically or merely as a consequence of other orders. Here we employ resonant x-ray scattering in stripeordered  $(\text{La,M})_2\text{CuO}_4$  to probe the relationship between electronic nematicity of the Cu  $3d$  orbitals, structure of the  $(\text{La,M})_2\text{O}_2$  layers and CDW order. We find distinct temperature dependencies of the structure of the  $(\text{La,M})_2\text{O}_2$  layers and the electronic nematicity of the  $\text{CuO}_2$  planes, with only the latter being enhanced by the onset of CDW order. These results suggest electronic nematicity is an order parameter that is distinct from a purely structural order parameter in underdoped cuprates.

**4:18PM H8.00010 Innovative uses of X-ray FEL and the pulsed magnets: High magnetic field X-ray scattering studies on quantum materials**, H. JANG, SLAC, H. NOJIRI, Tohoku Univ., S. GERBER, W.-S. LEE, D. ZHU, J.-S. LEE, C.-C. KAO, SLAC — X-ray scattering under high magnetic fields provides unique opportunities for solving many scientific puzzles in quantum materials, such as strongly correlated electron systems. Incorporating high magnetic field capability presents serious challenges at an x-ray facility, including the limitation on the maximum magnetic field even with a DC magnet (up to ~20 Tesla), expensive cost in development, radiation damage, and limited flexibility in the experimental configuration. These challenges are especially important when studying the symmetry broken state induced by the high magnetic field are necessary, for example, exploring intertwined orders between charge density wave (CDW) and high  $T_c$  superconductivity. Moreover, a gap in magnetic field strengths has led to many discrepancies and puzzling issues for understanding strongly correlated systems – is a CDW competing or more intimately intertwined with high-temperature superconductivity. To bridge this gap and resolve these experimental discrepancies, one needs an innovative experimental approach. Here, we will present a new approach to x-ray scattering under high magnetic field up to 28 Tesla by taking advantage of brilliant x-ray free electron laser (FEL). The FEL generates sufficiently high photon flux for single shot x-ray scattering experiment. In this talk, we will also present the first demonstration about the field induced CDW order in YBCO Ortho-VIII with 28 Tesla, which show the totally unexpected three-dimensional behavior.

**4:30PM H8.00011 Evidence for charge density wave order in the quasi-1D Superconductor  $\text{Ta}_4\text{Pd}_3\text{Te}_{16}$** , TONI HELM<sup>\*1</sup>, Lawrence Berkeley National Laboratory, University of California, Berkeley, CA, USA, ROBERT KEALHOFER, PHILIP J. W. MOLL\*, ZHENGLU LI, NICHOLAS P. BREZNAY, IAN HAYES, FELIX FLICKER, University of California, Berkeley, CA, USA, ROSS MACDONALD, LUIS BALICAS, National High Magnetic Field Laboratory, USA, STEVEN LUI, JAMES G. ANALYTIS, University of California, Berkeley, CA, USA — One dimensional metals are commonly susceptible to electronic instabilities such as density waves. Only recently the ternary Chalcogenide  $\text{Ta}_4\text{Pd}_3\text{Te}_{16}$  (TPT) was observed to superconduct below  $T_c = 4.6\text{ K}$  [1]. Band structure calculations predict a complex multiband Fermi surface in TPT, including strongly nested quasi 1D bands[2]. Despite this one-dimensional character, no evidence for a Peierls transition has been reported and its superconductivity below  $T_c$  was suggested to be unconventional. We investigate this puzzle by high-field quantum oscillation experiments and contrast them with first-principles band-structure calculations. Our quantum oscillation experiments in high magnetic fields confirmed the presence of 2D and 3D bands. Our magnetotransport measurements on microstructures fabricated by focused ion beam etching reveal an anomaly above  $T_c$ , suggesting the onset of charge density wave ordering. [1] W. H. Jiao et al. J. Am. Chem. Soc. 136, 1284 (2014) [2] D. Singh, PRB 90, 144501 (2014)

<sup>1\*</sup> Current address: Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany

**4:42PM H8.00012 Things that make  $\text{TiSe}_2$  superconducting**, IVO PLETIKOSIC, HUIXIA LUO, WEIWEI XIE, ELIZABETH SEIBEL, JASON KRIZAN, ROBERT CAVA, Princeton Univ, TONICA VALLA, Brookhaven National Laboratory — The unusual charge density wave phase in  $\text{TiSe}_2$  is accompanied by superconductivity when electron dopants like copper and palladium are intercalated between the layers of this transition-metal dichalcogenide. But when nominally one-electron donors like tantalum and niobium are brought in to replace titanium,  $\text{Ti}_{1-x}\text{Ta}_x\text{Se}_2$  is superconducting and  $\text{Ti}_{1-x}\text{Nb}_x\text{Se}_2$  not. We investigated by angle-resolved photoemission (ARPES) the origins of this behavior by comparing the electronic band structure of pristine  $\text{TiSe}_2$  and the two doped compounds. We question whether the effect can be attributed to the differences in electron doping only.

**4:54PM H8.00013 Resonance-state-induced superconductivity at high Indium contents in In-doped  $\text{SnTe}$** , NEEL HALDOLAARACHCHIGE, Saint Joseph's University, QUINN GOBSON, WEIWEI XIE, MORTEN NIELSEN, SATYA KUSHWAHA, ROBERT CAVA, Princeton University, CAVA'S GROUP TEAM — We report a reinvestigation of superconducting  $\text{Sn}_{1-x}\text{In}_x\text{Te}$  at both low and high In doping levels. Analysis of the superconductivity reveals a fundamental change as a function of  $x$ : the system evolves from a weakly coupled to a strongly coupled superconductor with increasing indium content. Hall Effect measurements further show that the carrier density does not vary linearly with Indium content; indeed at high Indium content, the samples are overall n-type, which is contrary to expectations of the standard picture of  $\text{In}^{1+}$  replacing  $\text{Sn}^{2+}$  in this material. Density functional theory calculations probing the electronic state of In in  $\text{SnTe}$  show that it does not act as a trivial hole dopant, but instead forms a distinct, partly filled In  $5s$  - Te  $5p$  hybridized state centered around  $E_F$ , very different from what is seen for other nominal hole dopants such as Na, Ag, and vacant Sn sites. We conclude that superconducting In-doped  $\text{SnTe}$  therefore cannot be considered as a simple hole doped semiconductor.

**5:06PM H8.00014 Fermiology of the low carrier density superconductor Tl-doped  $\text{PbTe}$ , and its non-superconducting analog, Na-doped  $\text{PbTe}$ .**, PAULA GIRALDO-GALLO, Stanford University and National High Magnetic Field Laboratory, PHILIP WALMSLEY, Stanford University, BORIS SANGIORGIO, MICHAEL FECHNER, ETH Zurich, LISA BUCHAUER, BENOIT FAUQUE, ESPCI, Paris, France, SCOTT RIGGS, National High Magnetic Field Laboratory, ROSS MCDONALD, Los Alamos National Laboratory, THEODORE GEBALLE, Stanford University, NICOLA SPALDIN, ETH Zurich, KAMRAN BEHNIA, ESPCI, Paris, France, IAN FISHER, Stanford University —  $\text{PbTe}$  is a narrow band gap semiconductor, which can be electron- or hole-doped, obtaining typical carrier densities of the order of  $1 \times 10^{20} \text{ cm}^{-3}$ . The only impurity known to produce superconductivity in this host material is Tl, resulting in a maximum critical temperature of 1.5K - an order of magnitude higher than the  $T_c$  observed in similar low carrier density semiconductors. In this work we performed a full Fermi surface characterization of  $\text{Pb}_{1-x}\text{Tl}_x\text{Te}$ , as well as its non-superconducting analog,  $\text{Pb}_{1-x}\text{Na}_x\text{Te}$ , via Shubnikov de Haas oscillations in magnetotransport, for magnetic fields up to 35T (DC). Our results show that beyond a critical impurity concentration close to the emergence of superconductivity, there are clear differences in the normal-state carriers. In non-superconducting  $\text{Pb}_{1-x}\text{Na}_x\text{Te}$ , all carriers reside at four ellipsoidal pockets of the Fermi surface, while in superconducting  $\text{Pb}_{1-x}\text{Tl}_x\text{Te}$ , there is an additional set of carriers, consistent with incoherent resonant impurity levels. The presence or absence of these states at or near the Fermi energy is intimately connected to the presence or absence of superconductivity in doped  $\text{PbTe}$ .

we would like to present back-to-back with the following contribution:

Paula Giraldo-Gallo et al., "Fermiology of the low carrier density superconductor Tl-doped  $\text{PbTe}$ , and its non-superconducting analog, Na-doped  $\text{PbTe}$ "

### 5:18PM H8.00015 First-principles Fermi surface of doped

Zurich, PAULA GIRALDO-GALLO, Stanford University, MICHAEL FECHNER, Materials Theory, ETH Zurich — PbTe is a narrow-gap semiconductor and one of the few materials where a superconducting state is observed. When doped with Tl atoms an unusual superconducting state is observed that persists to  $\sim 1.5$  K, the nature of the superconductivity is not well understood, with a charge Kondo effect suggested as the origin. We will discuss the electronic properties - in particular the Fermi surface - of doped PbTe using first-principles calculations. We compute de Haas-van Alphen frequencies and compare them to recent quantum-oscillations experiments. We confirm the usefulness of the rigid-band approximation for Na impurities. In contrast, we find for Tl impurities: a narrow "impurity band" (originating from hybridization between Tl  $s$  and Te  $p$  orbitals) and a charge disproportionation instability, such as a charge disproportionation, which is likely relevant for the superconductivity.

Thank you very much!

## Tuesday, March 15, 2016 2:30PM - 5:18PM –

Session H11 DMP: Correlations and Superconductivity in Fe Chalcogenides | 307 - Amalia Coldea, Oxford University

### 2:30PM H11.00001 Systematic investigation of the electron Fermi surface dominated FeSe

based systems, DONGLAI FENG, Dept. of Physics, Fudan University — FeSe-based superconductors exhibit very rich phenomena. We systematically investigate the behavior of isovalent doping and electron carrier doping effects in a variety of FeSe-based superconductors with angle-resolved photoemission spectroscopy (ARPES). For the isovalent-doped  $A_x\text{Fe}_2(\text{Se}, \text{S/Te})_2$ , a continuous decreasing bandwidth is observed from the heavily S doped side to the highly Te doped side, while the system ground state evolves from a metal to a superconductor, and eventually to a correlation-driven insulator. On the other hand, when electron doping is introduced by surface K dosing on bulk FeSe or thick FeSe films, the system ground state evolves from a nematic metal to a superconductor, and then an insulator before it becomes a metal again. Correlation is found to increase with electron doping as well. These two intriguing phase diagrams of FeSe-based superconductors highlight the important role of correlations on the ground state, and provide a microscopic understanding of various FeSe-based superconductors, including the recently discovered  $(\text{Li,Fe})\text{OHFeSe}$ . Reference [1] X. H. Niu et al. Phys. Rev. B 92, 060504(R) (2015). [2] C. H. P. Wen et al. arXiv:1508.05848. [3] X. H. Niu et al. arXiv:1506.04018.

### 3:06PM H11.00002 Observation of two distinct $dxz/dyz$ band splittings in FeSe

, PENG ZHANG, TIAN QIAN, PIERRE RICHARD, Institute of Physics, CAS, XIAOPING WANG, Department of Physics, Tsinghua University, HU MIAO, BAIQING LV, BINBIN WU, Institute of Physics, CAS, THOMAS WOLF, CHRISTOPH MEINGAST, Institut für Festkörperphysik, Karlsruhe Institute of Technology, XIANXIN WU, Institute of Physics, CAS, ZIJIANG WANG, Department of Physics, Boston College, JIANGPING HU, HONG DING, Institute of Physics, CAS — We report the temperature evolution of the detailed electronic band structure in FeSe single crystals measured by angle-resolved photoemission spectroscopy (ARPES), including the degeneracy removal of the  $dxz$  and  $dyz$  orbitals at the  $\Gamma$  and M points, and the orbital-selective hybridization between the  $dxz$  and  $dyz$  orbitals. The temperature dependences of the splittings at the  $\Gamma$  and M points are different, indicating that they are controlled by different order parameters. The splitting at the M point is closely related to the structural transition and is attributed to orbital ordering defined on Fe-Fe bonds with a d-wave form in the reciprocal space that breaks the rotational symmetry. In contrast, the band splitting at the  $\Gamma$  points remains at temperature far above the structural transition. Although the origin of this latter splitting remains unclear, our experimental results exclude the previously proposed ferro-orbital ordering scenario.

### 3:18PM H11.00003 The effects of local correlations on the electronic structure of FeSe<sup>1</sup>

, MATTHEW WATSON, TIMUR KIM, Diamond Light Source, Harwell Campus, Didcot, OX11 0DE, AMIR HAGHIGHIRAD, AMALIA COLDEA, Clarendon Laboratory, Department of Physics, University of Oxford, Parks Road, Oxford OX1 3PU — FeSe is structurally the simplest of Fe-based superconductors, but its complex and unique properties pose important theoretical questions. One important aspect of the physics of FeSe is the understanding of the strength and effects of electronic correlations. In order to explore this, we have performed angle-resolved photo-emission spectroscopy (ARPES) measurements on high quality bulk single crystals of FeSe over a wide range of binding energies, in different scattering geometries and with varying incident photon energies, analysing the quasiparticle renormalisations, scattering rates and degree of coherence. We find that FeSe exhibits moderately strong, orbital-dependent correlation effects which are understood to arise primarily due to local electron-electron interactions on the Fe sites. We conclude that electronic correlations constitute a key ingredient in understanding the electronic structure of FeSe.

<sup>1</sup>Part of this work was supported by EPSRC, UK (EP/I004475/1, EP/I017836/1). We thank Diamond Light Source for access to Beamline I05.

### 3:30PM H11.00004 Magnetic interactions in FeSe studied by first principle calculations<sup>1</sup>

, SHUAI WANG, FA WANG, Peking Univ — Based on first principle calculations we have investigated the evolution of magnetism in free-standing monolayer FeSe with respect to lattice constant and magnetism in bulk FeSe. The computational results show that the magnetic order in free-standing monolayer FeSe will change from anti-ferromagnetic pair-checkboard order to stripe collinear order along with enlarging lattice constant. The magnetic order in bulk FeSe will change from stripe collinear order to anti-ferromagnetic pair-checkboard order only if structure reconstruction is allowed. We use  $J_1$ - $J_2$ - $K_1$  model to fit the calculated total energies of different magnetic orders to study magnetic interaction strengths in FeSe. The fitting results of  $J_1$ - $J_2$ - $K_1$  indicate that magnetic interactions in FeSe are quite strong and highly frustrated, and increase slowly with enlarging lattice parameter.

<sup>1</sup>This work was supported by the National Key Basic Research Program of China (Grant No. 2014CB920902) and the National Science Foundation of China (Grant No. 11374018).

**3:42PM H11.00005 Highly accurate calculation of the magnetic properties of FeSe and FeTe using first principles quantum Monte Carlo<sup>1</sup>**, BRIAN BUSEMEYER, University of Illinois at Urbana-Champaign, MARIO DAGRADA, SANDRO SORELLA, University Pierre et Marie Curie, MICHELE CASULA, SISSA, LUCAS K. WAGNER, University of Illinois at Urbana-Champaign — While the origin of superconductivity in the iron-based materials is still controversial, the proximity of the superconductivity to magnetic order is suggestive that magnetism may be important. We use first principles quantum Monte Carlo (QMC) techniques to obtain an accurate microscopic picture of the effects of magnetic configurations on the electronic structure of FeSe under pressure. The QMC calculations reproduce experimental values for bulk modulus, lattice constants, bandwidth, and lowest energy magnetic ordering. The relative energy of magnetic orderings is rather different from standard density functional theory calculations, which may warrant a reassessment of the role of magnetism in this material. We analyze the correlated wave functions to obtain a microscopic explanation for the spontaneous  $S_4$  symmetry-breaking in this material, and contrast these results with the non-superconducting case of FeTe.

<sup>1</sup>This presentation is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research, Scientific Discovery through Advanced Computing (SciDAC) program under Award Number FG02-12ER46875

**3:54PM H11.00006 Quadrupolar Spin Orders in FeSe**, ZHENTAO WANG, ANDRIY NEVIDOMSKYY, Department of Physics and Astronomy, Rice University — Motivated by the absence of long-range magnetic order and the strong spin fluctuations observed in the Fe-based superconductor FeSe, we study spin-1 model on a square lattice up to next-nearest neighbor Heisenberg and biquadratic spin exchanges. The zero-temperature variational phase diagram gives the conventional antiferromagnetic order and also more exotic quadrupolar spin phases. These quadrupolar phases do not host long-range magnetic order and preserve time-reversal symmetry, but break the spin  $SU(2)$  symmetry. In particular, we observe a robust ferroquadrupolar order (FQ) in immediate proximity to the columnar AFM phase. We envision that FeSe may be positioned within the FQ phase close to the phase boundary. Using the flavor-wave technique, we calculate the structure factor inside the FQ phase and find a Goldstone mode emerging from  $Q = (0, 0)$ , which however bears zero spectral weight at  $\omega = 0$  due to time reversal symmetry. At the same time, we observe strong spin fluctuations near  $(\pi, 0)/(0, \pi)$ , which agrees with the recent neutron scattering experiments. Further, we calculate the higher order interactions between the  $(\pi, 0)$  and  $(0, \pi)$  spin fluctuations inside the FQ phase, which may shed light on the  $C_4$  symmetry breaking in the nematic phase of FeSe.

**4:06PM H11.00007 Electronic correlations and topological Fermi surface transition in the iron-based chalcogenides**, S. SKORNYAKOV, Institute of Metal Physics, Yekaterinburg, Russia and Ural Federal Univ., Yekaterinburg, Russia, I. LEONOV, Theoretical Physics III, Center for Electronic Correlations and Magnetism, Univ. Augsburg, Germany, V.I. ANISIMOV, Institute of Metal Physics, Yekaterinburg, Russia and Ural Federal Univ., Yekaterinburg, Russia, D. VOLLHARDT, Theoretical Physics III, Center for Electronic Correlations and Magnetism, Univ. Augsburg, Germany — We present results of a theoretical investigation of the electronic structure and phase stability of paramagnetic FeSe obtained within a combination of *ab initio* methods for calculating band structure and dynamical mean-field theory. Our results reveal an entire reconstruction of the Fermi surface topology upon a moderate expansion of the lattice (Lifshitz transition), with a change of magnetic correlations from the in-plane magnetic wave vector  $(\pi, \pi)$  to  $(\pi, 0)$ . We attribute this behavior to a correlation-induced shift of the Van Hove singularity originating from the  $xy$  and  $xz/yz$  bands at the M-point across the Fermi level. Our results predict a structural transition of FeSe upon a ca. 10 % expansion of the lattice volume as well as a topological change of the Fermi surface of FeSe upon partial substitution Se by Te, which is accompanied with a sharp increase of the local moments. We expect that these changes are responsible for the experimentally observed increase of  $T_c$  in FeSe upon doping with Te. The microscopic origin for superconductivity in this system is then due to a Van Hove singularity close to the Fermi level. This identification may open a new route to increase  $T_c$  even further.

**4:18PM H11.00008 Effect of hydrostatic pressure on the structural and magnetic transitions in FeSe**, K. KOTHAPALLI\*, A. E. BÖHMER\*, W. T. JAYASEKARA\*, P. DAS\*, A. SAPKOTA\*, B. G. UELAND\*, V. TAUFOR\*, S. L. BUD'KO\*, P. C. CANFIELD\*, Y. XIAO<sup>+</sup>, A. I. GOLDMAN, A. KREYSSIG\*, \*Ames Laboratory, Dept. of Phys. and Astro., Iowa State University, IA, USA; <sup>+</sup>Argonne National Laboratory, Argonne, IL, USA — The phase diagram of FeSe is unique among all the iron-based superconductors. At ambient pressure, FeSe undergoes a tetragonal-to-orthorhombic structural phase transition at  $T_s = 90$  K, and becomes superconducting below  $T_c = 8$  K. Unlike other iron-based materials, it does not magnetically order down to the lowest measured temperature ( $T$ ). However, under the application of hydrostatic pressure ( $p$ ), a new magnetic phase is stabilized starting from  $\sim 1$  GPa. Higher pressure increases  $T_c$ , whose maximum onset reaches a surprising 37 K at  $\sim 7$  GPa. We investigate the  $p$ - $T$  phase diagram using high-quality vapor-grown single crystals, which shows features not seen previously in powder and mixed-phase samples. Specifically, using high-pressure low-temperature diffraction and synchrotron Mössbauer we elucidate the effect of pressure - evolution of orthorhombic distortion and emergence of magnetic ordering - in the vicinity of the crossover region of the structural, magnetic and superconducting transitions. Work at Ames Lab. was supported by the DOE, BES, Division of Materials Sciences & Engineering, under Contract No. DEAC02-07CH11358. This research used resources at Argonne National Lab.

**4:30PM H11.00009 Neutron Scattering Study of Low Energy Magnetic Excitation in superconducting Te-vapor annealed under-doped FeTeSe**, ZHIJUN XU, MING YI, UC Berkeley, GUANGYONG XU, J. A. SHNEELOCH, Brookhaven National Laboratory, MASAOKI MATSUDA, SONGXUE CHI, Oak Ridge National Laboratory, GENDA GU, J. M. TRANQUADA, Brookhaven National Laboratory, R.J. BIRGENEAU, UC Berkeley — To study the interplay between magnetism and superconductivity, we have performed neutron scattering and magnetization measurements on a Te vapor annealed single crystal  $\text{Fe}_{1-y}\text{Te}_{0.85}\text{Se}_{0.2}$  ( $T_c \sim 13$ K) sample. Te vapor annealed process is found to reduce/remove the excess Fe in the as-grown sample and make the under-doped originally non-superconducting sample become good superconducting sample. Our neutron scattering studies show both spin gap and spin resonance found in the Te vapor annealed superconducting sample. Comparing to commensurate spin resonance in as-grown optimal-doped sample, the spin resonance of Te annealed sample only shows up at the clearly incommensurate positions. The temperature and energy dependence of low energy magnetic excitations are also measured in the sample. This work is supported by the Office of Basic Energy Sciences, DOE.

**4:42PM H11.00010 Thermal evolution of antiferromagnetic correlations and tetrahedral bond angles in superconducting  $\text{FeTe}_{1-x}\text{Se}_x$** , GUANGYONG XU, Brookhaven National Laboratory, ZHIJUN XU, UC Berkeley, JOHN SCHNEELOCH, Brookhaven National Laboratory, JINSHENG WEN, Nanjing University, EMIL BOZIN, Brookhaven National Laboratory, BARRY WINN, M. FEYGENSON, Oak Ridge National Laboratory, R. J. BIRGENEAU, UC Berkeley, GENDA GU, IGOR ZALIZNYAK, JOHN TRANQUADA, Brookhaven National Laboratory — We will present neutron scattering measurements of low energy magnetic excitations from superconducting  $\text{FeTe}_{1-x}\text{Se}_x$  samples. A model with short-range correlated spin plaquettes characterized by particular antiferromagnetic wave vectors is used to describe the measured magnetic scattering data in the (HK0) plane. We show that the characteristic antiferromagnetic wave vector evolves from that characteristic of the bicollinear structure characteristic of  $\text{FeTe}_{1-x}\text{Se}_x$  (at high temperature) to that associated with the stripe structure of antiferromagnetic iron arsenides (at low temperature). We also present powder neutron diffraction results for lattice parameters in  $\text{FeTe}_{1-x}\text{Se}_x$  indicating that the tetrahedral bond angle tends to increase towards the ideal value on cooling, with a corresponding reduction in crystal-field splitting of the Fe 3d orbitals. We suggest that the thermal change in spin correlations implies a relative change among the exchange couplings, and that this is associated with changes in orbital occupancies. Finally, while the magnitude of the low energy magnetic spectral weight is substantial at all temperatures, it actually weakens somewhat at low temperature, where the charge carriers become more itinerant.

**4:54PM H11.00011 Physical properties of superconducting single crystal iron sulfide**, EFRAIN E. RODRIGUEZ, CHRISTOPHER K. H. BORG, XIUQUAN ZHOU, JOHNPierre PAGLIONE, University of Maryland, UNIVERSITY OF MARYLAND COLLABORATION — Recently, the simple binary tetragonal iron sulfide, FeS, was found to be a superconductor with a  $T_c = 5\text{K}$ . [1] We have prepared single crystals of tetragonal iron sulfide through hydrothermal de-intercalation of  $\text{K}_x\text{Fe}_{2-y}\text{S}_2$ . The  $\text{K}_x\text{Fe}_{2-y}\text{S}_2$  single crystal precursors were grown by slow cooling of stoichiometric melts of K, Fe and S. The silver, plate-like FeS single crystals were highly crystalline with a superconducting transition temperature ( $T_c$ ) of 4 K. The high quality of the FeS crystals revealed highly anisotropic nature of the magnetic and electronic properties intrinsic to FeS. The physical properties and thermal stability of single crystal FeS will be discussed in detail. [1] Lai X, et al., *JACS* **2015** 137 (32)

**5:06PM H11.00012 Structure and Magnetic Interactions in FeS: A low- $T_c$  superconductor**, S. J. KUHN, University of Notre Dame and Oak Ridge National Laboratory, M. R. ESKILDSEN, University of Notre Dame, L. DEBEER-SCHMITT, L. LI, C. DE LA CRUZ, A. S. SEFAT, Oak Ridge National Laboratory (ORNL) — Tetragonal-phase iron sulfide (FeS), with the same structure as the well-known superconductor FeSe ( $T_c \sim 8\text{K}$ ), was recently discovered as a superconductor with a  $T_c$  of  $\sim 5\text{K}$  [1]. Although it has been difficult to synthesize this binary in pure tetragonal, crystalline, and superconducting form by various methods (e.g. [2]), the simple low-temperature hydrothermal method yields pure FeS products. Careful composition and particle size analyses, in addition to the results of neutron diffraction and magnetization across transition temperature(s), will be presented. Preliminary results show high sensitivity of pure products to synthesis procedure, particle sizes of  $\sim 40\text{nm}$ , and phase transitions in addition to  $T_c$ . We explain reasons for superconductivity. [1] Lai, X. et al, *Jour. Amer. Chem. Soc.*, 137, 10148 (2015). [2] Sines, I. T. et al. *Jour. Sol. Stat. Chem.*, 196, 17 (2012). The work of AS, LL, and SJK is supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES); SJK is supported by the DOE, Office of Science Graduate Student Research (SCGSR) Award. MRE is funded by the Office of BES (DE-FG02-10ER46783). The work at ORNLs High Flux Isotope Reactor (HFIR) was sponsored by the Scientific User Facilities Div., BES (LDS, CC)

## Tuesday, March 15, 2016 2:30PM - 5:30PM –

### Session H12 FIAP GMAG: Beyond STT-MRAM: Future Perspective for Spintronics Devices

308 - Ernesto E. Marinero, Supriyo Datta, Purdue University

**2:30PM H12.00001 Magnetic skyrmions : new solitons on the track for future memories and logic applications.**, VINCENT CROS, Unit Mixte de Physique CNRS/Thales — Magnetic skyrmions are arguably the smallest topologically non-trivial magnetic configurations [1]. These solitons are nanoscale spin configurations that hold promise as information carriers in ultra-dense memory and logic devices owing to the extremely low threshold currents densities for initiating their dynamics [2]. Up to now however magnetic skyrmions have been observed mostly at very low temperature in a few exotic materials and ultra-thin films. Here, I will illustrate the wealth of skyrmions with some of our recent experimental and numerical results stabilized at room temperature in magnetic multilayers due to interfacial chiral interaction. This discovery of stable sub-100 nm individual skyrmions at room temperature [3,4] in a technologically relevant material opens the way for the development of several concepts of skyrmion based memory devices going from race-track memory type to MRAMS, rf devices, logic gates, transistors. [1] Bogdanov, A. N. and Roessler, U. K. *Phys. Rev. Lett.* 87, 037203 (2001). ; [2] N. Nagaosa, Y. Tokura, *Nature Nanotech.* 8, 899 (2013), [3] J. Sampaio, et al, *Nat. Nanotech.* 8, 839 (2013). ; [4] C. Moreau-Luchaire et al, arXiv: 1502.07853. — Authors : V. Cros1, C. Moreau-Luchaire1, C. Moutafis2,3, N. Reyren1, J. Sampaio1,5, C.A.F. Vaz2, P. Warnicke2, D. Maccariello1, N. Vanhorne1, F. Garcia-Sanchez3, K. Bouzehouane1, K. Garcia1, C. Deranlot1, S. Rohart4, J.M. George1, J. Raabe2, J.V. Kim3, A. Thiaville4, A. Fert1 1 Unité Mixte de Physique CNRS Thales, Univ. Paris-Sud, Université Paris-Saclay, Palaiseau, France 2 Swiss Light Source, Paul Scherrer Institute, Villigen, Switzerland 3 School of Computer Science, University of Manchester, Manchester, UK 4 Institut d'Electronique Fondamentale, Univ. Paris-Sud, CNRS, Orsay, France 5 Lab. de Physique des Solides, CNRS, Univ. Paris-Sud, Orsay, France — Acknowledgements : ANR ULTRASKY and EU grant MAGicSky No. FET-Open-665095 are acknowledged for financial support.

**3:06PM H12.00002 Novel spintronics devices for memory and logic: prospects and challenges for room temperature all spin computing**, JIAN-PING WANG, Electrical and Computer Engineering Dept., Univ of Minnesota — An energy efficient memory and logic device for the post-CMOS era has been the goal of a variety of research fields. The limits of scaling, which we expect to reach by the year 2025, demand that future advances in computational power will not be realized from ever-shrinking device sizes, but rather by innovative designs and new materials and physics. Magnetoresistive based devices have been a promising candidate for future integrated magnetic computation because of its unique non-volatility and functionalities. The application of perpendicular magnetic anisotropy for potential STT-RAM application was demonstrated and later has been intensively investigated by both academia and industry groups, but there is no clear path way how scaling will eventually work for both memory and logic applications. One of main reasons is that there is no demonstrated material stack candidate that could lead to a scaling scheme down to sub 10 nm. Another challenge for the usage of magnetoresistive based devices for logic application is its available switching speed and writing energy. Although a good progress has been made to demonstrate the fast switching of a thermally stable magnetic tunnel junction (MTJ) down to 165 ps, it is still several times slower than its CMOS counterpart. In this talk, I will review the recent progress by my research group and my C-SPIN colleagues, then discuss the opportunities, challenges and some potential path ways for magnetoresistive based devices for memory and logic applications and their integration for room temperature all spin computing system.

**3:42PM H12.00003 In Search of New Spintronic Devices Using the Modular Approach<sup>1</sup>**, KEREM YUNUS CAMSARI, Purdue University — There has been enormous progress in the last two decades, effectively combining spintronics and magnetism into a powerful force that is shaping the field of memory devices. At the same time, new materials and phenomena continue to be discovered at a very fast pace, providing an ever-increasing set of building blocks that could be exploited in designing functional devices of the future. Through careful benchmarking against available theory and experiment we recently established a set of “elemental” circuit modules representing a diverse range of materials and phenomena [1], which are continually updated [2]. We will first show how these elemental modules can be integrated seamlessly to model both spintronic transport and nanomagnetic dynamics, starting from basic spin-valves and extending to complex experimental structures. We will then show how this framework can be used to design transistor-like spintronic devices to provide novel functionality compared to a standard complementary metal oxide semiconductor (CMOS) device. This approach allows us to incorporate the detailed physics of diverse sophisticated phenomena accurately into detailed circuit-level simulations to provide reliable estimates for the switching energy and delay of carefully designed devices.

[1] K.Camsari et al., *Scientific Reports*, 5, 10571 (2015)

[2] <https://nanohub.org/groups/spintronics>

<sup>1</sup>This work was supported in part by C-SPIN, one of six centers of STARnet, a Semiconductor Research Corporation program, sponsored by MARCO and DARPA and in part by the National Science Foundation through the NCN-NEEDS program, contract 1227020-EEC.

**4:18PM H12.00004 Spin Orbit Interaction Engineering for beyond Spin Transfer Torque memory**, KANG L. WANG, Electrical Engineering Dept., Univ of California, Los Angeles, CA 90095 — Spin transfer torque memory uses electron current to transfer the spin torque of electrons to switch a magnetic free layer. This talk will address an alternative approach to energy efficient non-volatile spintronics through engineering of spin orbit interaction (SOC) and the use of spin orbit torque (SOT) by the use of electric field to improve further the energy efficiency of switching. I will first discuss the engineering of interface SOC, which results in the electric field control of magnetic moment or magneto-electric (ME) effect. Magnetic memory bits based on this ME effect, referred to as magnetoelectric RAM (MeRAM), is shown to have orders of magnitude lower energy dissipation compared with spin transfer torque memory (STTRAM). Likewise, interests in spin Hall as a result of SOC have led to many advances. Recent demonstrations of magnetization switching induced by in-plane current in heavy metal/ferromagnetic heterostructures have been shown to arise from the large SOC. The large SOC is also shown to give rise to the large SOT. Due to the presence of an intrinsic extraordinarily strong SOC and spin-momentum lock, topological insulators (TIs) are expected to be promising candidates for exploring spin-orbit torque (SOT)-related physics. In particular, we will show the magnetization switching in a chromium-doped magnetic TI bilayer heterostructure by charge current. A giant SOT of more than three orders of magnitude larger than those reported in heavy metals is also obtained. This large SOT is shown to come from the spin-momentum locked surface states of TI, which may further lead to innovative low power applications. I will also describe other related physics of SOC at the interface of anti-ferromagnetism/ferromagnetic structure and show the control exchange bias by electric field for high speed memory switching. The work was in part supported by ERFC-SHINES, NSF, ARO, TANMS, and FAME

**4:54PM H12.00005 Rise of Racetrack Memory! Domain Wall Spin-Orbitronics**, STUART PARKIN, Max Planck Institute for Microstructure Physics & IBM Research - Almaden — Memory-storage devices based on the current controlled motion of a series of domain walls (DWs) in magnetic racetracks promise performance and reliability beyond that of conventional magnetic disk drives and solid state storage devices (1). Racetracks that are formed from atomically thin, perpendicularly magnetized nano-wires, interfaced with adjacent metal layers with high spin-orbit coupling, give rise to domain walls that exhibit a chiral Néel structure (2). These DWs can be moved very efficiently with current via chiral spin-orbit torques (2,3). Record-breaking current-induced DW speeds exceeding 1,000 m/sec are found in synthetic antiferromagnetic structures (3) in which the net magnetization of the DWs is tuned to almost zero, making them “invisible”. Based on these recent discoveries, Racetrack Memory devices have the potential to operate on picosecond timescales and at densities more than 100 times greater than other memory technologies. (1) S.S.P. Parkin et al., Science 320, 5873 (2008); S.S.P. Parkin and S.-H. Yang, Nat. Nano. 10, 195 (2015). (2) K.-S. Ryu et al., Nat. Nano. 8, 527 (2013). (3) S.-H. Yang, K.-S. Ryu and S.S.P. Parkin, Nat. Nano. 10, 221 (2015). (4) S.S.P. Parkin, Phys. Rev. Lett. 67, 3598 (1991).

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**  
**Session H13 DCOMP: Rahman Prize Lecture and Computational Design of New Topological Materials** 309 - Bluegel Stefan, Forschungszentrum Jülich GmbH

**2:30PM H13.00001 Designing topologicality using oxides<sup>1</sup>**, VICTOR PARDO, University of Santiago de Compostela — In this talk we will describe a series of ab initio calculations carried out on different oxide-based systems and their nanostructures that show emerging non-trivial topological properties or nodal Fermi surfaces. We will show that various well-known oxide structures with the appropriate filling host Dirac points at the Fermi level that could eventually respond to spin-orbit coupling. In particular, we will focus on the results obtained in rutile multilayers[1], perovskite bilayers[2] grown along the polar (111) direction and corundum-based multilayers[3]. Topologically non-trivial phases occur in various limits of spin-orbit coupling strength and on-site Coulomb repulsion, using different fillings of the d-shell for various 3d and 5d elements in the active layers. The different systems will be discussed and compared to try to understand the key ingredients that lead to non-trivial topological properties in oxides and how these can be enhanced or tuned. [1] V. Pardo, W.E. Pickett, Phys. Rev. Lett. 102, 166803 (2010). [2] J.L. Lado, V. Pardo, D. Baldomir, Phys. Rev. B 88, 155119 (2013). [3] J.F. Afonso, V. Pardo, arxiv/1507.08813 (2015).

<sup>1</sup>We acknowledge support of the MINECO through the Ramon y Cajal Program and Project No. MAT2013-44673-R and Xunta de Galicia through project no. EM2013/037.

**3:06PM H13.00002 Designing topological states by pressure, strain, and functionalization**, UDO SCHWINGENSCHLOGL, PSE Division, KAUST, Thuwal 23955, Saudi Arabia — Various examples of the design of topological states by means of first-principles calculations are discussed. The presentation focusses on the design parameters (1) pressure, (2) strain, and (3) functionalization.  $\text{TiTe}_2$  is found to be unusually accessible to strain effects and the first compound that under hydrostatic pressure (up to experimentally reasonable 30 GPa) is subject to a series of four topological phase transitions, which are related to band inversions at different points of the Brillouin zone. Therefore,  $\text{TiTe}_2$  enables experimental access to all these transitions in a single compound. Phase transitions in  $\text{TiBiS}_2$  and  $\text{TiSbS}_2$  are identified by parity analysis and by calculating the surface states. Zero, one, and four Dirac cones are found for the (111) surfaces of both  $\text{TiBiS}_2$  and  $\text{TiSbS}_2$  when the pressure grows, which confirms trivial-nontrivial-trivial phase transitions. The Dirac cones at the  $\bar{M}$  points are anisotropic with large out-of-plane component.  $\text{TiBiS}_2$  shows normal, topological, and topological crystalline insulator phases under hydrostatic pressure, thus being the first compound to exhibit a phase transition from a topological to a topological crystalline insulator. While monolayer arsenic and arsenic antimonide are semiconductors (direct band gap at the  $\Gamma$  point), fluorination results for both compounds in Dirac cones at the K points. Fluorinated monolayer arsenic shows a band gap of 0.16 eV due to spin-orbit coupling and fluorinated arsenic antimonide a larger band gap of 0.37 eV due to inversion symmetry breaking. Spin-orbit coupling induces spin splitting similar to monolayer  $\text{MoS}_2$ . Phonon calculations confirm that both materials are dynamically stable. Calculations of the edge states of nanoribbons by the tight-binding method demonstrate that fluorinated arsenic is topologically nontrivial in contrast to fluorinated arsenic antimonide.

**3:42PM H13.00003 High-Throughput Computational Design of Advanced Functional Materials: Topological Insulators and Two-Dimensional Electron Gas Systems**, KESONG YANG, Univ of California - San Diego — As a rapidly growing area of materials science, high-throughput (HT) computational materials design is playing a crucial role in accelerating the discovery and development of novel functional materials. In this presentation, I will first introduce the strategy of HT computational materials design, and take the HT discovery of topological insulators (TIs) as a practical example to show the usage of such an approach. Topological insulators are one of the most studied classes of novel materials because of their great potential for applications ranging from spintronics to quantum computers. Here I will show that, by defining a reliable and accessible descriptor, which represents the topological robustness or feasibility of the candidate, and by searching the quantum materials repository aflowlib.org, we have automatically discovered 28 TIs (some of them already known) in five different symmetry families. Next, I will talk about our recent research work on the HT computational design of the perovskite-based two-dimensional electron gas (2DEG) systems. The 2DEG formed on the perovskite oxide heterostructure (HS) has potential applications in next-generation nanoelectronic devices. In order to achieve practical implementation of the 2DEG in the device design, desired physical properties such as high charge carrier density and mobility are necessary. Here I show that, using the same strategy with the HT discovery of TIs, by introducing a series of combinatorial descriptors, we have successfully identified a series of candidate 2DEG systems based on the perovskite oxides. This work provides another exemplar of applying HT computational design approach for the discovery of advanced functional materials.

**4:18PM H13.00004 Materials discovery guided by data-driven insights**, MATTIAS KLINTENBERG, Uppsala University — As the computational power continues to grow systematic computational exploration has become an important tool for materials discovery. In this presentation the Electronic Structure Project (ESP/ELSA)[1-3] will be discussed and a number of examples presented that show some of the capabilities of a data-driven methodology for guiding materials discovery. These examples include topological insulators [4], detector materials and 2D materials. ESP/ELSA is an initiative that dates back to 2001 [5,6] and today contain many tens of thousands of materials that have been investigated using a robust and high accuracy electronic structure method (all-electron FP-LMTO [7]) thus providing basic materials first-principles data for most inorganic compounds that have been structurally characterized. The web-site containing the ESP/ELSA [1] data has as of today been accessed from more than 4,000 unique computers from all around the world.

[1] <http://www.materialsdesign.se>

[2] Our Fermi-surface database can be found at <http://gurka.fysik.uu.se/esp-fs>

[3] "Data mining and accelerated electronic structure theory as a tool in the search for new functional materials", C. Ortiz, O. Eriksson and M. Klintonberg. Comput. Mater. Sci. 44, 1042-1049 (2009)

[4] "The search for strong topological insulators", M. Klintonberg. Arxiv:1007.4838 (2010).

[5] "A systematic search for new scintillators using electronic structure calculations", M. Klintonberg, S. E. Derenzo and M. J. Weber, Nanotech, 2, 427 (2002). Technical Proceedings of the 2002 International Conference on Computational Nanoscience and Nanotechnology, <http://www.nsti.org/procs/ICCN2002/16/W62.11>

[6] "Potential new scintillators identified by electronic structure calculations", M. Klintonberg, S. E. Derenzo and M. J. Weber, Nucl. Inst. Meth. A, 486, 298 (2002)

[7] "Full-Potential Electronic Structure Method", J. M. Wills, M. Alouani, P. Andersson, A. Delin, O. Eriksson, O. Grechnev. Springer 2010. ISBN 978-3-642-15144-6.

**4:54PM H13.00005 Rahman Prize Talk: Pushing the frontier in the simulation of correlated quantum many body systems**, MATTHIAS TROYER, ETH Zurich — Amazing progress in the simulation of correlated quantum many body systems has been achieved in the past two decades by combining significant advances in new algorithms with efficient implementations on ever faster supercomputers. This has enabled the accurate simulation of an increasing number of problems and helped settle many open questions. I will review a selection of results that my collaborators and I have worked on, from quantum phase transitions in quantum magnets, over supersolidity of bosons in lattice models and Helium-4 to recent simulations of correlated fermions and quantum gases. I will then provide an outlook to the future and discuss how in the short term analog quantum simulators can help tackle problems for which no efficient simulation algorithms exist and how in the longer term quantum computers can be used to solve many of the still open questions in the field. I will finally connect to the topic of the remainder of this symposium by touching on how the design of new topological materials will help in the construction of these quantum computers.

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**

**Session H14 FEd: Reichert Award** 310 - Tim Stelzer, Univ of Illinois - Urbana

**2:30PM H14.00001 Jonathan F. Reichert and Barbara Wolff-Reichert Award for Excellence in Advanced Laboratory Instruction: Advanced Instructional Labs: Why Bother?**, VAN BISTROW, University of Chicago — What are we teaching about physics in the traditional lecture course? Plenty! By offering the Advanced Laboratory Course, we hope to shed light on the following questions: How do we develop a systematic process of doing experiments? How do we record procedures and results? How should we interpret theoretical concepts in the real world? What experimental and computational techniques are available for producing and analyzing data? With what degree of confidence can we trust our measurements and interpretations? How well does a theory represent physical reality? How do we collaborate with experimental partners? How do we best communicate our findings to others? These questions are of fundamental importance to experimental physics, yet are not generally addressed by reading textbooks, attending lectures or doing homework problems. Thus, to provide a more complete understanding of physics, we offer laboratory exercises as a supplement to the other modes of learning. The speaker will describe some examples of experiments, and outline the history, structure and student impressions of the Advanced Lab course at the University of Chicago Department of Physics.

**3:06PM H14.00002 Investigating Student Ownership of Projects in Upper-Division Physics Laboratory Courses<sup>1</sup>**, JACOB STANLEY, University of Colorado - Boulder — In undergraduate research experiences, student development of an identity as a scientist is coupled to their sense of ownership of their research projects. As a first step towards studying similar connections in physics laboratory courses, we investigate student ownership of projects in a lasers-based upper-division course. Students spent the final seven weeks of the semester working in groups on final projects of their choosing. Using data from the Project Ownership Survey and weekly student reflections, we investigate student ownership as it relates to students' personal agency, self-efficacy, peer interactions, and complex affective responses to challenges and successes. We present evidence of students' project ownership in an upper-division physics lab. Additionally, we propose a model for student development of ownership through cycles of frustration and excitement as students progress on their projects.

<sup>1</sup>This work was supported by NSF grant nos. DUE-1323101 and DUE-1334170.

**3:42PM H14.00003 8 Years of ALPhA's Impacts / 45 Years of Developing Experimentalists with Few Resources: A Talk in Two Parts<sup>1</sup>**, LOWELL MCCANN, Univ. of Wisconsin - River Falls — In 2007, faculty with a shared interest in the health of advanced physics laboratory courses (those offered beyond the first year of college) created ALPhA, the Advanced Laboratory Physics Association. Over the past 8 years, ALPhA activities have involved faculty from a sizeable fraction of the physics departments in the United States. In the first part of this talk, I will overview ALPhA's efforts and its impact. In the second part of the talk I will discuss the advanced laboratory curricula at the University of Wisconsin - River Falls, which was developed over several decades using minimal resources for maximum impact.

<sup>1</sup>Supported by NSF grant DUE-1122993.

**4:18PM H14.00004 Student-Driven Engagement: An Interdisciplinary-Team Research-Learning Renewable Energy Laboratory Experience for Undergraduates**, MARK TUOMINEN, University of Massachusetts Amherst — How does engagement and deep learning happen? Every science department seeks to cultivate an excellent level of scientific skills and knowledge in its undergraduate students. Yet, this is not sufficient to thrive as a professional. Engaging directly in real-world challenges can foster a professional attitude: a high level of self-efficacy, a genuine sense of relevance, and proactivity. This talk will describe pedagogical developments of a junior-year renewable energy laboratory course at the University of Massachusetts Amherst that is part of a four-year Integrated Concentration in Science (iCons) program. Over the four years, the interdisciplinary iCons students—from 24 various majors—work through case studies, selection and analysis of real-world problems, inception and development of potential solutions, integrative communication, experimental practice, and capstone research. The team dynamic is a central aspect of the experience, yielding significant educational and developmental benefits. The third-year energy course uses adopts a culture of a small vibrant R and D company (I3E – “Energy, Powered By Intelligence”), in which every person in the course has a vital responsibility and creative resourcefulness must be employed in the project work. The course emphasizes the practice of using reflection and redesign, as a means of generating better solutions and embedding the practice of learning in a real-world context. This work is supported in part by NSF grant DUE-1140805.

**4:54PM H14.00005 Open-ended projects in undergraduate optics and lasers courses**, CHAD HOYT, Bethel University — This talk will describe the format and experience of undergraduate Lasers and Optics courses at Bethel University. The courses, which include a rigorous lecture portion, are built on open-ended research projects that have a novel aspect. They begin with four weeks of small student groups rotating between several standard laser and optics laboratory exercises. These may include, for example, alignment and characterization of a helium neon laser and measurements with a Michelson interferometer or a scanning Fabry-Pérot optical cavity. During the following seven weeks of the course, student groups (2-4 people) choose and pursue research questions in the lab. Their work culminates in a group manuscript typeset in L<sup>A</sup>T<sub>E</sub>X and a twenty-minute presentation to the class. Projects in the spring, 2014 Optics course included experiments with ultracold lithium atoms in a magneto-optical trap, optical tweezers, digital holography and adaptive optics. Projects in the spring, 2015 Lasers course included ultrafast optics with a mode-locked erbium fiber laser, quantum optics, surface plasmon lasers (led by Nathan Lindquist) and a low-cost, near-infrared spectrometer. Several of these projects are related to larger scale, funded research in the physics department. The format and experience in Lasers and Optics is representative of other upper-level courses at Bethel, including Fluid Mechanics and Computer Methods. A physics education research group from the University of Colorado evaluated the spring, 2015 Lasers course. They focused on student experimental attitudes and measurements of student project ownership.

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**  
**Session H15 DMP: 2D and Graphene - Electronic and Atomic Structure** 314 -

**2:30PM H15.00001 One-dimensional metallic wires at phase-engineered boundaries in two-dimensional materials**, MARCO GIBERTINI, NICOLA MARZARI, Ecole Polytechnique Federale de Lausanne, Switzerland — At the interfaces between systems with different electric polarization, free carriers appear in order to screen the resulting polarization charges associated with the resulting polar discontinuity. This mechanism is believed to be at the origin of the two-dimensional electron gas emerging at oxide interfaces and provides the basis for manifold exciting novel phenomena. Recently, it has been shown that similar processes take place also in two-dimensional materials, where one-dimensional wires of free carriers are induced at planar interfaces between materials with different in-plane polarization or at the edges of polar nanoribbons. Here we show by first-principles simulations that some two-dimensional polar materials can display a metastable non-polar phase, so that boundaries between the stable and metastable phases support a polar discontinuity and the resulting one-dimensional metallic wires. We provide several approaches to engineer such phase boundaries by locally inducing metastable phases in a single parent crystal. We finally show how this novel strategy to engineer polar discontinuities in two dimensions offers unprecedented opportunities to efficiently manipulate and reconfigure the emerging one-dimensional metallic wires or switch their conducting state.

**2:42PM H15.00002 First-principles study of structural properties of SiO<sub>2</sub> bilayers**, ANDREI MALASHEVICH, SOHRAB ISMAIL-BEIGI, ERIC I. ALTMAN, Center for Research on Interface Structures and Phenomena and Department of Applied Physics, Yale University — Two dimensional (2D) materials draw a tremendous amount of interest because they exhibit unique physical properties due to reduced dimensionality. Recently, SiO<sub>2</sub> 2D bilayer systems were discovered. The structure of these bilayers is formed by two mirror-image planes of corner-sharing SiO<sub>4</sub> tetrahedra and does not have a direct relation to bulk SiO<sub>2</sub> systems. SiO<sub>2</sub> bilayers may be obtained in crystalline or amorphous forms. In the crystalline form, the bilayers are constructed from six-membered rings of corner-sharing SiO<sub>4</sub> tetrahedra. The amorphous form has rings of various sizes typically in the range from four to nine Si atoms in the ring. These structures may be of practical interest as atomically thin membranes and molecular sieves. In our work, we study the effect of strain and doping on the crystalline structure of SiO<sub>2</sub> bilayers using density functional theory. We analyze the stability of structures depending on the ring size and establish strain and doping conditions that may render the structures with large ring sizes stable. This work is supported by the National Science Foundation through grants MRSEC NSF DMR-1119826 and NSF DMR-1506800.

**2:54PM H15.00003 The Pyrite Structure of PdS<sub>2</sub> and PdSe<sub>2</sub> Monolayers**, ARUNIMA K. SINGH, National Institute of Standards and Technology, RICHARD G. HENNIG, University of Florida, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY COLLABORATION, UNIVERSITY OF FLORIDA COLLABORATION — There has been a rising interest in two-dimensional (2D) materials due to a range of extraordinary electronic, optical and mechanical properties which are different from their bulk counterparts. The structure, stability and electronic properties of 2D PdS<sub>2</sub> and PdSe<sub>2</sub> have been investigated in the past in the well-known hexagonal 1T and 2H structures. However, bulk PdS<sub>2</sub> and PdSe<sub>2</sub> are layered compounds with individual rhombohedral pyrite-type monolayers vertically stacked with van-der Waals forces. Using density functional theory simulations, and five different functionals, we compare the energetic stability of 2D PdS<sub>2</sub> and PdSe<sub>2</sub> pyrite structure with the 1T and 2H structures. We find that the PdS<sub>2</sub> is most stable in the pyrite structure, whereas the PdSe<sub>2</sub> is most stable in the 1T structure with the pyrite structure closely competing in energy. The fundamental band gap of these compounds as a function of the structure, number of layers, the stacking arrangement and in-layer strain has been investigated. The pyrite structures of PdS<sub>2</sub> and PdSe<sub>2</sub> are found to be semi-conducting with indirect band gaps, and effective masses comparable to that of monolayer MoS<sub>2</sub>; thus are potential candidates for nano-electronic applications.

**3:06PM H15.00004 Electronic and Mechanical Properties of Hydrogenated Irradiated and Amorphous Graphene**, ASANKA WEERASINGHE, Department of Physics, University of Massachusetts - Amherst, ASHWIN RAMASUBRAMANIAM, Department of Mechanical and Industrial Engineering, University of Massachusetts - Amherst, DIMITRIOS MAROUDAS, Department of Chemical Engineering, University of Massachusetts - Amherst — Defect engineering and chemical functionalization of graphene are promising routes for fabrication of carbon nanostructures and 2D metamaterials with unique properties and function. Here, we use hydrogenation of irradiated, including irradiation-induced amorphous, graphene as a means of studying chemical functionalization effects on its electronic structure and mechanical response. We use molecular-dynamics simulations based on a reliable bond-order potential to prepare the hydrogenated configurations and carry out dynamic deformation tests at constant strain rate and temperature. Our mechanical tests show that hydrogenation does not affect the ultimate tensile strength (UTS) of the irradiated graphene sheet if the hydrogenated C atoms remain sp<sup>2</sup>-hybridized; however, upon inducing sp<sup>3</sup> hybridization of these C atoms, UTS decreases by about 10 GPa. Furthermore, the fracture strain of the irradiated structure decreases by up to 30% upon hydrogenation independent of the hybridization type. We also report results for the electronic structure of hydrogenated configurations based on a density-functional tight-binding approach and assess the potential for tuning the electronic properties of these defective, functionalized graphenes.

**3:18PM H15.00005 Effect of radial stretch on vibration characteristics of single-layered circular graphene sheets**, GUNJAN PAHLANI, Mechanical Engineering, Indian Institute of Tech Hyderabad, DEEPTI VERMA, CEMS, University of Minnesota, SHAKTI GUPTA, Mechanical Engineering, Indian Institute of Tech Kanpur — Vibrations of single-layered circular graphene sheets are studied using molecular mechanics (MM) simulations. Interactions between bonded and non-bonded atoms are prescribed using MM3 potential. Frequencies of different modes of vibration are computed from the eigenvalues and eigen vectors of mass weighted Hessian of the system. This study is performed on graphene sheets of various diameters. A linear continuum membrane model for predicting vibrational frequencies is studied using finite element (FE) method. Frequencies for several modes computed from continuum and molecular model matched well for moderate values of radial stretch, however, with increased stretch those deviated from each other significantly. In particular for higher values of stretch the MM simulations predict considerably lower values of frequencies compared to that found from FE simulations. Also, at higher values of stretch the frequency vs. stretch curve obtained from MM simulations showed a hardening behavior which could not be captured by the linear continuum model. We have also found a similar behavior in two-layered graphene sheets using MM simulations.

**3:30PM H15.00006 A Tight Binding Approach to Strain in Monolayer Transition-Metal Dichalcogenides**, ALEXANDER PEARCE, GUIDO BURKARD, University of Konstanz, Germany — We present a model of the electronic properties of the monolayer transition-metal dichalcogenides based on a tight binding approach which includes the effects of strain and curvature of the crystal lattice. Mechanical deformations of the lattice change bond lengths leading directly to corrections in the electronic Hamiltonian, while curvature of the crystal lattice mixes the orbital structure of the electronic Bloch bands. We first present an effective low energy Hamiltonian describing the electronic properties near the K point in the Brillouin zone, then present the corrections to this Hamiltonian due to arbitrary mechanical deformations and curvature in a way which treats both effects on an equal footing. This analysis finds that local area variations of the lattice allow for tuning of the band gap and effective masses, where the application of uniaxial strain decreases the magnitude of the direct band gap at the K point. Additionally, strain induced bond length modifications create a fictitious gauge field but with a coupling that is smaller than seen in related materials like graphene. Whereas curvature of the lattice leads to appearance of both an effective in-plane magnetic field which couples to spin degrees of freedom and a Rashba-like spin-orbit coupling.

**3:42PM H15.00007 Effective tight-binding model for transition metal dichalcogenides<sup>1</sup>**, YEN-HUNG HO, MIGUEL CAZALILLA, National Tsing Hua University, TAIWAN, HECTOR OCHOA, University of California, Los Angeles, USA — For transition metal dichalcogenides, various band models have been developed to describe the novel subband features. In this work, we propose a new effective minimum-band model by preforming a canonical transformation on the full-band Hamiltonian. We found that, depending on the form of transformation, both the  $\Gamma$ - and  $K$ -valley electrons can be well captured, including the frequency and band effective mass. And, for the full-band parameters used, starting from Wannier function basis set leads to a better result than from Slater-Koster basis set. A close inspection of the transformation projection also enables us to extract the modification on the site energy, as well as the orbital hopping between several nearest neighboring atoms. Instead of pure empirical fitting, our effective models preserve rich orbital physics inside, which is shown to be versatile in studying a variety of fundamental physical properties.

<sup>1</sup>Ministry of Science and Technology of Taiwan (NSC 102-2112-M-007-024-MY5)

**3:54PM H15.00008 Structural and electronic properties of a single layered  $\alpha$ -tetragonal B<sub>50</sub> sheet.**, CHERNO KAH, MING YU, CHAKRAM S JAYANTHI, SHIYU WU, Univ of Louisville — Ultrathin single-crystalline boron nanosheets with  $\alpha$ -tetragonal B<sub>50</sub> symmetry ( $\alpha$ -t-B<sub>50</sub>) have recently been synthesized [1]. In this presentation, the relaxed structure of this new type of boron sheet is determined using a robust self-consistent and environment-dependent semi-empirical Hamiltonian developed within the LCAO framework that includes MD and power quenching schemes. Upon relaxation, the sheet symmetry is broken and the icosahedral B<sub>12</sub> units in the sheet are found to be distorted. This stability of the sheet was investigated through a calculation of the vibrational frequencies. The sheet electronic density of states exhibits no energy gap at the Fermi level, suggesting a metallic character similar to that of the bulk  $\alpha$ -t-B<sub>50</sub>. Finally, the cohesive energy of the  $\alpha$ -t-B<sub>50</sub> sheet is found to be higher than that of the recently reported icosahedral B<sub>12</sub>-O<sub>6</sub> sheet [2]. [1] Adv. Sci. 2, 1500023 (2015) [2] Nanotechnology 26, 405701 (2015)

**4:06PM H15.00009 Ab Initio Based 2D Continuum Mechanics – Sensitivity Prediction for Contact Resonance Atomic Force Microscopy Based Structure Fingerprints**, QING TU, BJÖRN LANGE, MEMS Department, Duke University, Durham, NC 27708, J. MARCELO J. LOPES, Paul-Drude-Institut für Festkörperelektronik, D-10117 Berlin, Germany, STEFAN ZAUSCHER, VOLKER BLUM, MEMS Department, Duke University, Durham, NC 27708 — Contact resonance AFM is demonstrated as a powerful tool for mapping differences in the mechanical properties of 2D materials and heterostructures, permitting to resolve surface and subsurface structural differences of different domains. Measured contact resonance frequencies are related to the contact stiffness of the combined tip-sample system. Based on first principles predicted elastic properties and a continuum approach to model the mechanical impedance, we find contact stiffness ratios between different domains of few-layer graphene on 3C-SiC(111) in excellent agreement with experiment. We next demonstrate that the approach is able to quantitatively resolve differences between other 2D materials domains, e.g., for h-BN, MoS<sub>2</sub> and MoO<sub>3</sub> on graphene on SiC. We show that the combined effect of several materials parameters, especially the in-plane elastic properties and the layer thickness, determines the contact stiffness, therefore boosting the sensitivity even if the out-of-plane elastic properties are similar.

**4:18PM H15.00010 Substrate induced phase transformation of monolayer transition metal dichalcogenides**, SHUDUN LIU, University of Louisville, XIAOJUN FU, WENGUANG ZHU, University of Science and Technology of China — Using density functional theory calculations, we investigate the effects of a metal substrate on the structural and electronic properties of a monolayer of transition metal dichalcogenide (TMD). We find that a suitable choice of substrate can induce a transformation of the phase of the monolayer from 2H to 1T. We will discuss the impact of the results on some earlier studies of TMD/metal contacts as well as potential applications of our system in catalysis.

**4:30PM H15.00011 DFT calculation of Landau levels in 2D crystals: from black phosphorus to dichalcogenides<sup>1</sup>**, JOSE LADO, JOAQUIN FERNANDEZ ROSSIER, International Iberian Nanotechnology Laboratory — We present a method to calculate the Landau levels and the corresponding edge states of two dimensional (2D) crystals using as a starting point their electronic structure as obtained from standard density functional theory (DFT). The DFT Hamiltonian is represented in the basis of maximally localized Wannier functions [1]. This defines a tight-binding Hamiltonian for the bulk that can be readily used to describe other structures, such as ribbons, provided that atomic scale details of the edges are ignored. The effect of the orbital magnetic field is described using the Peierls substitution. By implementing this approach in a ribbon geometry we recover known results for graphene, MoS<sub>2</sub> [2] and black phosphorous [3]. We apply this method to predict the Landau level spectrum of MoSSe. Our procedure can readily be used in any other 2D crystal, and provides an alternative to effective mass descriptions. [1] A. A. Mostofi, J. R. Yates, Y.-S. Lee, I. Souza, D. Vanderbilt and N. Marzari Comput. Phys. Commun. 178, 685 (2008) [2] Habib Rostami and Reza Asgari, Phys. Rev. B 91, 075433 (2015) [3] J. M. Pereira, Jr. and M. I. Katsnelson, Phys. Rev. B 92, 075437 (2015)

<sup>1</sup>We acknowledge financial support from SPINOGRAPH

**4:42PM H15.00012 A tight-binding model for MoS<sub>2</sub> monolayers<sup>1</sup>**, EMILIA RIDOLFI, Universidade Federal Fluminense, DUY LE, TALAT RAHMAN, EDUARDO MUCCIOLO, University of Central Florida, CAIO LEWENKOPF, Universidade Federal Fluminense — We propose an accurate tight-binding parametrization for the band structure of MoS<sub>2</sub> monolayers near the main energy gap. We introduce a generic and straightforward derivation for the band energies equations that could be employed for other monolayer dichalcogenides. A parametrization that includes spinorbit coupling is also provided. The proposed set of model parameters reproduce both the correct orbital compositions and location of valence and conduction band in comparison with ab initio calculations. The model gives a suitable starting point for realistic large-scale atomistic electronic transport calculations.

<sup>1</sup>Supported by the Brazilian funding agencies CNPq, CAPES, FAPERJ, and the Ciencia sem Fronteiras program. DL and TSR are supported in part by the DOE grant DE-FG02-07ER46354.

**4:54PM H15.00013 Probing the uniaxial strains in MoS<sub>2</sub> using polarized Raman spectroscopy: A first-principles study<sup>1</sup>**, DANNA DORATOTAJ, JEFFREY R. SIMPSON, JIA-AN YAN, Towson University — Characterization of strain in two-dimensional crystals is important for understanding their properties and performance. Using first-principles calculations, we study the effects of uniaxial strain on the Raman-active modes in monolayer MoS<sub>2</sub>. We show that the in-plane  $E'$  mode at 384 cm<sup>-1</sup> and the out-of-plane  $A'_1$  mode at 403 cm<sup>-1</sup> can serve as fingerprints for the uniaxial strain in this material. Specifically, under a uniaxial strain, the doubly degenerate  $E'$  mode splits into two non-degenerate modes: the  $E'_{||}$  and  $E'_{\perp}$  modes. The frequency of the  $E'_{||}$  mode blue-shifts for a compressive strain, but red-shifts for a tensile strain. In addition, due to the strain-induced anisotropy in the MoS<sub>2</sub> lattice, the polarized Raman spectra of the  $E'_{||}$  and  $E'_{\perp}$  modes exhibit distinct angular dependence for specific laser polarization setups, allowing for a precise determination of the direction of the strain with respect to the crystallographic orientation. Furthermore, we find that the polarized Raman intensity of the  $A'_1$  mode also shows evident dependence on the applied strain, providing additional effective clues for determining the direction of the strain even without knowledge of the crystallographic orientation. Thus, polarized Raman spectroscopy offers an efficient non-destructive way to characterize the uniaxial strains in monolayer MoS<sub>2</sub>.

<sup>1</sup>This research was supported by the FCSM Undergraduate Research Committee, the FCSM Fisher General Endowment and the FDRC grant (OSPR No. 140269) at Towson University. This work used the computing resources of Carver at NERSC.

**5:06PM H15.00014 Computational study of electronic and thermal properties of single-layer molybdenum disulphide folded nanostructure**, JIE PENG, PETER CHUNG, Univ of Maryland-College Park — Single-layer Molybdenum disulphide (*SLMoS<sub>2</sub>*), a two-dimensional transition-metal dichalcogenide with a large band gap and high mobility, is considered to be a next generation material for transistors and optoelectronic devices. We present recent results on the electronic and thermal behavior of *SLMoS<sub>2</sub>* folded nanostructures. Through an approach that uses both molecular dynamics (MD) and density functional theory (DFT), we estimate the stable equilibrium structure of folded sheets as well as the related phonon and electronic band structures. The MD simulations are based on a Stillinger-Weber potential and the DFT simulations employ projector augmented wave (PAW) pseudopotentials using generalized gradient approximation (GGA) and local density approximation (LDA). The structure is examined as a function of folding orientation, layer number and system size. Mechanisms of the phonon transport and electronic band gap properties in such a mechanically distorted atomic-layer nanostructure will be discussed.

**5:18PM H15.00015 Tight binding approach to study electronic properties of MoS<sub>2</sub>/WS<sub>2</sub> heterostructure**, NAMITA NARENDRA, KI WOOK KIM, North Carolina State University — The heterostructure interface of MoS<sub>2</sub>/WS<sub>2</sub> is being increasingly studied in recent years for its electronic and optical properties. The ability to tune properties of few-layer transition metal dichalcogenides (TMDs) by strain engineering provides a significant incentive to further explore these material interfaces. It has been shown that misorientation in bulk MoS<sub>2</sub> and WS<sub>2</sub> can also alter the electronic properties. Tight binding allows us to calculate the transport properties of MoS<sub>2</sub>/WS<sub>2</sub> interface for all the angles of misorientation, unlike the computationally limited first principles approach. In this work, the tight binding parameters for the bulk are extracted from first principles and the heterostructure model is verified. A detailed study of variation of electronic properties of MoS<sub>2</sub>/WS<sub>2</sub> interface with respect to addition of strain and number of layers of MoS<sub>2</sub> and WS<sub>2</sub> is carried out. The extension of tight binding model to misoriented MoS<sub>2</sub>/WS<sub>2</sub> interface is demonstrated.

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**

**Session H16 DMP: 2D Devices: Electronics and Optoelectronics** 315 - Jonathan Bird, University at Buffalo

**2:30PM H16.00001 Nano-scale electronic and optoelectronic devices based on 2D crystals**, WENJUAN ZHU, University of Illinois at Urbana-Champaign — In the last few years, the research community has been rapidly growing interests in two-dimensional (2D) crystals and their applications. The properties of these 2D crystals are diverse — ranging from semi-metal such as graphene, semiconductors such as MoS<sub>2</sub>, to insulator such as boron nitride. These 2D crystals have many unique properties as compared to their bulk counterparts due to their reduced dimensionality and symmetry. A key difference is the band structures, which lead to distinct electronic and photonic properties. The 2D nature of the material also plays an important role in defining their exceptional properties of mechanical strength, surface sensitivity, thermal conductivity, tunable band-gap and their interaction with light. These unique properties of 2D crystals open up a broad territory of applications in computing, communication, energy, and medicine. In this talk, I will present our work on understanding the electrical properties of graphene and MoS<sub>2</sub>, in particular current transport and band-gap engineering in graphene, interface between gate dielectrics and graphene, and gap states in MoS<sub>2</sub>. I will also present our work on the nano-scale electronic devices (RF and logic devices) and photonic devices (plasmonic devices and photo-detectors) based on these 2D crystals.

**3:06PM H16.00002 Direct Visualization of Edge States and Electrical Inhomogeneity in MoS<sub>2</sub> Field Effect Transistors**, DI WU, LAN LUAN, ZHAODONG CHU, XIAOYU WU, KEJI LAI, Department of Physics, University of Texas at Austin — Ultrathin transition metal dichalcogenides (TMDs) with layer-dependent bandgaps, relatively high carrier mobilities, and valley pseudospins are promising material platforms for novel electronics. It is of great importance to microscopically probe the TMD-based electronic devices for understanding and improving their performances in relation to metal contacts, interfaces, and defects. Here, we report the electrical imaging of the channel conductance of few-layer MoS<sub>2</sub> field-effect transistors by microwave impedance microscopy (MIM). A systematic evolution of the local conductance of exfoliated MoS<sub>2</sub> back-gated devices was captured during the insulator-to-metal transition induced by electrostatic gating. Interestingly, when the transistors were gradually turned on, the carriers were first accumulated at the edges of MoS<sub>2</sub> flakes, as indicated by the higher local conductivity in MIM images. At the same time, we have also observed strong local conductance fluctuation, which are presumably due to the charged impurities in the flakes or defects at the interfaces. The MIM images can thus provide us the microscopic understanding of how the device performance is influenced by the local defects and edge states.

**3:18PM H16.00003 Tunnelling in van der Waals heterostructures**, ARTEM MISHCHENKO, KOSTYA NOVOSELOV, ANDRE GEIM, School of Physics And Astronomy, The University of Manchester, LAURENCE EAVES, The University of Nottingham, VLADIMIR FALKO, School of Physics And Astronomy, The University of Manchester — When graphene and other conductive two-dimensional (2D) materials are separated by an atomically thin insulating 2D crystal, quantum mechanical tunnelling leads to appreciable current between two 2D conductors due to the overlap of their wavefunctions. These tunnel devices demonstrate interesting physics and potential for applications: such effects as resonant tunnelling, negative differential conductance, light emission and detection have already been demonstrated. In this presentation we will outline the current status and perspectives of tunnelling transistors based on 2D materials assembled into van der Waals heterostructures. Particularly, we will present results on mono- and bilayer graphene tunnelling, tunnelling in 2D crystal-based quantum wells, and tunnelling in superconducting 2D materials. Such effects as momentum and chirality conservation, phonon- and impurity-assisted tunnelling will also be discussed. Finally, we will ponder the implications of discovered effects for practical applications.

**3:30PM H16.00004 Fabrication and characterization of graphene PN junctions<sup>1</sup>**, DENNIS WANG, XIAODONG ZHOU, ALI DADGAR, Columbia Univ, PRATIK AGNIHOTRI, JI UNG LEE, The State University of New York, Albany, MARK REUTER, FRANCES ROSS, IBM T.J. Watson Research Center, ABHAY PASUPATHY, Columbia Univ — Theoretical predictions of relativistic Klein tunneling and Veselago lensing in graphene have inspired efforts to fabricate graphene p-n junctions where such phenomena could be realized and studied via electronic transport or scanning tunneling microscopy (STM). Here we will discuss the interplay between device geometry and our measurements in a 4-probe STM, which allows for simultaneous back gating, biasing, and scanning of a micromechanically exfoliated graphene sample. A sharp p-n junction is essential to the manifestation of these aforementioned effects, and we examine the benefits and drawbacks of several routes toward this goal from a fabrication standpoint. These methods include lithographically pre-patterned substrates and the stacking of vertical heterostructures. Finally, we will describe our subsequent characterization results for each, including information about topography and spatial mapping of the density of states.

<sup>1</sup>This work is supported by NSF IGERT (DGE-1069240)

**3:42PM H16.00005 Graphene – ferroelectric and MoS<sub>2</sub> – ferroelectric heterostructures for memory applications.**, ALEXEY LIPATOV, PANKAJ SHARMA, ALEXEI GRUVERMAN, ALEXANDER SINITSKII, University of Nebraska - Lincoln — In recent years there has been an unprecedented interest in two-dimensional (2D) materials with unique physical and chemical properties that cannot be found in their three-dimensional (3D) counterparts. One of the important advantages of 2D materials is that they can be easily integrated with other 2D materials and functional films, resulting in multilayered structures with new properties. We fabricated and tested electronic and memory properties of field-effect transistors (FETs) based on a single-layer graphene combined with lead zirconium titanate (PZT) substrate. Previously studied graphene-PZT devices exhibited an unusual electronic behavior such as clockwise hysteresis of electronic transport, in contradiction with counterclockwise polarization dependence of PZT. We investigated how the interplay of polarization and interfacial phenomena affects the electronic behavior and memory characteristics of graphene-PZT FETs, explain the origin of unusual clockwise hysteresis and experimentally demonstrate a reversed polarization-dependent hysteresis of electronic transport. In addition we fabricated and tested properties of MoS<sub>2</sub>-PZT FETs which exhibit a large hysteresis of electronic transport with high ON/OFF ratios. We demonstrate that MoS<sub>2</sub>-PZT memories have a number of advantages over commercial FeRAMs, such as nondestructive data readout, low operation voltage, wide memory window and the possibility to write and erase them both electrically and optically.

**3:54PM H16.00006 Programmable Schottky Junctions Based on Ferroelectric Gated MoS<sub>2</sub> Transistors.**, ZHIYONG XIAO, JINGFENG SONG, STEPHEN DRCHARME, XIA HONG, Univ of Nebraska-Lincoln — We report a programmable Schottky junction based on MoS<sub>2</sub> field effect transistors with a SiO<sub>2</sub> back gate and a ferroelectric copolymer poly(vinylidene-fluoride-trifluoroethylene) (PVDF) top gate. We fabricated mechanically exfoliated single layer MoS<sub>2</sub> flakes into two point devices via e-beam lithography, and deposited on the top of the devices ~20 nm PVDF thin films. The polarization of the PVDF layer is controlled locally by conducting atomic force microscopy. The devices exhibit linear  $I_D$ - $V_D$  characteristics when the ferroelectric gate is uniformly polarized in one direction. We then polarized the gate into two domains with opposite polarization directions, and observed that the  $I_D$ - $V_D$  characteristics of the MoS<sub>2</sub> channel can be modulated between linear and rectified behaviors depending on the back gate voltage. The nonlinear  $I_D$ - $V_D$  relation emerges when half of the channel is in the semiconductor phase while the other half is in the metallic phase, and it can be well described by the thermionic emission model with a Schottky barrier of ~0.5 eV. The Schottky junction can be erased by re-write the entire channel in the uniform polarization state. Our study facilitates the development of programmable, multifunctional nanoelectronics based on layered 2D TMDs..

**4:06PM H16.00007 Control of Rewriteable Doping Patterns in Graphene/Boron Nitride Heterostructures**, SALMAN KAHN, JAIRO VELASCO JR., DILLON WONG, JUWON LEE, HSIN ZON TSAI, University of California - Berkeley, LONG JU, Cornell University, LILI JIANG, ZHIWEN SHI, University of California - Berkeley, PAUL ASHBY, Molecular Foundry, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, ALEX ZETTL, FENG WANG, MICHAEL CROMMIE, University of California - Berkeley — Spatial control of charge doping in 2D materials is a promising technique for designing future electronic devices and understanding novel physics. Electrostatic gating and chemical doping are common methods to achieve control of charge doping in 2D materials. However, these approaches suffer from complicated fabrication processes that introduce impurities, change material properties irreversibly, and lack flexibility. Here, we introduce a new method for patterning rewriteable doping profiles with local interface charge transfer from defects in a tunable BN substrate into an adjacent layer of graphene. We characterize these spatial doping patterns through local probe and transport techniques. This technique enables many novel device designs for 2D materials, including atomically thin p-n junctions and rewriteable memory devices.

**4:18PM H16.00008 Spatially inhomogeneous barrier height in graphene/MoS<sub>2</sub> Schottky junctions<sup>1</sup>**, DUSHYANT TOMER, SHIVANI RAJPUT, LIAN LI, University of Wisconsin, Milwaukee — Graphene interfaced with a semiconductor forms a Schottky junction with rectifying properties. In this study, graphene Schottky junctions are fabricated by transferring CVD monolayer graphene on mechanically exfoliated MoS<sub>2</sub> multilayers. The forward bias current-voltage characteristics are measured in the temperature range of 210–300 K. An increase in the zero bias barrier height and decrease in the ideality factor are observed with increasing temperature. Such behavior is attributed to Schottky barrier inhomogeneities possibly due to graphene ripples and ridges at the junction interface as suggested by atomic force microscopy. Assuming a Gaussian distribution of the barrier height, mean barrier of 0.970.10 eV is found for the graphene MoS<sub>2</sub> junction. Our findings provide significant insight on the barrier height inhomogeneities in graphene/two dimensional semiconductor Schottky junctions.

<sup>1</sup>U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering Award No. DEFG02-07ER46228

**4:30PM H16.00009 Phase change memory devices formed by using 2 dimensional layered Graphene-In<sub>2</sub>Se<sub>3</sub> van der Waals heterostructure.**<sup>1</sup>, MIN SUP CHOI, CHENXI YANG, CHANG HO RA, WON JONG YOO<sup>2</sup>, Sungkyunkwan Univ., SKKU Advanced Institute of Nano-Technology — Indium selenide (In<sub>2</sub>Se<sub>3</sub>) is one of the unique materials which have both a layered structure and phase change property. One of the advantages of using 2 dimensional (2D) materials is their potential to form van der Waals heterostructures which enable unique physical properties and novel quantum device functions, which cannot be achieved in 2D material alone. In this study, we fabricated vertically stacked graphene-In<sub>2</sub>Se<sub>3</sub> heterostructured memory devices. The fabricated devices showed a rapid increase of current conduction, which is attributed to the phase transition of In<sub>2</sub>Se<sub>3</sub>. The TEM images demonstrated that In<sub>2</sub>Se<sub>3</sub> transformed from polycrystalline to layered structure thanks to the effective thermal confinement effect between graphene and In<sub>2</sub>Se<sub>3</sub>, attributed to the low thermal conductivity of layered materials in vertical direction. In addition, the current conduction could be controlled effectively by applying different pulse voltages, showing stable retention and endurance characteristics. It is thought that the differently bonded states contribute to this control process. This study demonstrates the possibility of Graphene-In<sub>2</sub>Se<sub>3</sub> van der Waals heterostructure as 2D based future memory electronics.

<sup>1</sup>This work was supported by the National Research Foundation of Korea(NRF) grant funded by the Korea government(MEST) (No. 2013R1A2A2A01015516).

<sup>2</sup>Corresponding author

**4:42PM H16.00010 Optoelectronic devices based on MoTe<sub>2</sub> p-n junction.**, YA-QING BIE, Condensed Matter Physics, MIT, MIKKEL HEUCK, EECS, MIT, MARCO FURCHI, Condensed Matter Physics, MIT, GABRIELE GROSSO, EECS, MIT, JIABAO ZHENG, Columbia University, YUAN CAO, Condensed Matter Physics, EECS, MIT, EFREN NAVARRO-MORATALLA, Condensed Matter Physics, MIT, DIRK ENGLUND, EECS, MIT, PABLO JARILLO-HERRERO, Condensed Matter Physics, MIT — 2D transition metal dichalcogenides (2D-TMD), such as MoS<sub>2</sub>, have been verified with many remarkable physical properties, which include an indirect to direct band transition as a function of thickness and a valley dependent spin polarization. One of the 2D-TMD family members, 2H-MoTe<sub>2</sub> has been shown to be a direct bandgap semiconductor as a monolayer and bilayer with a near infrared (NIR) bandgap of about 1.1eV. However, optoelectronic devices based on MoTe<sub>2</sub> were so far not experimentally demonstrated. Here, we will present a high on-off ratio MoTe<sub>2</sub> p-n junction enabled by a hexagonal boron nitride encapsulation technique. Our study of the MoTe<sub>2</sub> p-n junction devices sheds light on designing efficient NIR optoelectronic devices such as photodetectors and energy harvesting cells and light emitters.

**4:54PM H16.00011 Polarization and resistive switching behavior of ferroelectric tunnel junctions with transition metal dichalcogenides**, TAO LI, ALEXEY LIPATOV, University of Nebraska-Lincoln, PANKAJ SHARMA, University of New South Wales, HYUNGWOO LEE, CHANG-BEOM EOM, University of Wisconsin-Madison, ALEXANDER SINITSKII, ALEXEI GRUVERMAN, University of Nebraska-Lincoln, ALEXEI GRUVERMAN TEAM, ALEXANDER SINITSKII TEAM, CHANG-BEOM EOM TEAM — Transition metal dichalcogenides (TMDs) are emerging 2-dimensional (2D) materials of the MX<sub>2</sub> type, where M is a transition metal atom (Mo, W, Ti, Sn, Zr, etc.) and X is a chalcogen atom (S, Se, or Te.). Comparing to graphene, TMDs have a sizable band gap and can be metal, half-metal, semiconductor or superconductor. Their band structures can be tuned by external bias voltage, mechanical force, or light illumination. Their rich physical properties make TMDs potential candidates for a variety of applications in nanoelectronics and optoelectronics. Ferroelectric tunnel junctions (FTJs) are actively studied as a next-generation of non-volatile memory elements. An FTJ comprises a ferroelectric tunnel barrier sandwiched between two electrodes. In this work, we investigate the resistive switching behavior of MoS<sub>2</sub>/BaTiO<sub>3</sub>-based FTJs. The ON/OFF ratio can be modulated via electric or mechanical control of the switched polarization fraction opening a possibility of tunable electroresistance effect. Effect of optical illumination on the polarization reversal dynamics has been observed and analyzed based on the polarization-induced modulation of the MoS<sub>2</sub> layered electronic properties.

**5:06PM H16.00012 Atomic-scaled characterization of graphene PN junctions**, XIAODONG ZHOU, Department of Physics, Columbia University, New York, New York 10027, USA, DENNIS WANG, Department of Applied Physics and Mathematics, Columbia University, New York, New York 10027, USA, ALI DADGAR, Department of Physics, Columbia University, New York, New York 10027, USA, PRATIK AGNIHOTRI, JI UNG LEE, College of Nanoscale Science and Engineering, The State University of New York, Albany, New York 12203, USA, MARK C. REUTER, FRANCES M. ROSS, IBM T.J. Watson Research Center, Yorktown Heights, New York 10598, USA, ABHAY N. PASUPATHY, Department of Physics, Columbia University, New York, New York 10027, USA — Graphene p-n junctions are essential devices for studying relativistic Klein tunneling and the Veselago lensing effect in graphene. We have successfully fabricated graphene p-n junctions using both lithographically pre-patterned substrates and the stacking of vertical heterostructures. We then use our 4-probe STM system to characterize the junctions. The ability to carry out scanning electron microscopy (SEM) in our STM instrument is essential for us to locate and measure the junction interface. We obtain both the topography and *dI/dV* spectra at the junction area, from which we track the shift of the graphene chemical potential with position across the junction interface. This allows us to directly measure the spatial width and roughness of the junction and its potential barrier height. We will compare the junction properties of devices fabricated by the aforementioned two methods and discuss their effects on the performance as a Veselago lens.

**5:18PM H16.00013 Two-dimensional transition metal dichalcogenides based magnetic tunneling junctions**, ZHENG YANG, BO HSU, University of Illinois at Chicago, DEPARTMENT OF ELECTRICAL AND COMPUTER ENGINEERING TEAM — The transport properties of magnetic tunneling junctions (MTJ) using two-dimensional (2D) transition metal dichalcogenide monolayers MX<sub>2</sub> (M=Mo, W; X=S, Se) as tunnel layer are reported. The 2D MX<sub>2</sub> were grown using chemical vapor deposition. As-grown 2D MX<sub>2</sub> were transferred and lithographic fabricated into MTJ devices with MX<sub>2</sub> sandwiched within two ferromagnetic material layers. The magnetoresistance of the MTJs were studied at different temperatures.

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**

**Session H17 DMP: Transition Metal Dichalcogenides: Defects and Degradation** 316 - Chongwu Zhou, University of Southern California

**2:30PM H17.00001 TMD 2D Materials: Defects, Passivation, Functionalization and Device Impact**<sup>1</sup>, ROBERT WALLACE, Depts. of Materials Science and Engineering and Physics, The University of Texas at Dallas, Richardson, TX — Transition metal dichalcogenides (TMDs) such as MoS<sub>2</sub> have become popular in "beyond CMOS" device concepts and research due to their band structure in two-dimensional layers – viz. a significant band gap. Various device demonstrations have been reported utilizing exfoliated and synthesized single/few layer TMDs for possible electronic and photonic applications. The performance of such devices will also necessarily depend upon the TMD layer quality. The impact of defects and impurities on device transport characteristics is of interest, as well as methods to passivate and minimize their effects. The interaction of the TMDs with component materials, such as dielectrics and contacts, is also an important aspect. This talk will present our recent work using in-situ and ex-situ methods to understand the physics and chemistry of TMDs and their associated interfaces.

<sup>1</sup>This work was supported in part by the LEAST Center, one of the six SRC STARnet Centers, sponsored by MARCO and DARPA; the SWAN Center sponsored by the SRC NRI and NIST, and the NSF under award ECCS-1407765.

**3:06PM H17.00002 Effects of High-Energy X-Ray Radiation on MoS<sub>2</sub> FETs**, AMRITESH RAI, Univ of Texas, Austin, LAXMAN THOUTAM, WEI ZHANG, Materials Science Division, Argonne National Laboratory, Argonne, IL, KIRAN KOVI, Center for Nanoscale Materials, Argonne National Laboratory, Argonne, IL, SANJAY BANERJEE, Univ of Texas, Austin, SAPTARSHI DAS, Center for Nanoscale Materials, Argonne National Laboratory, Argonne, IL — FETs based on semiconducting MoS<sub>2</sub> nanosheets are currently being extensively explored for various nanoelectronic device applications. In real-life, several of these applications mandate the exposure of devices to X-ray radiation. In this study, we investigate the effects of high-energy X-ray radiation on few-layer MoS<sub>2</sub> transistors. Back-gated MoS<sub>2</sub> FETs on SiO<sub>2</sub> substrates were fabricated and exposed to X-ray radiation in an enclosed X-ray tube utilizing tungsten as the X-ray source. The devices were exposed to successive radiation doses up to a cumulative dose of 1500 kilorads (Krad). Even after high radiation doses, the devices maintained acceptable electrical performance with high  $I_{ON}/I_{OFF}$  ratios and good current saturation. The subthreshold swing remained similar to initial values. There was, however, a slight reduction in the ON-currents after each successive radiation, concomitant with a positive threshold voltage shift that can be attributed to the formation of negative-fixed charges in the substrate. Moreover, the maximum transconductance ( $g_m$ ) of the devices decreased slightly with increasing radiation dose. Finally, Raman spectroscopy revealed practically no change in the in-plane and out-of-plane Raman modes of MoS<sub>2</sub> after radiation.

**3:18PM H17.00003 Raman shifts and in situ TEM electrical degradation of electron-irradiated monolayer MoS<sub>2</sub>**<sup>1</sup>, WILLIAM M. PARKIN, ADRIAN BALAN, Univ of Pennsylvania, LIANGBO LIANG, Rensselaer Polytechnic Institute, PAUL MASIH DAS, Univ of Pennsylvania, MICHAEL LAMPARSKI, Rensselaer Polytechnic Institute, CARL NAYLOR, JULIO A. RODRIGUEZ-MANZO, ALAN T. JOHNSON, Univ of Pennsylvania, VINCENT MEUNIER, Rensselaer Polytechnic Institute, MARIJA DRNDIC, Univ of Pennsylvania — We report how the presence of electron-beam-induced vacancies affects first-order Raman modes and correlate this effect with the evolution of in situ TEM two-terminal conductivity of monolayer MoS<sub>2</sub> under electron irradiation. We observe a redshift in the E' Raman peak and a less pronounced blueshift in the A'1 peak with increasing electron dose. Using energy-dispersive X-ray spectroscopy, we show that irradiation causes partial removal of sulfur and correlate the dependence of the Raman peak shifts with S vacancy density (a few percent), which is confirmed by first-principles density functional theory calculations. *In situ* device current measurements show exponential decrease in channel current upon irradiation. Our analysis demonstrates that the observed frequency shifts are intrinsic properties of the defective systems and that Raman spectroscopy can be used as a quantitative diagnostic tool to accurately characterize MoS<sub>2</sub>-based transport channels.

<sup>1</sup>This work was supported by the NIH Grant R21HG004767 and NIH Grant R21HG007856. Theoretical work at RPI was supported the NYSTAR program C080117 and the Office of Naval Research. C.H.N. and A.T.C.J. acknowledge support from UES/Air Force Research Lab.

**3:30PM H17.00004 Spin- and Valley-Polarized Transport across Line Defects in Monolayer MoS<sub>2</sub>**<sup>1</sup>, ARTEM PULKIN, OLEG YAZYEV, Institute of Theoretical Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland — We address ballistic transmission of charge carriers across ordered line defects in monolayer transition metal dichalcogenides. Our study reveals the presence of a transport gap driven by spin-orbit interactions, spin and valley filtering, both stemming from a simple picture of spin and momentum conservation, as well as the electron-hole asymmetry of charge-carrier transmission. Electronic transport properties of experimentally observed ordered line defects in monolayer MoS<sub>2</sub>, in particular the vacancy lines and inversion domain boundaries, are further investigated using first-principles Green's function methodology. Our calculations demonstrate the possibility of achieving nearly complete spin polarization of charge carriers in nanoelectronic devices based on engineered periodic line defects in monolayer transition metal dichalcogenides, thus suggesting a novel practical scheme for all-electric control of spin transport.

<sup>1</sup>We acknowledge support from ERC project "TopoMat" (grant No. 306504) and the Swiss NSF (grant No. PP00P2\_133552).

**3:42PM H17.00005 Electronic and Optical properties of Vacancy Defects in two dimensional monolayer Transition metal Dichalcogenides**, MAHTAB KHAN, MIKHAIL EREMENTCHOUK, MICHAEL LEUENBERGER, University of Central Florida — Defects play an important role in tailoring electronic and optical properties of two-dimensional monolayer transition metal dichalcogenides (TMDCs). Recently it has been shown that the presence of vacancy defects (VDs) in two-dimensional monolayer MoS<sub>2</sub> induces localized states which give rise to extra resonance peaks in both in-plane  $\chi_{||}$  and out-of-plane  $\chi_{\perp}$  susceptibilities.<sup>1</sup> In-plane  $\chi_{||}$  and out-of-plane  $\chi_{\perp}$  susceptibilities are related to the presence of even and odd states with respect to the Mo plane, respectively<sup>1</sup>. Moreover, monolayer TMDCs have a large spin orbit coupling (SOC), originating from d-orbitals of heavy transition metals and being of the order of a few 100 meV. We present a more general picture of the electronic and optical properties of defected monolayer TMDCs. In particular, we consider MoS<sub>2</sub>, MoSe<sub>2</sub>, WS<sub>2</sub> and WSe<sub>2</sub> with three types of VDs (i) Mo, W vacancy, (ii) S<sub>2</sub>, Se<sub>2</sub> vacancy, and (iii) S, Se vacancy. In addition, we investigate the effects of SOC on the band structures and the optical susceptibilities of VDs in TMDCs. 1. Mikhail Erementchouk, M. A. Khan, and Michael N. Leuenberger, Phys. Rev. B 92, 121401(R) (2015).

**3:54PM H17.00006 Ab-initio study of gold nanoparticles supported on defect-laden single-layer MoS<sub>2</sub>**<sup>1</sup>, TAKAT B. RAWAL, DUY LE, TALAT S. RAHMAN, University of Central Florida — We have investigated the geometry, electronic structure, and catalytic properties of gold nanoparticles on defect-laden single-layer MoS<sub>2</sub> using density functional theory (DFT) based calculations with semi-empirical van der Waals interaction (DFT-D3). Our results show that the two-dimensional planar structure, the most favorable one for unsupported Au<sub>13</sub> nanoparticle, transforms into a distorted three-dimensional (3D) structure when supported on single-layer MoS<sub>2</sub> with single S-vacancy which is more favorable than the icosahedral, decahedron and cuboctahedron forms. The MoS<sub>2</sub> support substantially alters the electronic structure of Au<sub>13</sub> nanoparticle near the Fermi level, owing to the strong interaction of MoS<sub>2</sub> support with Au<sub>13</sub> in the presence of an S-vacancy. The modified electronic structure remarkably affects the catalytic activity of the MoS<sub>2</sub>-supported Au<sub>13</sub>, offering enhanced activity towards methanol synthesis reaction via CO hydrogenation reaction - a contrast from that of titania-supported Au<sub>13</sub> nanoparticle [1] which promotes methanol decomposition. [1] S. Hong and T. S. Rahman, JACS, 135, 7629 (2013)

<sup>1</sup>This work is supported in part by U.S. Department of Energy (DOE DE-FG02-07ER15842)

**4:06PM H17.00007 Growth and optical characterization of distorted octahedral (T') WTe<sub>2</sub> and MoTe<sub>2</sub>**, SHAO-YU CHEN, THOMAS GOLDSTEIN, JUN YAN, Univ of Mass - Amherst, UNIV OF MASS - AMHERST TEAM — The polymorph of transition metal dichalcogenide (TMDC) has recently attracted great attention due to its novel physical properties. We grow distorted octahedral (T') WTe<sub>2</sub> and MoTe<sub>2</sub> by chemical vapor transport and rapid thermal quenching methods. The bulk and few layer samples exhibit distinct optical properties as compared with the well-investigated semiconducting hexagonal (H) TMDCs. We observe sharp intralayer, as well as interlayer optical phonon modes, that display angular dependent intensities consistent with the estimation by Raman tensor calculation. We also demonstrate *in-situ* phase transition of MoTe<sub>2</sub> from H to T' via rapid annealing in an electrically heated microfurnace. This enables ramping of the temperature from above 900C to room temperature within seconds. This well-controlled annealing process is promising for innovative fabrication of novel 2D materials devices.

**4:18PM H17.00008 Alloy Engineering of Defect Properties in Semiconductors: Suppression of Deep Levels in Transition-Metal Dichalcogenides**, BING HUANG, Beijing Computational Science Research Center, MINA YOON, BOBBY SUMPTER, Oak Ridge National Lab, SUHUI WEI, Beijing Computational Science Research Center, FENG LIU, University of Utah — Developing practical approaches to effectively reduce the amount of deep defect levels in semiconductors is critical for their use in electronic and optoelectronic devices, but this still remains a very challenging task. In this talk, we propose that specific alloying can provide an effective means to suppress the deep defect levels in semiconductors while maintaining their basic electronic properties. Specifically, we demonstrate that for transition-metal dichalcogenides, such as MoSe<sub>2</sub> and WSe<sub>2</sub>, where anion vacancies are the most abundant defects that can induce deep levels, the deep levels can be effectively suppressed in MoWSe<sub>2</sub> alloys at low W concentrations. This surprising phenomenon is associated with the fact that the band edge energies can be substantially tuned by the global alloy concentration, whereas the defect level is controlled locally by the preferred locations of Se vacancies around W atoms. Our findings illustrate a concept of alloy engineering and provide a promising approach to control the defect properties of semiconductors.

**4:30PM H17.00009 Focused helium-ion beam irradiation effects on electrical properties of multi-layer WSe<sub>2</sub>**, PUSHPA RAJ PUDASAINI, MICHAEL STANFORD, NICK CROSS, GERD DUSCHER, DAVID MANDRUS<sup>1</sup>, PHILIP RACK<sup>2</sup>, The University of Tennessee — Atomically thin transition metal dichalcogenides (TMDs) are currently receiving great attention due to their excellent opto-electronic properties. Tuning optical and electrical properties of mono and few layers TMDs, such as Tungsten diselenide (WSe<sub>2</sub>), by controlling the defects, is an intriguing opportunity to fabricate the next generation opto-electronic devices. Here, we report the effects of focused helium ion beam irradiation on structural, optical and electrical properties of few layer WSe<sub>2</sub>, via high resolution scanning transmission electron microscopy, Raman spectroscopy and electrical measurements. By controlling the ion irradiation dose, we selectively introduced precise defects in few layer WSe<sub>2</sub> thereby locally tuning the electrically resistivity of the material. Hole transport in the few layer WSe<sub>2</sub> is severely affected compared to electron transport for the same dose of helium ion beam irradiation studied. Furthermore, by selectively exposing the ion beams, we demonstrate the lateral p-n junction in few layer WSe<sub>2</sub> flakes, which constitute an important advance towards two dimensional opto-electronic devices.

<sup>1</sup>Materials Science and Technology Division, ORNL, Oak Ridge, TN 37831, USA

<sup>2</sup>Center for Nanophase Materials Sciences, ORNL, Oak Ridge, TN 37831, USA

**4:42PM H17.00010 Interplay of magnetic order and defect modulation in monolayer FeSe<sup>1</sup>**, JUNQIANG LU, University of Puerto Rico at Mayaguez, PENGFEI ZHANG, JIAN WU, Tsinghua University — We investigate the role of the defects (vacancy and anti-site) at the Fe-site on the magnetic order in monolayer FeSe. Experimental STM studies of defect states reveal that two type dumbbell-like dimers are formed at the surface of monolayer FeSe. We perform first-principles calculations of the magnetic structure of FeSe monolayer in the presence of defects in order to identify the origin of the STM observations. We consider various distribution of the defects and compare the checkerboard and collinear antiferromagnetic orders. Our results show that a single defect can give a dimer in STM image. A preliminary analysis show that both dimers are centered at the defects with their bright ends positioned on two adjacent Se atoms. We show that the two magnetic orders give rise to two distinct dimers types, in agreement with experiments.

<sup>1</sup>This work was supported by the NSF EPSCOR (grant 1010094).

**4:54PM H17.00011 Spatially Correlated Disorder in Epitaxial van der Waals Heterostructures<sup>1</sup>**, NOUAMANE LAANAIT, Center for Nanophase Materials Sciences, Oak Ridge National Lab, ZHAN ZHANG, Argonne National Lab, CHRISTIAN SCHLEPUTZ, Paul Sherrer Institute, YING LIU, University of Wisconsin, Milwaukee, MICHAEL WOJCIK, Argonne National Lab, RACHAEL MYERS-WARD, D. KURT GASKILL, U.S Naval Research Lab, PAUL FENTER, Argonne National Lab, LIAN LI, University of Wisconsin, Milwaukee — The structural cohesion of van der Waals (vdW) heterostructures relies upon a cooperative balance between strong intra-layer bonded interactions and weak inter-layer coupling. The confinement of extended defects to within a single vdW layer and competing interactions introduced by epitaxial constraints could generate fundamentally new structural disorders. Here we report on the presence of spatially correlated and localized disorder states that coexist with the near perfect crystallographic order along the growth direction of epitaxial vdW heterostructure of Bi<sub>2</sub>Se<sub>3</sub>/graphene/SiC grown by molecular beam epitaxy. With the depth penetration of hard X-ray diffraction microscopy and high-resolution surface scattering, we imaged local structural configurations from the atomic to mesoscopic length scales, and found that these disorder states result as a confluence of atomic scale modulations in the strength of vdW layer-layer interactions and nanoscale boundary conditions imposed by the substrate. These findings reveal a vast landscape of novel disorder states that can be manifested in epitaxial vdW heterostructures.

<sup>1</sup>Supported by the Wigner Fellowship program at Oak Ridge Nat'l Lab.

**5:06PM H17.00012 Defect-induced multiphoton absorption and photoluminescence in BN for bio-imaging**, MEHMET KARAKAYA, YONGCHANG DONG, RAMAKRISHNA PODILA, APPARAO RAO, Clemson Univ — Emerging two-dimensional materials are known for their excellent optical properties. Boron nitride (BN) is the only 2D material which exhibits multi-photon absorption. This combined with tunable defect-induced photoluminescence in BN could be used for multi-photon bio-imaging. Previously, a two-photon absorption process was proposed for explaining non-linear optical absorption in BN. However, as discussed in this talk, we show that defects (such as C and O) in BN result in mid-gap states that enable three-photon absorption in addition to tunable emission. The non-linear optical properties of BN could be used for bio-imaging at longer wavelengths which facilitate higher penetration depth and the resolution in vivo.

**5:18PM H17.00013 Impurity-mediated early charge density wave condensation in the oxygen-adsorbed In/Si(111)-(4×1)/(8×2) nanowire array**, STEFAN WIPPERMANN, Max-Planck-Institut fuer Eisenforschung, ANDREAS LUECKE, WOLF GERO SCHMIDT, Paderborn University, DEOK MAHN OH, HAN WOONG YEOM, Pohang University — The self-assembled In/Si(111)-(4×1) nanowire array is an extremely popular model system for one-dimensional electronic systems and features a reversible temperature-induced phase transition into a charge density wave (CDW) ordered ground state. While impurities have been widely known to affect this phase transition, the atomistic mechanisms have rarely been elucidated. Here we present a joint experimental and *first principles* study, demonstrating oxygen impurity atoms to condense the In/Si(111) nanowire array locally into its CDW ground state, even above the transition temperature. Interestingly, CDW ordering is induced only by a concerted effect of multiple impurities. The mechanism is explained as a subtle interplay between coherent superposition of local impurity-induced lattice strain, a strong coupling between electronic and lattice degrees of freedom, and phononic effects on the free energy. Funding from DFG FOR1700 is gratefully acknowledged.

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**

**Session H18 GMAG DMP FIAP: Spins in Reduced Dimensional Semiconductors** 317 - Scott Crooker, Los Alamos National Laboratory

**2:30PM H18.00001 ABSTRACT WITHDRAWN –**

**2:42PM H18.00002 Spin-orbit interaction in monolayer (group-III) metal-monochalcogenides**, PENGKE LI, IAN APPELBAUM, Univ of Maryland-College Park, PHYSICS DEPARTMENT TEAM — Beginning with an analysis of the fundamental symmetries of monolayer (group-III) metal-monochalcogenides (such as GaSe), we examine various spin-dependent properties of this new series of 2D semiconductors. Interesting features resulting from spin-orbit interaction include broken valence band degeneracy, cubic Dresselhaus spin splitting, and eigenstate spin-mixing. The latter two control the type and magnitude of dominant spin relaxation pathways and influence the 'caldera' shape valence band edge. Further phenomena endowed by spin-orbit interaction include a modest orbital contribution to the Lande g-factors and the possibility of optical orientation via band-edge photoexcitation spectroscopy, which shows an energy-dependent reversal of conduction electron spin polarization. Based on this analysis, we propose an experiment to use optically-driven spin dynamics to quantify different spin lifetimes for electron and holes. Reference: arXiv:1508.06963

**2:54PM H18.00003 Controlling spin lifetime with Dresselhaus and Rashba fields in the 2D semiconductor  $MX^1$** , IAN APPELBAUM, PENGKE LI, Univ of Maryland-College Park — It is widely believed that whenever spin encodes logic state in a semiconductor device, transport channel materials with the longest spin lifetime are the most suitable choice. However, once a logic operation is completed, residual spins can and will interfere with those involved in future operations. We propose to solve this problem by utilizing the unique properties of spin-orbit effects in the electronic structure of monolayer of group-III metal-monochalcogenide ( $MX$ ) semiconductors. The interplay of Dresselhaus and Rashba effective magnetic fields in these materials will be shown to provide effective external control over spin polarization lifetime, potentially useful for future spin-enabled digital devices.

<sup>1</sup>Based upon: Pengke Li and Ian Appelbaum, arxiv:1508.06963 (to appear in Phys. Rev. B). We acknowledge support from NSF, DTRA, and ONR.

**3:06PM H18.00004 Long-lived Spin Relaxation and Spin Coherence of Electrons in Monolayer  $MoS_2^1$** , LUYI YANG, National High Magnetic Field Laboratory, Los Alamos — Monolayer  $MoS_2$  and related transition metal dichalcogenides (TMDs) are direct-gap semiconductors in which strong spin-orbit coupling and a lack of structural inversion symmetry give rise to new coupled spin-valley physics. Although robust spin and valley degrees of freedom have been inferred from polarized photoluminescence (PL) studies of *excitons*, PL timescales are necessarily constrained by short (3–100 ps) electron-hole recombination. Direct probes of spin/valley dynamics of resident carriers in electron (or hole)-doped TMDs, which may persist long after recombination ceases, are still at an early stage. Here we directly measure the coupled spin-valley dynamics of *resident* electrons in *n*-type monolayer  $MoS_2$  using optical Kerr-rotation spectroscopy [1], and reveal very long spin lifetimes exceeding 3ns at 5K (orders of magnitude longer than typical exciton lifetimes). In contrast with conventional III-V or II-VI semiconductors, spin relaxation accelerates rapidly in small transverse magnetic fields. This suggests a novel mechanism of electron spin dephasing in monolayer TMDs, driven by rapidly-fluctuating internal spin-orbit fields due to fast intervalley scattering. Additionally, a small but very long-lived oscillatory signal is observed, indicating spin coherence of localized states [2]. These studies provide direct insight into the physics underpinning the spin and valley dynamics of electrons in monolayer TMDs. [1] L. Yang *et al.*, *Nature Physics* **11**, 830 (2015). [2] L. Yang *et al.*, *submitted*.

<sup>1</sup>In collaboration with S.A. Crooker & N.A. Sinitsyn (Los Alamos), W. Chen, J. Yuan, J. Zhang & J. Lou (Rice University), K.M. McCreary & B.T. Jonker (Naval Research Lab), and supported by the Los Alamos LDRD program.

**3:42PM H18.00005 Spin Transport in Single Layer Transition Metal Dichalcogenides<sup>1</sup>**, MICHAEL PHILLIPS, VIVEK AJI<sup>2</sup>, Univ of California - Riverside — Inversion symmetry breaking and strong spin orbit coupling in two dimensional transition metal dichalcogenides leads to interesting new phenomena such as the valley hall and spin hall effects. The nontrivial Berry curvature of the bands yields transverse spin currents in applied field. In this talk we characterize the spin transport in hole-doped systems. Due to the large spin-splitting, time-reversal invariance, and the large separation of hole pockets in momentum space, spin flip scattering involves inter-valley processes with large momentum. As such, one expects large spin life times and a large spin hall angle. We analyze the robustness of the phenomena to various scattering processes and explore the viability of transition metal dichalcogenides for spintronic applications.

<sup>1</sup>We acknowledge the support of the NSF via grant NSF DMR-1506707.

<sup>2</sup>PI

**3:54PM H18.00006 Spin polarized transport in  $MoS_2$** , ANDRÉ DANKERT, PARHAM PASHAEI, VENKATA KAMALAKAR MUTTA, SAROJ PRASAD DASH, Chalmers University of Technology, SPINTRONIC SPD TEAM — The two-dimensional (2D) semiconductor  $MoS_2$  possesses a high potential for spintronic devices due to a rich spin-valley physics and large spin-orbit coupling. While there have been significant advances in studying the spin and valley dynamics in  $MoS_2$  using optical spectroscopy techniques, electronic spin transport in semiconducting  $MoS_2$  or its heterostructures have not yet been demonstrated. Here we report the electronic and spin transport properties in  $MoS_2$  employing ferromagnetic electrodes in a vertical device geometry. Such vertical devices with  $MoS_2$  channel length defined by the thickness of the 2D layer allow to investigate the spin injection, transport and detection. We observe a magnetoresistance effect over a large temperature range up to 300 K and investigate the temperature and bias dependence behavior. Using magnetotransport data and calculations we extract spin parameters in the  $MoS_2$  spin valve devices. These findings can open new avenues for exploring spin functionalities in 2D semiconductor heterostructures for spin logic applications.

**4:06PM H18.00007 Novel valley depolarization dynamics and valley Hall effect of exciton in mono- and bilayer  $MoS_2$** , T. YU, M. W. WU, University of Science and Technology of China, Physics Department — We investigate the valley depolarization dynamics and valley Hall effect of exciton due to the electron-hole exchange interaction in mono- and bilayer  $MoS_2$ . For the valley depolarization dynamics, in the monolayer  $MoS_2$ , it is found that in the strong scattering regime, the conventional motional narrowing picture is no longer valid, and a novel valley depolarization channel is opened. For the valley Hall effect of exciton, in both the mono- and bilayer  $MoS_2$ , with the exciton equally pumped in the K and K' valleys, the system can evolve into the equilibrium state with the valley polarization parallel to the effective magnetic field due to the exchange interaction. With the drift of this equilibrium state by applied uniaxial strain, the *momentum-dependent* valley/photoluminescence polarization is induced by the exchange interaction, which leads to the valley/photoluminescence Hall current. Specifically, the disorder strength dependence of the valley Hall conductivity is revealed. In the strong scattering regime, the valley Hall conductivity decreases with the increase of the disorder strength; whereas in the weak scattering regime, it saturates to a constant, which can be much larger than the one in Fermi system due to the absence of the Pauli blocking.

**4:18PM H18.00008 Spin-orbit coupling and spin relaxation in phosphorene**, MARCIN KURPAS, MARTIN GMITRA, JAROSLAV FABIAN, Physics Department, University of Regensburg, 93040 Regensburg, Germany — We employ first principles density functional theory calculations to study intrinsic and extrinsic spin-orbit coupling in monolayer phosphorene. We also extract the spin-mixing amplitudes of the Bloch wave functions to give realistic estimates of the Elliott-Yafet spin relaxation rate. The most remarkable result is the striking anisotropy in both spin-orbit coupling and spin relaxation rates, which could be tested experimentally in spin injection experiments. We also identify spin hot spots in the electronic structure of phosphorene at accidental bands anticrossings. We compare the Elliott-Yafet with Dyakonov-Perel spin relaxation times, obtained from extrinsic couplings in an applied electric field. We also compare the results in phosphorene with those of black phosphorous. This work is supported by the DFG SPP 1538, SFB 689, and by the EU Seventh Framework Programme under Grant Agreement No. 604391 Graphene Flagship.

**4:30PM H18.00009 Probing Hole Spins in an InAs/GaAs Quantum Dot Molecule subject to Lateral Electric Fields**, XIANGYU MA, Univ of Delaware, GARNETT BRYANT, National Institute of Standards and Technology, MATTHEW DOTY, Univ of Delaware — Quantum dot molecules (QDMs) are structures in which coherent interactions between two or more adjacent quantum dots (QDs) can lead to unique, tunable electronic and spin properties. We explore computationally spin-mixing interactions in the molecular states of single holes confined in vertically-stacked InAs/GaAs self-assembled QDMs. We consider the spin properties of the hole states subject to electric fields that have components both parallel and perpendicular to the molecular stacking axis. We compute the energies of the QDM hole states under various electric and magnetic fields with a combination of full tight binding atomistic calculations and approximate atomistic results using eigenstates found at particular fields as a basis to extrapolate to other fields. We observe a relatively large Stark shift in hole states with the application of lateral electric fields, as well as a quenching of the Zeeman splitting. Most importantly, we observe that lateral electric fields induce hole spin mixing with a magnitude that increases with increasing lateral electric field over a moderate range. These results suggest that applied lateral electric fields provide an opportunity to fine-tune and manipulate, in situ, the energy levels and spin properties of single holes confined in QDMs.

**4:42PM H18.00010 Spin Dynamics of Tellurium Isoelectronic Centers Bound Excitons in Zn-Se-Te Nanostructures**<sup>1</sup>, VASILIOS DELIGIANNAKIS, The City College of New York of CUNY, SIDDHARTH DHOMKAR, Queens College of CUNY, DANIELA PAGLIERO, The City College of New York of CUNY, HAOJIE JI, Queens College of CUNY, MARIA TAMARGO, The City College of New York of CUNY, IGOR KUSKOVSKY, Queens College of CUNY, CARLOS MERILES, The City College of New York of CUNY — Three-dimensionally confined structures such as quantum dots (QDs) have been of considerable interest due to their ability to closely imitate isolated atoms on mesoscopic length scales. Recently, single impurity states in bulk semiconductors have also attracted attention due to their ability to optically address quantum states. Here we show results pertaining to the optical and spin properties of Te isoelectronic centers present in type-II sub-monolayer QDs within a ZnSe matrix. Time resolved Kerr rotation (TRKR) measurements were performed using a degenerate pump-and-probe setup. Attempts to probe the QDs by direct optical excitation did not show any results most likely due to the weak oscillator strength of this transition resulting from their type-II nature. Centering the pump and probe pulses around the band edge of ZnSe and performing TRKR vs energy measurements we were able to address the spin dynamics of Te-isoelectronic centers present in the spacer layer. Results show that the  $\tau^2$  lifetimes exhibit a bi-exponential decay and persist up to 1 ns. Further measurements will be done on samples with varying Te concentration, as well as a function of the applied magnetic-field to understand the spin properties of this defect.

<sup>1</sup>U.S. Department of Energy Award No. DE- SC003739

**4:54PM H18.00011 Self-consistent Theory of Magnetic Polarons in Semiconductor Quantum Dots**<sup>1</sup>, DAN REDERTH, RAFAL OSZWALDOWSKI, SDSMT Physics, A. G. PETUKHOV, NASA Ames Research Center — Nanostructures based on dilute magnetic semiconductors indicate paths towards novel devices that could employ carrier spin [1-2]. Magnetic quantum dots (QDs) are an example of such structures. We use a robust numerical method, based on the Luttinger-Kohn Hamiltonian and suitable for realistic self-assembled QD geometries [3], to study electronic structure and magnetism of p-type II-VI quantum dots doped with Mn magnetic ions. Our method relies on self-consistent treatment of exchange coupling of holes and magnetic ions within the mean-field approximation [4]. It explicitly takes into account multi-band character of the hole kinetic energy operator. We demonstrate formation of the hole magnetic polarons, which manifests itself in self-induced splitting of the hole levels in absence of an external magnetic field [5]. Furthermore, we conduct detailed studies of the magnetically-ordered QD ground state. The structure of the ground state reveals highly anisotropic, as well as, position- and temperature-dependent self-induced magnetization. [1] Semiconductor spintronics and quantum computation, D.D. Awschalom, D. Loss, and N. Samarth eds., (Springer, Berlin, 2002). [2] J. Fabian, A. Matos-Abiad, C. Ertler, et al., Acta Phys. Slov 57, 565 (2007). [3] H. Kirmse, R. Schneider, M. Rabe, et al., Appl. Phys. Lett. 72, 1329 (1998). [4] R. Oszwaldowski, P. Stano, A. Petukhov, and I. Zutic, Phys. Rev. B 86, 201408 (2012). [5] Seufert, J., Bacher, G., Scheibner, et al., Phys. Rev. Letters 88, 27402 (2002).

<sup>1</sup>Supported by DOE DE-SC00004890

**5:06PM H18.00012 Modeling of magnetic polaron properties in (Zn,Mn)Te quantum dots**<sup>1</sup>, JAMES PIENKA, St. Bonaventure University, B. BARMAN, L. SCHWEIDENBACK, A.H. RUSS, Y. TSAI, J.R. MURPHY, A.N. CARTWRIGHT, I. ZUTIC, B.D. MCCOMBE, A. PETROU, SUNY Buffalo, W-C. CHOU, W. C. FAN, National Chiao Tung University, I.R. SELLERS, University of Oklahoma, A.G. PETUKHOV, R. OSZWALDOWSKI, South Dakota School of Mines and Technology — Magnetic polarons in (Zn,Mn)Te quantum dots (QD) show unconventional behavior [1]. These structures exhibit a small red shift of the photoluminescence peak energy in the presence of a magnetic field  $B$  and they also have a weak dependence of the polaron energy  $E_{MP}$  on temperature  $T$  and  $B$ . We attribute these properties to a large molecular field  $B_m$  that is proportional to the heavy holes spin density [2]. We have calculated  $B_m$  using the QD diameter and height as adjustable parameters. Assuming hole localization, this calculation yields values of  $B_m > 20$  T. The assumption that the hole localization diameter can be smaller than the QD diameter is justified due to alloy and spin disorder scattering [3]. Using the magnetic polaron free energy, we calculate  $E_{MP}$  as function of  $T$  and  $B$  for a variety of  $B_m$  values. To get a weak dependence of  $E_{MP}$  on  $T$  and  $B$  we must assume that the polaron temperature is higher than  $T$ . [1] B. Barman et al., Phys. Rev. B 92, 035430 (2015). [2] J. M. Pientka et al., Phys. Rev. B 92, 155402 (2015). [3] K. V. Kavokin et al., Phys. Rev. B 60, 16499 (1999).

<sup>1</sup>This work was supported by U.S. DOE BES, Award DE-SC0004890, NSF DMR-1305770 and U.S. ONR N000141310754.

**5:18PM H18.00013 Gate-tuned spin to charge conversion in semiconducting single-walled carbon nanotubes**, EI SHIGEMATSU, HIROSHI NAGANO, Kyoto Univ, SERGEY DUSHENKO, Osaka Univ, YUICHIRO ANDO, Kyoto Univ, TETSUYA TSUDA, SUSUMU KUWABATA, Osaka Univ, TAISHI TAKENOBU, Waseda Univ, TAKESHI TANAKA, HIROMICHI KATAURA, AIST, TERUYA SHINJO, MASASHI SHIRAIISHI, Kyoto Univ — Interconversion of spin and charge current is a hot topic in the molecular spintronics. It was achieved for the first time in a conducting conjugated polymer<sup>1</sup>, and shortly followed by spin-charge conversion in graphene. However, control over carrier type has not been shown yet. In this study we focused on single-walled carbon nanotubes (SWNT). Spin injection into semiconductor from metal ferromagnet is challenging due to the presence of Schottky barrier and conductance mismatch problem. To bypass it, we used ionic liquid electric gate and ferrimagnetic insulator. We prepared SWNT layer on top of ferrimagnetic yttrium iron garnet substrate. Using spin pumping we successfully observed spin-charge conversion in metallic SWNT. As for a semiconducting SWNT, we applied a top gate using ionic liquid. The drain-source current vs. gate voltage dependence showed tuning of the Fermi level and changing of carrier type. Under gate voltage application we measured electromotive force induced by spin pumping. Detected voltage changed its sign together with carrier type. This is first evidence of spin-charge conversion in carbon nanotubes<sup>2</sup>.

<sup>1</sup> K. Ando et al., Nature Mater. 12, 622 (2013).

<sup>2</sup> E. Shigematsu et al., submitted.

**Tuesday, March 15, 2016 2:30PM - 5:18PM –**  
**Session H19 GMAG DMP FIAP: Spin-Order and Half-Metallicity of Magnetic Thin Films** 318 -  
 Chiara Ciccarelli, University of Cambridge

**2:30PM H19.00001 Influence of interstitial Mn on spin order and dynamics in the room-temperature ferromagnet  $\text{Mn}_{1+\delta}\text{Sb}$** , ALICE TAYLOR, Oak Ridge National Laboratory —  $\text{Mn}_{1+\delta}\text{Sb}$  is a well-known, high Curie temperature, ferromagnetic metal. It has particular importance because it, and closely related MnBi, show promise as alternatives to rare-earth-containing permanent magnets, and as magneto-optic media. To exploit these materials useful properties, it is desirable to tune and optimize the magnetic properties [1]. To achieve this, the magnetic interactions, and the effects of doping and defects must be understood. In  $\text{Mn}_{1+\delta}\text{Sb}$  the magnetic order is highly sensitive to the interstitial Mn ion content,  $\delta$ , suggesting a route to tune the properties [2]. However, detailed theoretical and experimental investigations of the effect of the interstitial ion, Mn2, have been lacking, probably due to a prevailing view in the literature that the Mn2 site is nonmagnetic [3,4]. We examine the magnetic state of Mn2, and its influence on the magnetic properties of  $\text{Mn}_{1+\delta}\text{Sb}$ . We use a combination of neutron scattering techniques alongside detailed calculations to show that the Mn2 site is in-fact magnetic, and has a dramatic impact on the magnetic dynamics in  $\text{Mn}_{1+\delta}\text{Sb}$ . An unusual, broad, intense feature is identified in the magnetic dynamics which cannot be explained by the long-range symmetry of the material. This reveals an area in which current theoretical/modeling techniques limit our ability to understand the magnetic excitations revealed by neutron scattering. This investigation elucidates important aspects of the behavior of  $\text{Mn}_{1+\delta}\text{Sb}$ , whilst highlighting requirements for future research to understand the major influence of the interstitial ion on the magnetic properties. [1] A. E. Taylor et al., Phys. Rev. B, 91, 224418 (2015). [2] T. Okita and Y. Makino, J. Phys. Soc. Jpn. 25, 120 (1968). [3] Y. Yamaguchi et al., J. Phys. Soc. Jpn. 45, 846 (1978). [4] W. Reimers et al., J. Phys. Chem. Solids 44, 195 (1983).

**3:06PM H19.00002 Magnetic Structure and Dynamics in the Itinerant High-Temperature Ferromagnet MnBi**, TRAVIS WILLIAMS, ALICE TAYLOR, ANDREW CHRISTIANSON, STEVEN HAHN, RANDY FISHMAN, MICHAEL MCGUIRE, BRIAN SALES, MARK LUMSDEN, Oak Ridge National Laboratory — The high-temperature ferromagnet MnBi has been receiving much attention as a rare-earth-free permanent magnet to replace more costly rare-earth-containing magnets in applications above room temperature. This is due to MnBi containing strong Mn moments and large energy products. The synthesis of MnBi also allows for crystals that are free from interstitial Mn, allowing for the study of a more fundamental member of this family of binary Mn-based ferromagnets. In this work, we use polarized neutron diffraction to measure the magnetic moments of Mn and Bi, and find that the Bi atoms also have a magnetic moment, but 2 orders of magnitude smaller than Mn. We study their behavior through the spin reorientation that occurs at  $T_S \approx 100$  K, finding that both moments reorient simultaneously. We also use inelastic neutron scattering to measure the spin waves of MnBi in order to determine the magnetic exchange at low temperatures. Consistent with the strongly temperature-dependent magnetic anisotropy, we find that the spin gap is very small, and so the magnetic order arises from the strongly ferromagnetic nearest-neighbor term, but interactions up to sixth nearest neighbor are required to fully characterize the spin waves, suggesting that the Mn moments are strongly itinerant.

**3:18PM H19.00003 Electronic and magnetic properties of ferromagnetic interfaces for spin injection applications: metallic and semiconducting cases<sup>1</sup>**, E. A. ALBANESI, IFIS-CONICET-UNL and FI-UNER, Santa Fe, Argentina, L. MAKINISTIAN, INFAP-CONICET-UNSL, San Luis, Argentina, C. I. ZANDALAZINI, IFIS-CONICET-UNL, Santa Fe, Argentina, R. M. OSZWALDOWSKI, SDSMT, Rapid City, SD, A. G. PETUKHOV, NASA Ames Research Center, Moffett Field, CA 94035 — Robust and reliable operation of spintronic devices is determined by the quality of interfaces between magnetic and nonmagnetic materials. In order to get insights in the tuning of the magnetic properties of such interfaces we present comparative studies of two important cases relevant to applications in spin injection devices. We performed ab-initio calculations of the electronic and magnetic properties, of the ferromagnetic metallic interface of  $\text{Co}_2\text{MnAl}$  and gold, and of the interfaces of non- and of magnetic II-VI semiconductors and their quantum wells. In the case of the Heusler alloy  $\text{Co}_2\text{MnAl-Au}$ , two structural models are implemented: one with the ferromagnet slab terminated in a pure cobalt plane ( $\text{Co}_2\text{-t}$ ), and the other with it terminated with a plane of MnAl ( $\text{MnAl-t}$ ). The electric in-plane and averaged potential are resolved and analyzed layer by layer through the interface. We predict that both terminations are to be expected to display sensibly different spin injection performances. On the example of magnetic quantum wells of  $\text{ZnSe/Zn}_x\text{Mn}_{1-x}\text{Te/ZnSe}$ , we study the variations in the spin resolved density of states, and the potential energy along the junctions.

<sup>1</sup>We acknowledge financial support from SDSMT (USA), and CONICET, FIUNER, of Argentina

**3:30PM H19.00004 Structural and magnetic properties of a prospective spin gapless semiconductor MnCrVAL<sup>1</sup>**, Y HUH, S GILBERT, P KHAREL, Department of Physics, South Dakota State University, Brookings, SD 57007, Y JIN, Department of Physics and Astronomy, University of Nebraska, Lincoln, NE 68588, P LUKASHEV, Department of Physics, University of Northern Iowa, Cedar Falls, IA 50614, S VALLOPILLY, D. J. SELLMYER, Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, NE 68588 — Recently a new class of material, spin gapless semiconductors (SGS), has attracted much attention because of their potential for spintronic devices. We have synthesized a Heusler compound, MnCrVAL, which is theoretically predicted to exhibit SGS by arc melting, rapid quenching and thermal annealing. First principles calculations are employed to describe its structural, electronic and magnetic properties. X-ray diffraction indicates that the rapidly quenched samples crystallize in the disordered cubic structure. The crystal structure is stable against heat treatment up to 650°C. The samples show very small saturation magnetization, 0.3 emu/g, at room temperature under high magnetic field, 30 kOe. Above room temperature, the magnetization increases with increasing temperature undergoing a magnetic transition at 560°C, similar to an antiferromagnetic-to-paramagnetic transition. The prospect of this material for spintronic applications will be discussed.

<sup>1</sup>This research is supported by SDSU Academic/Scholarly Excellence Fund, and Research/Scholarship Support Fund. Research at UNL is supported by DOE (DE-FG02-04ER46152, synthesis, characterization), NSF (ECCS-1542182, facilities), and NRI.

**3:42PM H19.00005 Enhancement of ferromagnetism by Ag doping in Ni-Mn-In-Ag Heusler alloys**, SUDIP PANDEY, ABDIEL QUETZ, ANIL ARYAL, IGOR DUBENKO, DIPANJAN MAZUMDAR, Southern Illinois University, SHANE STADLER, Louisiana State University, NAUSHAD ALI, Southern Illinois University — The effect of Ag on the structural, magnetocaloric, and thermomagnetic properties of  $\text{Ni}_{50}\text{Mn}_{35}\text{In}_{15-x}\text{Ag}_x$  ( $x=0.1, 0.2, 0.5$ , and 1) Heusler alloys was studied. The magnitude of the magnetization change at martensitic transition temperature ( $T_M$ ) decreases with increasing Ag concentration. A smaller magnetic entropy changes ( $\Delta S_M$ ) for the alloys with higher Ag concentration is observed. A shift of  $T_M$  by about 25 K to a higher temperature was detected for  $P = 6.6$  kbar with respect to ambient pressure. Large drop of resistivity is observed with the increase of Ag concentration. The magnetoresistance is dramatically suppressed with increasing Ag concentration due to the weakening of the antiferromagnetic interactions in the martensitic phase. The experimental results demonstrate that Ag substitution in  $\text{Ni}_{50}\text{Mn}_{35}\text{In}_{15-x}\text{Ag}_x$  Heusler alloys suppresses the AFM interactions and enhances the FM interactions in the alloys. The possible mechanisms responsible for the observed behavior are discussed. Acknowledgement: This work was supported by the Office of Basic Energy Sciences, Material Science Division of the U.S. Department of Energy (DOE Grant No. DE-FG02-06ER46291 and DE-FG02-13ER46946).

**3:54PM H19.00006 Probing the magnetic structure of  $\text{Co}_2\text{Fe}_x\text{Mn}_{1-x}\text{Si}$  thin films by XAS/XMCD**, ADAM J. HAUSER, JOSHUA PHILLIPS, Department of Physics, The University of Alabama, MIHIR PENDHARKAR, SAHILL J. PATEL, CHRIS J. PALMSTROM, Materials Department, University of California-Santa Barbara, Santa Barbara, California 93106, USA — We have analyzed the magnetic configuration for highly ordered epitaxial thin films across the  $\text{Co}_2\text{Fe}_x\text{Mn}_{1-x}\text{Si}$  compositional series ( $x = 0, 0.3, 0.7, 1$ ) by x-ray circular magnetic dichroism (XMCD) and x-ray absorption spectroscopy (XAS). These measurements give the element-specific electronic structure of each film, as well as the spin and orbital moments. We will present our observations at the Co, Mn, and Fe L-edges to explain the significant changes in intermediate stoichiometries as compared with the parent  $\text{Co}_2\text{MnSi}$  and  $\text{Co}_2\text{FeSi}$  systems.

**4:06PM H19.00007 Growth of Cr<sub>2</sub>CoGa and inverse Heusler thin films using Molecular Beam Epitaxy<sup>1</sup>**, MICHELLE JAMER, MATTHEW DECAPIUA, GABRIEL PLAYER, DON HEIMAN, Northeastern University — Theoretical calculations have predicted the existence of inverse Heusler compounds that exhibit zero-moment magnetization while retaining their half-metallicity. These unique compounds have been labeled spin gapless semiconductors (SGS), where the density of states (DOS) can behave as a half-metal or gapless semiconductor.[1] There is a special interest for zero-moment SGS compounds since traditional antiferromagnets cannot be spin-polarized.[2] Such compounds are experimentally attractive for future spintronic devices due to their large magnetic transition temperature (400-800 K).[3] This work focuses on zero-moment inverse Heusler compounds including Cr<sub>2</sub>CoGa and Mn<sub>3</sub>Al. Thin films have been grown using MBE and their magnetic, structural, and electrical properties of these compounds have been characterized by various techniques, including XMCD and magnetometry. The atomic moments are found to be large, but significant cancellations lead to small average moments. [1] M.E. Jamer, B.A. Assaf, T. Devakul and D. Heiman, Appl. Phys. Lett. **103**, 142403 (2013). [2] M.E. Jamer, B.A. Assaf, G.E. Sterbinsky, D. Arena, L.H. Lewis, A.A. Saúl, G. Radtke, D. Heiman, Phys. Rev. B **91**, 094409 (2015). [3] M.E. Jamer, L.G. Marshall, G.E. Sterbinsky, L.H. Lewis, D. Heiman, J. Magn. Magn. Mater. (2015).

<sup>1</sup>Supported by NSF grant ECCS-1402738

**4:18PM H19.00008 Large magnetoresistance induced by crystallographic defects in Fe<sub>x</sub>TaS<sub>2</sub> single crystals<sup>1</sup>**, CHIH-WEI CHEN, EMILIA MOROSAN, Rice University, MOROSAN'S GROUP TEAM — The search for the materials that show large magnetoresistance and the mechanisms that induce it remains challenging in both experimental and theoretical aspects. The giant magnetoresistance in one class of materials, ferromagnetic conductors, is generally attributed to the misalignments of magnetic moments, which cause spin disorder scattering. Recently, very large magnetoresistance (>60%) was discovered in the ferromagnetic Fe-intercalated transition metal dichalcogenide, Fe<sub>0.28</sub>TaS<sub>2</sub> [Phys. Rev. B **91**, 054426(2015)]. The mechanism that led to this large magnetoresistance was suggested to be due to the deviation of Fe concentration from commensurate values (1/4 or 1/3), which caused magnetic moments misalignments. Here we report a study of Fe<sub>x</sub>TaS<sub>2</sub> crystals with *x* close to the commensurate values. Our results qualitatively demonstrate that crystallographic defects significantly affect magnetoresistance in Fe<sub>x</sub>TaS<sub>2</sub>. This provides a way to search for large magnetoresistance in more intercalated transition metal dichalcogenides.

<sup>1</sup>This work is supported by the Department of Defense PECASE.

**4:30PM H19.00009 Development of spin-gapless semiconductivity and half metallicity in Ti<sub>2</sub>MnAl by substitutions for Al<sup>1</sup>**, PAVEL LUKASHEV, University of Northern Iowa, SIMEON GILBERT, South Dakota State University, BRADLEY STATEN, NOAH HURLEY, University of Northern Iowa, RYAN FUGLSBY, PARASHU KHAREL, YUNG HUH, South Dakota State University, SHAH VALLOPILLY, WENYONG ZHANG, University of Nebraska, Lincoln, K. YANG, Hohai University, DAVID J. SELLMYER, University of Nebraska, Lincoln — In recent years, ever increasing interest in spin-based electronics has resulted in the search for a new class of materials that can provide a high degree of spin polarized electron transport. An ideal candidate would act like insulator for one spin channel and a conductor or semiconductor for the opposite spin channel (e.g., half metal (HM), spin-gapless semiconductor (SGS)). Here, we present the combined computational, theoretical, and experimental study of Ti<sub>2</sub>MnAl, a Heusler compound with potential application in the field of spintronics. We show that in the ground state this material is metallic, however it becomes a SGS when 50% of Al is substituted with In (e.g., Ti<sub>2</sub>MnAl<sub>0.5</sub>In<sub>0.5</sub>), and a HM when 50% of Al is substituted with Sn (e.g., Ti<sub>2</sub>MnAl<sub>0.5</sub>Sn<sub>0.5</sub>). Detailed study of the structural, electronic, and magnetic properties of these materials is presented.

<sup>1</sup>Financial support: DOE/BES (DE-FG02-04ER46152); NSF NNCI: 1542182; NRI; Academic and Scholarly Excellence Funds, Office of Academic Affairs, SDSU; UNI Faculty Summer Fellowship; Program for Outstanding Innovative Talents in Hohai University.

**4:42PM H19.00010 Antiferromagnetic-domain-dependent magnetoresistance in Pt/Fe<sub>2</sub>Mo<sub>3</sub>O<sub>8</sub> interface**, TOSHIYA IDEUE, University of Tokyo, TAKASHI KURUMAJI, RIKEN Center for Emergent Matter Science (CEMS), SHINTARO ISHIWATA, University of Tokyo, YOSHINORI TOKURA, University of Tokyo, RIKEN Center for Emergent Matter Science (CEMS), UNIVERSITY OF TOKYO TEAM, RIKEN CENTER FOR EMERGENT MATTER SCIENCE (CEMS) TEAM — Interface between nonmagnetic metal and magnetic insulator has been extensively studied, exploiting a variety of new exotic spin transports. Among them, magnetoresistance in Pt/YIG interface attracts intense experimental and theoretical interest. The resistance of Pt layer reflects the magnetization of YIG in spite of the insulating nature of YIG, which has been explained by the spin current across the Pt/YIG interface or the magnetic proximity effect. So far, such anomalous magnetoresistance have been reported only in the interface between nonmagnetic metal and ferrimagnetic insulator. In this work, we have studied the transport properties of Pt on the antiferromagnetic insulator Fe<sub>2</sub>Mo<sub>3</sub>O<sub>8</sub>. Fe<sub>2</sub>Mo<sub>3</sub>O<sub>8</sub> shows the metamagnetic phase transition under the magnetic field by which we can control the two different antiferromagnetic domains. Interestingly, transverse magnetoresistance in Pt/Fe<sub>2</sub>Mo<sub>3</sub>O<sub>8</sub> interface shows the distinct behaviors depending on the field cooling process which result in the different antiferromagnetic domains. This implies that the spin transport or proximity effect at the interface is different between two domains and can be probed by the resistance of nonmagnetic Pt.

**4:54PM H19.00011 Magnetic properties of Cr<sub>3</sub>Te<sub>4</sub> doped with transition metals: An *ab initio* study**, NABIL AL-AQTASH, The Hashemite University, RENAT SABIRIANOV, University of Nebraska at Omaha — We report density functional theory (DFT) study of the magnetic properties of Cr<sub>3</sub>Te<sub>4</sub> doped with transition metals (TM) (Co, Fe, Ni, V and Mn), TM ions doped in Cr sites, Cr<sub>3-x</sub>(TM)<sub>x</sub>Te<sub>4</sub> (*x* = 0.5 and 1). We performed screening of the exchange coupling interaction and magnetization modifications upon the substitution of Cr by 3d-transition metals at various Cr sites in the Cr<sub>3</sub>Te<sub>4</sub> structure. Our calculation show that Cr<sub>3</sub>Te<sub>4</sub> has ferromagnetic coupling and large magnetization (Magnetization per unit cell is 18.24μB). Magnetocrystalline anisotropy (MAE) of this material is also large (MAE= 1.67MJ/m<sup>3</sup>). Our calculations show that the increase in interlayer spacing strengthen ferromagnetism of Cr<sub>3</sub>Te<sub>4</sub>. Doping with Mn increases Cr<sub>3</sub>Te<sub>4</sub> magnetization, but reduces the exchange coupling energy which means reducing Curie temperature (T<sub>c</sub>). We find that doping with 3d-TM elements decreases the magnetocrystalline anisotropy energies (MAE) of Cr<sub>3</sub>Te<sub>4</sub>.

**5:06PM H19.00012 Magnetic properties and stability of the atomic laminate Mn<sub>2</sub>GaC.**, MARTIN DAHLQVIST, ÅRNI INGASON, Linköping University, Sweden, GUNNAR PÁLSSON, Uppsala University, Sweden, BJÖRN ALLING, IGOR ABRIKOSOV, JOHANNA ROSEN, Linköping University, Sweden — Using first-principles calculations, we predicted the thermodynamically stable magnetic Mn<sub>2</sub>GaC and subsequently synthesized it as a heteroepitaxial thin film. It belongs to a class of atomically laminated compounds with a unique combination of metallic and ceramic properties. They have a common formula *M*<sub>*n*+1</sub>*A*X<sub>*n*</sub>M<sub>*n*+1</sub>S<sub>*n*</sub> (n = 1-3), where M is an early transition metal, A is an A-group element, and X is carbon or nitrogen. Using density functional theory (DFT) and Heisenberg Monte Carlo (HMC) for a magnetic ground state search, several collinear and noncollinear low energy magnetic spin configurations have been identified, some with different symmetries compared to the non-magnetic crystal structure. Around 240 K X-ray diffraction and magnetic measurements display a sharp contraction of the lattice in the c-direction coinciding with a sharp magnetic transition. Neutron diffraction measurements displays diffraction peaks consistent with long-ranged antiferromagnetic order with a repetition distance of two structural unit cells (25 Å). This is consistent with theoretically predicted structural changes between different, close to degenerate, magnetic ground states, and it is the first unambiguous evidence of long ranged AFM order in MAX phase materials.

**Tuesday, March 15, 2016 2:30PM - 5:30PM —**

**Session H20 GSCCM DCOMP DMP: Materials in Extremes: Novel Energetic Materials 319 -**

Elissaios Stavrou, Lawrence Livermore National Laboratory

**2:30PM H20.00001 The Promise and Challenge of Extended Solids of Nitrogen**, JENNIFER CIEZAK-JENKINS, US Army Research Laboratory — The extended solids of nitrogen are of considerable interest as high-energy-density materials, as it has been projected a transformation from a single-bonded polymeric-like material back to the more stable triply-bonded diatomic phase would release over 2.3 eV/atom, which is significantly higher than conventional energetic materials. Although a transformation to the single bonded cubic gauche structure was experimentally confirmed in 2005, efforts to recover this material to ambient conditions have been challenging and unsuccessful to date. In an effort to increase the metastability of the extended solid, recent studies have focused on mixing, or doping, the nitrogen with small amounts of secondary gases, such as hydrogen or carbon monoxide. It was been postulated the secondary gas would passivate the terminal ends thus increasing the stability of the nitrogen extended solid. Our group was the first to demonstrate such an approach could be used successfully to decrease the transition pressure for the formation of the nitrogen extended solid through doping with hydrogen. Although recent studies on nitrogen/hydrogen mixtures by other research groups have also observed several non-molecular nitrogen/hydrogen structures, recovery of these materials to ambient conditions has not yet been demonstrated. In this talk, I will describe our progress in the study of the synthesis, characterization, and recovery of extended solids of nitrogen from high pressure conditions from nitrogen/carbon monoxide mixtures. I will also detail results from our closely coupled modeling and simulation efforts and discuss how these results help guide our experimental efforts. New opportunities and challenges that have arisen in the course of our studies that will be pursued in the future will also be presented.

**3:06PM H20.00002 Sodium Pentazolate: a Nitrogen Rich Energetic Material**, IVAN OLEJNIK, BRAD STEELE, University of South Florida — Sodium pentazolates  $\text{NaN}_5$  and  $\text{Na}_2\text{N}_5$ , new energetic materials, are discovered using first principles crystal structure search for the compounds of varying amounts of elemental sodium and nitrogen. The pentazole anion ( $\text{N}_5^-$ ) is stabilized in the condensed phase by sodium  $\text{Na}^+$  cations at pressures exceeding 20 GPa, and becomes metastable upon release of pressure, i.e. at ambient conditions. The sodium azide ( $\text{NaN}_3$ ) precursor for the new compounds is predicted to undergo a chemical transformation above 50 GPa into sodium pentazolates  $\text{NaN}_5$  and  $\text{Na}_2\text{N}_5$ . The calculated Raman spectrum of  $\text{NaN}_5$  is in agreement with the experimental Raman spectrum of a previously unidentified substance appearing upon compression and heating of  $\text{NaN}_3$  precursor, thus confirming the appearance of the new compound.

**3:18PM H20.00003 Modeling of formation of extended NH solids under high pressure.**, ISKANDER G. BATYREV, US Army Research Laboratory — Structure of N-H extended network under high pressure was modelled using the evolutionary algorithm program USPEX based on plane wave DFT calculations (VASP). Concentration ratio of  $\text{N}_2$  to  $\text{H}_2$  gases was 3:1, 4:1, and 9:1. Range of the studied pressures was 10 – 50 GPa on compression, and from 50 to 1 GPa on isotropic decompression of the extended network. Formation of an extended network with covalent bonds occurs between 30-50 GPa. Higher concentration of N requires higher pressure to form a covalent bond network. New structure of NH extended solids with covalent bonds are predicted: with P-1(CI-1) symmetry group for 9:1 ratio, with PBAM ( $\text{D}_{2\text{H}+9}$ ) symmetry group for 4:1 ratio, and with P-1(CI-1) for 3:1 ratio of  $\text{N}_2$  to  $\text{H}_2$  gas. Calculations of the mixtures of  $\text{N}_2$  and  $\text{H}_2$  gases at pressures in the range of 10-20 GPa resulted in a variety of structures without a covalent network, but consisting of nitrogen-containing molecules. For example, the lowest energy structure for a 3:1 ratio of N to H atoms consists of tetrazene and  $\text{N}_2$  molecules. At 10 GPa the lowest energy structure appears to be a combination of protonated ammonia and  $\text{N}_2$  molecules.

**3:30PM H20.00004 Computational design of fused heterocyclic energetic materials<sup>1</sup>**, ROMAN TSYSHEVSKIY, University of Maryland College Park, PHILIP PAGORIA, Lawrence Livermore National Laboratory, ISKANDER BATYREV, US Army Research Laboratory, MAIJA KUKLJA, University of Maryland College Park — A continuous traditional search for effective energetic materials is often based on a trial and error approach. Understanding of fundamental correlations between the structure and sensitivity of the materials remains the main challenge for design of novel energetics due to the complexity of the behavior of energetic materials. State of the art methods of computational chemistry and solid state physics open new compelling opportunities in simulating and predicting a response of the energetic material to various external stimuli. Hence, theoretical and computational studies can be effectively used not only for an interpretation of sensitivity mechanisms of widely used explosives, but also for identifying criteria for material design prior to its synthesis and experimental characterization. We report here, how knowledge on thermal stability of recently synthesized materials of LLM series is used for design of novel fused heterocyclic energetic materials, including DNBTT (2,7-dinitro-4H,9H-bis([1,2,4]triazolo)[1,5-b:1',5'-e][1,2,4,5]tetrazine), compound with high thermal stability, which is on par or better than that of TATB.

<sup>1</sup>This research is supported by ONR (Grant N00014-12-1-0529), NSF XSEDE resources (Grant DMR-130077) and DOE NERSC resources (Contract DE-AC02-05CH11231)

**3:42PM H20.00005 Metalloid Clusters as Novel Energetic Materials: Progress and Challenges.**, SUFIAN ALNEMRAT, JOSEPH HOOPER, Naval Postgraduate School — Integration of combustible metals is a standard route for increasing the energy density of explosive and propellant formulations. Bulk metals, however, have well-known limitations. As a rather different route, we have been studying molecular scale metalloid clusters that contain a core of low-valence metal surrounded by a layer of organic ligands. These materials may retain the high energy density of bulk metals but offer substantially faster reaction kinetics. In this talk we present recent computational results on the stability and decomposition of these clusters. We compare molecular dynamics simulations of the oxidation of a prototype aluminum metalloid cluster to recent experimental thermally programmed reaction data; both show that oxygen reacts with the metal core and not the ligands. As a route to larger-scale fabrication of these clusters, we present simulations of the nucleation and growth of small metalloid systems on functionalized graphene layers. The simulations demonstrate that spontaneous cluster nucleation and growth is favorable on many graphene defects, suggesting a means of templated growth of clusters and nanoparticles.

**3:54PM H20.00006 Novel LLM series high density energy materials: Synthesis, characterization, and thermal stability<sup>1</sup>**, PHILIP PAGORIA, MAOXI ZHANG, Lawrence Livermore National Laboratory, ROMAN TSYSHEVSKIY, MAIJA KUKLJA, University of Maryland College Park — Novel high density energy materials must satisfy specific requirements, such as an increased performance, reliably high stability to external stimuli, cost-efficiency and ease of synthesis, be environmentally benign, and be safe for handling and transportation. During the last decade, the attention of researchers has drifted from widely used nitroester-, nitramine-, and nitroaromatic-based explosives to nitrogen-rich heterocyclic compounds. Good thermal stability, the low melting point, high density, and moderate sensitivity make heterocycle materials attractive candidates for use as oxidizers in rocket propellants and fuels, secondary explosives, and possibly as melt-castable ingredients of high explosive formulations. In this report, the synthesis, characterization, and results of quantum-chemical DFT study of thermal stability of LLM-191, LLM-192 and LLM-200 high density energy materials are presented.

<sup>1</sup>Work performed under the auspices of the DOE by the LLNL (Contract DE-AC52-07NA27344). This research is supported in part by ONR (Grant N00014-12-1-0529) and NSF. We used NSF XSEDE (Grant DMR-130077) and DOE NERSC (Contract DE-AC02-05CH11231) resources

**4:06PM H20.00007 ABSTRACT WITHDRAWN —**

**4:18PM H20.00008 Mixed Nitrogen-Methane Solids at High Density**, SERGE DESGRENIERS, Laboratoire de physique des solides denses, University of Ottawa — Mixing different molecular species may yield weakly bound compounds or van der Waals solids upon the application of high pressure. Van der Waals solids differ in physical properties from solids formed by pure molecular species at comparable thermodynamic conditions. In this contribution, we present results of the formation of binary methane-nitrogen compounds at high density. Methane and nitrogen, with similar potentials and molecular size, are expected to be partly miscible in the condensed state. Using single crystal and powder X-ray diffraction with synchrotron radiation and vibrational spectroscopy, the pressure-concentration phase diagram for this system has been explored from 1 to 16 GPa, at room temperature. The existence of van der Waals solid phases for samples with concentrations above 10% (methane per volume) is demonstrated. For example, at 7.6 GPa and at room temperature, whereas pure nitrogen and methane exist in cubic and in rhombohedral structures, respectively, our study indicates that a methane-nitrogen sample with 60% nitrogen by volume exhibits, under the same conditions, a novel phase with a tetragonal symmetry. Other novel structures in methane-nitrogen samples with different concentrations under varying pressure conditions have also been observed and will be discussed.

**4:30PM H20.00009 High Pressure Structures and Equations of State of HIO3 and HIO3O8<sup>1</sup>**, JOSEPH ZAUG, ELISSAIO STAVROU, Lawrence Livermore National Laboratory, BRIAN LITTLE, AFRL/RWM, SORIN BASTEA, JONATHAN CROWHURST, Lawrence Livermore National Laboratory, CHEMICAL ENERGETICS COLLABORATION — Knowledge of high-pressure thermodynamic properties of iodine containing oxides and acids is important toward improving the accuracy of semi-empirical predictions of extreme condition explosive and combusive chemistry of iodine containing formulations. Here we report on the synthesis of explosive chemical products HIO3 and HIO3O8 and on the structures and isotropic equations of state up to 35 and 45 GPa respectively. EOS model parameters are provided including parametrized exponential-6 interatomic potential values used to conduct thermochemical calculations of iodine containing reactants.

<sup>1</sup>This work was performed under the auspices of the U.S. Department of Energy jointly by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344

**4:42PM H20.00010 Harvesting materials formed under extreme conditions: Synthesis and isolation of nanocarbons derived from detonation of high explosives**, MILLICENT FIRESTONE, BRYAN RINGSTRAND, RACHEL HUBER, DANA DATTELBAUM, RICHARD GUSTAVSON, DAVID PODLESÁK, Los Alamos Natl Lab — High explosive detonation products are primarily composed of molecular gases and solid carbon products. Recent studies have shown that the solid carbon condensate morphologies can vary depending on the high explosive and / or the pressure, temperature, or environment of the detonation. These studies have revealed, for example, unique carbon nanoparticles possessing novel morphologies, such as ones composed of hollow cores surrounded by lamellar structured graphitic shells. Despite these observations little work has been done to isolate these particles from the recovered post-detonation soot. This lack of effort to isolate and purify these products limits our understanding of their materials properties and, ultimately our ability to adapt them for useful materials. Herein, we report our recent studies directed at the production of nano-carbons through the detonation of a high explosive (e.g., composition B) under a range of experimental conditions. We further describe work directed at isolation and purification of the carbon nanoparticles.

**4:54PM H20.00011 Simulation of Initiation in Hexanitrostilbene<sup>1</sup>**, AIDAN THOMPSON, TZU-RAY SHAN, COLE YARRINGTON, RYAN WIXOM, Sandia National Laboratories — We report on the effect of isolated voids and pairs of nearby voids on hot spot formation, growth and chemical reaction initiation in hexanitrostilbene (HNS) crystals subjected to shock loading. Large-scale, reactive molecular dynamics simulations are performed using the reactive force field (ReaxFF) as implemented in the LAMMPS software. The ReaxFF force field description for HNS has been validated previously by comparing the isothermal equation of state to available diamond anvil cell (DAC) measurements and density function theory (DFT) calculations. Micron-scale molecular dynamics simulations of a supported shockwave propagating in HNS crystal along the [010] orientation are performed ( $u_p = 1.25$  km/s,  $U_s = 4.0$  km/s,  $P = 11$  GPa.) We compare the effect on hot spot formation and growth rate of isolated cylindrical voids up to 0.1  $\mu$ m in size with that of two 50nm voids set 100nm apart. Results from the micron-scale atomistic simulations are compared with hydrodynamics simulations.

<sup>1</sup>Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. DOE National Nuclear Security Administration under contract DE-AC04-94AL85000

**5:06PM H20.00012 Large-Amplitude Deformation and Bond Breakage in Shock-Induced Reactions of Explosive Molecules**, JEFFREY KAY, Sandia National Laboratories — The response of explosive molecules to large-amplitude mechanical deformation plays an important role in shock-induced reactions and the initiation of detonation in explosive materials. In this presentation, the response of a series of explosive molecules (nitromethane, 2,4,6-trinitrotoluene [TNT], and 2,4,6-triamino-1,3,5-trinitrobenzene [TATB]) to a variety of large-amplitude deformations are examined using ab initio quantum chemical calculations. Large-amplitude motions that result in bond breakage are described, and the insights these results provide into both previous experimental observations and previous theoretical predictions of shock-induced reactions are discussed.

**5:18PM H20.00013 Reactive Force Field for Liquid Hydrazoic Acid with Applications to Detonation Chemistry<sup>1</sup>**, DAVID FURMAN, Hebrew University of Jerusalem and NRCN, Israel, FAINA DUBNIKOVA, Hebrew University of Jerusalem, Israel, ADRI VAN DUIN, Penn. State University, Pennsylvania, USA, YEHUDA ZEIRI, Ben Gurion University, Israel and NRCN, Israel, RONNIE KOSLOFF, Hebrew University of Jerusalem, Israel — The development of a reactive force field (ReaxFF formalism) for hydrazoic acid (HN3), a highly sensitive liquid energetic material, is reported. The force field accurately reproduces results of density functional theory (DFT) calculations. The quality and performance of the force field are examined by detailed comparison with DFT calculations related to uni, bi and trimolecular thermal decomposition routes. Reactive molecular dynamics (RMD) simulations are performed to reveal the initial chemical events governing the detonation chemistry of liquid HN3. The outcome of these simulations compares very well with recent results of tight-binding DFT molecular dynamics and thermodynamic calculations. Based on our RMD simulations, predictions were made for the activation energies and volumes in a broad range of temperatures and initial material compressions.

<sup>1</sup>Work Supported by The Center of Excellence for Explosives Detection, Mitigation and Response, Department of Homeland Security

**Tuesday, March 15, 2016 2:30PM - 5:30PM —**

**Session H21 GMAG DMP: 1D Gapped Antiferromagnets** 320 - Vivien Zapf, NHMFL-LANL

**2:30PM H21.00001 Spectroscopic Investigation of the Origin of Magnetic Bistability in Molecular Nanomagnets<sup>1</sup>**, JORIS VAN SLAGEREN, University of Stuttgart — Molecular nanomagnets (MNM)s are coordination complexes consisting of one or more transition metal and/or f-element ions bridged and surrounded by organic ligands. Some of these can be magnetized in a magnetic field, and remain magnetized after the field is switched off. Because of this, MNMs have been proposed for magnetic data storage applications, where up to 1000 times higher data densities than currently possible can be obtained. Other MNMs were shown to display quantum coherence, and, as a consequence, are suitable as quantum bits. Quantum bits are the building blocks of a quantum computer, which will be able to carry out calculations that will never be possible with a conventional computer. The magnetic bistability of MNMs originates from the magnetic anisotropy of the magnetic ions, which creates an energy barrier between up and down orientations of the magnetic moment. Currently, most work in the area focuses on complexes of either lanthanide ions or low-coordinate transition metal ions. Synthetic chemical efforts have led to a large number of novel materials, but the rate of improvement has been slow. Therefore a better understanding of the origin of the magnetic anisotropy is clearly necessary. To this end we have applied a wide range of advanced spectroscopic techniques, ranging from different electron spin resonance techniques at frequencies up to the terahertz domain to optical techniques, including luminescence and magnetic circular dichroism spectroscopy. We will discuss two examples, one from the area of lanthanide MNMs [1], one a transition metal MNM (unpublished). [1] . Rechkemmer, J.E. Fischer, R. Marx, M. Dörfel, P. Neugebauer, S. Horvath, M. Gysler, T. Brock-Nannestad, W. Frey, M.F. Reid, J. van Slageren\*, "Comprehensive Spectroscopic Determination of the Crystal Field Splitting in an Erbium Single-Ion Magnet", J. Am. Chem. Soc., 137, 13114–13120 (2015).

<sup>1</sup>This work was financially supported by DFG, DAAD and COST CM1006 EUFEN

**3:06PM H21.00002 Conditions for the appearance of boundary modes in topological phases of Heisenberg spin ladders**, NEIL ROBINSON, Brookhaven Natl Lab, ALEXANDER ATLAND, Universität zu Köln, REINHOLD EGGER, HHU Düsseldorf, NKILAS GERGS, Utrecht University, ROBERT KONIK, Brookhaven Natl Lab, WEI LI, LMU München, DIRK SCHURICHT, Utrecht University, ALEXEI TSVELIK, Brookhaven Natl Lab, ANDREAS WEICHSELBAUM, LMU München — We consider the problem of delineating the necessary conditions for the appearance of boundary modes in extended  $SU(2)$  Heisenberg spin ladders. Specifically, we study Heisenberg ladders with rung exchange,  $J_{\perp}$ , and ring exchange,  $J_{\chi}$ , that admit a field theoretic description in terms of Majorana fermions in the continuum limit. In this description there are four Majorana fermions, arranged in a triplet and a singlet. This suggests there are four distinct phases, corresponding to the configurations of the signs of the triplet  $m_t$  and singlet  $m_s$  masses. We label these phases as: Haldane ( $m_t > 0, m_s < 0$ ), rung singlet ( $m_t < 0, m_s > 0$ ),  $VBS_+$  ( $m_t, m_s > 0$ ) and  $VBS_-$  ( $m_t, m_s < 0$ ). Topologically, we find two of these phases support gapless boundary modes: the Haldane phase (the triplet forms a spin-1/2 degree of freedom at the ends of the ladder) and the  $VBS_+$  phase, where all the Majorana fermions have gapless boundary modes. The absence of a gapless boundary mode in the rung singlet phase is surprising; we find that the singlet mode can become gapless if open boundary conditions are replaced with a continuous change in lattice parameters. We suggest a symmetry-allowed modification to the low-energy effective theory which may be responsible for this behavior.

**3:18PM H21.00003 The pressure effects on the antiferromagnetic orders in iron-based ladder compounds  $BaFe_2S_3$** , SONGXUE CHI, Quantum Condensed Matter Division, Oak Ridge National Laboratory, YOSHIYA UWATOKO, None, YASUYUKI HIRATA, KENYA OHGUSHI, Institute for Solid State Physics (ISSP), University of Tokyo — The ladder compounds have recently become a new test ground for the studies on Fe-based superconductors. The building block for such materials, the two-leg Fe ladder surrounded by edge-sharing chalcogen tetrahedra, has provided a quasi-one-dimensional channel for the remaining critical issues in this field. Recently, superconductivity was successfully induced by pressure in one of such compounds,  $BaFe_2S_3$ . The knowledge of the pressure effect on its antiferromagnetic order is crucial in understanding the superconductivity in the low-dimensional system. I will present the results of our neutron diffraction studies on the evolution of the magnetic phase under hydraulic pressure in single crystalline  $BaFe_2S_3$ .

**3:30PM H21.00004 Neutron scattering study of magnetic structure in triangle spin tube  $CsCrF_4$** , MASATO HAGIHALA, ISSP, Univ. of Tokyo, MAXIM AVDEEV, Bragg Institute, ANSTO, HIROTAKA MANAKA, Kagoshima Univ., TAKAT-SUGU MASUDA, ISSP, Univ. of Tokyo — Triangle spin tube viewed from tube direction is topologically equivalent to kagom lattice. The rung ( $J_1$ ) and inter-tube ( $J_2$ ) interactions on triangle spin tube correspond respectively to the next nearest neighbor and the nearest neighbor interactions on kagom lattice. In the case of  $J_1 > 0$  (Antiferromagnetic) and  $J_1 \gg |J_2|$ , the ground state is  $q = 0, 120^\circ$  structure with  $J_2 > 0$  or Cuboc state that represented multi- $q$  ( $q = 2\pi(1/2, 0)$  and two symmetric-equivalent vectors) with  $J_2 < 0$  [1].  $CsCrF_4$  is a perfect triangle spin tube material with antiferromagnetic intra-tube and rung interactions [2]. Neutron diffraction measurement revealed magnetic long-range order at  $T = 1.5$  K. Contrary to the expectation, the magnetic structure was determined  $q = 2\pi(1/2, 0, 1/2)$ ,  $120^\circ$  structure by Rietveld refinement. We also confirmed that this structure was stabilized by Dzyaloshinskii-Moriya interaction and small anisotropy that obeyed the three-fold symmetry at Cr sites by calculation. [1] H. Ishikawa et al., JPSJ 83, 043703 (2014). [2] H. Manaka et al., JPSJ 78, 093701 (2009).

**3:42PM H21.00005 Dielectric effects at a magnetic Bose-Einstein condensation<sup>1</sup>**, KIRILL POVAROV, AARON REICHERT, ERIK WULF, ANDREY ZHELUDEV, Neutron Scattering and Magnetism Group, ETH Zürich, Switzerland — In the presence of magnetoelectric coupling one can expect non-trivial dielectric properties at a magnetic quantum phase transition. A "toy model" here is a spin spiral undergoing a field-induced transition into a quantum-disordered phase. In the incommensurate phase the in-plane spin rotational symmetry is protected, making the analogy between the magnetic long-range ordering and BEC exact, but the spin spiral may also host an electric polarization complicating the picture. We have experimentally studied this transition in the spin tube material  $Sr_{1-x}Cu_2Cl_4$  [1] to understand if it can be described as a magnetic BEC. We have found that indeed it can. Dielectric spectroscopy results combined with calorimetric measurements, clearly show the absence of polarization fluctuations in the disordered phase down to the very critical point. At the same time the ordered phase shows a huge nonlinearity in dielectric permittivity even for small electric fields. The phase boundary shows beautiful consistency with the 3D BEC universality class. We conclude, that although magnetoelectric coupling does not alter the nature of the transition, it gives rise to complex magnetoelectric effects in the helimagnetically ordered phase.

[1] K. Povarov et al.; Phys. Rev. B 92 140410 (2015)

<sup>1</sup>This work was supported by the Swiss National Science Foundation, Division 2

**3:54PM H21.00006 Optical spin excitations in quantum spin ladders**, GEDIMINAS SIMUTIS, SEVERIAN GVASALIYA, NSM laboratory, ETH Zurich, FAN XIAO, Department of Physics, Durham University, CHRISTOPHER LANDEE, Department of Physics, Clark University, ANDREY ZHELUDEV, NSM laboratory, ETH Zurich — We present a Raman spectroscopy study of magnetic excitations in quantum spin ladders. We start with a strong-rung ladder  $Cu(Qnx)(Cl_{1-x}Br_x)_2$ . It has recently attracted attention due to proposal that the ratio of leg to rung exchange can be varied continuously by substituting Br for Cl. We have measured the Raman spectra for the hole doping series and report on the scattering from two magnons [1]. We extract the onset and cutoff of the scattering for the whole series and compare it to the estimates from previous bulk measurements as well as numerical calculations. We find that the magnetic spectrum indeed varies continuously as the halogen ions are exchanged. The general behavior is found to be consistent with expectations, however small systematic deviations persist. The difference can potentially be explained by the existence of three-dimensional coupling, however more systematic computational studies are needed to ascertain the origin of the inconsistencies. Having established the analysis using the strong rung case, we then turn our attention to other ladder systems. Unusual magnetic signal is found in a strong leg spin ladder, which is discussed in terms of selection rules and an unexpected energy scale. [1] G. Simutis *et al.* arXiv:1510.06360

**4:06PM H21.00007 ESR modes in a Strong-Leg Ladder in the Tomonaga-Luttinger Liquid Phase<sup>1</sup>**, S. ZVYAGIN, HLD-HZDR, D-01328 Dresden, Germany, M. OZEROV, Radboud University, 6525 ED Nijmegen, The Netherlands, M. MAKSYMENKO, Weizmann Institute of Science, Rehovot 76100, Israel, J. WOSNITZA, HLD-HZDR, D-01328 Dresden, Germany, A. HONECKER, Université de Cergy-Pontoise, F-95302 Cergy-Pontoise Cedex, France, C.P. LANDEE, M. TURNBULL, Clark University, Worcester, MA 01060, USA, S.C. FURUYA, T. GIAMARCHI, University of Geneva, CH-1211 Geneva, Switzerland — Magnetic excitations in the strong-leg quantum spin ladder compound  $(\text{C}_7\text{H}_{10}\text{N})_2\text{CuBr}_4$  (known as DIMPY) in the field-induced Tomonaga-Luttinger spin liquid phase are studied by means of high-field electron spin resonance (ESR) spectroscopy. The presence of a gapped ESR mode with unusual non-linear frequency-field dependence is revealed experimentally. Using a combination of analytic and exact diagonalization methods, we compute the dynamical structure factor and identify this mode with longitudinal excitations in the antisymmetric channel. We argue that these excitations constitute a fingerprint of the spin dynamics in a strong-leg spin-1/2 Heisenberg antiferromagnetic ladder and owe its ESR observability to the uniform Dzyaloshinskii-Moriya interaction.

<sup>1</sup>This work was partially supported by the DFG and Helmholtz Gemeinschaft (Germany), Swiss SNF under Division II, and ERC synergy UQUAM project. We acknowledge the support of the HLD at HZDR, member of the European Magnetic Field Laboratory (EMFL).

**4:18PM H21.00008 Field-induced spontaneous magnon decay in a spin-1/2 coupled two-leg ladder antiferromagnet  $\text{C}_9\text{H}_{18}\text{N}_2\text{CuBr}_4$  with small Ising anisotropy**, TAO HONG, Quantum Condensed Matter Division, Oak Ridge National Laboratory, Y. QIU, National Institute of Standards and Technology, D. A. TENNANT, Quantum Condensed Matter Division, Oak Ridge National Laboratory, K. COESTER, K. P. SCHMIDT, Lehrstuhl für Theoretische Physik I, TU Dortmund, F. F. AWWADI, Department of Chemistry, The University of Jordan, M. M. TURNBULL, Carlson School of Chemistry, Clark University — We present the high-resolution neutron scattering study in magnetic fields applied perpendicular to an easy-axis (Ising type) on the  $S = 1/2$  coupled two-leg ladder antiferromagnet (dimethylammonium)(3,5-dimethylpyridinium) $\text{CuBr}_4$ . At finite fields, the magnetic structure becomes noncollinear canted and the observed intriguing spontaneous magnon decays over a large region of Brillouin Zone in the excitation spectra can be well explained by the mechanism where the process of one-magnon decays into two-magnon continuum is kinematically allowed [1]. [1] M. E. Zhitomirsky and A. L. Chernyshev, Rev. Mod. Phys. **85**, 219 (2013).

**4:30PM H21.00009 Local structure of spin Peierls compound  $\text{TiPO}_4$ :  $^{47/49}\text{Ti}$  and  $^{31}\text{P}$  NMR study<sup>1</sup>**, RAIVO STERN<sup>2</sup>, IVO HEINMAA, ALEXANDER LEITME, ENNO JOON, ALEXANDER TSIRLIN, Natl Inst of Chem Phy & Bio, REINHARD KREMER, MPI Stuttgart, ROBERT GLAUM, Universitt Bonn —  $\text{TiPO}_4$  structure is made of slightly corrugated  $\text{TiO}_2$  ribbon chains of edge-sharing  $\text{TiO}_6$  octahedra. The almost perfect 1D spin  $\text{Ti}^{3+}$  chains are well separated by  $\text{PO}_4$  tetrahedra. By magnetic susceptibility and MAS-NMR measurements [1] it was shown that  $\text{TiPO}_4$  has nonmagnetic singlet ground state with remarkably high Spin-Peierls (SP) transition temperature. The high-T magnetic susceptibility of  $\text{TiPO}_4$  follows well that of a  $S = 1/2$  Heisenberg chain with very strong nearest-neighbor AF spin-exchange coupling constant of  $J = 965\text{K}$ . On cooling  $\text{TiPO}_4$  shows two successive phase transitions at 111K and 74K, with incommensurate (IC) SP phase between them. We studied local structure and dynamics in  $\text{TiPO}_4$  single crystal using  $^{47/49}\text{Ti}$  and  $^{31}\text{P}$  NMR in the temperature range 40K to 300K, and determined the principal values and orientation of the magnetic shift tensors for  $^{31}\text{P}$  and  $^{47,49}\text{Ti}$  nuclei. Since  $^{47,49}\text{Ti}$  ( $S = 5/2$  and  $S = 7/2$ , respectively) have quadrupolar moments, we also found the principal axis values and orientations of the electric field gradient (efg) tensor in SP phase and at 295K. In SP phase the structure contains 2 magnetically inequivalent P sites and only one Ti site. From the T-dependence of the relaxation rate of  $^{31}\text{P}$  and  $^{47}\text{Ti}$  nuclei we determined activation energy  $E_a = 550\text{K}$  for spin excitations in SP phase.

<sup>1</sup>J. Law et al., PRB 83, 180414(R) (2011)

<sup>2</sup>Support from ETAg by PUT210 and IUT23-3 is acknowledged.

**4:42PM H21.00010 Pressure-Induced Order in the Gapped Quantum Magnet DTN**, ALEXANDRA MANNIG, JOHANNES MOELLER, ANDREY ZHELUDEV, ETH Zurich, Neutron Scattering and Magnetism Group, Laboratory for Solid State Physics, Zurich, Switzerland, V. OVIDIU GARLEA, CLARINA DELA CRUZ, Oak Ridge National Laboratory, Quantum Condensed Matter Division, Oak Ridge, Tennessee, USA, ZURAB GUGUCHIA, RUSTEM KHASANOV, ELVEZIO MORENZONI, Paul Scherrer Institute, Laboratory for Muon Spin Spectroscopy, Villigen-PSI, Switzerland — We present muon-spin relaxation, neutron diffraction and magnetic susceptibility data under applied hydrostatic pressure on the organometallic  $S = 1$  quantum magnet  $\text{NiCl}_2 \cdot 4[\text{SC}(\text{NH}_2)_2]$ . The material consists of weakly coupled antiferromagnetic chains and has a spin gap resulting from a large single-ion anisotropy. Our muon spin rotation experiments provide local field dependencies on temperature as well as pressure and allow for the mapping of a detailed phase diagram up to 22 kbar. Thus, we demonstrate that the compound may be driven through two subsequent pressure-induced transitions into apparently distinct magnetically ordered phases. Neutron diffraction and susceptibility measurements support those results and show the potential of low-pressure transitions to be investigated by various techniques.

**4:54PM H21.00011 Unusual Magnetic-Pressure Response of an  $S = 1$  Antiferromagnetic Linear-Chain near the  $D/J \approx 1$  Critical Point.<sup>1</sup>**, M. K. PEPRAH, P. A. QUINTERO, J. S. XIA, J. M. PÉREZ, M. W. MEISEL, Dept. of Physics and NHMFL, Univ. of Florida, A. GARCIA, S. E. BROWN, Dept. of Physics, UCLA, J. L. MANSON, Dept. of Chemistry, Eastern Washington Univ. — An  $S = 1$  chain,  $[\text{Ni}(\text{HF}_2)(3\text{-Cpy})_4]\text{BF}_4$  (py = pyridine), has been identified to have nearest-neighbor antiferromagnetic interaction  $J/k_B = 4.86\text{K}$  and single-ion anisotropy  $D/k_B = 4.3\text{K}$ , while avoiding long-range order to 25 mK.<sup>2</sup> With  $D/J = 0.88$ , this system is close to the  $D/J \approx 1$  gapless quantum critical point between the Haldane and Large- $D$  phases. The magnetization was studied at  $50\text{mK} \leq T \leq 1\text{K}$  and with  $B \leq 10\text{T}$ .<sup>3</sup> Using a magnetometer equipped with a pressure cell, the low-field (0.1 T), high temperature ( $T \geq 2\text{K}$ ) magnetic susceptibility was studied to 1.47 GPa. These data suggest the response at ambient pressure<sup>2</sup> changes between 0.24 GPa and 0.35 GPa. These studies are being extended by  $^1\text{H}$  NMR experiments capable of varying the pressure and of spanning from 300 K to below 100 mK.

<sup>1</sup>Supported by the NSF via DMR-1202033 (MWM), DMR-1410343 (SEB), DMR-1306158 (JLM), DMR-1461019 (UF Physics REU support for JMP), and DMR-1157490 (NHMFL), and by the State of Florida.

<sup>2</sup>J.L. Manson *et al.*, Inorg. Chem. **51** (2012) 7520.

<sup>3</sup>J.-S. Xia *et al.*, arxiv.1409.5971 (2014).

**5:06PM H21.00012 High-pressure neutron scattering of Prussian blue analogue magnets**, DANIEL PAJEROWSKI, Oak Ridge National Laboratory — Pressure sensitive magnetism is known to be useful in sensors, and while applications tend to use metallic alloys, molecule based magnets (MBMs) have been shown to have large inverse magnetostrictive (IMS) response. A promising group of MBMs are the Prussian blue analogues (PBAs), in which magnetic ordering can be tuned by external stimuli such as light, electric field, and pressure. Previously, high pressure neutron scattering of nickel hexacyanochromate hydrate has shown direct evidence for isomerization of the cyanide linkage with applied pressure. Other probes have suggested a similar effect in iron hexacyanochromate hydrate, although there has yet to be direct crystallographic evidence. Neutron diffraction is sensitive to organic elements, even while in the presence of metals, and we have performed experiments above 1 GPa to look for linkage isomerism in iron hexacyanochromate. These results are supported by bulk probes and calculations.

**5:18PM H21.00013 Changes in the unoccupied electronic structure of the spin crossover molecule [Co(dpzca)<sub>2</sub>]**, YANG LIU, XIN ZHANG, AXEL ENDERS, PETER DOWBEN, JIAN LUO, JIAN ZHANG, Univ of Nebraska - Lincoln, ALPHA NDIAYE, LBNL, Advanced Light Source — We have investigated the changes in the unoccupied electronic structure of the spin crossover molecule - [Co(dpzca)<sub>2</sub>] using X-ray absorption spectroscopy (XAS) and have compared the results with magnetometry (SQUID) measurements. The studies of the variable temperature of the electronic structure of this cobalt complex with symmetric pyrazine imide ligands, -(2-pyrazylcarbonyl)-2-pyrazinecarboxamide, i.e. [Co(dpzca)<sub>2</sub>], are consistent with density functional theory (DFT). The temperature dependence of the occupancy of the high-spin state and low-spin state molecular orbital states, the unoccupied  $e_g/t_{2g}$  ratio from XAS and high spin state to low spin state ratio from molecular magnetic susceptibility  $\chi_M T$  indicates that the low spin state is not a zero spin state, but simply a lower moment state that would occur below the spin crossover transition of [Co(dpzca)<sub>2</sub>].

**Tuesday, March 15, 2016 2:30PM - 5:18PM –**

**Session H22 DCOMP: Theory and Simulations of Novel Superconductors** 321 - Barry Klein, University of California, Davis

**2:30PM H22.00001 Computational search of novel superconductors**, ZHIPING YIN, The Center of Advanced Quantum Studies, Beijing Normal University — The recently discovered 200 K high temperature superconductivity in the hydrogen sulfur material under high pressure was first successfully predicted by first-principles computation in a quantitative fashion, demonstrating the power of computation in the search of new superconductors. With the rapid advancement of theory, algorithm, and computer power, computation will play an increasingly important role. In this talk, I will first summarize the key features of different families of high temperature superconductors, including the iron pnictide and chalcogenide superconductors, the transition metal chloronitrides, and Bi-based superconductors. Then I will show how to use the key features as guidance to design novel candidate materials of high temperature superconductivity by utilizing a combination of different computational methods and tools, including evolutionary structural search method, density functional theory and dynamical mean field theory. A few candidate materials will be given towards the end of the talk for interested experimentalists and theorists to test and explore

**3:06PM H22.00002 Superconductivity in compressed sulfur hydride: Dependences on pressure, composition, and crystal structure from first principles**, RYOSUKE AKASHI, The University of Tokyo — The recent discovery of high-temperature superconductivity in sulfur hydride under extreme pressure has broken the long-standing record of superconducting transition temperature ( $T_c$ ) in the Hg-cuprate. According to the isotope effect measurement and theoretical calculations, the superconducting transition is mainly ascribed to the conventional phonon-mediated pairing interaction. It is, however, not enough for understanding the high- $T_c$  superconductivity in the sulfur hydride. To elucidate various possible effects on  $T_c$  with accuracy, we have analyzed  $T_c$  with first-principles methods without any empirical parameters. First, for various pressures and theoretically proposed crystal structures, we calculated  $T_c$  with the density functional theory for superconductors (SCDFT) to examine which structure(s) can explain experimentally measured  $T_c$  data [Akashi et al., PRB 91, 224513(2015)]. We next solved the Eliashberg equations without introducing the renormalized Coulomb parameter  $\mu^*$ , which is the Green-function-based counterpart of the SCDFT, and evaluated the effects of rapidly varying electron density of states, atomic zero-point motion, and phonon anharmonic corrections on  $T_c$  [Sano et al, in preparation]. In the talk, we review these results and discuss the dominant factors for the  $T_c$  and their relation to the experimental results. We also report some crystal structures that we recently found with first-principles calculations, which could have a key role for the pressure-induced transformation to the high- $T_c$  phase.

**3:42PM H22.00003 van Hove Singularities and Spectral Smearing in High Temperature Superconducting H<sub>3</sub>S<sup>1</sup>**, YUNDI QUAN, Physics Department, UC Davis & CAQS, Beijing Normal Univ., WARREN E. PICKETT, Physics Department, UC Davis — The superconducting phase of hydrogen sulfide at  $T_c=200$  K observed by Drozdov and collaborators at pressures around 200 GPa is simple bcc  $Im\bar{3}m$  H<sub>3</sub>S reopens questions about what is achievable in high  $T_c$ . The various "extremes" that are involved – pressure, implying extreme reduction of volume, extremely high H phonon energy scale around 1400K, extremely high temperature for a superconductor – necessitate a close look at new issues raised by these characteristics in relation to high  $T_c$ . We have applied first principles methods to analyze the H<sub>3</sub>S electronic structure, particularly the van Hove singularities (vHs) and the effect of sulfur. Focusing on the two closely spaced vHs near the Fermi level that give rise to the impressively sharp peak in the density of states, the implications of strong coupling Migdal-Eliashberg theory are assessed. The electron spectral density smearing due to virtual phonon emission and absorption, as done in earlier days for A15 superconductors, must be included explicitly to obtain accurate theoretical predictions and a correct understanding. Means for increasing  $T_c$  in H<sub>3</sub>S-like materials will be mentioned.

<sup>1</sup>NSF DMR Grant 1207622

**3:54PM H22.00004 Structure, lattice dynamics, and high- $T_c$  superconductivity in hydrogen sulfide under high pressure**, LINDA HUNG, TANER YILDIRIM, NIST Center for Neutron Research — The recent discovery of superconductivity near 200 K in hydrogen sulfide under pressures 200 GPa has sparked interest in the search for hydrogen-rich superconducting materials. The observed large isotope effect and earlier first-principles calculations convincingly suggest that the high  $T_c$  is due to strong electron-phonon coupling, i.e., that hydrogen sulfide is a conventional superconductor. Hence, first-principles predictions of phonon properties can be used in the search for new phases that can superconduct at even higher temperatures and lower pressures. In this talk, we present structural and lattice dynamics calculations of various phases of H<sub>2</sub>S/H<sub>3</sub>S, examining the electron-phonon coupling and superconductivity in each phase using the finite-displacement and frozen-phonon approaches. The effect of anharmonicity on electron-phonon coupling, isotope effect, and superconducting temperature is discussed. Finally, we explore the properties of potential new hydrogen-sulfide-based materials.

**4:06PM H22.00005 Hydrogen bond symmetrization by proton quantum motion and high  $T_c$  superconductivity in Sulfur hydrides at high pressure.**, ION ERREA, University of the Basque Country and Donostia International Physics Center, MATTEO CALANDRA, CNRS and Université P. et M. Curie, CHRIS PICKARD, University College London, JOSEPH NELSON, RICHARD NEEDS, Cavendish Laboratory Cambridge, Y LI, HANYU LIU, University of Saskatchewan, YUNWEY ZHANG, YAMMING MA, State Key Laboratory of Superhard Materials,, FRANCESCO MAURI, CNRS and Université P. et M. Curie — Atoms in a crystal are quantum particles differing substantial from classical particles. The vibrational energy associated to the quantum oscillations can strongly modify the static energy landscape, even changing the ground state derived from the Born-Oppenheimer energy surface (BOES) minimum. Here, making use of density-functional theory and of the Stochastic Self-consistent Harmonic Approximation, we show that the ground state of the high  $T_c$  superconductor hydrogen sulfide at 155 GPa is completely determined by quantum fluctuations. Indeed, despite the minimum of the BOES is obtained for a rhombohedral structure with covalently bonded H<sub>3</sub>S units and hydrogen bonds between them, quantum fluctuations favor a fully symmetric cubic structure in which the covalent and hydrogen bonds equalize. The quantum hydrogen-bond symmetrization and the large anharmonic effects are crucial to understand the pressure dependence of the observed extraordinary  $T_c=205$  K at 155 GPa. We finally show how, the dependence of  $T_c$  as a function of pressure can be completely explained in the framework of a phonon mediated pairing mechanism in the presence of large anharmonic effects.

**4:18PM H22.00006 Novel properties of Tungsten ditelluride**, HUIMEI LIU, Nanjing Univ, NATIONAL LABORATORY OF SOLID STATE MICROSTRUCTURES, SCHOOL OF PHYSICS, COLLABORATIVE INNOVATION CENT COLLABORATION — Tungsten ditelluride has attracted intense research interest due to the recent discovery of its large unsaturated magnetoresistance up to 60 Tesla. By using density functional theory calculations, we qualitatively reproduced the observed spin texture. Since the spin texture would forbid back scatterings that are directly involved in the resistivity, we suggest that the SOC and the related spin and orbital angular momentum textures may play an important role in the anomalously large magnetoresistance of WTe<sub>2</sub>. Motivated by the presence of a small, sensitive Fermi surface of 5d electronic orbitals, we also boost the electronic properties by applying a high pressure, and introduce superconductivity successfully.

**4:30PM H22.00007 Superconductivity in organic conductors: ab-initio results from parallel DMRG**, ADRIAN KANTIAN, Nordita, KTH Stockholm, MICHELE DOLFI, MATTHIAS TROYER, ETH Zurich, THIERRY GIAMARCHI, Université de Genève — The U-V model at quarter filling is considered the canonical minimal model to explain unconventional superconductivity in the organic Bechgaard and Fabre salts [1]. Yet it has so far resisted solution to show that it actually can support superconducting order. Here, we use a heavily parallelized version of the density-matrix renormalization group (DMRG) to provide the first ab-initio solutions for the U-V model in the regime suspected to support superconducting order. Our results support the existence of a phase marked by spin-singlet pairing, thus ruling out antiferromagnetic order (the usual close competitor to unconventional superconductivity). In this phase we will extend our analysis by studying the response to explicit bias fields. Our work is complemented by analysis of the two-leg U-V ladder through a combination of DMRG and analytical RG of a bosonized low-energy theory. [1] C. Bourbonnais, D. Jerome, The Physics of Organic Superconductors and Conductors (ed. Lebed, A.) pp. 358 (Springer, 2007).

**4:42PM H22.00008 Exchange and correlation effects on the superconducting transition of two-dimensional multivalley semiconductors<sup>1</sup>**, BETUL PAMUK, CNRS and Université Pierre et Marie Curie, JACOPO BAIMA, ROBERTO DOVESI, Università di Torio, MATTEO CALANDRA, FRANCESCO MAURI, CNRS and Université Pierre et Marie Curie — It has recently been shown that the enhancement in the superconducting temperature of two-dimensional semiconductors at low doping is linked to the electron-electron interaction enhancing the response to the valley polarization that is due to the electron-phonon coupling [1]. In this work, we extend this study to analyze the exchange and correlation effects on the electronic, magnetic, and vibrational properties of Li-doped ZrNCI and HfNCI - typical examples of two-dimensional two-valley semiconductors. We show that these properties can be calculated by *ab initio* density functional theory only by using approximations beyond the generalized gradient approximation. Finally, we present the link between the enhancement of the spin susceptibility and superconducting temperature by demonstrating that the electron-phonon coupling is acting as a pseudo-magnetic field causing the valley polarization. [2] [1] M. Calandra, P. Zocante and F. Mauri, Phys. Rev. Lett. 114, 077001 (2015) [2] B. Pamuk *et al.*, in preparation

<sup>1</sup>This work is supported by the Graphene Flagship and by Agence Nationale de la Recherche under reference ANR-13-IS10-0003-01.

**4:54PM H22.00009 Correlated properties of the doped Hubbard model on a honeycomb lattice**, TIANXING MA, LUFENG ZHANG, Beijing Normal University, HAI-QING LIN, Beijing Computational Science Research Center — Low doped graphene has a finite density of state, while heavily doped graphene have a Van Hove singularity in the density of states, in combination with pronounced antiferromagnetic spin fluctuations close to half filling, and strong ferromagnetic correlation as doping is below the location of Van Hove singularity, which may lead to different unconventional superconductivity. We performed a systematic quantum Monte Carlo study of the pairing correlation in the Hubbard model on a honeycomb lattice. Close to half filling, we find that pairing with d+id symmetry dominates over pairing with extended-s symmetry. When the next-nearest-neighbor  $t'$  is larger than  $t/6$ , the single-particle spectrum is featured by the continuously distributed Van Hove saddle points at the band bottom, where the density of states diverges in a power law. We investigate possible unconventional superconductivity in such systems with the Fermi level close to the band bottom by employing both random-phase-approximation and determinant quantum Monte Carlo approaches. Our study reveals a possible triplet p+ip superconductivity with appropriate interactions in low-filled graphene. We also explore the effect of the disorder and spin-orbit coupling on the magnetic correlation in doped graphene.

**5:06PM H22.00010 Helical Majorana fermions in d+id'-wave topological superconductivity of doped correlated quantum spin Hall insulators<sup>1</sup>**, CHUNG-HOU CHUNG, National Chiao-Tung University, Taiwan, SHIH-JYE SUN, National University of Kaohsiung, Taiwan, YUNG-YEH CHANG, National Chiao-Tung University, Taiwan, WEI-FENG TSAI, National Sun Yat-Sen University, Taiwan, FUCHUN ZHANG, Zhejiang University, China — Large Hubbard  $U$  limit of the Kane-Mele model on a zigzag ribbon of honeycomb lattice near half-filling is studied via a renormalized mean-field theory. The ground state exhibits time-reversal symmetry (TRS) breaking  $d_{x^2-y^2} + id_{xy}$ -wave superconductivity. At large spin-orbit coupling, the  $Z_2$  topological phase with non-trivial spin Chern number in the pure Kane-Mele model is persistent into the TRS broken state (called "spin-Chern phase"), and has two pairs of counter-propagating helical Majorana modes at the edges. As the spin-orbit coupling is reduced, the system undergoes a topological quantum phase transition from the spin-Chern to chiral superconducting states. Possible relevance of our results to adatom-doped graphene and iridate compounds is discussed. Ref.: Shih-Jye Sun, Chung-Hou Chung, Yung-Yeh Chang, Wei-Feng Tsai, and Fu-Chun Zhang, arXiv:1506.02584.

<sup>1</sup>CHC acknowledges support from NSC grant No.98-2918-I-009-06, No.98-2112-M-009-010-MY3, the NCTU-CTS, the MOE-ATU program, the NCTS of Taiwan, R.O.C.

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**  
**Session H23 DMP DCOMP: Computational Materials Discovery and Design - Materials for Catalysis** 322 - David Strubbe, Massachusetts Institute of Technology

**2:30PM H23.00001 First-principles data-driven discovery of transition metal oxides for artificial photosynthesis**, QIMIN YAN, Molecular Foundry, Lawrence Berkeley National Laboratory; Department of Physics, University of California, Berkeley — We develop a first-principles data-driven approach for rapid identification of transition metal oxide (TMO) light absorbers and photocatalysts for artificial photosynthesis using the Materials Project. Initially focusing on Cr, V, and Mn-based ternary TMOs in the database, we design a broadly-applicable multiple-layer screening workflow automating density functional theory (DFT) and hybrid functional calculations of bulk and surface electronic and magnetic structures. We further assess the electrochemical stability of TMOs in aqueous environments from computed Pourbaix diagrams. Several promising earth-abundant low band-gap TMO compounds with desirable band edge energies and electrochemical stability are identified by our computational efforts and then synergistically evaluated using high-throughput synthesis and photoelectrochemical screening techniques by our experimental collaborators at Caltech. Our joint theory-experiment effort has successfully identified new earth-abundant copper and manganese vanadate complex oxides that meet highly demanding requirements for photoanodes, substantially expanding the known space of such materials. By integrating theory and experiment, we validate our approach and develop important new insights into structure-property relationships for TMOs for oxygen evolution photocatalysts, paving the way for use of first-principles data-driven techniques in future applications. This work is supported by the Materials Project Predictive Modeling Center and the Joint Center for Artificial Photosynthesis through the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract No. DE-AC02-05CH11231. Computational resources also provided by the Department of Energy through the National Energy Supercomputing Center.

**3:06PM H23.00002 Computational Nano-materials Design for Spinodal Nanotechnology as a New Class of Bottom-up Nanotechnology**, HIROSHI KATAYAMA-YOSHIDA, TETSUYA FUKUSHIMA, Graduate School of Engineering Science, Osaka University, KAZUNORI SATO, Graduate School of Engineering, Osaka University — Based on the spinodal nano-decomposition (SND) of dilute magnetic semiconductors (DMS) [1,2], we generalized the SND to the application of catalysis [3,4] and photovoltaic solar-cells [5], where nano-scale particle formation in catalysis and nano-scale separation of electrons and holes are essential in order to enhance the efficiency. First, we summarize the shape control (Konbu- & Dairiseki-Phases) and dimensionality dependence of crystal growth condition on SND in DMS. Second, we discuss the application of SND for the formation of nano-particles and the self-regeneration in three-way catalysis for automotive emission control by Perovskite  $\text{La}(\text{Fe}, \text{Pd} \text{ or } \text{Rh})\text{O}_3$ . Third, we propose (i) self-regeneration mechanism and (ii) self-organized nano-structures by SND in chalcopyrite  $\text{Cu}(\text{In}, \text{Ga})\text{Se}_2$ , Kesterite  $\text{Cu}_2\text{ZnSnSe}_4$ , and Perovskite  $\text{CsSnI}_3$  for the low-cost, environment-friendly and high-efficiency photovoltaic solar cells using first-principles calculations. [1] K. Sato et al., Rev. Mod. Phys., 82, 1633 (2010). [2] T. Dietl, et al., Rev. Mod. Phys., (2015) in press. [3] H. Kizaki et al., Chem. Phys. Lett. 579, 85 (2013). [4] I. Hamada et al., J. Am. Chem. Soc. 133, 18506 (2011). [5] Y. Tani et al., Appl. Phys. Express, 3, 101201 (2010).

**3:18PM H23.00003 Simulation of Photo-isomerization of Functionalized Azobenzene Derivatives**, PEDRAM TAVAZOHI, ZACHARY HERBERGER, JAMES LEWIS, West Virginia Univ — Photo-isomerization is the process of changing the isomer (*cis*, *trans*) of a molecule using light. In azobenzene this process can be utilized in a Metal Organic Framework (MOF) for adsorption of  $\text{CO}_2$ . MOFs are created by two major components, metal ions, and organic molecules which are called linkers. The metal ions and linkers can be coordinated in a way that they form a porous material. In the *cis* isomer of azobenzene, the MOFs pore is available to be filled by  $\text{CO}_2$ , but in the *trans* isomer the pore is filled with a benzene ring. The change from *cis* to *trans* will evacuate the pore if  $\text{CO}_2$  is present. The important considerations in using azobenzene photo-isomerization as a photo-switch in MOFs are, the quantum yield of the process, and the wavelength of the light which triggers photo-isomerization. By substitution of the functional groups of azobenzene and using the fewest switches surface-hopping algorithm in FIREBALL to simulate the photo-isomerization process we can tune the properties of the molecule as we desire and predict the best substitution sites for azobenzene functional groups. We studied the effects of functionalizing the molecule with OH,  $\text{CH}_3$ ,  $\text{NH}_2$ ,  $\text{NO}_2$  and COOH on isomerization quantum yield.

**3:30PM H23.00004 Computational Design of Metal–Organic Frameworks with High Methane Deliverable Capacity**<sup>1</sup>, YI BAO, Rice University, RICHARD MARTIN, Lawrence Berkeley National Laboratory, CORY SIMON, University of California, Berkeley, MACIEJ HARANCZYK, Lawrence Berkeley National Laboratory, BEREND SMIT, University of California, Berkeley, MICHAEL DEEM, Rice University, DEEM TEAM, HARANCZYK TEAM, SMIT TEAM — Metal–organic frameworks (MOFs) are a rapidly emerging class of nanoporous materials with largely tunable chemistry and diverse applications in gas storage, gas purification, catalysis, etc. Intensive efforts are being made to develop new MOFs with desirable properties both experimentally and computationally in the past decades. To guide experimental synthesis with limited throughput, we develop a computational methodology to explore MOFs with high methane deliverable capacity. This *de novo* design procedure applies known chemical reactions, considers synthesizability and geometric requirements of organic linkers, and evolves a population of MOFs with desirable property efficiently. We identify about 500 MOFs with higher deliverable capacity than MOF-5 in 10 networks. We also investigate the relationship between deliverable capacity and internal surface area of MOFs. This methodology can be extended to MOFs with multiple types of linkers and multiple SBUs.

<sup>1</sup>DE-FG02- 12ER16362

**3:42PM H23.00005 Computational design of materials for solar hydrogen generation**, NAOTO UMEZAWA, National Institute for Materials Science — Photocatalysis has a great potential for the production of hydrogen from aqueous solution under solar light [1]. In this talk, two different approaches toward the computational materials design for solar hydrogen generation will be presented. Tin (Sn), which has two major oxidation states,  $\text{Sn}^{2+}$  and  $\text{Sn}^{4+}$ , is abundant on the earth's crust. Recently, visible-light responsive photocatalytic  $\text{H}_2$  evolution reaction was identified over a mixed valence tin oxide  $\text{Sn}_3\text{O}_4$  [2]. We have carried out crystal structure prediction for mixed valence tin oxides in different atomic compositions under ambient pressure condition using advanced computational methods based on the evolutionary crystal-structure search and density-functional theory. The predicted novel crystal structures realize the desirable band gaps and band edge positions for  $\text{H}_2$  evolution under visible light irradiation. It is concluded that multivalent tin oxides have a great potential as an abundant, cheap and environmentally-benign solar-energy conversion photofunctional materials [3]. Transition metal doping is effective for sensitizing  $\text{SrTiO}_3$  under visible light. We have theoretically investigated the roles of the doped Cr in STO based on hybrid density-functional calculations [4]. Cr atoms are preferably substituting for Ti under any equilibrium growth conditions. The lower oxidation state  $\text{Cr}^{3+}$ , which is stabilized under an n-type condition of STO, is found to be advantageous for the photocatalytic performance. It is further predicted that lanthanum is the best codopant for stabilizing the favorable oxidation state,  $\text{Cr}^{3+}$ . The prediction was validated by our experiments that La and Cr co-doped STO shows the best performance among examined samples [5]. This work was supported by the Japan Science and Technology Agency (JST) Precursory Research for Embryonic Science and Technology (PRESTO) and International Research Fellow program of Japan Society for the Promotion of Science (JSPS) through project P14207. [1] H. Tong, S. Ouyang, Y. Bi, N. Umezawa, M. Oshikiri, J. Ye, Adv. Mater. 24, 229 (2012). [2] Maidhily Manikandan, Toyokazu Tanabe, Peng Li, Shigenori Ueda, Gubbala V. Ramesh, Rajesh Kodyath, Junjie Wang, Toru Hara, Arivuoli Dakshanamoorthy, Shinsuke Ishihara, Katsuhiko Ariga, Jinhua Ye, Naoto Umezawa, and Hideki Abe, "Photocatalytic Water Splitting under Visible Light by Mixed-Valence  $\text{Sn}_3\text{O}_4$ " ACS Applied Materials & Interfaces, 6, 3790 (2014). [3] Junjie Wang, Naoto Umezawa\*, and Hideo Hosono, "Mixed Valence Tin Oxides as Novel van der Waals Materials: Theoretical Predictions and Potential Applications" Adv. Energy Mater. 2015, DOI: 10.1002/aenm.201501190 [4] P. Reunchan, N. Umezawa, S. Ouyang, J. Ye, Phys. Chem. Chem. Phys. 14, 1876 (2012). [5] P. Reunchan, S. Ouyang, N. Umezawa, H. Xu, Y. Zhang, and J. Ye, Journal of Materials Chemistry A, 1, 4221 (2013).

**4:18PM H23.00006 Understanding and controlling the water stability of MOF-74**<sup>1</sup>, SEBASTIAN ZULUAGA, Wake Forest University, ERIKA FUENTES, KUI TAN, University of Texas at Dallas, FENG XU, JING LI, Rutgers University, YVES CHABAL, University of Texas at Dallas, TIMO THONHAUSER, Wake Forest University — Metal organic framework (MOF) materials in general, and MOF-74 in particular, have promising properties for many technologically important processes. However, their instability under humid conditions severely restricts their practical use. In this work, we show that this instability and the accompanying reduction of the  $\text{CO}_2$  uptake capacity of MOF-74 under humid conditions originate in the dissociation of water molecules at the metal centers. In turn, the reduction in the  $\text{CO}_2$  uptake capacity occurs as the metal centers are occupied by the remaining OH groups after the water molecules dissociate. It follows that the reduction in  $\text{CO}_2$  uptake depends on the catalytic activity of MOF-74 towards the water dissociation reaction  $\text{H}_2\text{O} \rightarrow \text{OH} + \text{H}$ . On the other hand, we show that—while the water molecules themselves do only have a negligible effect on the crystal structure of MOF-74—the OH and H products of the dissociation reaction can significantly weaken the MOF framework and lead to the observed crystal structure breakdown. With this knowledge, we can now propose a way to suppress this particular reaction and therefore control the stability of the system under humid conditions.

<sup>1</sup>This work was supported in full by DOE Grant No. DE-FG02-08ER46491

**4:30PM H23.00007 High-throughput discovery of electrochemically stable photocatalysts for oxygen evolution.** , JIE YU, JCAP, Lawrence Berkeley National Laboratory, QIMIN YAN, WEI CHEN, ANUBHAV JAIN, Lawrence Berkeley National Laboratory, JOHN GREGOIRE, JCAP, California Institute of Technology, JEFFREY NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory, KRISTIN PERSSON, EETD, Lawrence Berkeley National Laboratory — Widespread use of artificial photosynthesis hinges upon development of photocatalysts and light absorbers with excellent electrochemical stability in aqueous solution. The poor stability of most semiconductors in the highly oxidizing environment of a solar fuels photoanode has been a key factor limiting the use of many candidates light absorbers. We assess the stability of candidate transition metal oxides (TMOs) in alkaline aqueous environments from calculated Pourbaix diagrams. Our analysis reveals interesting trends in the electrochemical stability of TMOs containing elements which have not traditionally been explored for photocatalysts. Utilizing the Pourbaix diagram analysis as the first screen-layer in a high-throughput workflow that incorporates automating density functional theory and hybrid functional calculations, we screen for electrochemically stable TMO compounds with low band gaps and optimal band edge energies. Applying our new data-driven approach, we successfully identify several new TMOs with promising band gaps and edges that are predicted to resist corrosion under aqueous conditions relevant to solar water splitting. Materials synthesis and electrochemical measurements confirm several predictions and demonstrate the utility of computational screening for identifying new solar fuels materials.

**4:42PM H23.00008 Rational Co-Design of Polymer Dielectrics for Energy Storage** , ARUN MANNODI-KANAKKITHODI, HUAN TRAN, University of Connecticut, GHANSHYAM PILANIA, TURAB LOOKMAN, Los Alamos National Laboratory, RAMPI RAM-PRASAD, University of Connecticut — While intuition-driven experiments and serendipity have guided traditional materials discovery, computational strategies have become increasingly important and a powerful complement to experiments in modern day materials research. With the example of polymer dielectrics for electrostatic energy storage applications, we demonstrate how a rational co-design approach—involving synergies between high-throughput computational screening and experimental synthesis and testing—can be harnessed for quick and efficient discovery. We highlight recent co-design efforts that can potentially lead to replacement of present-day “standard” polymer dielectrics (such as biaxially oriented polypropylene) not only by new organic polymer candidates within known generic polymer subclasses (e.g., polyurea, polythiourea, polyimide), but also by organometallic polymers, a hitherto untapped but promising chemical subspace. We also discuss the utilization of vast computational data (generated in the aforementioned process) towards the development of statistical learning models for relevant properties of dielectric polymers, which can further accelerate the guidance to experiments and thus the successful discovery of new materials.

**4:54PM H23.00009 Simulated synthesis of lithium manganese oxide nanostructures and their characterisation.**<sup>1</sup> , PHUTI NGOEPE, SYLVIA LEDWABA, University of Limpopo, Sovenga, 0727, South Africa., DEAN SAYLE, University of Kent, Canterbury, CT2 7NZ, UK — Simulated amorphisation/recrystallization methods, are now routinely used to generate models of various nano-architectures for metal oxides with complex microstructural details [1]. Nano-architectures, i.e. nano- sphere, sheet, porous and bulk, associated with the Li-Mn-O ternary were synthesised from amorphous spinel nanosphere. The resulting crystallised nanostructures are characterised from visual images, radial distribution functions, XRDs and simulated microstructures. An analysis of microstructures and simulated X-ray diffractions reveals the presence of the layered  $\text{Li}_2\text{MnO}_3$  and spinel  $\text{LiMn}_2\text{O}_4$  together with a wide variety of defects, including grain boundaries and ion vacancies. [1] T.X.T. Sayle, R.R. Maphanga, P. E. Ngoepe and D. C. Sayle, J. Am. Chem. Soc., **131** (2009), 6161-6173

<sup>1</sup> Acknowledge support from the National Research Fundation, Pretoria

**5:06PM H23.00010 Study of Hydrogen Adsorption in Titanium, Nickel and Pd Cluster Supported on Graphene Monovacancies** , CARLOS MANUEL RAMOS CASTILLO, ROMEO DE COSS GMEZ, Departament of Applied Physics Centro de Investigacion y Estudios Avanzados del Instituto Politecnico Nacional, Mexico, JOSE ULISES REVELES, Departament of Applied Physics Virginia Commonwealth University , VA USA — A detailed description of the atomic structure and the energetics of  $\text{H}_2$  adsorption on  $\text{Ti}_4$ ,  $\text{Ni}_4$ , and  $\text{Pd}_4$  clusters on graphene monovacancies is presented. The large binding energy of that clusters on vacancies is a result of strong hybridization between the unsaturated carbon. We found that the binding energy of a single  $\text{H}_2$  is strongly dependent on the specific cluster. In particular, the  $\text{H}_2$  bond cleavage is favored by titanium clusters. On the other hand, the Ni and Pd clusters favours the formation of Kubas complexes. The analysis of the adsorption energies and  $\text{H}_2$  average bond lengths suggests that supported  $\text{Ti}_4$  cluster is a potential hydrogen storage candidate, being able to hold up to 6 molecules covalently with moderate average binding energy within the optimal range for an efficient cyclic adsorption/desorption process at room temperature and moderate pressures. These results give physical insights about how the interaction between graphene monovacancies and metal clusters can be used to enhanced the hydrogen uptake, towards of design of new graphene-based material for hydrogen storage.

**5:18PM H23.00011 Using Cluster Expansions to Model Diffusion in Pt-Ni Nanoparticles** , THOMAS NILSON, TIM MUELLER, LIANG CAO, Johns Hopkins Univ — Pt-Ni alloys have been shown to have excellent catalytic activity for the oxygen reduction reaction. However in practice these particles suffer from Ni dissolution, degrading the performance of the catalyst over time. The exact mechanism by which this occurs is unknown and difficult to determine experimentally. Using density functional theory, we have calculated the energies of formation of several dozen  $\text{Pt}_x\text{Ni}_{1-x}$  nanoparticles with included vacancies and used this data to parametrize a cluster expansion. Because the activation energies for diffusion are included in the model, we are able to use the cluster expansion to rapidly predict the transition rates in a Pt-Ni nanoparticle as a function of particle shape, size, and local atomic order. By using the cluster expansion model in a kinetic Monte Carlo algorithm we are able to model the diffusion of Pt and Ni and provide insights into the dissolution of Ni from Pt-Ni nanoparticles.

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**  
**Session H24 DMP: Many-Body Perturbation Theory for Electronic Excitations: Excitonic Phenomena** 323 - Serdar Ogut, University of Illinois at Chicago

### **2:30PM H24.00001 A direct approach to the calculation of many-body Green's functions: quasi-particles and more<sup>1</sup>**

**LUCIA REINING, CNRS-Ecole Polytechnique** — Many-body perturbation theory is a powerful approach to describe many properties of materials. Most often one uses Dyson equations with self-energy kernels that are approximated to low order in the interaction. In Hedin's GW approximation, for example, the self-energy is a product of the one-body Green's function and the screened Coulomb interaction. This is the state-of-the-art method for bandstructure calculations in a wide range of materials. However, sometimes the GW approximation and related approaches are not sufficient, for example when one is interested in satellite structure beyond the quasi-particle peaks in the spectral function, or in the case of strong coupling, where the quasi-particle picture is no longer adequate. We explore an alternative route to the calculation of interacting electron Green's functions. It is based on a set of functional differential equations relating the one-body Green's function to its functional derivative with respect to an external perturbing potential [1]. This set of equations can be used to generate the perturbation series. Here we will show that working directly with the differential equations yields precious insight concerning some fundamental questions, guidelines for practical calculations, and methods that lead to an improved description of spectra, in particular advanced versions of the cumulant expansion. Results will be illustrated on various levels of approximation starting from simple models [2], but with a focus on full ab initio calculations [3] and comparison with, and interpretation of, experiment. In particular, we will discuss various kinds of photoemission satellites, and also address questions linked to strong correlation. [1] L.P. Kadanoff and G. Baym, Quantum Statistical Mechanics (New York: Benjamin, 1962) [2] A. Stan et al., New J. Phys. 17, 093045 (2015) [3] M. Guzzo et al., Phys. Rev. Lett. 107, 166401 (2011); Phys. Rev. B 89, 085425 (2014)

<sup>1</sup>This work has been carried out in collaboration with colleagues in the European Theoretical Spectroscopy Facility

### **3:06PM H24.00002 Multiple Exciton Generation in Semiconductor Nanostructures: DFT-based Computation**

**DEYAN MIHAYLOV, ANDREI KRYJEVSKI, DMITRI KILIN, SVETLANA KILINA, North Dakota State Univ, DAYTON VOGEL, University of South Dakota** — Multiple exciton generation (MEG) in nm-sized H-passivated Si nanowires (NWs), and quasi 2D nanofilms depends strongly on the degree of the core structural disorder as shown by the perturbation theory calculations based on the DFT simulations. In perturbation theory, we work to the 2<sup>nd</sup> order in the electron-photon coupling and in the (approximate) RPA-screened Coulomb interaction. We also include the effect of excitons for which we solve Bethe-Salpeter Equation. To describe MEG we calculate exciton-to-biexciton as well as biexciton-to-exciton rates and quantum efficiency (QE). We consider 3D arrays of Si<sub>29</sub>H<sub>36</sub> quantum dots, NWs, and quasi 2D silicon nanofilms, all with both crystalline and amorphous core structures. Efficient MEG with QE of 1.3 up to 1.8 at the photon energy of about  $3E_{gap}$  is predicted in these nanoparticles except for the crystalline NW and film where  $QE \simeq 1$ . MEG in the amorphous nanoparticles is enhanced by the electron localization due to structural disorder. The exciton effects significantly red-shift QE vs. photon energy curves. Nm-sized a-Si NWs and films are predicted to have effective MEG within the solar spectrum range. Also, we find efficient MEG in the chiral single-wall Carbon nanotubes and in a perovskite nanostructure.

### **3:18PM H24.00003 Excitons in solids with time-dependent density-functional theory: the bootstrap kernel and beyond<sup>1</sup>**

**YOUNG-MOO BYUN, Univ of Missouri - Columbia, ZENG-HUI YANG, Temple University, CARSTEN ULLRICH, Univ of Missouri - Columbia** — Time-dependent density-functional theory (TDDFT) is an efficient method to describe the optical properties of solids. Lately, a series of bootstrap-type exchange-correlation (xc) kernels have been reported to produce accurate excitons in solids, but different bootstrap-type kernels exist in the literature, with mixed results. In this presentation, we reveal the origin of the confusion and show a new empirical TDDFT xc kernel to compute excitonic properties of semiconductors and insulators efficiently and accurately. Our method can be used for high-throughput screening calculations and large unit cell calculations.

<sup>1</sup>Work supported by NSF Grant DMR-1408904

### **3:30PM H24.00004 Stability of excitonic complexes in a multi-valley/band semiconductor**

**HIROKI KATOW, University of Tokyo, JUNKO USUKURA, Tokyo University of Science, RYOSUKE AKASHI, University of Tokyo, KALMAN VARGA, Vanderbilt University, SHINJI TSUNEYUKI, University of Tokyo** — Whether bound states are present for few-particle quantum systems is far from axiomatic and has been a hot topic for decades. For example, three-positronium and -/hydrogen bound states are not present in the vacuum. On the other hand, it has also been proposed that three excitons can be bound with each other in multi-valley/band semiconductors [J. S. Wang & C. Kittel, Phys. Lett. 42A, No. 3 (1972)]. Indeed, an array of photoluminescence peaks have been recently observed in diamond [J. Omachi et al., Phys. Rev. Lett. 111, 026402(2013)], which could suggest the existence of possible multi-exciton bound states. We theoretically examine if such bound states are possible by a variational method. For the electron-hole Hamiltonian including the valley and band degrees of freedom, we expressed trial many-body wave function with the correlated Gaussian bases and optimized it with the stochastic variational method [J. Mitroy et al., Rev. of Mod. Phys., 85, 2013]. We have shown bound states for N-exciton systems with N more than two. In the talk, we discuss the dependence of the bound states on the model settings and its relation to the experimental observation.

### **3:42PM H24.00005 Exploring the nature of low-lying excited-states in molecular crystals from many-body perturbation theory beyond the Tamm-Dancoff Approximation<sup>1</sup>**

**TONATIUH RANGEL, Lawrence Berkeley Natl Lab; UC Berkeley, SAHAR SHARIFZADEH, Boston University, ANDRE RINN, Philipps-Universitt Marburg, FELIPE H. DA JORNADA, UC Berkeley; Lawrence Berkeley Natl Lab, MEIYUE SHAO, Lawrence Berkeley Natl Lab, GREGOR WITTE, Philipps-Universitt Marburg, CHAO YANG, Lawrence Berkeley Natl Lab, STEVEN G. LOUIE, UC Berkeley; Lawrence Berkeley Natl Lab, SANGAAM CHATTERJEE, Philipps-Universitt Marburg, LEEOR KRONIK, Weizmann Institute of Science, JEFFREY B. NEATON, Lawrence Berkeley Natl Lab; UC Berkeley** — Organic semiconductors have attracted attention due to their potential for optoelectronics and novel phenomena, such as singlet fission. Here, we use many-body perturbation theory to simulate neutral excitations in acene and perylene crystals. By diagonalizing the full Bethe-Salpeter (BSE) Hamiltonian beyond the Tamm-Dancoff approximation (TDA) [1], we find that both low-lying excitation energies and oscillator strengths are in improved agreement with experiments relative to the TDA. We characterize the low-lying excitons, focusing in the degree of charge-transfer and spatial delocalization, connecting their relevance to singlet fission. [2] For perylene, we find overall good agreement with absorption measurements, and we see evidence for the formation of an exciton-polariton band in  $\beta$ -perylene. 1. da Jornada, F. H. et al., to be submitted. 2. Sharifzadeh, S. et al., J. Phys. Chem. Lett. 4, 2197 (2013).

<sup>1</sup>This work is supported by the DOE.

### **3:54PM H24.00006 ABSTRACT WITHDRAWN —**

**4:06PM H24.00007 Effect of Crystal Packing on the Excitonic Properties of Rubrene Polymorphs**, XIAOPENG WANG, Tulane University, TAYLOR GARCIA, STEPHEN MONACO, Pennsylvania State University, BOHDAN SCHATTSCHNEIDER, California State Polytechnic University, Pomona, NOA MAROM, Tulane University — Singlet fission, the down-conversion of one singlet exciton into two triplet excitons, has been recently observed in molecular crystals of rubrene. The orthorhombic form of rubrene is the most stable in ambient conditions. However, rubrene has two additional known polymorphs, a triclinic form and a monoclinic form. To investigate the relative stability of the three polymorphs under different temperature and pressure conditions we use dispersion-inclusive density functional theory (DFT) with the pairwise Tkatchenko-Scheffler (TS) method and the many-body dispersion (MBD) method. Many-body perturbation theory is then employed to study the effect of crystal structure on the electronic and excitonic properties. Band structures are calculated within the GW approximation, where G is the one-particle Green's function and W is the screened Coulomb interaction, and optical properties are calculated by solving the Bethe-Salpeter equation (BSE). We find that crystal packing affects the band gaps, band dispersion, optical gaps, singlet-triplet gaps, and exciton localization in the three polymorphs of rubrene. Singlet fission efficiency may thus be improved by modulating the crystal packing.

**4:18PM H24.00008 Multiscale modeling of excitation dynamics in molecular materials with GW-BSE/MM**, BJOERN BAUMEIER, Department of Mathematics and Computer Science & Institute for Complex Molecular Systems, Eindhoven University of Technology — Processes involving electronic excitations govern the functionality of molecular materials in which the dynamics of excitons and charges is determined by an interplay of molecular electronic structure and morphological order. To understand, e.g., charge separation and recombination at donor-acceptor heterojunctions in organic solar cells, knowledge about the microscopic details influencing these dynamics in the bulk and across the interface is required. For heterojunctions of small-molecule donor materials with C60, we employ a hybrid QM/MM approach [JCTC 7, 3335 (2011)] linking density-functional and many-body Green's functions theory [JCTC 8, 2790 (2012)] (DFT/GW-BSE) to polarizable force-fields [JCTC 10, 3140 (2014)] and analyze the charged and neutral electronic excitations therein. We develop models for both static and dynamic properties of the excitations, including (a) the diffusion of Frenkel excitons and (b) the relative energies of Frenkel and charge-transfer excitations at the donor-acceptor interface and the resulting charge separation dynamics. Our simulations allow linking the molecular architecture of the donor material, its orientation on the fullerene substrate as well as mesoscale order [Nat. Mater. 14, 434 (2015)] to the solar cell performance.

**4:30PM H24.00009 Excited Biexcitons in Transition Metal Dichalcogenides**, DAVID ZHANG, Vanderbilt University — Recently, experimental measurements and theoretical modeling have been in a disagreement concerning the binding energy of biexcitons in transition metal dichalcogenides.<sup>1</sup> While theory predicts a smaller binding energy ( $\sim 20$  meV) that is, as logically expected, lower than that of the trion, experiment finds values much larger ( $\sim 60$  meV), actually exceeding those for the trion. In this work, we show that there exists an excited state of the biexciton which yields binding energies that match well with experimental findings and thus gives a plausible explanation for the apparent discrepancy. Furthermore, it is shown that the electron-hole correlation functions of the ground state biexciton and trion are remarkably similar, possibly explaining why a distinct signature of ground state biexcitons would not have been noticed experimentally.<sup>2</sup>

<sup>1</sup>Y. You, X.-X. Zhang, T. C. Berkelbach, M. S. Hybertsen, D. R. Reichman, T. F. Heinz, *Nat. Phys.* 11 477–481 (2015).

<sup>2</sup>D. K. Zhang, D. W. Kidd, K. Varga, *Nano. Lett.* Article ASAP (2015).

**4:42PM H24.00010 Exciton band structure in two-dimensional materials**, PIER LUIGI CUDAZZO, LSI Ecole Polytechnique France, LORENZO SPONZA, Kings College London UK, CHRISTINE GIORGETTI, LUCIA REINING, FRANCESCO SOTTILE, MATTEO GATTI, LSI Ecole Polytechnique France — In low-dimensional materials the screening of the Coulomb interaction is strongly reduced[1,2]. As a consequence, the binding energy of both Wannier and Frenkel excitons in the optical spectra is large and comparable in size. Therefore, contrarily to bulk materials, it cannot serve as a criterion to distinguish different kinds of excitons. Here we demonstrate that the exciton band structure, which can be accessed experimentally, instead provides a powerful way to identify the exciton character. By comparing the *ab initio* solution of the many-body Bethe-Salpeter equation for graphene and single-layer hexagonal BN, we draw a general picture of the exciton dispersion in two-dimensional materials, highlighting the different role played by the exchange electron-hole interaction and by the hopping terms related to the electronic band structure. 1 Pierluigi Cudazzo et. al. *Phys. Rev. Letter* 104 226804 (2010) 2 Pierluigi Cudazzo et. al. *Phys. Rev. B* 84, 085406 (2011)

**4:54PM H24.00011 Effect of Lattice Screening on Excitonic and Optical Properties in CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> Solar Cell Materials**<sup>1</sup>, JOSHUA LEVEILLE, ANDRE SCHLEIFE, Univ of Illinois - Urbana, ANDRE SCHLEIFE RESEARCH GROUP TEAM — Hybrid Organo-Metallic Perovskites have made great strides towards becoming a next generation solar cell material. Though high performing experimental devices have been constructed from these perovskites, the fundamental optical and electronic physics of these systems remains an active area of research. A large lattice dielectric constant in the Methylammonium(CH<sub>3</sub>NH<sub>3</sub>)-Lead(Pb)-Iodide(I<sub>3</sub>) system potentially contributes to the screening of the electron-hole interaction. The strongly increased dielectric screening due to lattice contributions has been suggested to reduce the exciton binding energy and strongly effects the optical band gap. In this study, we seek to understand, from first principles, the interplay between lattice screening and exciton binding energy. We use density functional theory for ground state calculations and the Bethe-Salpeter equation for the optical polarization function, from which we calculate optical spectra and excitonic properties. We will discuss differences between lattice and electronic screening and the effect on the optical properties of multiple CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> phases.

<sup>1</sup>supported by NSF grand number: CBET-1437230

**5:06PM H24.00012 Substrate-induced renormalization of the quasiparticle and optical gaps in monolayer transition metal dichalcogenides from GW and GW-BSE calculations.**, FELIPE H. DA JORNADA, CHIN SHEN ONG, DIANA Y. QIU, STEVEN G. LOUIE, UC Berkeley and Lawrence Berkeley National Lab — There has been a considerable effort to experimentally characterize the electronic and optical properties of novel atomically thin 2D semiconductors, such as mono- and few-layer transition metal dichalcogenides (TMDs). However, the role that different substrates play in these experiments still remains unclear. From a theoretical perspective, it is hard to include the substrate in an *ab initio* framework, while in experiments, it is often difficult to suspend these samples. Here, we present a new method to compute the substrate effect on the quasiparticle and optical properties of quasi-2D materials based on state-of-the-art *ab initio* GW and GW plus Bethe-Salpeter equation (GW-BSE) methods. We compute the effects of different metallic and semiconducting substrates, and show that the quasiparticle gap and exciton binding energy can be dramatically reduced even with semiconducting substrates. This work was supported by the National Science Foundation under Grant No. DMR15-1508412 and the DOE under Contract No. DE-AC02-05CH11231.

**5:18PM H24.00013 Nonanalyticity, Valley Quantum Phases, and Massless Excitons in Monolayer Transition Metal Dichalcogenides<sup>1</sup>**, DIANA Y. QIU, TING CAO, STEVEN G. LOUIE, University of California at Berkeley and Lawrence Berkeley National Laboratory — Exciton dispersion as a function of center-of-mass momentum  $\mathbf{Q}$  is essential to the understanding of exciton dynamics, relaxation, and condensation. We use the *ab initio* GW-Bethe-Salpeter equation (GW-BSE) method to calculate the dispersion of excitons in monolayer MoS<sub>2</sub> and find a nonanalytic lightlike dispersion. This behavior arises from the interplay of an unusual  $|\mathbf{Q}|$ -term in both the intra- and intervalley exchange of the electron-hole interaction, which concurrently gives rise to a valley quantum phase of winding number two. We have derived a simple, effective Hamiltonian and analytic solutions, which quantitatively describe this physics, and we predict that signatures of this unusual dispersion can be measured with a linearly polarized optical beam tilted away from normal incidence. The existence of a nonanalytic exciton dispersion can be generalized to other 2D semiconductors with excitons whose amplitudes are localized in a small region of the Brillouin zone.

<sup>1</sup>This work was supported by NSF grant No. DMR15-1508412 and U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by NERSC and XSEDE.

**Tuesday, March 15, 2016 2:30PM - 5:06PM –**  
**Session H25 DCMP: Josephson Tunneling: SQUIDS and Superconductor-ferromagnetic Interactions** 324 - Steven Anlage, University of Maryland

**2:30PM H25.00001 Controlling Hysteresis in Superconducting Weak Links and  $\mu$ -Superconducting Quantum Interference Devices.<sup>1</sup>**, NIKHIL KUMAR, Department of Physics, Indian Institute of Technology, Kanpur, India-208016, C.B. WINKELMANN, Institute Neel, CNRS and University Joseph Fourier, 25 Avenue des Martyrs, BP 166, 38042, Grenoble, France, SOURAV BISWAS, Department of Physics, Indian Institute of Technology, Kanpur, India-208016, H. COURTOIS, Institute Neel, CNRS and University Joseph Fourier, 25 Avenue des Martyrs, BP 166, 38042, Grenoble, France, ANJAN K. GUPTA, Department of Physics, Indian Institute of Technology, Kanpur, India-208016 — We have fabricated and studied the current-voltage characteristics of a number of niobium film based weak-link devices and  $\mu$ -SQUIDS showing a critical current and two re-trapping currents. We have proposed a new understanding for the re-trapping currents in terms of thermal instabilities in different portions of the device. We also find that the superconducting proximity effect and the phase-slip processes play an important role in dictating the temperature dependence of the critical current in the non-hysteretic regime. The proximity effect helps in widening the temperature range of hysteresis-free characteristics. Finally we demonstrate control on temperature-range with hysteresis-free characteristics in two ways: 1) By using a parallel shunt resistor in close vicinity of the device, and 2) by reducing the weak-link width. Thus we get non-hysteretic behavior down to 1.3 K temperature in some of the studied devices.

<sup>1</sup>We acknowledge the financial support from CSIR, India as well as CNRS-Institute Neel, Grenoble, France.

**2:42PM H25.00002 Phase-engineering artificial topology in a three-terminal Josephson interferometer.**, SOPHIE D'AMBROSIO, FRANCESCO VISCHI, ELIA STRAMBINI, FRANCESCO GIAZOTTO, NEST laboratory, GIAZOTTO GROUP TEAM — The fundamental aspects of Majoranas with their non-Abelian statistics offer great applications for the future of quantum computation. Current theories on multi-terminal Josephson junctions emphasize the possibility of engineering non trivial states in the spectrum of a proximized normal metal giving rise to an artificial topological superconductor which is able to support Majorana bound states, and points out the importance of a first experimental agreement with the theoretical speculations [1,2]. Here we report on the realization of a three-terminal Josephson interferometer based on proximity effect and fully controlled by phase-coherence. Our device shows a non trivial phase-tunable switch from a regime where the normal metal spectrum shows a gap in the density of states to a gapless regime in full agreement with recent predictions [1,2,3,4], and represents the first essential step towards phase engineering of an artificial topological superconductor hosting Majorana bound states. [1] arXiv:1508.00146. [2] arXiv:1503.06862. [3] Phys. Rev. B 90, 155450 (2014). [4] arXiv:1508.03289.

**2:54PM H25.00003 Tunable microstrip SQUID amplifiers for the Gen 2 Axion Dark Matter eXperiment (ADMX)**, SEAN O'KELLEY, UC Berkeley, GENE HILTON, NIST Boulder, JOHN CLARKE, UC Berkeley — We present a series of tunable microstrip SQUID amplifiers (MSAs) for installation in ADMX. The axion dark matter candidate is detected via Primakoff conversion to a microwave photon in a high-Q ( $\approx 100,000$ ) tunable microwave cavity cooled with a dilution refrigerator in the presence of a 7-tesla magnetic field. The microwave photon frequency  $\nu$  is a function of the unknown axion mass, so both the cavity and amplifier must be scanned over a wide frequency range. An MSA is a linear, phase-preserving amplifier consisting of a superconducting, resonant microstrip flux-coupled to a resistively-shunted dc SQUID biased into the voltage state. Tunability is achieved by terminating the microstrip with low inductance GaAs varactor diodes that operate below 100 mK. By varying the bias voltage of the varactors we vary their capacitance, allowing a reflected phase varying from nearly 0 to  $\pi$ , thus achieving a tunability close to a factor of 2. We demonstrate several devices operating below 100 mK, matched to the discrete operating bands of ADMX at frequencies ranging from 560 MHz to 1 GHz, that exhibit gains exceeding 20 dB. The associated noise temperatures, measured with a hot/cold load, approach the standard quantum limit ( $h\nu/k_B$ ) for a linear phase-preserving amplifier.

**3:06PM H25.00004 Transparency and Coherence in rf SQUID Metamaterials<sup>1</sup>**, STEVEN ANLAGE, MELISSA TREPANIER, DAIMENG ZHANG, University of Maryland — We have developed active metamaterials capable of quickly tuning their electrical and magnetic responses over a wide frequency range [1]. These metamaterials are based on superconducting elements to form low loss, physically and electrically small, highly tunable structures for fundamental studies of extraordinarily nonlinear media. The meta-atoms are rf superconducting quantum interference devices (SQUIDs) that incorporate the Josephson effect. RF SQUIDs have an inductance which is strongly tunable with dc and rf magnetic fields and currents. The rf SQUID metamaterial is a richly nonlinear effective medium introducing qualitatively new macroscopic quantum phenomena into the metamaterials community, namely magnetic flux quantization and the Josephson effect. The coherent oscillation of the meta-atoms is strongly sensitive to the environment and measurement conditions, and we have developed several strategies to improve the coherence experimentally by exploiting ideas from nonlinear dynamics [2]. The metamaterials also display a unique form of transparency whose development can be manipulated through multiple parametric dependences [3]. We discuss these qualitatively new metamaterial phenomena. [1] Melissa Trepanier, *et al.*, Phys. Rev. X 3, 041029 (2013). [2] Melissa Trepanier, *et al.*, in preparation. [3] Daimeng Zhang, *et al.*, Phys. Rev. X (in press). arXiv:1504.08301

<sup>1</sup>This work is supported by the NSF-GOALI and OISE Programs through Grant No. ECCS-1158644 and the Center for Nanophysics and Advanced Materials (CNAM).

**3:18PM H25.00005 Multi-tone response of Nonlinear rf-SQUID metamaterials<sup>1</sup>**, DAIMENG ZHANG, MELISSA TREPANIER, Univ of Maryland-College Park, OLEG MUKHANOV, Hypres Inc., THOMAS ANTONSEN, EDWARD OTT, STEVEN ANLAGE, Univ of Maryland-College Park — We study the multi-tone response over a broad microwave frequency range of a nonlinear superconducting meta-atom and a metamaterial composed of Radio Frequency Superconducting QUantum Interference Devices (rf-SQUIDs). Nonlinearity in the SQUID metamaterial gives rise to large-range tunable resonance via dc/rf magnetic field and temperature [1] [2], it also results in signal mixing through intermodulation distortion (IMD). Our metamaterial responds to multi-frequency signals and generates strong higher order intermodulation signals in a certain range of applied rf power. However, our meta-atom and metamaterial show a reduced third-order IMD generation around the resonance, which is unusual for typical nonlinear systems. The numerical simulation predicts the same IMD gap feature as in experiment. A comprehensive analytical model is applied to explain the phenomena, and methods to enhance, or reduce, intermodulation levels are explored. [1] M. Trepanier, Daimeng Zhang, Oleg Mukhanov, Steven M. Anlage, Phys. Rev. X 3, 041029 (2013). [2] Daimeng Zhang, M. Trepanier, Oleg Mukhanov, Steven. M. Anlage, Anlage, arXiv:1504.08301 (2015).

<sup>1</sup>This work is supported by the NSF-GOALI and OISE programs through grant ECCS-1158644, and CNAM.

**3:30PM H25.00006 Stochastic Resonance Magnetic Force Microscopy imaging of Josephson Arrays**, TYLER NAIBERT, HRYHORIY POLSHYN, BRIAN WOLIN, MALCOLM DURKIN, RITA GARRIDO MENACHO, IAN MONDRAGON SHEM, VICTOR CHUA, TAYLOR HUGHES, NADYA MASON, RAFFI BUDAKIAN, University of Illinois at Urbana-Champaign — Vortex interactions are key to explaining the behavior of many two dimensional superconducting systems. We report on the development of a technique to locally probe vortex interactions in a 2D array of Josephson junctions. Scanning a magnetic tip attached to an ultra-soft cantilever over the array produces changes in the frequency of the cantilever along certain lines, forming geometric patterns in the scans. Different tip-surface separations and external magnetic fields produce a number of different patterns. These patterns correspond to tip locations in which two configurations of vortices in the lattice have degenerate energies. By imaging the locations of these degeneracies, information on the local vortex interactions may be obtained.

**3:42PM H25.00007 Phase-coherent engineering of electronic heat currents with a Josephson modulator.**, ANTONIO FORNIERI, CHRISTOPHE BLANC, RICCARDO BOSISIO, SOPHIE D'AMBROSIO, FRANCESCO GIAZZOTTO, NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore — In this contribution we report the realization of the first balanced Josephson heat modulator designed to offer full control at the nanoscale over the phase-coherent component of electronic thermal currents.<sup>1</sup> The ability to master the amount of heat transferred through two tunnel-coupled superconductors by tuning their phase difference<sup>2</sup> is the core of coherent caloritronics, and is expected to be a key tool in a number of nanoscience fields, including solid state cooling, thermal isolation, radiation detection, quantum information and thermal logic. Our device provides magnetic-flux-dependent temperature modulations up to 40 mK in amplitude with a maximum of the flux-to-temperature transfer coefficient reaching 200 mK per flux quantum at a bath temperature of 25 mK. Foremost, it demonstrates the exact correspondence in the phase-engineering of charge and heat currents, breaking ground for advanced caloritronic nanodevices such as thermal splitters, heat pumps and time-dependent electronic engines.

<sup>1</sup>A. Fornieri *et al.*, arXiv:1507.00199, to be published in *Nature Nanotechnology*.

<sup>2</sup>F. Giazotto and M.-J. Martínez-Pérez, *Nature* **492**, 401-405 (2012).

**3:54PM H25.00008 Josephson current in parallel SFS junctions**, PAVEL IOSELEVICH, PAVEL OSTROVSKY, Max Planck Institute for Solid State Research, Stuttgart, Germany, YAKOV FOMINOV, MIKHAIL FEIGELMAN, Landau Institute for Theoretical Physics — We study a Josephson junction between superconductors connected by two parallel ferromagnetic arms. If the ferromagnets are fully polarised, supercurrent can only flow via Cooper pair splitting between the differently polarised arms. The disorder-average current is suppressed, but mesoscopic fluctuations lead to a significant typical current. We extract the typical current from a current-current correlator. The current is proportional to  $\sin^2 \alpha/2$ , where  $\alpha$  is the angle between the polarisations of the two arms, revealing the spin dependence of crossed Andreev reflection. Compared to an SNS device of the same geometry, the typical SFS current is small by a factor determined by the properties of the superconducting leads alone. The current is insensitive to the flux threading the area between the ferromagnetic arms of the junction. However, if the ferromagnetic arms are replaced by metal with magnetic impurities, or partially polarised ferromagnets, the Josephson current starts depending on the flux with a period of  $h/e$ , i.e. twice the superconducting flux quantum.

**4:06PM H25.00009 Critical Current Oscillations of Josephson Junctions with Ferromagnetic Layers<sup>1</sup>**, JOSEPH A. GLICK, MAZIN A. KHASAWNEH, BETHANY M. NIEDZIELSKI, REZA LOLOEE, W. P. PRATT JR., NORMAN O. BIRGE, Dept. of Physics and Astronomy, Michigan State University — Josephson junctions containing ferromagnetic layers are of considerable interest for the development of practical cryogenic memory and superconducting qubits. Such junctions exhibit a phase shift of  $\pi$  for certain ranges of ferromagnetic layer thickness. We present studies of Nb based micron-scale Josephson junctions using ferromagnetic layers of Ni, Ni<sub>81</sub>Fe<sub>19</sub>, or Ni<sub>65</sub>Co<sub>20</sub>Fe<sub>15</sub>. By applying an external magnetic field, the critical current of the junctions containing Ni<sub>81</sub>Fe<sub>19</sub> and Ni<sub>65</sub>Co<sub>20</sub>Fe<sub>15</sub> is found to follow a characteristic Fraunhofer pattern, and displays the clear switching behavior expected of single-domain magnets. However, the junctions containing Ni exhibit more complex behaviors. The maximum value of the critical current, extracted from the Fraunhofer patterns, oscillates as a function of the ferromagnetic layer thickness, indicating transitions in the phase difference across the junction between values of zero and  $\pi$ . We compare the data to previous work and to models of the  $0-\pi$  transitions based on existing clean and dirty limit theories.

<sup>1</sup>This work was supported by IARPA via ARO contract W911NF-14-C-0115.

**4:18PM H25.00010 Controlling the Phase of Ferromagnetic Josephson Junctions for Cryogenic Memory Applications<sup>1</sup>**, BETHANY NIEDZIELSKI, Michigan State University, ERIC GINGRICH, Northrop Grumman Systems Corporation, JOSEPH GLICK, Michigan State University, YIXING WANG, Seagate Technology, DON MILLER, Northrop Grumman Systems Corporation, REZA LOLOEE, WILLIAM PRATT JR., NORMAN BIRGE, Michigan State University — Josephson junctions containing ferromagnetic layers are currently of interest for use in cryogenic memory where either the phase or critical current can be switched between two distinct states. We present the first direct phase measurements of such a junction demonstrating control of the phase [1]. If a junction contains one ferromagnetic layer, the thickness of that layer dictates the ground state phase between the superconducting electrodes, which can be either 0 or  $\pi$ . If the junction contains two ferromagnetic layers and the layer thicknesses are carefully chosen, then the phase of a single junction can be switched between 0 and  $\pi$  by changing the relative magnetization directions of the two layers from antiparallel to parallel. We have successfully fabricated and directly measured the relative phase of two such spin valve junctions in a SQUID loop to confirm the phase change from  $\pi$  to 0 and back again of each junction. We report our continued progress in optimizing the control of such systems. [1] E. C. Gingrich, B. M. Niedzielski, J. A. Glick, Y. Wang, D. L. Miller, R. Loloee, W. P. Pratt Jr., and N. O. Birge, arXiv:1509.05368

<sup>1</sup>This work was supported by IARPA via ARO contract W911NF-14-C-0115.

**4:30PM H25.00011 Effects of a rotating magnetization on pair correlations in a ballistic regime Josephson Junction<sup>1</sup>**, ANDREAS BILL, LUIS LEAL, California State University Long Beach — Pair correlations in clean superconducting-magnetic proximity systems are studied with a focus on the singlet-triplet mixing resulting from magnetic inhomogeneities. The system is modeled in the clean limit using a tight-binding Hamiltonian and the Bogoliubov–de Gennes equations are solved to determine the Gor'kov functions of the system. Three different magnetic configurations are considered: an exchange spring, a helical magnet, and misaligned homogeneous ferromagnetic layers; each is sandwiched between two superconductors to form a Josephson junction. The goal of the study is to revisit how pair correlations are affected by different magnetization configurations and magnitudes in the clean limit. We discuss our results in the light of those obtained in the diffusive regime [1,2].

[1] T.E. Baker, A. Richie-Halford, A. Bill New J. Phys. 16, 093048 (2014).

T.E. Baker, A. Richie-Halford, O.E. Icreverzi, A. Bill Europhys. Lett., 107, 17001 (2014).

<sup>1</sup>We gratefully acknowledge support from the National Science Foundation under grant DMR- 1309341 and the ORSP Student Research Assistantship at CSU Long Beach.

**4:42PM H25.00012 Nanoscale investigation of mesoscopic phenomena in superconductor/ferromagnet hybrid structures using low-temperature scanning tunneling microscopy and spectroscopy<sup>1</sup>**, C. DI GIORGIO<sup>2</sup>, S. A. MOORE, A. PUTILOV<sup>3</sup>, E. LECHNER, Department of Physics, Temple University, Philadelphia, PA 19122, J. E. PEARSON, V. NOVOSAD, Materials Science Division, Argonne National Laboratory, Argonne, IL, G. KARAPETROV, Department of Physics, Drexel University, Philadelphia, PA 19104, M. IAVARONE, Department of Physics, Temple University, Philadelphia, PA 19122 — Superconductor/ferromagnet (S/F) heterostructures exhibit unique electronic phenomena which strongly depend on the nature of the constituent materials and the coupling between the layers. Using low-temperature scanning tunneling microscopy and spectroscopy we have investigated S/F structures in the regimes of magnetic and proximity coupling. Here, in the case of S/F systems made of conventional low- $T_c$  lead films with different ferromagnet materials, the spatial and temperature dependent effects on the local density of states which emerge at the nanoscale will be discussed.

<sup>1</sup>Work at Temple University was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-SC0004556.

<sup>2</sup>C.D.G. would like to acknowledge the partial support from MIUR (Ministry of Education, Universities and Research of the Italian Government

<sup>3</sup>Permanent address: Institute for Physics of Microstructures RAS, Nizhny Novgorod, Russia

**4:54PM H25.00013 Josephson critical current of long SNS junctions in the presence of a magnetic field**, HENDRIK MEIER, Department of Physics, Yale University, VLADIMIR I. FAL'KO, National Graphene Institute, University of Manchester, United Kingdom, LEONID I. GLAZMAN, Department of Physics, Yale University — We evaluate the Josephson critical current of a long and wide two-dimensional superconductor-normal metal-superconductor (SNS) junction, taking into account the effect of electron reflection off the side edges of the junction. Considering clean junctions, we find that the effect of edges alters the usual Fraunhofer-like dependence of the Josephson critical current  $I_c$  on the magnetic flux  $\Phi$ . At relatively weak fields,  $B\Phi_0/W^2$ , the edge effect lifts zeros of the  $I_c(\Phi)$  dependence and gradually shifts the maxima of that function by  $\Phi_0/2$ . (Here  $W$  is the width of the junction and  $\Phi_0$  the magnetic flux quantum.) At higher fields,  $B\Phi_0/W^2$ , the edge effect leads to an accelerated decay of the critical current  $I_c(\Phi)$  with increasing  $\Phi$ . Our results are robust with respect to the roughness of realistic boundaries. Finally, we discuss the role of mesoscopic fluctuations of  $I_c(\Phi)$  originating from the scattering off the edges, and compare our findings to recent experiments.

**Tuesday, March 15, 2016 2:30PM - 5:06PM –**

**Session H26 DCMP DMP: Graphene: Plasmons and Fluorescence** 325 - Abdel El Fatimy, Georgetown University

**2:30PM H26.00001 Plasmon damping in graphene out of equilibrium**, ZHIYUAN SUN, DIMITRI BASOV, MICHAEL FOGLER, Univ of California - San Diego — Motivated by recent experiments with graphene under high photoexcitation, we study theoretically plasmons of graphene in the two-temperature regime, i.e., the regime where electrons are much hotter than the lattice. We calculate the plasmon damping due to scattering of electrons by acoustic phonons, which is the dominant intrinsic contribution in clean graphene. As the system relaxes to equilibrium, the plasmon frequency adiabatically changes with time. We show that this causes a partial compensation of the plasmon damping. A similar mechanism may apply to another collective mode (the energy wave) predicted to exist in graphene in the low-frequency hydrodynamic regime. Implications for infrared and THz pump-probe experiments are discussed.

**2:42PM H26.00002 Plasmonics of graphene laced stratified media.**, UPALI APARAJITA, United States Military Academy:Department of Physics and Nuclear Engineering,753 Cullum Rd, West Point, NY 10996, OLEKSIY ROSLYAK, Physics and Engineering Physics Fordham University Freeman Hall 208 Bronx, NY 10458 - 5198 — Strong overlap of fields of graphene physics and photonics drawn a lot of attention recently. Not only graphene possesses intrinsic highly tunable plasmons but a combination of graphene with noble metal nano structures promises a variety of existing applications for conventional plasmonics, such as novel optical devices working in a broad range from THz to visible spectra. We report simulations of those devices using combination of discrete dipole approximation (DDA) and boundary element methods (BEM). While DDA is an essential tool for modeling large molecule polarizabilities and scattering the BEM provides necessary Green's function tensors when those molecules are in close proximity to the nano-structures. As an example of that technique we study electron energy loss and Raman spectra for complex molecules in presence of metal plasmon active nano particles embedded into a stratified graphene laced medium.

**2:54PM H26.00003 Nano-plasmonic phenomena in graphene nanoribbons**, ZHE FEI, Iowa State University, MICHAEL GOLDFLAM, JIHI-SHENG WU, SIYUAN DAI, MARTIN WAGNER, ALEX MCLEOD, University of California, San Diego, MENGKUN LIU, Stony Brook University, KIRK POST, University of California, San Diego, SHOU-EN ZHU, GUIDO JANSSEN, Delft University of Technology, MICHAEL FOGLER, DIMITRI BASOV, University of California, San Diego — We report on infrared nano-imaging studies of confined plasmon modes inside patterned graphene nanoribbons. The confined geometry of these ribbons leads to distinct mode patterns and strong field enhancement, both of which evolve systematically with the ribbon width and excitation laser frequency. In addition, broadband nano-imaging in a wide mid-infrared region allowed us to evaluate in real space the effect of the plasmon-phonon coupling. Our data and modeling show that the plasmon damping rate increases significantly when approaching the substrate phonon. Furthermore, we observed one-dimensional edge plasmons that propagate strictly along the edges of our patterned graphene nanostructures. These edge modes appear to have a relatively shorter wavelength compared to two-dimensional plasmons.

**3:06PM H26.00004 Resonantly Enhanced Nonlinear Response of Graphene Plasmons**, MOHAMMAD M. JADIDI, Univ of Maryland-College Park, JACOB KNIG-OTTO, STEPHAN WINNERL, Helmholtz-Zentrum Dresden-Rossendorf, Germany, ANDREI B. SUSHKOV, H. DENNIS DREW, THOMAS E. MURPHY, MARTIN MITTENDORFF, Univ of Maryland-College Park — Sub-wavelength graphene structures support plasmonic resonances in terahertz and mid-infrared part of the spectrum. The strong field confinement at plasmon resonance significantly enhances the light-graphene interaction and can lead to a very strong nonlinear optical response. This feature of graphene plasmons can enable nonlinear optics with low field intensity in miniaturized sub-wavelength devices. However, to date, the nonlinear response of graphene plasmons and their energy loss dynamics have not been studied experimentally. Here we present an experimental and theoretical study of the nonlinear terahertz response of plasmon resonances and their energy relaxation dynamics in graphene nanoribbons. Using THz pump-THz probe measurements at the plasmon frequency (9.4 THz), we observe a strong saturation of plasmon absorption followed by a 10 ps relaxation time. The observed nonlinearity is found to be significantly higher than that of graphene with no plasmon resonance. We further present a thermal model for nonlinear plasmonic absorption in graphene nanoribbons that supports the experimental results.

**3:18PM H26.00005 Fluorescence Intermittency and Nanodot Evolution in Graphene Oxide<sup>1</sup>**, ANTHONY RUTH, Univ of Notre Dame, HAYASHI MICHITOSHI, National Taiwan University, MATTHEW MCDONALD, JIXIN SI, YURI MOROZOV, Univ of Notre Dame, PETER ZAPOL, Argonne National Laboratory, MASARU KUNO, BOLDIZSAR JANKO, Univ of Notre Dame — In recent experiments, micron-sized reduced graphene oxide (rGO) flakes were observed to exhibit strong photoluminescence intensity fluctuations, or blinking. Although blinking has been observed in a wide variety of nanoscale emitters, and striking universalities exist across these very different systems, rGO is the first quasi-two dimensional emitter that shows blinking. Despite the widespread presence of blinking at nanoscale, a microscopic mechanism behind this phenomenon remains elusive. Here we provide density functional theory results, analytical calculations, and Monte Carlo simulations to connect the fluorescence trajectories observed in the experiment to microscopic processes. Through Monte Carlo simulations of chemical processes occurring on the graphene oxide surface, we observe the formation and destruction of carbon nanodots. Finally, we use emission characteristics of carbon nanodots from Ab Initio methods to reconstruct the photoluminescence of the macroscopic flake. In particular, we are investigating whether fluorescence intermittency in reduced graphene oxide is an intrinsic optoelectronic property of the nanodot constituents or the result of reversible chemical processes capable of changing the size and number of graphene nanodots.

<sup>1</sup>This work was supported by a NASA Space Technology Research Fellowship

**3:30PM H26.00006 Heterogeneous fluorescence intermittency in single layer reduced graphene oxide<sup>1</sup>**, JIXIN SI, Univ of Notre Dame, SANDOR VOLKAN-KACSO, California Institute of Technology, AHMED ELTOM, Oliver Wyman, YURII MOROZOV, Univ of Notre Dame, MATTHEW P. MCDONALD, Max Planck Institute for the Science of Light, ANTHONY RUTH, MASARU KUNO, BOLDIZSAR JANKO, Univ of Notre Dame — Fluorescence intermittency, or blinking, has been observed in a wide range of systems, including quantum dots, nanorods, and nanowires. Striking similarities have been documented in the optical response of these nanoscale emitters. However, the mechanism behind blinking still remains elusive. For the first time, blinking has been observed in a two-dimensional system in recent experiments on reduced graphene oxide (rGO). Here we reveal the power spectral density (PSD) of the blinking in rGO shares the same 1/f-like behavior of previously known blinking systems; meanwhile, the heterogeneous dynamic evolution and spatial correlation make rGO a unique blinking system. To investigate the origin of blinking, we self-consistently explain the evolution of rGO blinking using the phenomenological multiple recombination center (MRC) model that captures common features of nanoscale blinking. Furthermore, tight binding method and ab-initio method calculations of carbon nanodots are utilized to look for the microscopic structure corresponding to the RCs in the MRC model.

<sup>1</sup>M. K. thanks the American Chemical Society Petroleum Research Fund, the Army Research Office (W911NF-12-1-0578) for support. B.J. was supported in part by the U. S. DOE, Office of Science, Office of Basic Energy Sciences, under contract W-31-109-Eng-38.

**3:42PM H26.00007 Photoemission from Graphene on Copper and Cesium Antimonide: Theory and Experiment<sup>1</sup>**, DANIEL FINKENSTADT, US Naval Academy, KEVIN L. JENSEN, SAMUEL G. LAMBRAKOS, US Naval Research Laboratory, ANDREW SHABAEV, George Mason University, NATHAN A. MOODY, Los Alamos National Laboratory — The work function is calculated using DFT for a substrate of flat copper on which a single layer of graphene is deposited. These calculations show a reduced work function, compared to bare copper, when graphene is deposited on a cathode. Based on our DFT-calculated results, a simple model using the transfer matrix approach gives the transmission probability near and above the barrier maximum. An important element of our model is the DFT-calculated, macroscopically-averaged electrostatic potential. Using this potential, graphene behaves as a resonant well for electrons transmitted between the substrate and vacuum regions. Another system to be discussed is graphene atop cesium antimonide, which has very low work function making it technologically useful, in particular for the development of an x-ray free electron laser. On cesium antimonide, we examine whether graphene may allow for the retention of an underlying cesium layer that is often damaged in high-field applications. A discussion of these results in light of recent experimental characterization at LANL will be given.

<sup>1</sup>Funding and support provide by ONR and DOE.

**3:54PM H26.00008 Optical properties of graphene nanoribbons<sup>1</sup>**, FARHAD KARIMI, IRENA KNEZEVIC, Univ of Wisconsin, Madison — We calculate the dielectric function and optical conductivity of ultra-narrow armchair graphene nanoribbons (AGNRs) and zigzag graphene nanoribbons (ZGNRs) by a self-consistent-field approach within a Markovian master-equation formalism (SCF-MMEF) coupled with full-wave electromagnetic equations. Based on third-nearest-neighbor tight-binding, with appropriate modifications for AGNRs and ZGNRs, we calculate electron dispersions and Bloch wave functions in excellent agreement with the local spin-density approximation (LSDA) results. A generalized Markovian master equation of the Lindblad form, which maintains the positivity of the density matrix, is derived to describe the interaction of the electronic system with an external electromagnetic field (to first order) and with a dissipative environment (to second order). Not only does the SCF-MMEF capture the interband electron-hole-pair generation, but it also accurately accounts for concurrent interband and intraband electron scattering with phonons and impurities. We employ the SCF-MMEF to calculate the dielectric function, complex conductivity, and loss function for both suspended and supported AGNRs and ZGNRs with different widths. Then, we obtain the plasmon dispersion and propagation length from the loss-function maximum.

<sup>1</sup>Support by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-SC0008712

**4:06PM H26.00009 Thermally managed *f*s Z-scan methods investigation of the size-dependent nonlinearity of Graphene Oxide in different solvents**, PAUL BURKINS, ISAAC BASALDUA, ROBINSON KUIS, ANTHONY JOHNSON, University of Maryland, Baltimore County, SIVA RAM SWAMINATHAN, DAIJE ZHANG, SUDHIR TRIVEDI, Brimrose Corporation, UNIVERSITY OF MARYLAND, BALTIMORE MARYLAND TEAM, BRIMROSE CORPORATION OF AMERICA COLLABORATION — Acoustic and thermal diffusion effects are often ignored in Z-scan measurements resulting in misinterpretation of the nonlinear index of refraction and nonlinear absorption. Thermally managed Z-scan using a modified chopper was compared to utilizing a pulsepicker with the common calibration material CS<sub>2</sub> and then extended to Graphene Oxide (GO) in different solvents. The chopper reveals properties of the material in time and is an inexpensive alternative to changing the repetition rate with a pulsepicker. The pulsepicker allows for much faster rise-times and therefore measurements can be taken before thermal effects have overwhelmed the nonlinear electronic response. GO in DI water using pulsepicked *f*s laser excitation yielded a value of  $(-1.79 \pm .6) \times 10^{-15} \text{ cm}^2/\text{W}$  for nanometer particles and  $(-1.09 \pm .6) \times 10^{-15} \text{ cm}^2/\text{W}$  for micrometer sized particles. Open aperture Z-scan of GO in THF using the modified chopper shows a flip from reverse saturable absorption to saturable absorption in time, previously shown to be intensity dependent, potentially resulting from thermal effects. Both measurements indicate smaller particles have larger negative nonlinearities originating from thermal effects or from defects in lattice structure at the edges.

**4:18PM H26.00010 Infrared spectroscopy of vertical heterostructures of graphene and hexagonal boron nitride<sup>1</sup>**, MARCIN MUCHA-KRUCZYŃSKI, University of Bath, DAVID ABERGEL, NORDITA — We suggest that optical absorption of monolayer and bilayer graphene on hexagonal boron nitride will provide meaningful information about the moiré characteristics. In particular, study of the absorption spectrum as a function of the doping for an almost completely full first miniband will distinguish between various theoretical proposals for the physically realistic interaction. Also, for bilayer graphene, the ability to compare spectra for the opposite signs of the interlayer asymmetry induced by an external electric field might provide additional information about the moiré parameters.

<sup>1</sup>This research was funded by EPSRC Grant No. EP/L013010/1 (MM-K), and ERC project DM-321031 (DSLA),

**4:30PM H26.00011 Quantized beam shifts in graphene<sup>1</sup>**, WILTON KORT-KAMP, NIKOLAI SINITSYN, DIEGO DALVIT, Los Alamos National Laboratory — We show that the magneto-optical response of a graphene-on-substrate system in the presence of an external magnetic field strongly affects light beam shifts. In the quantum Hall regime, we predict quantized Imbert-Fedorov, Goos-Hänchen, and photonic spin Hall shifts. The Imbert-Fedorov and photonic spin Hall shifts are given in integer multiples of the fine structure constant  $\alpha$ , while the Goos-Hänchen ones in discrete multiples of  $\alpha^2$ . Due to time-reversal symmetry breaking the IF shifts change sign when the direction of the applied magnetic field is reversed, while the other shifts remain unchanged. We investigate the influence on these shifts of magnetic field, temperature, and material dispersion and dissipation. An experimental demonstration of quantized beam shifts could be achieved at terahertz frequencies for moderate values of the magnetic field.

<sup>1</sup>We acknowledge the LANL LDRD program for financial support.

**4:42PM H26.00012 Auger mediated positron sticking on graphene and highly oriented pyrolytic graphite.<sup>1</sup>**, V A CHIRAYATH, M CHRYSLER, A MCDONALD, Z LIM, K SHASTRY, R GLADEN, A FAIRCHILD, A KOYMEN, A WEISS, Univ of Texas, Arlington — Positron annihilation induced Auger electron spectroscopy (PAES) measurements on 6-8 layers graphene grown on polycrystalline copper and the measurements on a highly oriented pyrolytic graphite (HOPG) sample have indicated the presence of a bound surface state for positrons. Measurements carried out with positrons of kinetic energies lower than the electron work function for graphene or HOPG have shown emission of low energy electrons possible only through the Auger mediated positron sticking (AMPS) process. In this process the positron makes a transition from a positive energy scattering state to a bound surface state. The transition energy is coupled to a valence electron which may then have enough energy to get ejected from the sample surface. The positrons which are bound to surface state are highly localized in a direction perpendicular to surface and delocalized parallel to it which makes this process highly surface sensitive and can thus be used for characterizing graphene or graphite surfaces for open volume defects and surface impurities. The measurements have also shown an extremely large low energy tail for the C KVV Auger transition at 263eV indicative of another physical process for low energy emission.

<sup>1</sup>This work was supported by NSF grant No. DMR 1508719 and DMR 1338130

**4:54PM H26.00013 Impurity signatures in two-dimensional materials in atomic-resolution valence-electron-energy-loss spectroscopic maps.<sup>1</sup>**, MYRON KAPETANAKIS, MARK OXLEY, VANDERBILT UNIV. & ORNL, WU ZHOU, JUAN-CARLOS IDROBO, ORNL, SOKRATES PANTELIDES, VANDERBILT UNIV. & ORNL — The local atomic configurations and electronic states of impurities in 2D materials can be probed directly by several microscopy techniques. Probes of electronic excitations, however, lack spatial resolution. Here we demonstrate that valence-electron energy-loss spectroscopy in an aberration-corrected scanning transmission electron microscope yields atomic-resolution maps of electronic excitations that provide unique signatures of distinct bonding configuration impurities in 2D materials. We report simulations of the maps based on density functional theory and dynamical scattering theory, which agree with and provide direct interpretation of the observed features. The maps differentiate between different bonding configurations of impurities in graphene and hexagonal boron nitride. The theoretical analysis yields information on local electronic excitations, corresponding to impurity-induced bound, resonant and antiresonant states. The method stands to benefit from new monochromators and detectors that enhance spatial and energy resolution and constitutes a powerful alternative to optical spectroscopies for probing electronic and magnetic signatures related with impurities and defects.

<sup>1</sup>Supported by DOE grant DE-FG02-0946554 and by DOE BES MSed

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**

**Session H28 DMP: Topological Crystalline Insulators and Quantum Hall Effects.** 327 - Vidya Madhavan, University of Illinois, Urbana-Champaign

**2:30PM H28.00001 Identification of odd-parity nematic superconductivity in doped topological insulators**, LIANG FU, MIT, Physics Department — I will review our theoretical proposal [1] that  $\text{Cu}_x\text{Bi}_2\text{Se}_3$ , a doped topological insulator that becomes superconducting below  $T_c = 3.8\text{K}$ , may have an odd-parity superconducting order parameter emerging from a strongly spin-orbit-coupled band structure. I will discuss recent experimental discovery of spontaneously rotational symmetry breaking in the superconducting state of  $\text{Cu}_x\text{Bi}_2\text{Se}_3$  [2], which provides strong evidence for a two-component odd-parity order parameter leading to nematic superconductivity [3]. Our theoretical analysis shows that this nematic superconductor is stabilized by spin-orbit coupling [4], exhibits a variety of novel thermodynamic properties [5], and realizes a time-reversal-invariant topological superconductor. [1] L. Fu and E. Berg, PRL 105, 097001 (2010) [2] K. Matano, M. Kriener, K. Segawa, Y. Ando and G. Zheng, arXiv:1512.07086 [3] L. Fu, PRB, 90, 100509 (2014) [4] J. Venderbos, V. Kozii, and L. Fu, arXiv:1512.04554 [5] J. Venderbos, V. Kozii, and L. Fu, to appear

**3:06PM H28.00002 Two-dimensional Topological Crystalline Insulator Phase in Sb/Bi Planar Honeycomb with Tunable Dirac Gap**, CHIA-HSIU HSU, ZHI-QUAN HUANG, CHRISTIAN CRISOSTOMO, LIANG-ZI YAO, FENG-CHUAN CHUANG, Natl. Sun Yat-sen U., YU-TZU LIU, BAO-KAI WANG, CHUANG-HAN HSU, CHI-CHENG LEE, HSIN LIN, Natl. U. of Singapore, ARUN BANSIL, Northeastern U. — We predict planar Sb/Bi honeycomb to harbor a two-dimensional (2D) topological crystalline insulator (TCI) phase based on first-principles computations. Although buckled Sb and Bi honeycombs support 2D topological insulator (TI) phases, their structure becomes planar under tensile strain. The planar Sb/Bi honeycomb structure restores the mirror symmetry, and is shown to exhibit non-zero mirror Chern numbers, indicating that the system can host topologically protected edge states. Our computations show that the electronic spectrum of a planar Sb/Bi nanoribbon with armchair or zigzag edges contains two Dirac cones within the band gap and an even number of edge bands crossing the Fermi level. Lattice constant of the planar Sb honeycomb is found to nearly match that of hexagonal-BN. The Sb nanoribbon on hexagonal-BN exhibits gapped edge states, which we show to be tunable by an out-of-the-plane electric field, providing controllable gating of edge state important for device applications.

### 3:18PM H28.00003 Topological crystalline insulators and superconductors with order-two nonsymmorphic symmetry

KEN SHIOZAKI, Department of Physics, University of Illinois at Urbana Champaign, MASATOSHI SATO, Yukawa Institute for Theoretical Physics, Kyoto University, KIYONORI GOMI, Department of Mathematical Sciences, Shinshu University — Topological crystalline insulators (TCIs) and topological crystalline superconductors (TCSCs) are symmetry protected topological phases of free fermions with space group symmetry. Like conventional topological insulators and superconductors, TCIs and TCSCs support stable gapless boundary states associated with bulk topological nontriviality, when the additional symmetry is compatible with the boundary. Using the twisted equivariant K-theory, we complete the classification of TCIs and TCSCs in the presence of additional order-two nonsymmorphic space group (NSG) symmetry, which includes half lattice translation with  $Z_2$  spin flip, glide, two-fold screw rotation, and their magnetic symmetries. From isomorphisms connecting different space dimensions, the K-groups are evaluated by those in one-dimension. The resultant topological table shows several interesting features: (1) The NSGs allow various  $Z_2$  topological phases, even in the absence of time-reversal and/or particle-hole symmetries. Their boundary states are detached from the bulk spectrum in the direction of the non-primitive lattice translation. (2)  $Z_4$  phases are found to be realized. Especially, the TCI with the glide and the time-reversal symmetry in three-dimensions shows the  $Z_4$  phase.

### 3:30PM H28.00004 Anion-Anion Bonding and Topology in Ternary Iridium Tin Selenides<sup>1</sup>

BENJAMIN TRUMP, JAKE TUTMAHER, TYREL MCQUEEN, Johns Hopkins University — Iridium compounds have been under intense scrutiny due to strong relativistic effects (spin-orbit coupling) which have comparable energy scales to crystal field stabilization and electron correlations, which could lead to non-trivial behavior. Here we report the synthesis, characterization, and physical properties of two new, and one known, Ir-Sn-Se compounds. Resistivity, specific heat, and magnetization measurements show that all three have insulating and diamagnetic behavior, indicative of low spin  $5d^6$  Ir<sup>3+</sup>. Furthermore, electronic structures calculations on Ir<sub>2</sub>Sn<sub>3</sub>Se<sub>3</sub> show a single, spherical, non-spin-orbit split valence band that supports mobile p-type carriers, and imply that Ir<sub>2</sub>Sn<sub>3</sub>Se<sub>3</sub> is topologically non-trivial under tensile strain, due to inversion of Ir-*d* and Se-*p* states.

<sup>1</sup>Work supported by NSF, Division of Materials Research (DMR), Solid State Chemistry (SSMC), CAREER grant under Award DMR-1253562, and the ICDD Ludo Frevel Crystallography Scholarship.

### 3:42PM H28.00005 Helical Quantum Edge Gears in 2D Topological Insulators

YANG-ZHI CHOU, Rice University, ALEX LEVCHENKO, University of Wisconsin - Madison, MATTHEW FOSTER, Rice University — A remarkable and as-yet-unexploited aspect of topological insulator (TI) physics is the topology of the edge states, i.e. the fact that the edge liquid of a 2D TI forms a closed, unbreakable loop in the absence of electrical contacts or magnetic fields. We propose a novel experimental setup in which edge loops rotate as interlocking gears through Coulomb drag, in TIs with Rashba spin-orbit coupling. We show that two-terminal transport can measure the Luttinger liquid parameter  $K$ , a quantity that is otherwise notoriously difficult to measure. In the low-temperature ( $T \rightarrow 0$ ) perfect drag regime, the conductance is  $(e^2/h)(2K+1)/(K+1)$ . At higher  $T$  we predict a conductivity  $\sim T^{-4K+3}$ . Our results should trigger new experiments and may open a new venue for edge gear-based electronic devices.

Ref: Phys. Rev. Lett. 115, 186404 (2015)

### 3:54PM H28.00006 Quantum anomalous Hall effect with field-tunable Chern number near $Z_2$ topological critical point<sup>1</sup>

LE QUY DUONG, HSIN LIN, WEI-FENG TSAI, YUAN PING FENG, National University of Singapore — We study the practicability of achieving quantum anomalous Hall (QAH) effect with field-tunable Chern number in a magnetically doped, topologically trivial insulating thin film. Specifically in a candidate material, TlBi(S<sub>1- $\delta$</sub> Se <sub>$\delta$</sub> )<sub>2</sub>, we demonstrate that the QAH phases with different Chern numbers can be achieved by means of tuning the exchange field strength or the sample thickness near the  $Z_2$  topological critical point. Our physics scenario successfully reduces the necessary exchange coupling strength for a targeted Chern number. This QAH mechanism differs from the traditional QAH picture with a magnetic topological insulating thin film, where the “surface” states must involve and sometimes complicate the realization issue. Furthermore, we find that a given Chern number can also be tuned by a perpendicular electric field, which naturally occurs when a substrate is present.[1] High-Chern number QAH phase obtained from magnetically doped topological crystalline insulator thin films will also be discussed.

REF: [1] Le Quy Duong, Hsin Lin, Wei-Feng Tsai, and Y. P. Feng, Phys. Rev. B 92, 115205 (2015).

<sup>1</sup>Support by the Singapore National Research Foundation under NRF Award No. NRF-NRFF2013-03 is acknowledged.

### 4:06PM H28.00007 Zero-field Dissipationless Chiral Edge Current in Quantum Anomalous Hall State

CUI-ZU CHANG, Massachusetts Inst of Tech-MIT, WEIWEI ZHAO, DUK Y. KIM, The Center for Nanoscale Science and Department of Physics, The Pennsylvania State University, PENG WEI, Francis Bitter Magnet Lab and Physics Department, Massachusetts Institute of Technology, J. K. JAIN, CHAOXING LIU, MOSES H. W. CHAN, The Center for Nanoscale Science and Department of Physics, The Pennsylvania State University, JAGADEESH S. MOODERA, Francis Bitter Magnet Lab and Physics Department, Massachusetts Institute of Technology — The quantum anomalous Hall (QAH) state is predicted to possess, at zero magnetic field, chiral edge channels that conduct spin polarized current without dissipation, and thus holds great promise for future high-performance information processing. In this talk, we will discuss our transport experiments that probe the QAH state with gate bias and temperature dependences, by local and nonlocal magnetoresistance measurements. This allows us to unambiguously distinguish the dissipationless edge transport from transport via other dissipative channels in the QAH system. Our experiments confirm a fundamental feature of the QAH state, namely the dissipationless transport by edge channels in zero applied fields, which will be crucial for future chiral interconnected electric and spintronic applications. This research is supported by the NSF grants (DMR-1420620, Penn State MRSEC; in MIT by DMR-1207469 and the STC Center for Integrated Quantum Materials under NSF grant DMR-1231319) and by ONR Grant N00014-13-1-0301.

### 4:18PM H28.00008 Anomalous Hall Effect on the surface of topological Kondo insulators

ELIO KÖNIG, University of Wisconsin-Madison, PAVEL OSTROVSKY, Max Planck Institute for Solid State Research, Stuttgart, Germany, MAXIM DZERO, Kent State University, ALEX LEVCHENKO, University of Wisconsin-Madison — We calculate the anomalous Hall conductivity  $\sigma_{xy}$  of surface states on three dimensional topological Kondo insulators with cubic symmetry and multiple Dirac cones. We treat a generic model in which the Fermi velocity, the Fermi momentum and the Zeeman energy in different pockets may be unequal and in which the microscopic impurity potential is short ranged on the scale of the smallest Fermi wavelength. Our calculation of  $\sigma_{xy}$  to the zeroth (i.e. leading) order in impurity concentration is based on the Kubo-Smrcka-Streda diagrammatic approach. It also includes certain extrinsic contributions with a single cross of impurity lines, which are of the same order in impurity concentration and were, to the best of our knowledge, scrutinized in a single band model, only. We discuss various special cases of our result and the experimental relevance of our study in the context of recent hysteretic magnetotransport data in SmB<sub>6</sub> samples.

### 4:30PM H28.00009 Intrinsic Quantum Anomalous Hall Effect in the Kagome Lattice

Cs<sub>2</sub>LiMn<sub>3</sub>F<sub>12</sub>, GANG XU, BIAO LIAN, SHOU-CHENG ZHANG, Stanford Univ, ZHANG'S GROUP TEAM — In a kagome lattice, the time reversal symmetry can be broken by a staggered magnetic flux emerging from the ferromagnetic ordering and intrinsic spin-orbit coupling, leading to several well-separated nontrivial Chern bands and intrinsic quantum anomalous Hall effect. Based on this idea and *ab initio* calculations, we propose the realization of the intrinsic quantum anomalous Hall effect in the single layer Cs<sub>2</sub>Mn<sub>3</sub>F<sub>12</sub> kagome lattice and on the (001) surface of a Cs<sub>2</sub>LiMn<sub>3</sub>F<sub>12</sub> single crystal by modifying the carrier coverage on it, where the band gap is around 20 meV. Moreover, a simplified tight binding model based on the inplane  $dd\sigma$  antibonding states is constructed to understand the topological band structures of the system.

**4:42PM H28.00010 Giant tunneling anomalous Hall conductance in topological insulators<sup>1</sup>**, ALEX MATOS-ABIAGUE, BENEDIKT SCHARF, JONG E. HAN, State University of New York at Buffalo, EWELINA M. HANKIEWICZ, University of Würzburg, IGOR ZUTIC, State University of New York at Buffalo — We theoretically investigate the tunneling transport across a magnetic barrier modulated by a top gate potential on the surface of a three-dimensional topological insulator. In the presence of a magnetization component along the bias direction, a finite tunneling anomalous Hall conductance (TAHC), transverse to the applied bias, develops. Depending on the strengths of the magnetization and gate potential, the system can exhibit a giant anomalous Hall angle, with the TAHC exceeding the longitudinal tunneling conductance. Moreover, we predict the existence of a negative differential TAHC even when the longitudinal differential conductance remains positive.

<sup>1</sup>This work was supported by U.S. ONR Grant No. N000141310754 (A.M.-A., B.S.), DFG Grant No. SCHA 1899/1-1 (B.S.), DFG Grant No. HA 5893/4-1 within SPP 1666 (E.M.H.), and U.S. DOE, Office of Science BES, under Award DE-SC0004890 (I.Z.)

**4:54PM H28.00011 Effective boundary theory of the quantized thermal Hall effect**, RYOTA NAKAI, Tohoku University, SHINSEI RYU, University of Illinois, KENTARO NOMURA, Tohoku University — We study the effective gravitational field theory that accounts for the quantized thermal Hall effect. The effective theory is microscopically derived from the one-dimensional massless boundary fermion, which is a manifestation of the two-dimensional bulk Dirac fermion with nontrivial energy band topology. The gravitational response of the boundary effective theory explains the bulk quantized thermal Hall effect through the Stréda formula.

**5:06PM H28.00012 Quantum tunneling between Chern states in a Topological Insulator<sup>1</sup>**, MINHAO LIU, WUDI WANG, Princeton Univ, ANTHONY R. RICARDELLA, ABHINAV KANDALA, Pennsylvania State Univ, JIAN LI, ALI YAZDANI, Princeton Univ, NITIN SAMARTH, Pennsylvania State Univ, N. P. ONG, Princeton Univ — The tunneling of a macroscopic object through a barrier is a quintessentially quantum phenomenon important in field theory, low-temperature physics and quantum computing. Progress has been achieved in experiments on Josephson junctions, molecular magnets, and domain wall dynamics. However, a key feature - rapid expansion of the true vacuum triggered by a tunneling event is virtually unexplored. Here we report the detection of large jumps in the Hall resistance  $R_{xy}$  in a magnetized topological insulator which result from tunneling out of a metastable topological state. In the TI, the conducting electrons are confined to surface Dirac states. When magnetized, the TI enters the quantum anomalous Hall insulator state in which  $R_{xy}$  is strictly quantized. If the magnetic field is reversed, the sample is trapped in a metastable state. We find that, below 145 mK,  $R_{xy}$  exhibits abrupt jumps as large as one quantum unit on time-scales under 1 ms. If the temperature is raised, the escape rate is suppressed consistent with tunneling in the presence of dissipation. The jumps involve expansion of the thermodynamically stable state bubble over macroscopic lengths, but dissipation limits the final size. The results uncover novel effects of dissipation on macroscopic tunneling.

<sup>1</sup>We acknowledge support from DARPA SPAWAR (N66001-11-1-4110) and the Gordon and Betty Moore Foundations (GBMF4539).

**5:18PM H28.00013 Entanglement Spectra of Gapped One-dimensional Field Theories and Symmetry-Protected Topological Phases**, GIL YOUNG CHO, Department of Physics, Korea Advanced Institute of Science and Technology, KEN SHIOZAKI, Department of Physics, University of Illinois at Urbana-Champaign, ANDREAS LUDWIG, Department of Physics, University of California, Santa Barbara., SHINSEI RYU, Department of Physics, University of Illinois at Urbana-Champaign — We discuss the entanglement spectrum (ES) of (1+1)d gapped Lorentz invariant field theories in the vicinity of a conformal field theory (CFT). In particular, for a gapped theory obtained by perturbing a CFT in infinite space by relevant perturbations, we show that the low-lying ES for the half-line is equal to the physical spectrum of the gapless CFT defined on a finite interval of length  $L = \log(\xi/a)$ , which is the spectrum of a boundary CFT. Here  $\xi$  is the correlation length,  $a$  a microscopic lattice scale, and our result applies in the "scaling limit" where  $\xi \gg a$ . A similar property has been known to hold for Baxter's Corner Transfer Matrices of a class of very special, namely integrable lattice models, for the entire ES and independent of the scaling limit. In contrast, our result applies to completely general gapped Lorentz invariant theories in the scaling limit, without the requirement of integrability, for the low-lying ES. As a consequence, while on a finite interval of length  $2R$  the physical spectrum of the gapped theory is known to undergo a dramatic reorganization as  $2R$  crosses  $\xi$ , the bipartite ES remains unchanged up to an overall scale. We apply these to (1+1)d symmetry-protected topological phases and symmetry-protected degeneracy of ES.

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**  
**Session H29 DCMP DMP: Two-dimensional Topological Insulators: InAs/GaSb Quantum Wells and Beyond** 328 - Xiao Li, University of Maryland

**2:30PM H29.00001 Topologically nontrivial Fermi regions and their novel electromagnetic response properties**, CHING HUA LEE, Institute of High Performance Computing, Singapore, XIAO ZHANG, Sun Yat-Sen University, China — In the last decade, there has been a surge of interest in the application of topology to condensed matter physics. So far, most studies have been concerned with the novel properties that arise due to nontrivial band topology, i.e Quantum Anomalous Hall and Z2 topological insulators (TIs). In this talk, I shall describe another context where nontrivial topology also leads to interesting, measurable effects. Within the semi-classical Boltzmann approach, it can be shown that a topologically nontrivial Fermi sea region generically exhibits a non-monotonic nonlinear electromagnetic response in the limit of low chemical potential. Such topologically nontrivial regions of filled states can arise in experimentally realized TI heterostructures or materials with large Rashba splitting, i.e. BiTeI, where the Fermi sea is not simply connected. A non-monotonic electromagnetic response implies regimes of negative differential resistance, which have important applications in technologies involving microwave generation, like motion sensing and radio astronomy. We hope that nontrivial Fermi sea topology will hence provide another route for the realization of such technologies.

**2:42PM H29.00002 Response of Helical Luttinger Liquid in InAs/GaSb Edges to a Magnetic Field<sup>1</sup>**, TINGXIN LI, BINGBING TONG, XIAOXUE LIU, ZHONGDONG HAN, CHI ZHANG, ICQM, Peking University, GERARD SULLIVAN, Teledyne Scientific and Imaging, RUI-RUI DU, Rice University — Electron-electron interactions have been shown to play an important role in InAs/GaSb quantum spin Hall (QSH) edge states, leading to power-law behaviors of the helical edge conductance as a function of temperature and bias voltage (Li *et al*, Phys. Rev. Lett. **115** 136804). A variety of inelastic and/or multiparticle backscattering processes could occur in helical edges when taking electron-electron interactions into account. On the other hand, in the presence of an external magnetic field, single-particle elastic backscattering is also allowed in QSH edge due to the breaking of time-reversal symmetry (TRS). It would be interesting to pursue experimental investigations for the combined effect of electron-electron interactions and TRS breaking on QSH edge transport. We report work in progress for low temperature conductance measurements of the helical edge in InAs/GaSb under perpendicular or in-plane magnetic fields. We found that the magnetic field responses are generally correlated with the interaction strength in the edge states.

<sup>1</sup>The work at Peking University were supported by NBRPC Grants (No. 2012CB921301 and No. 2014CB920901), and by Collaborative Innovation Center of Quantum Matter.

**2:54PM H29.00003 Mapping the topological-to-normal insulator phase transition in InAs/GaSb bilayers by heterostructure variation<sup>1</sup>**, BORZOYEH SHOJAEI, Materials Department, University of California at Santa Barbara, ANTHONY P. MCFADDEN, Department of Electrical and Computer Engineering, University of California at Santa Barbara, JOON SUE LEE, California NanoSystems Institute, MIHIR PENDHARKAR, Department of Electrical and Computer Engineering, University of California at Santa Barbara, CHRIS J. PALMSTRM, Materials Department, Department of Electrical and Computer Engineering, University of California at Santa Barbara — When 2D electron and hole subbands in InAs/GaSb bilayers are tuned to the inverted regime the system is predicted to exhibit an insulating bulk and counter propagating helical 1D edge states. This work presents a dual-gate mapping of the topological-to-normal insulator phase transition for several InAs/GaSb bilayers wherein the InAs and GaSb layer thicknesses are varied. In-plane and out-of-plane magnetotransport experiments reveal the effect of heterostructure geometry on the magnitudes of the longitudinal and Hall magnetoresistances and on the shape and temperature dependence of the gate-tuned resistance map in the vicinity of the phase transition.

<sup>1</sup>This work was supported by Microsoft Research

**3:06PM H29.00004 Gate-Tuned Mott Transition in Dilute InAs/GaSb Quantum Wells**, LINGJIE DU, Department of Physics and Astronomy, Rice University, WENKAI LOU, KAI CHANG, Institute of Semiconductors, Chinese Academy of Sciences, GERARD SULLIVAN, Teledyne Scientific and Imaging, RUI-RUI DU, Department of Physics and Astronomy, Rice University — We investigate the origin of the bulk gap in inverted InAs/GaSb quantum wells (QWs) that host spatially-separated electrons and holes using charge-neutral point (CNP) density ( $n_o \sim p_o$ ) in gated devices as a tuning parameter. We find two distinct gap regimes: for I),  $n_o \gg 5 \times 10^{10}/\text{cm}^2$ , a soft gap opens predominately by hybridization, which closes under  $B_{\parallel} > 10\text{T}$ ; for II), approaching the dilute limit  $n_o \sim 5 \times 10^{10}/\text{cm}^2$ , a hard gap opens leading to a true bulk insulator with quantized helical edges, continuously for  $B_{\parallel}$  up to 35T. Our results confirm that hard gap is associated with the Quantum Spin Hall (QSH) effect but cannot be explained by single-particle band theory. Instead it originates from many-body correlations. The data are remarkably consistent with a Mott insulator bulk state in the dilute InAs/GaSb bilayers. Specifically, spontaneous exciton binding is a viable mechanism for driving the Mott transition. Our results point to the importance of charge interactions in properties of QSHE in InAs/GaSb, in addition to single-particle band theories. The work in Rice was supported by DOE (measurements) and NSF (materials).

**3:18PM H29.00005 Spin-orbit interaction in InAs/GaSb heterostructures**, FANMING QU, ARJAN J. A. BEUKMAN, FOKKO K. DE VRIES, JASPER VAN VEEN, STEVAN NADJ-PERGE, MICHAEL WIMMER, RAFAL J. SKOLASINSKI, DAVID DE VRIES, Delft University of Technology, BINH-MINH NGUYEN, WEI YI, JACOB THORP, MARKO SOKOLICH, HRL Laboratories, MICHAEL J. MANFRA, Purdue University, CHARLES M. MARCUS, University of Copenhagen, LEO P. KOUWENHOVEN, Delft University of Technology — We investigated spin-orbit interaction (SOI) in InAs/GaSb double quantum wells. A combination of dual-gating and spatially separated electron and hole gases allows for in situ engineering of the band structure. In both the trivial and inverted band alignment regimes, zero-field spin splitting due to SOI was extracted from the beating of the Shubnikov-de Haas oscillations. Deep in the electron regime, we observed anomalous magnetoresistance that points to a highly anisotropic Fermi surface as a result of the intermixing of Dresselhaus and Rashba SOI. In the inverted regime close to the hybridization gap, we obtained an oscillating spin-splitting as a function of electron density, as expected from the band structure calculation.

**3:30PM H29.00006 Electric control of inverted gap and hybridization gap in type II InAs/GaSb quantum wells**, LUN-HUI HU, Department of Physics, Zhejiang University, Hangzhou 310027, China, CHAO-XING LIU, Department of Physics, The Pennsylvania State University, University Park, Pennsylvania 16802, USA, DONG-HUI XU, Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong, China, FU-CHUN ZHANG, YI ZHOU, Department of Physics, Zhejiang University, Hangzhou 310027, China — The quantum spin Hall effect has been predicted theoretically and observed experimentally in InAs/GaSb quantum wells as a result of inverted band structures, for which electron bands in InAs layers are below heavy hole bands in GaSb layers in energy. The hybridization between electron bands and heavy hole bands leads to a hybridization gap away from  $k = 0$ . A recent puzzling observation in experiments is that when the system is tuned to more inverted regime by a gate voltage (a larger inverted gap at  $k = 0$ ), the hybridization gap decreases. Motivated by this experiment [ref. 1], we explore the dependence of hybridization gap as a function of external electric fields based on eight-band Kane model. We identify two regimes when varying electric fields: (1) both inverted and hybridization gaps increase and (2) inverted gap increases while hybridization gap decreases. We analyze the effective model and find that light-hole bands in GaSb layers play an important role in determining hybridization gap. In addition, large external electric field can induce strong Rashba splitting and also influence hybridization gap. Our results are consistent with experimental observations. Reference: [1] Lingjie Du, et.al., arXiv:1508.04509 (2015).

**3:42PM H29.00007 Image potential states in the topological semimetal Sb<sup>1</sup>**, YAU CHUEN YAM, YANG HE, PENGCHENG CHEN, ZHIHUAI ZHU, MOHAMMAD HAMIDIAN, Harvard University, MARCEL FRANZ, University of British Columbia, JENNIFER HOFFMAN, Harvard University, HOFFMAN LAB TEAM, MARCEL FRANZ COLLABORATION — Topological materials host protected surface states with locked spin and momentum degrees of freedom that have been predicted to give rise to several exotic excitations such as Majorana fermions and magnetic monopoles. The topological semimetal antimony (Sb) offers a pristine platform in which to search for these excitations. Here we present scanning tunneling microscopy and spectroscopy studies of Sb at high energy where quantized image potential states form due to the binding between the tunneling electron and the polarized surface. These states allow exploration of the image charge geometry necessary to realize a magnetic monopole.

<sup>1</sup>Acknowledge funding from the National Science Foundation DMR-1410480.

**3:54PM H29.00008 Two-Dimensional Oxide Topological Insulator With LiFeAs Structure**, QIUNAN XU, ZHIDA SONG, SIMIN NIE, HONGMING WENG, ZHONG FANG, XI DAI, Chinese Academy of Sci (CAS), KEY LABORATORY OF CONDENSED MATTER THEORY AND COMPUTATION, CHINESE ACADEMY OF SCI, T03 GROUP TEAM — Using first-principles calculations, we propose that ZrSiO can be viewed as a three-dimensional (3D) oxide weak topological insulator (TI) with  $Z_2$  invariants (0; 001). Further calculations show that the single layer of such material is a long-sought-after 2D oxide TI with a band gap around 10 meV. Furthermore, we also find that there are many other isostructural compounds, which can host similar electronic structure and form a 'WHM' material family with 'W' being Zr, Hf or La, 'H' being group IV or group V element, and 'M' being group VI one.

**4:06PM H29.00009 ab initio based tight-binding investigation of quantum spin Hall effect in InAs/GaSb quantum wells**, QUANSHENG WU, ALEXEY SOLUYANOV, MATTHIAS TROYER, ETH Zurich — Quantum spin Hall state is a topologically non-trivial quantum state, which can be used for designing various quantum devices including those potentially useful for quantum computing. Type-II InAs/GaSb semiconductor quantum well was predicted to realize this state of matter. In this work, we systematically investigate topological properties of this system using symmetrized Wannier-based tight-binding models. The model parameters are derived from first-principles hybrid functional calculations, which capture the right band gap and effective masses of both InAs and GaSb. By varying the thickness of InAs and GaSb layers, three possible phases are obtained: normal insulator, quantum spin Hall insulator, and semimetal, allowing us to optimize the growth conditions for the quantum spin Hall phase realization. Most importantly, we identify optimal growth directions, showing that a significant increase of the topological gap can be obtained by growing the quantum well in the [111]-direction. Phase diagrams are obtained for different layer thicknesses and growth directions. Effects of strain and applied electric fields are also discussed.

#### 4:18PM H29.00010 Zero bias conductance peak on the surface of topological semimetal Sb.<sup>1</sup>

PENGCHENG CHEN, Department of Physics, Harvard University; Department of Physics & Astronomy, University of British Columbia, YANG HE, Department of Physics, Harvard University, YAU CHUEN YAM, Department of Physics, Harvard University; Department of Physics & Astronomy, University of British Columbia, SHIANG FANG, Department of Physics, Harvard University, MARCEL FRANZ, Department of Physics & Astronomy, University of British Columbia, MOHAMMAD HAMIDIAN, Department of Physics, Harvard University; Department of Physics & Astronomy, University of British Columbia; LASSP, Department of Physics, Cornell U, JENNIFER HOFFMAN, Department of Physics, Harvard University; Department of Physics & Astronomy, University of British Columbia, HOFFMAN'S LAB TEAM, MARCEL FRANZ COLLABORATION, SHIANG FANG COLLABORATION — Topological materials host protected surface states with locked spin and momentum degrees of freedom that have been predicted to give rise to several exotic excitations such as Majorana fermions and magnetic monopoles. The topological semimetal antimony (Sb) offers a pristine platform in which to search for these excitations. Sb has a bilayer crystal structure; here we obtained both inter-bilayer cleaved and intra-bilayer cleaved terminations. Using scanning tunneling spectroscopy techniques, we observed a robust zero bias conductance peak on the rarer intra-bilayer cleaved surface.

<sup>1</sup>Acknowledge funding from the National Science Foundation DMR-1410480

#### 4:30PM H29.00011 Understanding Magnetic Proximity in Topological Insulators with Raman<sup>1</sup>

GAVIN OSTERHOUDT, KENNETH BURCH, Boston Coll, JAGADEESH MOODERA COLLABORATION, FERHAT KATMIS COLLABORATION — The magnetic proximity effect in Topological Insulators has been extensively studied due to predictions of quantum anomalous Hall effect and numerous applications in spintronics. Nonetheless, the origin of the proximity effect remains unclear. To uncover the role of the lattice we have used Raman scattering to investigate the magnetic proximity effect of thin film ferromagnetic insulator EuS grown by MBE on the topological insulator Bi<sub>2</sub>Se<sub>3</sub>. Through these measurements we are able to probe the magnetic fluctuations in the EuS. We will discuss the results of our measurements and their implications for the role of strain in ferromagnetic/topological insulator heterostructures.

<sup>1</sup>We gratefully acknowledge support from the National Science Foundation (Grant No. DMR-1410846)

#### 4:42PM H29.00012 Visualization of superparamagnetic dynamics in magnetic topological insulators

E. LACHMAN, Weizmann Institute of Science, A. F. YOUNG, University of California Santa Barbara, A. RICHARDELLA, The Pennsylvania State University, J. CUPPENS, N. HR, Y. ANAHORY, A. Y MELTZER, Weizmann Institute of Science, A. KANDALA, S. KEMPINGER, The Pennsylvania State University, Y. MYASOEDOV, Weizmann Institute of Science, M. E. HUBER, University of Colorado Denver, N. SAMARTH, The Pennsylvania State University, E. ZELDOV, Weizmann Institute of Science — Magnetically doped topological insulators have recently been shown to host a quantum anomalous Hall (QAH) state at low temperatures. Using scanning nanoSQUID magnetic imaging on a Cr-doped (Bi,Sb)<sub>2</sub>Te<sub>3</sub> thin film<sup>[1]</sup>, we reveal that the magnetic structure of magnetically doped topological insulators is not ferromagnetic as assumed so far. In fact it is superparamagnetic, formed by weakly interacting magnetic domains. These domains have a characteristic size of a few tens of nanometers, and undergo random reversals which drive the electronic state from one Hall plateau to the other. The superparamagnetic state is metastable, with small energy barriers to relaxation. We observe magnetic relaxation even at 300 mK, evident also in transport measurements. Unexpectedly, magnetic relaxation can also be induced by varying the gate voltage, and we propose a mechanism for the influence of the electronic phase on the magnetic relaxation. We speculate that the dynamic nature of magnetic disorder in QAH systems may contribute to the observed fragility of the QAH state at elevated temperatures. [1] Lachman *et al*, *arXiv:1506.05114*

#### 4:54PM H29.00013 1-D Modes on Step-edges of the Putative Weak Topological Insulator

BI<sub>2</sub>TeI, NURIT AVRAHAM, ANDREW NORRIS, Weizmann Atomic Scale Physics Lab / Weizmann Institute of Science, Israel, LIN PAN, SHU-CHUN WU, CLAUDIA FELSER, BINGHAI YAN, Max Planck Institute for Chemical Physics of Solids, Dresden Germany, HAIM BEIDENKOPF, Weizmann Atomic Scale Physics Lab / Weizmann Institute of Science, Israel — Weak topological insulators are layered materials that possess surfaces with an even number of Dirac cones and surfaces that are fully gapped. This inherent anisotropy provides them with unique properties such as sensitivity to the parity of the number of layers and absence of localization of their surface states. We use scanning tunneling microscopy to study the topological properties of stacked Bi<sub>2</sub>TeI, a promising candidate for weak topological insulator. We report the observation of the bulk energy gap on terraces perpendicular to the stacking direction and signatures of 1D intra-gap topological edge states along step-edges. The rich structure of quasi 2D terraces and Islands obtained on such cleaved Bi<sub>2</sub>TeI surfaces provides an excellent playground to explore some of the most fundamental concepts of TIs such as their Z<sub>2</sub> classification, “partner switching” of Kramer’s degenerate pairs, and helical modes along dislocation lines.

#### 5:06PM H29.00014 Optical conductivity of topological surface states with emergent supersymmetry<sup>1</sup>

JOSEPH MACIEJKO, University of Alberta, WILLIAM WITCZAK-KREMPA, Harvard University — Topological states of electrons present new avenues to explore the rich phenomenology of correlated quantum matter. Topological insulators (TIs) in particular offer an experimental setting to study novel quantum critical points (QCPs) of massless Dirac fermions, which exist on the samples surface. Here, we obtain exact results for the zero- and finite-temperature optical conductivity at the semimetal-superconductor QCP for these topological surface states. This strongly interacting QCP is described by a scale invariant theory with emergent supersymmetry, which is a unique symmetry mixing bosons and fermions. We show that supersymmetry implies exact relations between the optical conductivity and two otherwise unrelated properties: the shear viscosity and the entanglement entropy. We discuss experimental considerations for the observation of these signatures in TIs.

<sup>1</sup>This work was supported by NSERC, CRC, CIFAR, and the University of Alberta.

#### 5:18PM H29.00015 Proximity-induced global time-reversal symmetry (TRS) breaking and enhanced surface ferromagnetism mediated by Dirac fermions in bilayers of magnetic topological insulators (TIs)

C.-C. CHEN, M. L. TEAGUE, W. FAN, N.-C. YEH, Dept. of Physics, Caltech, Pasadena, CA 91125, L. HE, X. KOU, M. LANG, K.-L. WANG, Dept. of Elec. Eng., UCLA, Los Angeles, CA 90095 — Proximity-induced magnetic effects on the surface Dirac spectra of TIs are investigated by scanning tunneling spectroscopic (STS) studies of bilayer structures consisting of an undoped TI layer Bi<sub>2</sub>Se<sub>3</sub> and (Bi<sub>1-x</sub>Sb<sub>x</sub>)<sub>2</sub>Te<sub>3</sub> on top of a Cr-doped, magnetic TI of 6 quintuple-layer (QL) thickness.<sup>1</sup> For all samples with the top layer thinner than 4-QL, a surface gap  $\Delta$  opens up below  $T_c^{2D}$ , much higher than the bulk Curie temperature  $T_c^{3D}$  derived from the anomalous Hall resistance. The temperature ( $T$ ) evolution of  $\Delta$  shows an initial increase below  $T_c^{2D}$ , followed by a ‘dip’ near  $T_X$ , and then rises again, reaching maximum at  $T \ll T_c^{3D}$ . The gap is spatially inhomogeneous, and its average value and spatial homogeneity at low  $T$  increases with applied magnetic field  $H$  and Cr-doping level  $x$ . The appearance of massive Dirac spectra below  $T_c^{2D}$  is the result of global TRS breaking in the surface state of TIs. The non-monotonic  $T$ -dependence of  $\Delta$  and the finding of  $T_c^{2D} \gg T_c^{3D}$  may be attributed to proximity magnetism induced by a 3D contribution from the bulk magnetism that dominates at low  $T$ , and a 2D contribution from the RKKY interaction mediated by surface Dirac fermions, which dominates at  $T_c^{3D} \ll T_X < T < T_c^{2D}$  and can significantly enhance the surface magnetism due to the long wavelengths of Dirac fermions.

<sup>1</sup>C.-C. Chen et al., New J. Phys. (2015); arXiv:1506.06841

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**

**Session H30 DMP: Novel Behavior at Oxide Interfaces** 329 - Beatriz Noheda, University of Groningen

**2:30PM H30.00001 Interfaces between strongly correlated oxides : controlling charge transfer and induced magnetism by hybridization<sup>1</sup>**, MANUEL BIBES, CNRS/Thales, Univ. Paris-Saclay, Palaiseau (FRANCE) — At interfaces between conventional materials, band bending and alignment are controlled by differences in electrochemical potential. Applying this concept to oxides in which interfaces can be polar and cations may adopt a mixed valence has led to the discovery of novel two-dimensional states between simple band insulators such as  $\text{LaAlO}_3$  and  $\text{SrTiO}_3$ . However, many oxides have a more complex electronic structure, with charge, orbital and/or spin orders arising from correlations between transition metal and oxygen ions. Strong correlations thus offer a rich playground to engineer functional interfaces but their compatibility with the classical band alignment picture remains an open question. In this talk we will show that beyond differences in electron affinities and polar effects, a key parameter determining charge transfer at correlated oxide interfaces is the energy required to alter the covalence of the metal-oxygen bond. Using the perovskite nickelate ( $\text{RNiO}_3$ ) family as a template, we have probed charge reconstruction at interfaces with gadolinium titanate  $\text{GdTiO}_3$  using soft X-ray absorption spectroscopy and hard X-ray photoemission spectroscopy. We show that the charge transfer is thwarted by hybridization effects tuned by the rare-earth (R) size. Charge transfer results in an induced ferromagnetic-like state in the nickelate (observed by XMCD), exemplifying the potential of correlated interfaces to design novel phases. Further, our work clarifies strategies to engineer two-dimensional systems through the control of both doping and covalence.

<sup>1</sup>Work supported by ERC CoG MINT 615759

**3:06PM H30.00002 Electric field effect on magneto-thermopower in oxide interface  $\text{LaAlO}_3/\text{SrTiO}_3$** , TOMOYA ASABA, GANG LI, Univ of Michigan - Ann Arbor, PASCAL WITTLICH, JOCHEN MANNHART, Max Planck Institute for Solid State Research, LU LI, Univ of Michigan - Ann Arbor — Oxide interface  $\text{LaAlO}_3/\text{SrTiO}_3$  has been attracting huge interest as it shows 2-dimensional electron liquid behavior, negative compressibility and coexistence of magnetism and superconductivity. In this study we measured the magneto-thermoelectric effect and report the observation of the quantum oscillation in the thermopower. Backing gating through  $\text{SrTiO}_3$  tunes the carrier density and the oscillation pattern in the thermoelectric signal. At low carrier density, the oscillation frequency decreases when more electrons are populated, which directly indicates the negative capacitance. At high carrier density regime, both of magneto-thermopower and Nernst effect show the nonlinear behavior which suggests a Lifshitz transition. These results point to the unique multiband electronic structure of oxide interface.

**3:18PM H30.00003 Spin transport in  $\text{LaAlO}_3/\text{SrTiO}_3$  heterostructures**, THACH D. N. NGO, Korea Research Institute of Standards and Science, JUNGWON CHANG, Korea University, KYUJOON LEE, Sogang University, SEUNGJU HAN, JOONSUNG LEE, Korea University, YOUNGHEON KIM, Korea Research Institute of Standards and Science, MYUNGHWA JUNG, Sogang University, YONGJOO DOH, MAHNSOO CHOI, Korea University, JONGHYUN SONG, Chungnam National University, JINHEE KIM, Korea Research Institute of Standards and Science — Since the discovery in 2004, the 2-dimensional electron gas at the  $\text{LaAlO}_3/\text{SrTiO}_3$  heterointerfaces has attracted considerable attentions because of the fascinating physical phenomena and their strong tuneability. However, the manipulation of the spin degree of freedom in this oxide structure is still unattainable. Here, we report the spin-dependent electrical transport in hybrid magnetic tunnel junctions based on the ferromagnetism at the oxide interface. The Ohmic spin injection into the  $\text{LaAlO}_3/\text{SrTiO}_3$  heterostructure is feasible due to the insertion of an approximately thin Ti layer between the oxide and ferromagnetic metal (Co). The observed tunnel magnetoresistive effect shows such a strong anisotropy that the magnitude and even sign of the tunneling magnetoresistance ratio are dramatically modulated by a rotational, in-plane magnetic field. This is attributable to the strong Rashba-type spin-orbit coupling in the oxide structure. In addition, the spin transport is also associated with the tetragonal domain configuration of the  $\text{SrTiO}_3$  substrate. These results provide a further support for the existence of the macroscopic ferromagnetism at  $\text{LaAlO}_3/\text{SrTiO}_3$  interface.

**3:30PM H30.00004 Scanning SQUID measurements of magnetism in  $\text{LaAlO}_3/\text{SrTiO}_3$  heterostructures**, H. NOAD, E. M. SPANTON, J. A. BERT, B. KALISKY, K. C. NOWACK, C. BELL, M. KIM, Y. HIKITA, M. HOSODA, H. K. SATO, SIMES, SLAC National Laboratory, Y. XIE, Department of Applied Physics, Stanford University, P. WITTLICH, Max Planck Institute for Solid State Research, Stuttgart, H. Y. HWANG, SIMES, SLAC National Laboratory, J. MANNHART, Max Planck Institute for Solid State Research, Stuttgart, K. A. MOLER, SIMES, SLAC National Laboratory —  $\text{LaAlO}_3$  and  $\text{SrTiO}_3$  are both nonmagnetic band insulators. It is therefore surprising that signatures of magnetism in  $\text{LaAlO}_3/\text{SrTiO}_3$  heterostructures (LAO/STO) have been seen in a wide variety of experiments. Using scanning superconducting quantum interference device (SQUID) microscopy we previously found that, above a critical thickness of three unit cells of LAO, there can be heterogeneous patches of ferromagnetism. The observed ferromagnetic patches are sparse, and many samples show very few ferromagnetic patches. Scanning SQUID observations suggest that, although ferromagnetic patches can arise, the ground state of LAO/STO is not strongly ferromagnetic. In the few samples studied at millikelvin temperatures, we also observed a relatively homogeneous paramagnetic response with a  $1/T$ -like dependence, suggesting a landscape of localized spins. Theoretical proposals for the origin of magnetism in LAO/STO include intrinsic spin polarization near the interface and cation or oxygen vacancy defects. Measurements on samples with deliberately tuned oxygen content will help us to evaluate these proposals.

**3:42PM H30.00005 Correlations between magnetic and piezoelectric response at gated  $\text{LaAlO}_3/\text{SrTiO}_3$  interfaces<sup>1</sup>**, QING GUO, JIANAN LI, MENGCHEN HUANG, University of Pittsburgh, HYUNGWOO LEE, CHANG-BEOM EOM, University of Wisconsin-Madison, PATRICK IRVIN, JEREMY LEVY, University of Pittsburgh — The interface between perovskite oxide semiconductors  $\text{LaAlO}_3$  and  $\text{SrTiO}_3$  exhibits remarkable conducting, superconducting, magnetic, and spintronic properties that are strongly influenced by electron density. Scanning probe methods have the ability to probe local properties of interest. For example, magnetic force microscopy (MFM) has been used to measure magnetism at the  $\text{LaAlO}_3/\text{SrTiO}_3$  interface<sup>2</sup>, while piezoelectric force microscopy has been used to measure the local electron density<sup>3</sup>. Here we directly compare these two methods to provide further insight into the relationship between electron density and magnetic properties.

<sup>1</sup>We gratefully acknowledge support from NSF DMR-1104191 (JL, CBE), AFOSR FA9550-12-1-0057 (JL, CBE) and ONR N00014-15-1-2847

<sup>2</sup>F. Bi, *et al.*, Nat. commun. **5**, 5019 (2014); F. Bi, *et al.*, Appl. Phys. Lett.. **107**, 082402 (2015).

<sup>3</sup>M. Huang, *et al.*, APL Mater. **1**, 052110 (2013).

**3:54PM H30.00006 Magneto-optical Kerr probing of LAO/STO interface ferromagnetism<sup>1</sup>**, JIANAN LI, QING GUO, FENG BI, MENGCHEN HUANG, Univ of Pittsburgh, HYUNGWOO LEE, CHANG-BEOM EOM, Univ of Wisconsin-Madison, PATRICK IRVIN, JEREMY LEVY, Univ of Pittsburgh — Interfacial ferromagnetism in  $\text{LaAlO}_3/\text{SrTiO}_3$  (LAO/STO) heterostructures has been probed by a variety of techniques. Recently, magnetic force microscopy (MFM) was used to image ferromagnetic domains that are electrically tunable at room temperature<sup>2</sup> when the samples were grown in certain conditions. Optical techniques provide powerful tools for probing magnetic phenomena, and recently magnetic circular dichroism has been observed in reduced bulk STO crystals<sup>3</sup>. Here we describe a scanning magneto-optical Kerr imaging system that could achieve sub-micrometer precision and  $10^{-4}$  rad/ $\sqrt{\text{Hz}}$  sensitivity with a 150 fs pulsed-laser centered at 425 nm. Such capability would make pump and probe measurement on the gate-tunable LAO/STO ferromagnetism and ultrafast imaging of domain dynamics possible.

<sup>1</sup>We gratefully acknowledge support from NSF DMR-1104191 (JL, CBE), AFOSR FA9550-12-1-0057 (JL, CBE).

<sup>2</sup>F. Bi, *et al.* Nat. commun. **5**, 5019 (2014)

<sup>3</sup>W. D. Rice, *et al.* Nat. mater. **13**, 481487 (2014)

**4:06PM H30.00007 Surface chemically-switchable ultraviolet luminescence from interfacial two-dimensional electron gas**, JONATHAN E SPANIER, MOHAMMAD I ISLAM, Drexel University, DIOMEDES SALDANA-GRECO, University of Pennsylvania, ZONGQUAN GU, Drexel University, FENG GONG WANG, University of Pennsylvania, ERIC BRECKENFELD, University of Illinois at Urbana-Champaign, QINGYU LEI, Temple University, RUIJUAN XU, University of California at Berkeley, CHRISTOPHER J HAWLEY, Drexel University, XIAOXING XI, Temple University, LANE W MARTIN, University of California at Berkeley, ANDREW M RAPPE, University of Pennsylvania — We report intense, narrow-linewidth, surface chemisorption-activated and reversible ultraviolet (UV) photoluminescence from radiative recombination of the two-dimensional electron liquid with photo-excited holes at the  $\text{LaAlO}_3/\text{SrTiO}_3$  interface. The switchable luminescence arises from an electron transfer-driven modification of the electronic structure via H-chemisorption onto  $\text{AlO}_2$ -terminated  $\text{LaAlO}_3$ , at least 2 nm away from the interface. Control of the onset of emission and its intensity are functionalities that go beyond the luminescence of compound semiconductor quantum wells. Connections between reversible chemisorption, fast electron transfer, and quantum-well luminescence suggest a new model for surface chemically reconfigurable solid-state UV optoelectronics and molecular sensing. Work supported by NSF under DMR 1124696, DoE BES under DE-FG02-07ER46453, DE-FG-2-07ER15920, and DE-SC0004764, and by ONR under N00014-12-1-1033 and N00014-11-1-0664.

**4:18PM H30.00008 Ferroelectric Tunnel Junction with a Semiconductor Electrode**, XIAOHUI LIU, J.D. BURTON, EVGENY TSYMBAL, University of Nebraska-Lincoln — Realizing a large tunneling electroresistance (TER) is crucial for the application of ferroelectric tunnel junctions (FTJs) for device applications. FTJs are typically composed of a thin ferroelectric layer sandwiched by two metallic electrodes, where TER generally results from the dependence of the effective tunneling barrier height on the ferroelectric polarization. Since the resistance depends exponentially not only on barrier height but also on barrier width, TER is expected to be greatly enhanced when one of the electrodes is a semiconductor where the depletion region near the interface can be controlled via ferroelectric polarization. To explore this possibility, we perform studies on a  $\text{SrRuO}_3/\text{BaTiO}_3/n\text{-SrTiO}_3$  FTJ using first-principles density functional theory (DFT). We analyze the effect of ferroelectric polarization on the barrier width and transport properties. Our studies show that, in addition to modulation of the depletion region in  $n\text{-SrTiO}_3$ , layers in the  $\text{BaTiO}_3$  barrier near the interface become conducting for one polarization orientation leading to a large TER effect. Additional DFT+U calculations reveal that this effect is insensitive to the bandgap of the barrier, indicating that this should be a robust mechanism to realize large TER in FTJs.

**4:30PM H30.00009 Effect of epitaxial strain on tunneling electroresistance in ferroelectric tunnel junctions<sup>1</sup>**, ANDREI SOKOLOV, OHHEUM BAK, HAIDONG LU, EVGENY TSYMBAL, ALEXEI GRUVERMAN, University of Nebraska at Lincoln — We present the effect of compressive strain on the tunneling electroresistance (TER) effect in  $\text{BaTiO}_3/\text{SrRuO}_3$  (BTO/SRO) heterostructures. The films were prepared using PLD technique and characterized by XRD and RHEED methods. We performed comprehensive study of ferroelectric and transport properties of obtained structure and find that epitaxial strain imposed by the mismatch of  $\text{NdGaO}_3$  and  $\text{SrTiO}_3$  lattice parameters with the BTO and SRO layers improves ferroelectric polarization of BTO and concurrently promotes the metallicity of the SRO films. While the enhanced polarization is beneficial for the TER magnitude, the reduced asymmetry in the tunneling barrier due to the shortened screening length of SRO is detrimental for the effect. Thus, a combined effect of strain on the polarization of the ferroelectric barrier and the screening properties of the electrodes needs to be taken into account when considering and predicting the TER effect in ferroelectric tunnel junctions

<sup>1</sup>NSF MRSEC DMR-1420645, US DoE (DE-SC0004876), NSF DMR-1310542

**4:42PM H30.00010 Reversible Magnetoelectric Control of Exchange Coupling in Monodomain  $\text{BiFeO}_3$  Heterostructures<sup>1</sup>**, J IRWIN, W SAENRANG, Univ of Wisconsin, Madison, B.A. DAVIDSON, CNR-Istituto Officina dei Materiali, Trieste, Italy, J.E. PODKAMINER, KJ REIERSON, Univ of Wisconsin, Madison, F MACCHEROZZI, S DHESI, Diamond Light Source, Harwell Campus, Didcot, UK, J. W. FREELAND, Advanced Photon Source, Argonne National Laboratory, US, M.S. RZCHOWSKI, C. B. EOM, Univ of Wisconsin, Madison — The electric field control of ferromagnetism has exciting applications in spintronic devices such as magnetic tunnel junctions. We investigate reversible rotation of the magnetization of a Co overlayer on a heterostructure with a monodomain thin film of the multiferroic  $\text{BiFeO}_3$  (BFO). For different electric polarization directions of the BFO film we observe a rotation in Co magnetization direction by photoelectron emission microscopy (PEEM). This effect is robust over at least 100 cycles of the BFO electric polarization. According to anisotropic magnetoresistance (AMR) and magneto-optic Kerr effect (MOKE) measurements performed at room temperature, the easy magnetic direction for the Co layer rotates in plane when the electric polarization of the BFO is switched. Additionally, X-ray linear dichroism (XLD) measurements verify the presence of a magnetoelectric effect in the BFO and suggest magnetic coupling between the BFO and Co layers.

<sup>1</sup>This work is supported by the Army Research Office under Grant No. W911NF-10-0382

**4:54PM H30.00011 Rashba type band splittings in ferroelectric semiconductor  $\alpha\text{-GeTe}(111)$** , BEOMYOUNG KIM, HYUNGJU OH, YEONGKWAN KIM, JONATHAN DENLINGER, Lawrence Berkeley Natl Lab, CHANGYOUNG KIM, Department of Physics and Astronomy, Seoul National University, Seoul 151747, Republic of Korea — There has been significant increase in the research of spin orbit coupling (SOC) induced exotic phenomena. The Rashba effect, theoretically predicted to exist, is one of the SOC related phenomena. The phenomenon was later experimentally observed in the surface states of metals and topological insulators as well as interfaces of hetero structures that have inversion symmetry breaking (ISB). Even bulk states with intrinsic ISB such as  $\text{BiTeI}$  is found to have Rashba split bands. It was very recently proposed that ferroelectric GeTe has Rashba effect in the bulk. This is a unique situation where ISB is provided not by the structure ISB but by an electrical polarization. We have performed angle-resolved photoemission spectroscopy (ARPES) on GeTe single crystals to investigate the unique bulk Rashba state. Our results indeed show the existence of a Rashba-type band splitting as theoretically predicted. We discuss various aspect of the Rashba states in ferroelectric semiconductor  $\alpha\text{-GeTe}(111)$ .

### 5:06PM H30.00012 Effect of charge on the ferroelectric field effect in strongly correlated oxides

XUEGANG CHEN, ZHIYONG XIAO, XIAOZHE ZHANG, LE ZHANG, WEIWEI ZHAO, Department of Physics & Astronomy, University of Nebraska-Lincoln, NE 68588, XIAOSHAN XU, XIA HONG, Department of Physics & Astronomy and Nebraska Center for Materials and Nanoscience, University of Nebraska-Lincoln, NE 68588 — We present a systematic study of the effect of charge on the ferroelectric field effect modulation of various strongly correlated oxide materials. We have fabricated high quality epitaxial heterostructures composed of a ferroelectric  $\text{Pb}(\text{Zr,Ti})\text{O}_3$  (PZT) gate and a correlated oxide channel, including  $\text{Sm}_{0.5}\text{Nd}_{0.5}\text{NiO}_3$  (SNNNO),  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$  (LSMO), SNNNO/LSMO bilayers, and  $\text{NiCo}_2\text{O}_4$  (NCO). The Hall effect measurements reveal a carrier density of  $\sim 4$  holes/u.c. ( $0.4 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ ) for SNNNO to  $\sim 2$  holes/u.c. ( $27 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ ) for NCO. We find the magnitude of the field effect is closely related to both the intrinsic carrier density and carrier mobility of the channel material. For devices employing the SNNNO/LSMO bilayer channel, we believe the charge transfer between the two correlated oxides play an important role in the observed resistance modulation. The screening capacitor of the channel materials and the interfacial defect states also have significant impact on the retention characteristics of the field effect. Our study reveals the critical role of charge in determining the interfacial coupling between ferroelectric and magnetic oxides, and has important implications in developing ferroelectric-controlled Mott memory devices.

### 5:18PM H30.00013 Band offset measurement of oxygen annealed $\text{SrTiO}_3/\text{Si}$

ERIC JIN, LIOR KORNBLUM, CHARLES AHN, FRED WALKER, Yale Univ — Integration of the perovskite oxide  $\text{SrTiO}_3$  (STO) with silicon by molecular beam epitaxy (MBE) was initially developed for new high-K gate dielectrics, and more recently as a means to combine the multifunctional properties of oxide heterostructures with the well-established silicon platform. The band alignment at an oxide-semiconductor junction is critical in determining its electrical properties, and control over the conduction band offset is a fundamental goal of materials science. Density functional theory calculations have shown that an interface dipole forms at the STO-Si interface, with the magnitude of this dipole determined by the exact composition of the interface. If the interface is oxygen deficient, the band alignment is type II. If the interface is modified via the addition of a monolayer of oxygen atoms, the predicted heterojunction becomes type-I. We characterize the band alignment of MBE-grown STO-Si films by x-ray photoemission spectroscopy and show that the conduction band offset is negative between STO and Si. We demonstrate an experimental  $\sim 0.5$  eV increase in the conduction band offset for in-situ oxygen-annealed films, in close agreement with theoretical predictions. By careful control of the interface atomic structure, we show an approach toward tuning the band offset of the STO-Si system to modify electronic transport for a variety of device applications.

## Tuesday, March 15, 2016 2:30PM - 5:30PM –

Session H31 DCP: Advances in Density Functional Theory IV 331 - Adam Wasserman, Purdue University

### 2:30PM H31.00001 Extensions of time density functional theory to QED: QED-Chemistry

ANGEL RUBIO, Max Planck Institute for the Structure and Dynamics of Matter — In this talk we will review the recent advances within density-functional and many-body based schemes to describe spectroscopic properties of complex systems with special emphasis to modelling time and spatially resolved electron spectroscopies. We will discuss the theoretical approaches developed in the group for the characterisation of matter out of equilibrium, the control material processes at the electronic level and tailor material properties, and master energy and information on the nanoscale to propose new devices with capabilities. We will focus on examples linked to the efficient conversion of light into electricity or chemical fuels ("artificial photosynthesis") and the design on new nanostructured based optoelectronic devices based on inorganic nanotubes, among others. The goal is to provide a detailed, efficient, and at the same time accurate microscopic approach for the ab-initio description and control of the dynamics of decoherence and dissipation in quantum many-body systems. With the help of quantum optimal control (QOC) theory and the mastery over spectroscopy we could direct the movement of electrons, selectively trigger chemical reactions and processes, and create new materials

### 3:06PM H31.00002 Advances in time-dependent current-density functional theory<sup>1</sup>

ARJAN BERGER, University of Toulouse III - Paul Sabatier — In this work we solve the problem of the gauge dependence of molecular magnetic properties (magnetizabilities, circular dichroism) using time-dependent current-density functional theory [1]. We also present a new functional that accurately describes the optical absorption spectra of insulators, semiconductors and metals [2]

N. Raimbault, P.L. de Boeij, P. Romaniello, and J.A. Berger Phys. Rev. Lett. 114, 066404 (2015)

J.A. Berger, Phys. Rev. Lett. 115, 137402 (2015)

<sup>1</sup>This study has been partially supported through the Grant NEXT No. ANR-10-LABX-0037 in the framework of the Programme des Investissements d'Avenir.

### 3:18PM H31.00003 The particle-particle random phase approximation and beyond – insight from the superconductive Gorkov perspective and implications of an efficient truncation scheme

DU ZHANG, WEITAO YANG, Duke University, WEITAO YANG GROUP TEAM — As an excited-state electronic structure method, the particle-particle random phase approximation (ppRPA) satisfactorily resolves many challenges for the time-dependent density functional theory (TDDFT)/particle-hole (ph) RPA, e.g. absence of double excitations, diradicals, singlet-to-triplet instability, etc. Given that the ppRPA equation has been derived from the pairing potential linear response, we derive it using the propagator approach using the superconductive Gorkov formalism. Systematic higher-order contributions are added to the ppRPA, yielding the pp Bethe-Salpeter equation (BSE). This development can be combined with our recently proposed truncation scheme, which makes typical ppRPA calculations up to 100 times faster than the Davidson's algorithm. Since the electron correlation is important in yielding good excitation energies for the ppRPA (the superiority of DFT reference states over Hartree-Fock ones, esp. for large systems), combining the two developments allows us to add the electron correlation into the ppRPA calculation at a modest formal scaling of  $O(N^4)$ , pushing the excitation energy calculations towards both larger systems and higher accuracy.

### 3:30PM H31.00004 Calculating excitation energies with particle-particle and particle-hole random phase approximation using accurate optimized effective potentials

YE JIN, YANG YANG, DEGAO PENG, WEITAO YANG, Duke University — With an accurate electron density, one can calculate the optimized effective potential (OEP) which gives Kohn-Sham energies and eigenvectors accurately. Such Kohn-Sham energies and eigenvectors are developed here for applications in excited state calculations. In this work, Kohn-Sham results from OEP with an accurate input electron density, i.e. CCSD density, are used in excitation energy calculations, within the particle-particle and particle-hole random phase approximation (pp-, ph-RPA). Tests on small molecules, for example, BH and  $\text{CH}^+$ , matches well with the EOM-CCSD calculation for low energy excited states. For  $\text{N}_2$ , CO and  $\text{H}_2\text{O}$ , our method describes the lower excitations well compared with the experimental data and improves the results from pp- and ph-RPA based on approximate density functional approximations. This approach is thus promising for applications in calculating accurate excitation energies.

**3:42PM H31.00005 Singlet–Triplet Energy Gaps for Diradicals from Particle–Particle Random Phase Approximation**, YANG YANG, DEGAO PENG, Duke Univ, ERNEST DAVIDSON, University of Washington, WEITAO YANG, Duke Univ — The particle–particle random phase approximation (pp-RPA) has been applied to the calculation of vertical and adiabatic singlet–triplet energy gaps for a variety of categories of diradicals, including diatomic diradicals, carbene-like diradicals, disjoint diradicals, four- $\pi$ -electron diradicals, and benzynes are calculated. Except for some excitations in four- $\pi$ -electron diradicals, where four-electron correlation may play an important role, the singlet–triplet gaps are generally well predicted by pp-RPA. With a relatively low  $O(r^4)$  scaling, the pp-RPA with DFT references outperforms spin-flip configuration interaction singles. It is similar to or better than the (variational) fractional-spin method. For small diradicals such as diatomic and carbene-like ones, the error of pp-RPA is slightly larger than noncollinear spin-flip time-dependent density functional theory (NC-SF-TDDFT) with LDA or PBE functional. However, for disjoint diradicals and benzynes, the pp-RPA performs much better and is comparable to NC-SF-TDDFT with long-range corrected  $\omega$ PBEh functional and spin-flip configuration interaction singles with perturbative doubles (SF-CIS(D)). In particular, with a correct asymptotic behavior and being almost free from static correlation error, the pp-RPA with DFT references can well describe the challenging ground state and charge transfer excitations of disjoint diradicals in which almost all other DFT-based methods fail. Therefore, the pp-RPA could be a promising theoretical method for general diradical problems.

**3:54PM H31.00006 Thermal connection formula and linear response time-dependent density functional theory for thermal ensembles**, AURORA PRIBRAM-JONES, Lawrence Livermore National Lab and Department of Chemistry, University of California, Berkeley, PAUL GRABOWSKI, Department of Chemistry, University of California, Irvine, KIERON BURKE, Departments of Physics and Chemistry, University of California, Irvine — The finite-temperature adiabatic connection formula is cast as an integral over the temperature and used to write new relations between correlation components in terms of temperature and the coupling constant. Next, the van Leeuwen proof of time-dependent density functional theory is generalized to thermal ensembles, along with the Gross-Kohn relation and the fluctuation-dissipation theorem. These results are combined with the thermal connection formula to produce a method for generating new exchange-correlation approximations.

**4:06PM H31.00007 Solid-state optical absorption from optimally tuned time-dependent range-separated hybrid density functional theory<sup>1</sup>**, SIVAN REFAELY-ABRAMSON, Molecular Foundry, LBNL and Dept. of Physics, UC-Berkeley, MANISH JAIN, Dept. of Physics, IISc, Bangalore, India, SAHAR SHARIFZADEH, Dept. of Electrical and Computer Engineering and Physics Division of MSE, Boston University, JEFFREY B. NEATON, Molecular Foundry, LBNL, Dept. of Physics, UC-Berkeley and Kavli ESNi at Berkeley, LEEOR KRONIK, Dept. of Materials and Interfaces, Weizmann Institute — We present a framework for obtaining solid-state charge and optical excitations and spectra from optimally tuned range-separated hybrid density functional theory, which allows for the accurate prediction of exciton binding energies. We demonstrate our approach through calculations of one- and two-particle excitations in pentacene, a molecular semiconducting crystal, where we find excellent agreement with experiments and prior computations. We show that with one adjustable parameter, our method accurately predicts band structures and optical spectra of Si and LiF, prototypical covalent and ionic solids. For a range of extended bulk systems, this method may provide a computationally inexpensive alternative to many-body perturbation theory, opening the door to studies of materials of increasing size and complexity [Phys. Rev. B 92, 081204(R), 2015].

<sup>1</sup>This work was supported by DOE

**4:18PM H31.00008 Exploring Level Alignment in Molecule-Metal Interfaces with Optimally-Tuned Range-Separated Hybrid Functionals**, ZHENFEI LIU, Lawrence Berkeley National Lab, DAVID A. EGGER, Weizmann Institute of Science, SIVAN REFAELY-ABRAMSON, Lawrence Berkeley National Lab, LEEOR KRONIK, Weizmann Institute of Science, JEFFREY B. NEATON, Lawrence Berkeley National Lab — Molecule-metal interfaces are ubiquitous in nanoscale functional materials and energy related applications. Characterizing the electronic structure at molecule-metal interfaces, especially the level alignment between molecular frontier orbitals and the Fermi level of the combined system, is crucial for understanding charge dynamics. Density functional theory (DFT) has been successful in computing binding geometries and adsorption energies, but much less successful in predicting level alignment. This is because the latter depends on quasiparticle excitation energies, typically believed to be outside the reach of DFT. In this work, we apply the recently developed optimally-tuned range-separated hybrid functional to the electronic structure of a model molecule-metal interface - benzene on graphite - and elucidate parameters leading to agreement with experiment and with many-body perturbation theory.

**4:30PM H31.00009 Chemically accurate description of aromatic rings interaction using quantum Monte Carlo**, SAM AZADI, Department of Physics and Thomas Young Centre, University College London — We present an accurate study of interactions between benzene molecules using wave function based quantum Monte Carlo (QMC) methods [1]. We compare our QMC results with density functional theory (DFT) using various van der Waals (vdW) functionals. This comparison enables us to tune vdW functionals. We show that highly optimizing the wave function and introducing more dynamical correlation into the wave function are crucial to calculate the weak chemical binding energy between benzene molecules. The good agreement among our results, experiments and quantum chemistry methods, is an important sign of the capability of the wave function based QMC methods to provide accurate description of very weak intermolecular interactions based on vdW dispersive forces. [References:1] Sam Azadi, and R. E. Cohen, J. Chem. Phys. **143**, 104301 (2015).

**4:42PM H31.00010 Study of a Quantum Dot in an Excited State**, MARLINA SLAMET, Sacred Heart University, VIRAH T SAHNI, CUNY-Brooklyn Coll — We have studied the first excited singlet state of a quantum dot via quantum density functional theory (QDFT). The quantum dot is represented by a 2D Hooke's atom in an external magnetostatic field. The QDFT mapping is from an excited singlet state of this interacting system to one of noninteracting fermions in a singlet ground state. The results of the study will be compared to (a) the corresponding mapping<sup>1</sup> from a ground state of the quantum dot and (b) to the similar mapping<sup>2</sup> from an excited singlet state of the 3D Hooke's atom. <sup>1</sup> T. Yang, X.-Y. Pan, and V. Sahni, PRA **83**, 042518 (2011) <sup>2</sup> M. Slamet and V. Sahni, IJQC **85**, 436 (2001)

**4:54PM H31.00011 First-principles photoemission spectroscopy in DNA and RNA nucleobases from Koopmans-compliant functionals**, NGOC LINH NGUYEN, Theory and Simulations of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), EPFL, GIOVANNI BORGHI, ANDREA FERRETTI, Centro S3, CNR-Istituto Nanoscienze, 41125 Modena, Italy, NICOLA MARZARI, Theory and Simulations of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), EPFL — The determination of spectral properties of the DNA and RNA nucleobases from first principles can provide theoretical interpretation for experimental data, but requires complex electronic-structure formulations that fall outside the domain of applicability of common approaches such as density-functional theory. In this work, we show that Koopmans-compliant functionals [1], constructed to enforce piecewise linearity in energy functionals with respect to fractional occupation-i.e., with respect to charged excitations-can predict not only frontier ionization potentials and electron affinities of the nucleobases with accuracy comparable or superior with that of many-body perturbation theory and high-accuracy quantum chemistry methods, but also the molecular photoemission spectra are shown to be in excellent agreement with experimental ultraviolet photoemission spectroscopy data. The results highlight the role of Koopmans-compliant functionals as accurate and inexpensive quasiparticle approximations to the spectral potential, which transform DFT into a novel dynamical formalism where electronic properties, and not only total energies, can be correctly accounted for. Reference [1] N.L. Nguyen et al., PRL (2015).

**5:06PM H31.00012 van der Waals Density Functional Theory vdW-DFq for Semihard Materials<sup>1</sup>**, QING PENG, SUVVANU DE, Rensselaer Polytechnic Institute — There are a large number of materials with mild stiffness, which are not as soft as tissues and not as strong as metals. These semihard materials includes energetic materials, molecular crystals, layered materials, and van der Waals crystals. The integrity and mechanical stability are mainly determined by the interactions between instantaneously induced dipoles, the so called London dispersion force or van der Waals force. It is challenging to accurately model the structural and mechanical properties of these semihard materials in the frame of density functional theory where the non-local correlation functionals are not well known. Here we propose a van der Waals density functional named *vdW-DFq* to accurately model the density and geometry of semihard materials. Using  $\beta$ -cyclotetramethylene tetranitramine as a prototype, we adjust the enhancement factor of the exchange energy functional with generalized gradient approximations. We find this method to be simple and robust over a wide tuning range when calibrating the functional on-demand with experimental data. With a calibrated value  $q = 1.05$ , the proposed *vdW-DFq* method shows good performance in predicting the geometries of 11 common energetic material molecular crystals and 3 typical layered van der Waals crystals.

<sup>1</sup>The authors would like to acknowledge the generous financial support from the Defense Threat Reduction Agency (DTRA) Grant HDTRA1-13-1-0025

**5:18PM H31.00013 A non-empirical, parameter-free, hybrid functional for accurate calculations of optoelectronic properties of finite systems<sup>1</sup>**, NICHOLAS BRAWAND, Institute for Molecular Engineering, University of Chicago, MÁRTON VÖRÖS, Materials Science Division, Argonne National Laboratory and Institute for Molecular Engineering, University of Chicago, MARCO GOVONI, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago — The accurate prediction of optoelectronic properties of molecules and solids is a persisting challenge for current density functional theory (DFT) based methods. We propose a hybrid functional where the mixing fraction of exact and local exchange is determined by a non-empirical, system dependent function. This functional yields ionization potentials, fundamental and optical gaps of many, diverse systems in excellent agreement with experiments, including organic and inorganic molecules and nanocrystals. We further demonstrate that the newly defined hybrid functional gives the correct alignment between the energy level of the exemplary TTF-TCNQ donor-acceptor system.

<sup>1</sup>DOE-BES: DE-FG02-06ER46262

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**  
**Session H32 DCP: Theoretical Modeling of Materials for Solar Energy Conversion** 332 - Giulia Galli, University of Chicago

**2:30PM H32.00001 Predicting materials for solar energy conversion: ab-initio spectroscopy of heterogeneous interfaces**, GIULIA GALLI, University of Chicago — We will discuss some progress in predicting materials for solar energy conversion using ab initio calculations, in particular we will focus on heterogeneous interfaces between photo-electrodes and water and between nanocomposites. We will also address the problem of building much needed tighter connections between computational and laboratory experiments.

**3:06PM H32.00002 Ultrafast carrier dynamics in BiVO<sub>4</sub> thin film photoanode material: time-resolved THz spectroscopic study.**, WESLEY BELLEMAN, Department of Physics, Worcester Polytechnic Institute, L. ZHOU, B. GIRI, Department of Mechanical Engineering, Worcester Polytechnic Institute, B.J. DRINGOLI, Department of Physics, Worcester Polytechnic Institute, P.M. RAO, Department of Mechanical Engineering, Worcester Polytechnic Institute, L.V. TITOVA, Department of Physics, Worcester Polytechnic Institute — Recent demonstrations of 3% solar conversion efficiency in thin film BiVO<sub>4</sub> make it a promising photoanode material for photoelectrochemical water oxidation [1]. With a bandgap of 2.4 eV, it strongly absorbs UV and visible light up to 520 nm. However, its efficiency is limited by extremely poor carrier mobility, with values from 0.01 to 1 cm<sup>2</sup>/Vs reported in the literature, and often attributed to formation of small polarons [2]. The precise nature of conductivity in BiVO<sub>4</sub> is, however, not well-established. We use time-resolved terahertz (THz) spectroscopy as a non-contact probe of microscopic photoconductivity of a 100 nm-thick BiVO<sub>4</sub> film. THz spectroscopy allows probing the dynamics of photo-injected carriers over nanometer length scales, and thus provides insight about transport of carriers inside the 100-200 nm grains. We find that intra-grain mobility may be as much as several orders of magnitude higher than macroscopic mobility that is affected by the grain boundaries. References [1] P. M. Rao et al., Nano Lett. 14, 1099 (2014) [2] A.J.E. Rettie et al., Appl. Phys. Lett. 106, 022106 (2015).

**3:18PM H32.00003 Emerging materials with novel electronic properties for solar light harvesting and conversion**, IFFAT NAYYAR, TIFFANY KASPAR, MARTIN MCBRIARTY, SARA CHAMBERLIN, NIRANJAN GOVIND, SCOTT CHAMBERS, PETER SUSHKO, Pacific Northwest National Laboratory, Richland, WA — The optical absorption and electronic transport in complex oxides can be tuned by judicious selection of the lattice structure and control of chemical composition and prevalent oxidation state of the transition metal species. Optical spectra for solid solutions of metal oxides are complex; we focus on revealing the electronic structure and orbital nature of the transitions, which is crucial for rational materials design. We applied state-of-the-art *ab initio* methods, including time-dependent DFT, to screen thermodynamically favorable configurations and determine the effects of the local environment on the transition energies and relative intensities. Here we focus on the magnetite-type Fe<sub>3-x</sub>Cr<sub>x</sub>O<sub>4</sub> mixed spinel solid-solutions, which can only be doped to  $x \leq 2$ , since Cr strongly prefers to occupy octahedral sites. In the interval of  $0 \leq x \leq 2$ , the electronic structure of Fe<sub>3-x</sub>Cr<sub>x</sub>O<sub>4</sub> undergoes transformations resulting in several qualitatively different types of optical transitions sensitive to the Cr concentration. We find the lowest band gap and high room-temperature conductivity, in agreement with experiment, for  $x=1$  (Fe<sub>2</sub>CrO<sub>4</sub>), and attribute this conductivity to the thermally-driven electron hopping between the octahedral-site Fe<sup>2+</sup> and tetrahedral-site Fe<sup>3+</sup>. We compare Fe<sub>3-x</sub>Cr<sub>x</sub>O<sub>4</sub> with the corundum  $\alpha$ -(Fe<sub>1-x</sub>Cr<sub>x</sub>)<sub>2</sub>O<sub>3</sub> and  $\alpha$ -(Fe<sub>1-x</sub>V<sub>x</sub>)<sub>2</sub>O<sub>3</sub>, where electron transfer from the Cr and V 3d to the unoccupied Fe 3d\* orbitals reduces the band gap to 1.6 and 0.6 eV (from 2.1 eV in  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>).

**3:30PM H32.00004 New quaternary semiconductor Cu<sub>2</sub>MgSnS<sub>4</sub> and Cu<sub>2</sub>MgSnSe<sub>4</sub> for photovoltaics<sup>1</sup>**, KINFAL TSE, Chinese Univ of Hong Kong, GUOHUA ZHONG, Chinese Academy of Sciences, Shenzhen, YIYOU ZHANG, Chinese Univ of Hong Kong, XIAO GUANG LI, CHUNLEI YANG, Chinese Academy of Sciences, Shenzhen, JUNYI ZHU, Chinese Univ of Hong Kong, ZHI ZENG, Chinese Academy of Sciences, Hefei, ZHENYU ZHANG, University of Science and Technology of China, Hefei, XUDONG XIAO, Chinese Univ of Hong Kong — Element substitution of Zn by Mg and Ca is attempted to overcome the problem of potential fluctuation in Cu<sub>2</sub>ZnSnS<sub>4</sub> and Cu<sub>2</sub>ZnSnSe<sub>4</sub> (CZTSs) due to prevalence of Cu<sub>Zn</sub>+Zn<sub>Cu</sub> defect complex. Through density function theory calculation with hybrid functional, we have shown that Cu<sub>2</sub>MgSnS<sub>4</sub> and Cu<sub>2</sub>MgSnSe<sub>4</sub> (CMTSs) are stable with respect to secondary phases considered under suitable chemical potential. Stannite CMTSs is thermodynamically more favorable over the kesterite structure. The alternating Cu and Mg/Sn cation layer of stannite structure may suppress the formation of Mg<sub>Cu</sub> antisite due to large stress induced. The electronic and optical properties of CMTSs are similar to that of CZTSs with comparable absorption coefficient at the band-edge suggests CMTSs to be a promising photovoltaic material.

<sup>1</sup>The work was supported by the National Major Science Research Program of China under Grant no. 2012CB933700, the Natural Science Foundation of China (Grant nos. 61274093, 61574157, 11274335, 11504398, 51302303, and 51474132), and the Shenzhen Basic Research

**3:42PM H32.00005 Controlling defects and secondary phases of CZTS by surfactant Potassium<sup>1</sup>**, JUNYI ZHU, YIOU ZHANG, KINFAT TSE, XUDONG XIAO, Department of Physics, Chinese University of Hong Kong — Cu<sub>2</sub>ZnSnS<sub>4</sub> (CZTS) is a promising photovoltaic absorber material with earth abundant and nontoxic elements. However, the detrimental native defects and secondary phases of CZTS will largely reduce the energy conversion efficiencies. To understand the origin of these problems during the growth of CZTS, we investigated the kinetic processes on CZTS (-1-1-2) surface, using first principles calculations. A surface Zn atom was found to occupy the subsurface Cu site easily due to a low reaction barrier, which may lead to a high ZnCu concentration and a secondary phase of ZnS. These n-type defects may create deep electron traps near the interface and become detrimental to device performance. To reduce the population of ZnCu and the secondary phase, we propose to use K as a surfactant to alter surface kinetic processes. Improvements on crystal quality and device performance based on this surfactant are consistent with early experimental observations.

<sup>1</sup>Computing resources were provided by the High Performance Cluster Computing Centre, Hong Kong Baptist University. This work was supported by the start-up funding at CUHK.

**3:54PM H32.00006 Metal Disorder in Cu<sub>2</sub>ZnSnS<sub>4</sub> (CZTS) Solar Cells from Multi-Scale Simulations**, SUZANNE WALLACE, JARVIST FROST, ARON WALSH, University of Bath — Kesterite-structured Cu<sub>2</sub>ZnSnS<sub>4</sub> (CZTS) is a promising earth-abundant and non-toxic material for the active layer of thin-film solar cells due to its high optical absorption coefficient of  $> 10^4 \text{ cm}^{-1}$  and sunlight matched band gap of 1.5 eV. Device efficiencies are hampered by low open circuit voltage ( $V_{OC}$ ) compared to the optical band gap. One possible origin of this is disorder amongst the Cu and Zn ions. Such disorder could lead to sub band-gap recombination centres due to fluctuations in electrostatic potential from the presence of charged defects. Understanding the origin of these sub-gap states, and the resulting impediment on device performance, is essential to discover design and processing rules for high efficiency kesterite, and other multi-component semiconductor, devices. We investigate this by writing custom Monte-Carlo codes to simulate the on-lattice disorder. A generalised Ising Hamiltonian is parameterised with hybrid density functional theory (DFT) total-energy calculations on defect pairs. The resulting disorder is simulated as a function of temperature, and the order-disorder behaviour and resulting local and long-range electrostatic potential variation due to Cu-Zn disorder is quantified.

**4:06PM H32.00007 First principles investigations on the stability and catalytic reactivity of Cu<sub>2</sub>O surfaces**, LIANG LI, YIMIN WU, TIJANA RAJH, IAN MCNULTY, ZHONGHOU CAI, JEFF GUEST, YUZI LIU, MARIA CHAN, Argonne National Laboratory — Cu<sub>2</sub>O is an attractive candidate as a next-generation photocatalyst for CO<sub>2</sub> reduction because of its high solar spectrum absorption coefficient and small electron affinity. It is observed experimentally, by Electron Paramagnetic Resonance (EPR) and Scanning x-ray fluorescence microscopy (SXFEM), that the surface Cu atoms have various oxidation states, and different sites have different affinities for CO<sub>2</sub> and intermediate products. In this work, we employ first principles density functional theory (DFT) calculations to calculate the free energies of various low-index Cu<sub>2</sub>O surfaces and further identify the change of surface Cu oxidation states upon the creation of surface defects and during the photocatalytic process. The reactivity of Cu<sub>2</sub>O surfaces with various defect types and concentrations are also predicted.

**4:18PM H32.00008 *Ab initio* electron paramagnetic resonance study of 3C-SiC/SiO<sub>2</sub> interfaces in SiC-nanofiber based solar cells<sup>1</sup>**, TAUFIK ADI NUGRAHA, Max-Planck-Institut fuer Eisenforschung, UWE GERSTMANN, WOLFGANG GERO SCHMIDT, University of Paderborn, STEFAN WIPPERMANN, Max-Planck-Institut fuer Eisenforschung — Semiconducting nanocomposites, e. g. hybrid materials based on inorganic semiconducting 3C-SiC nanofibers and organic surfactants, provide genuinely novel pathways to exceed the Shockley-Queisser limit for solar energy conversion. The synthesis of such functionalized fibers can be performed completely using only inexpensive wet chemical solution processing. During synthesis a thin passivation layer is introduced between the SiC-fiber and surfactants, e. g. the native oxide, whose atomistic details are poorly understood. In this study, we utilize unpaired spins in interfacial defects to probe the local chemical environment with *ab initio* EPR (Electron Paramagnetic Resonance) calculations, which can be directly compared to experiment. Considering a wide variety of possible interfacial structures, a grand canonical approach is used to generate a phase diagram of the 3C-SiC/SiO<sub>2</sub> interface as a function of the chemical potentials of Si, O and H, to provide favorable interfacial structures for *g*-tensor calculations. This study provides directions about specific types of interfacial defects and their impact on the electronic properties of the interface. The authors wish to thank S. Greulich-Weber for helpful discussions.

<sup>1</sup>S. W. acknowledges BMBF NanoMatFutur Grant No. 13N12972.

**4:30PM H32.00009 Porphyrin-based polymeric nanostructures for light harvesting applications: *Ab initio* calculations**, WALTER ORELLANA<sup>1</sup>, Universidad Andres Bello — The capture and conversion of solar energy into electricity is one of the most important challenges to the sustainable development of mankind. Among the large variety of materials available for this purpose, porphyrins concentrate great attention due to their well-known absorption properties in the visible range. However, extended materials like polymers with similar absorption properties are highly desirable. In this work, we investigate the stability, electronic and optical properties of polymeric nanostructures based on free-base porphyrins and phthalocyanines (H<sub>2</sub>P, H<sub>2</sub>Pc), within the framework of the time-dependent density functional perturbation theory. The aim of this work is the stability, electronic, and optical characterization of polymeric sheets and nanotubes obtained from H<sub>2</sub>P and H<sub>2</sub>Pc monomers. Our results show that H<sub>2</sub>P and H<sub>2</sub>Pc sheets exhibit absorption bands between 350 and 400 nm, slightly different than the isolated molecules. However, the H<sub>2</sub>P and H<sub>2</sub>Pc nanotubes exhibit a wide absorption in the visible and near-UV range, with larger peaks at 600 and 700 nm, respectively, suggesting good characteristic for light harvesting. The stability and absorption properties of similar structures obtained from ZnP and ZnPc molecules is also discussed.

<sup>1</sup>Departamento de Ciencias Físicas, República 220, 037-0134 Santiago, Chile

**4:42PM H32.00010 Fundamental Insights into Aqueous Electrochemical Reduction of CO<sub>2</sub> on the Ligand-Protected Charged Au<sub>25</sub> Clusters**, DOMINIC ALFONSO, DOUGLAS KAUFFMAN, CHRISTOPHER MATRANGA, National Energy Technology Laboratory - Department of Energy, MATERIALS FUNDAMENTAL TEAM — Recent breakthroughs in electrochemical studies in our group showed aqueous CO<sub>2</sub> reduction to CO on atomically precise, inherently charged Au<sub>25</sub> clusters occurring at low overpotentials. Using first-principles density functional theory and continuum solvation models, the role of the cluster in the reduction process was examined. Free energies of species that were proposed as intermediates in its mechanism were determined. Contrary to previous assumptions, our results show that the fully ligand protected version of the cluster can be ruled out as an active participant. In particular, COOH species on the intact cluster should not be expected to form unless very high potentials are applied. Instead, the calculations suggest that the reduction process would likely occur on a dehiolated gold site. These findings point to the crucial role of such reaction center on the Au<sub>25</sub> clusters in facilitating the CO<sub>2</sub> conversion via the formation of low energy COOH intermediates.

**4:54PM H32.00011 First principle simulations of a bias-dependent electrochemical cell<sup>1</sup>**, LUANA PEDROZA, Univ Federal do ABC, Brazil, PEDRO BRANDIMARTE, CFM CSIC-UPV/EHU and DIPC, Spain, MARIVI FERNANDEZ-SERRA, Stony Brook University, USA, ALEXANDRE R. ROCHA, IFT-UNESP, Brazil — Understanding the local structure of water molecules at the interfaces of metallic electrodes is a key problem in many electrochemical problems. Notably the system is under an external potential bias, which makes the task of simulating this setup difficult. To correctly compute the effect of an external bias potential applied to electrodes, we combine density functional theory and non-equilibrium Green's functions methods, with and without van der Waals interactions. In this work, we apply this methodology to study the electronic properties and forces of water molecules at the interface of different metallic electrodes. We find that the water molecule is sensitive to the sign and magnitude of the applied bias. We also show that it changes the position and orientation of the most stable configuration indicating that the external bias plays an important role in the structural properties of the interface.

<sup>1</sup>The authors thank FAPESP and CNPq for financial support

**5:06PM H32.00012 Photoemission spectra of aqueous solutions of salts from many-body perturbation theory<sup>1</sup>**, ALEX P. GAIDUK, JONATHAN H. SKONE, MARCO GOVONI, GIULIA GALLI, University of Chicago — The computational design of electrode materials for energy conversion and storage processes requires an accurate description of the energy levels of the electrolyte and of electrolyte/electrode interfaces. Conventional density-functional approximations are in general not well suited for this task as they yield inaccurate orbital energies. Many-body perturbation theory (MBPT) predicts vertical ionization potentials and energy gaps in better agreement with experiments, providing the possibility for an accurate description of the electronic properties of electrolytes. We coupled *ab initio* molecular dynamics [1] with MBPT calculations [2] to investigate the photoemission spectra of a 1 M aqueous solution of NaCl. For the first time we were able to determine the absolute positions of the spectra peaks, with excellent agreement with experiments for both the solute and solvent peak positions. The best results were obtained using wavefunctions obtained from dielectric-dependent [3] hybrid calculations as a starting point for MBPT.

[1] A. P. Gaiduk, C. Zhang, F. Gygi, G. Galli, *Chem. Phys. Lett.* 604, 89 (2014); [2] M. Govoni and G. Galli, *J. Chem. Theory Comput.* 11, 2680 (2015); [3] J. H. Skone, M. Govoni, G. Galli, *Phys. Rev. B* 89, 195112 (2014).

<sup>1</sup>Work supported by DOE BES DE-SC0008938. Computer time provided by the Argonne Leadership Computing Facility through the INCITE program.

**5:18PM H32.00013 Coupled experimental and theoretical study of photon absorption and charge transport in BiVO<sub>4</sub> photoanodes for solar water splitting<sup>1</sup>**, YUAN PING, California Institute of Technology, TAE WOO KIM, University of Wisconsin, Madison, GIULIA GALLI, University of Chicago, KYOUNG-SHIN CHOI, University of Wisconsin, Madison — Bismuth vanadate (BiVO<sub>4</sub>) has been identified as one of the most promising photoanode materials for water-splitting photoelectrochemical cells. The major limitations of BiVO<sub>4</sub> are its relatively wide bandgap ( 2.5 eV) and low electron mobility ( 0.2 cm<sup>2</sup>V<sup>-1</sup>S<sup>-1</sup>), which limit its solar-to-hydrogen conversion efficiency. In this talk we will present the results of a coupled experimental and *ab initio* theoretical study showing that nitrogen doping together with extra oxygen vacancies lead to both a reduction of BiVO<sub>4</sub> band gap and to an increase of the majority carrier density and mobility. In turn these improvements lead to the applied bias photon-to-current efficiency over 2%, a record for a single oxide photon absorber, to the best of our knowledge[1]. The codoping method adopted in our work could also be applied to simultaneously enhance photon absorption and charge transport in other oxides, providing new possibilities for photocatalytic materials. [1] T. Kim, Y. Ping, G. Galli and K. Choi, *Nature Communications*, 6,8769, (2015).

<sup>1</sup>This work was supported by the National Science Foundation (NSF) under the NSF Center (CHE-1305124). Computer time was provided by NERSC.

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**  
**Session H33 DPOLY FIAP DCOMP: Where Simulation, Theory, and Experiment Meet Across Time Scales** 336 - K. Michael Salerno, Sandia National Laboratory

**2:30PM H33.00001 Simulation of chain diffusion in diblock copolymer microstructures using dynamical self-consistent mean-field theory**, DOUGLAS GRZETIC, ROBERT WICKHAM, University of Guelph — We simulate chain diffusion in ordered phases of a diblock copolymer melt, using our recently-developed dynamical self-consistent mean-field theory [*J. Chem. Phys.* **140**, 244907 (2014)]. This theory enables us to study large length and time scales in these dense systems, while remaining connected, in a self-consistent manner, to the microscopic physics of Brownian chains whose beads interact via a species-dependent modified Lennard-Jones potential. In the LAM and HEX phases, chain diffusion perpendicular to the microdomain interface is exponentially suppressed with increasing segregation, while parallel diffusion is unaffected. In the BCC phase, diffusion is isotropic and is gradually suppressed with increasing segregation. Chain diffusion is also isotropic in the gyroid phase, but does not vanish with increasing segregation. Instead, the diffusion constant asymptotes to a value consistent with chain diffusion being restricted to the interface of the three-dimensional gyroid network of struts, characterized by a network tortuosity value of 1.72. Finally, we measure the out-of-equilibrium evolution of the anisotropy in the chain diffusion as metastable LAM transforms to stable HEX over long times.

**2:42PM H33.00002 Effects of Structured Ionomer Interfaces on Water Diffusion: Molecular Dynamics Simulation Insight<sup>1</sup>**, DIPAK ARYAL, DVORA PERAHIA, Clemson University, GARY GRETT, Sandia National Laboratory — The dynamics of solvent molecules across structured ionomers interfaces is crucial to innovative technologies with selective controlled transport. These polymers consist of ionizable blocks facilitating transport tethered to mechanical stability enhancing ones, where their incompatibility drives compounded interfaces. Here water penetration through the interface of an A-B-C-B-A co-polymer is probed by atomistic molecular dynamics simulations where C is a randomly sulfonated polystyrene with sulfonation fractions  $f = 0$  to 0.55, B is poly (ethylene-r-propylene) and A is poly (t-butyl styrene). For  $f > 0$ , a two-step process with slow diffusion at the early stages is observed where water molecules transverse the hydrophobic rich surface before reaching the hydrophilic regime. Water molecules then diffuse along the percolating network of the ionic center block. Increasing the temperature and sulfonation fraction enhances both the rate of diffusion and the overall water uptake.

<sup>1</sup>This work is partially supported by DOE: DE-SC007908.

**2:54PM H33.00003 Towards a Modeling Framework for Thermodynamics and Transport Coefficients in Polyelectrolyte Assemblies**, RONALD LARSON, ALI SALEHI, University of Michigan — A continuum description of polyelectrolyte (PE) equilibrium gelation, and the kinetics of assembly is developed, accounting for PE chain diffusion, complexation, network relaxation is reported here. Using a combination of Flory-Huggins and Flory-Rehner free energy model, an upper-convected Maxwell model to describe polyelectrolyte gel stress and relaxation, and a Poisson equation for the electrostatic potential profiles, we develop a model that can account for both equilibrium properties of PE gels and for transport of PE's and ions during layer-by-layer assembly. As PE chains diffuse, counterions readjust themselves to minimize the net local charge, but fail to do so completely as they would have to pay a significant entropic penalty. Diffusion of PE chains predominantly driven by the electrostatic field induced by the entropy of counterions is characterized by pulse-like PE composition profiles. Even without considering chain complexation, we demonstrate that it is possible to at least qualitatively explain the non-monotonic variation of PEM growth kinetics versus salt concentration, observed experimentally.

**3:06PM H33.00004 Topological Constraints in Directed Polymer Melts**, ADAM NAHUM<sup>1</sup>, Massachusetts Institute of Technology, PABLO SERNA, University of Oxford, GUY BUNIN, Massachusetts Institute of Technology — Polymers in a melt may be subject to topological constraints, as in the example of unlinked polymer rings. How to do statistical mechanics in the presence of such constraints remains a fundamental open problem. We study the effect of topological constraints on a melt of directed polymers, using simulations of a simple quasi-2D model. We find that fixing the global topology of the melt to be trivial drastically changes both the static and dynamic properties. Polymers wander in the transverse direction by a distance which is only logarithmic in their length, and monomers subdiffuse logarithmically slowly. This is in sharp contrast to expectations from existing theories. To cast light on the suppression of the strands' wandering, we also analyse the topological complexity of subregions of the melt, finding it is also logarithmically small. We comment on insights the results give for 3D melts, directed and non-directed.

<sup>1</sup>Membership Pending

**3:18PM H33.00005 Scaling of viscosity with rate, pressure, and temperature: Linking simulations to experiments**<sup>1</sup>, VIKRAM JADHAO, MARK ROBBINS, The Johns Hopkins University — Elastohydrodynamic lubrication (EHL) is important in many practical devices and produces extreme pressures ( $> 1$  GPa) and shear rates ( $10^5 - 10^7$  s<sup>-1</sup>). This makes EHL fluids ideal candidates for bridging the gap between experimental and simulation studies of viscosity. There is an ongoing debate about whether the high-rate response of simple molecules like squalane follows a power-law Carreau model or a thermal activation based Eyring model. We use molecular dynamics simulations to investigate the rheological response of squalane for a wide range of rates ( $10^5 - 10^{10}$  s<sup>-1</sup>), pressures (0.1 MPa to 3 GPa), and temperatures (100 – 313 K). We find that experimental and theoretical results can be collapsed onto a master curve consistent with Eyring theory over more than 20 orders of magnitude in rate. Extrapolating Eyring fits to simulations at  $10^7$  s<sup>-1</sup> and above yields Newtonian viscosities  $\eta_0$  that are consistent with available low-rate experiments, and allows predictions to much higher pressures and lower temperatures. There is no indication of a diverging viscosity at finite stress, since  $\log \eta_0$  rises sublinearly with pressure up to 6 GPa and  $\eta_0 > 10^{12}$  Pa-s. Correlations between chain conformations and Eyring parameters are also presented.

<sup>1</sup>This research was performed within the Center for Materials in Extreme Dynamic Environments (CMEDE) under the Hopkins Extreme Materials Institute at Johns Hopkins University. Financial support was provided by grant W911NF-12-2-0022.

**3:30PM H33.00006 Unified force-level theory of multiscale transient localization and emergent elasticity in polymer solutions and melts**, ZACHARY E. DELL, KENNETH S. SCHWEIZER, University of Illinois at Urbana-Champaign — A unified, microscopic, theoretical understanding of polymer dynamics in concentrated liquids from segmental to macromolecular scales remains an open problem. We have formulated a statistical mechanical theory for this problem that explicitly accounts for intra- and inter-molecular forces at the Kuhn segment level. The theory is self-consistently closed at the level of a matrix of dynamical second moments of a tagged chain. Two distinct regimes of isotropic transient localization are predicted. In semidilute solutions, weak localization is predicted on a mesoscopic length scale between segment and chain scales which is a power law function of the invariant packing length. This is consistent with the breakdown of Rouse dynamics and the emergence of entanglements. The chain structural correlations in the dynamically arrested state are also computed. In dense melts, strong localization is predicted on a scale much smaller than the segment size which is weakly dependent on chain connectivity and signals the onset of glassy dynamics. Predictions of the dynamic plateau shear modulus are consistent with the known features of emergent rubbery and glassy elasticity. Generalizations to treat the effects of chemical crosslinking and physical bond formation in polymer gels are possible.

**3:42PM H33.00007 Failure of Tube Models to Predict the Linear Rheology of Star/Linear Blends**, RYAN HALL, PRIYANKA DESAI, University of Michigan, BEOMGOO KANG, University of Tennessee, MARIA KATZAROVA, Illinois Institute of Technology, QIFAN HUANG, University of Michigan, SANGHOON LEE, TAIHYUN CHANG, Pohang University of Science and Technology, DAVID VENERUS, Illinois Institute of Technology, JIMMY MAYS, University of Tennessee, JAY SCHIEBER, Illinois Institute of Technology, RONALD LARSON, University of Michigan — We compare predictions of two of the most advanced versions of the tube model, namely the Hierarchical model by Wang et al. (J. Rheol. 54:223, 2010) and the BOB (branch-on-branch) model by Das et al. (J. Rheol. 50:207-234, 2006), against linear viscoelastic data on blends of monodisperse star and monodisperse linear polybutadiene polymers. The star was carefully synthesized/characterized by temperature gradient interaction chromatography, and rheological data in the high frequency region were obtained through time-temperature superposition. We found massive failures of both the Hierarchical and BOB models to predict the terminal relaxation behavior of the star/linear blends, despite their success in predicting the rheology of the pure star and pure linear. This failure occurred regardless of the choices made concerning constraint release, such as assuming arm retraction in fat or skinny tubes, or allowing for disentanglement relaxation to cut off the constraint release Rouse process at long times. The failures call into question whether constraint release can be described as a combination of constraint release Rouse processes and dynamic tube dilation within a canonical tube model of entanglement interactions.

**3:54PM H33.00008 Challenging Slip-Link Models: Predicting the Linear Rheology of 1,4-Polybutadiene Blends of Well-Characterized Star and Linear 1,4-Polybutadienes**, MARIA KATZAROVA, Illinois Institute of Technology, PRIYANKA DESAI, University of Michigan, BEOMGOO KANG, University of Tennessee, RYAN HALL, QIFAN HUANG, University of Michigan, SANGHOON LEE, TAIHYUN CHANG, Pohang University of Science and Technology, DAVID VENERUS, Illinois Institute of Technology, JIMMY MAYS, University of Tennessee, JAY SCHIEBER, Illinois Institute of Technology, RONALD LARSON, University of Michigan — The discrete slip-link model (DSM) is a single-chain mean-field model for entanglement-dominated polymer dynamics. The model has been used successfully to make predictions about the linear and nonlinear rheology of monodisperse homopolymer melts, polydisperse melts, or blends. By using recent advances in coarse-graining, hierarchical modeling, and graphics processors, the model is amenable to predictions of well-entangled branched polymers. Here, the parameters of the most coarse-grained member of the hierarchy are fit to the dynamic modulus of monodisperse linear chains and applied to symmetric 4-arm polybutadiene (PBd) star-linear blends with roughly 20 entanglements per star arm, but with no parameter adjustment. Agreement with data is quantitative. This detailed model is further used to examine assumptions and approximations typically made in tube models for blending, including factorization in the time domain. Failure of these assumptions point towards possible fixes to tube models.

**4:06PM H33.00009 Multiscale simulations of polymer melt flow in an abrupt contraction and expansion channel<sup>1</sup>**, TAKASHI TANIGUCHI, KOHEI HARADA, Department of Chemical Engineering, Kyoto University, T.TANIGUCHI TEAM — We investigated a flow of a polymer melt with a molecular weight distribution in a channel with 4:1:4 contraction and expansion geometry by using a multi-scale simulation (MSS) method here a macroscopic model and microscopic molecular model are directly connected through the velocity gradient field and stress field. In the MSS method, we introduced Lagrangian particles which contain many chains to precisely maintain the microscopic states. As the microscopic polymer model, a slip-link model is used. As a result, we clarified the relation between the macroscopic flow behavior and molecular level information such as a local polymer configuration and spatial distribution of number of entanglements per chain.

<sup>1</sup>The present work is partially supported by KAKENHI No.15H03708 and No.15K13549.

**4:18PM H33.00010 Modeling Structure Property Relations and Failure Mechanisms of PPTA Fibers using Reactive Molecular Dynamics<sup>1</sup>**, DUNDAR YILMAZ, Zirve University — Failure mechanisms of poly(p-phenylene terephthalamide (PPTA) under extreme tensile deformation has been studied using reactive potentials with molecular dynamics simulations. Amorphous PPTA systems with different molecular weights generated using an in-house developed amorphous builder. Tensile modulus of amorphous PPTA has been calculated as up to 6.7 GPa. Nitrogen and carbon vacancy defects were introduced to both crystalline and amorphous systems. The tensile modulus of defects-free crystalline PPTA calculated as 350 GPa. Introduction of 5% nitrogen vacancy defects reduced the tensile modulus to 197 GPa. PPTA fibers generated with skin core structure where skin region composed of PPTA chains in crystalline order and core region was composed of unordered PPTA chains vice versa. Relation between ratios of skin and core regions and mechanical properties of the fiber studied. Tensile load was mostly accommodated through stretching of bonds between amide group and phenyl groups. Under extreme tensile deformation PPTA chains failed at these C-N bonds.

<sup>1</sup>TUBITAK GRANT NO: 113F358

**4:30PM H33.00011 Chain Ends and the Ultimate Tensile Strength of Polyethylene Fibers<sup>1</sup>**, THOMAS C. O'CONNOR, MARK O. ROBBINS, Johns Hopkins University — Determining the tensile yield mechanisms of oriented polymer fibers remains a challenging problem in polymer mechanics. By maximizing the alignment and crystallinity of polyethylene (PE) fibers, tensile strengths  $\sigma \sim 6 - 7$  GPa have been achieved. While impressive, first-principal calculations predict carbon backbone bonds would allow strengths four times higher ( $\sigma \sim 20$  GPa) before breaking. The reduction in strength is caused by crystal defects like chain ends, which allow fibers to yield by chain slip in addition to bond breaking. We use large scale molecular dynamics (MD) simulations to determine the tensile yield mechanism of orthorhombic PE crystals with finite chains spanning  $10^2 - 10^4$  carbons in length. The yield stress  $\sigma_y$  saturates for long chains at  $\sim 6.3$  GPa, agreeing well with experiments. Chains do not break but always yield by slip, after nucleation of 1D dislocations at chain ends. Dislocations are accurately described by a Frenkel-Kontorova model, parametrized by the mechanical properties of an ideal crystal. We compute a dislocation core size  $\xi = 25.24 \text{ \AA}$  and determine the high and low strain rate limits of  $\sigma_y$ . Our results suggest characterizing such 1D dislocations is an efficient method for predicting fiber strength.

<sup>1</sup>This research was performed within the Center for Materials in Extreme Dynamic Environments (CMEDE) under the Hopkins Extreme Materials Institute at Johns Hopkins University. Financial support was provided by grant W911NF-12-2-0022.

**4:42PM H33.00012 Microscopic deformation mechanisms in model thermoplastic elastomers by molecular dynamics simulation**, AMANDA PARKER, JÖRG RÖTTLER, University of British Columbia — Thermoplastic elastomers (TPEs) can be formed by exploiting the nanostructured morphology of triblock copolymers. Glassy end-blocks phase separate to form spherical regions which act as physical cross-links for the soft rubbery phase. Molecular dynamics simulations of TPEs allow us to relate the microscopic mechanisms active during plastic deformation to the macroscopic stress response. A coarse-grained bead-spring model of linear ABA triblock copolymers which forms the desired spherical morphology is used for pure stress and pure strain uniaxial deformations. The systems are first equilibrated using a soft pair potential. We observe increased strain hardening in triblocks when compared to homopolymers of the same chain length in accordance with experiments. We connect variations in the stress response for systems of different chain lengths to the non-affine deformation of chains and to the scale of phase separated regions. The stress response is also compared to rubbery elasticity models, taking into account the evolution of chain entanglements during deformation. We observe void formation at the interfaces of glassy regions or where these regions have broken up at large strain.

**4:54PM H33.00013 Computer-Aided Design of Photocured Polymer Networks**, SWARNAVO SARKAR, SHENG LIN-GIBSON, MARTIN CHIANG, NIST - Natl Inst of Stds & Tech — Light-initiated free radical polymerization is widely used for manufacturing biomaterials, scaffolds for micromolding, and is being developed as a method for fast 3D fabrication. This process has a large set of control parameters in the composition of the photocurable matrix and the photocuring conditions. But a quantitative map between the choice of parameters and the properties of the resultant polymer is currently unavailable. We present a computational approach to simulate the growth of a polymer network using the stochastic differential equations of reactions and diffusion for a photocuring system. This method allows us to sample trajectories of a growing polymer network in silico. Thus, we provide a computational alternative to synthesize and probe a polymer network for properties like the degree of conversion, structure factor, density of states, and viscosity. We present simulation results that agree with the universal features observed in photopolymerization. Our proposed method enables a thorough and systematic search over the entire parameter space to discover interesting combinations for synthesis.

**5:06PM H33.00014 Molecular Description of Yield in Densely Crosslinked Epoxy Thermosets**, SANDIPAN CHATTARAJ, Centre for Research in Nanotechnology and Science, Indian Inst of Tech-Bombay, PRITA PANT, Metallurgical Engineering and Materials Science, Indian Inst of Tech-Bombay, DNYANESH PAWASKAR, Department of Mechanical Engineering, Indian Inst of Tech-Bombay, HEMANT NANAVATI, Department of Chemical Engineering, Indian Inst of Tech-Bombay — In densely crosslinked networks, macroscopic yield is a transition from deformations of bond lengths and angles, to cooperative deformation of multiple effective network chains via bond torsions. In this work, we examine this yield in terms of the "activation number",  $\nu$ , of microscopic effective chains between crosslinks.  $\nu$  is the number of effective network chains, in one Eyring activation volume,  $V^*$ . It is thus a measure of the number of network chains activated at yield, for cooperative deformation. Microcompression experiments have been performed on SU-8 micropillars, to determine its  $V^*$  value. SU-8 is an important epoxy thermoset, which is used extensively in the microelectronics industry, in microfluidics and microelectromechanical systems (MEMS). The effective chain length based on Arruda and Boyce's 8-chain model, compares well with the rms length, obtained by chain conformer analyses. We find that  $\nu \sim 2-4$ , at room temperature, for DGEBA-based epoxies including SU-8 and DGEBA-amine networks, over a range of network junction functionalities and  $V^*$ . That  $\nu$  corresponds very well with the reduced temperature,  $T/T_g$ , also demonstrates its viability as a molecular descriptor of yield in densely crosslinked thermosets.

**5:18PM H33.00015 Toward a predictive model for elastomer seals.** , NICOLA MOLINARI, MUSAB KHAWAJA, ADRIAN SUTTON, ARASH MOSTOFI, Department of Physics and the Thomas Young Centre for Theory and Simulation of Materials, Imperial College London, UK — Nitrile butadiene rubber (NBR) and hydrogenated-NBR (HNBR) are widely used elastomers, especially as seals in oil and gas applications. During exposure to well-hole conditions, ingress of gases causes degradation of performance, including mechanical failure. We use computer simulations to investigate this problem at two different length and time-scales. First, we study the solubility of gases in the elastomer using a chemically-inspired description of HNBR based on the OPLS all-atom force-field. Starting with a model of NBR, C=C double bonds are saturated with either hydrogen or intramolecular cross-links, mimicking the hydrogenation of NBR to form HNBR. We validate against trends for the mass density and glass transition temperature for HNBR as a function of cross-link density, and for NBR as a function of the fraction of acrylonitrile in the copolymer. Second, we study mechanical behaviour using a coarse-grained model that overcomes some of the length and time-scale limitations of an all-atom approach. Nanoparticle fillers added to the elastomer matrix to enhance mechanical response are also included. Our initial focus is on understanding the mechanical properties at the elevated temperatures and pressures experienced in well-hole conditions.

**Tuesday, March 15, 2016 2:30PM - 5:18PM –**

**Session H34 GSOFD DBIO GSNP/DFD: Active Matter V** 337 - Erik Luijten, Northwestern University

**2:30PM H34.00001 Active colloids propelled by induced-charge electrophoresis** , MING HAN, ERIK LUIJTEN, Northwestern University — Populations of motile organisms exhibit a variety of collective behaviors, ranging from bacterial colony formation to the flocking of birds. Current understanding of these active motions, which are typically far from equilibrium and based on the collective behavior of self-propelled entities, is far from complete. One approach is to reproduce these observations in systems of synthetic active colloids. However, one of the standard self-propulsion mechanisms, induced-charge electrophoresis (ICEP) of a dielectric Janus colloid remains not fully understood by itself, especially the strong dependence of the resultant particle motion on the frequency of the external field. Resolution of this outstanding problem requires detailed study of the time-resolved dielectric response of the colloid and the dynamics of the electric double layer. Through molecular dynamics simulations coupled with an efficient dielectric solver, we elucidate the underlying mechanism of the frequency dependence of ICEP and the polarization of a metalodielectric Janus colloid.

**2:42PM H34.00002 Driving magnetic colloidal polymers<sup>1</sup>** , JOSHUA DEMPSTER, Northwestern University, MONICA OLVERA DE LA CRUZ, Northwestern University Department of Materials Science — Magnetic colloids are of growing interest for applications such as drug delivery and in vitro tissue growth. Recent experiments have synthesized 1D chains of magnetic colloids into permanent colloidal polymers. We study magnetic colloidal polymers theoretically and computationally under the influence of time-varying external fields and find a rich set of controllable, dynamic conformations. By iterating through a sequence of conformations, these polymers can perform mechanical functions. We discuss possible roles for these polymers beyond those considered for single colloids.

<sup>1</sup>This work was supported as part of the Center for Bio-Inspired Energy Science, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award DE-SC0000989

**2:54PM H34.00003 Broken detailed balance observed for hydrodynamically coupled colloidal particles in two optical traps** , CHRISTOPH F. SCHMIDT, JANNES GLADROW, Universitt Gttingen, NIKTA FAKHRI, Massachusetts Institute of Technology, CHASE P. BROEDERSZ, Ludwig-Maximilians-Universitt Mnchen — Optical traps can be approximated as harmonic potentials for refractile colloidal particles. If two particles are trapped by two optical traps at close distance, particles remain hydrodynamically coupled. With two traps at different laser powers, one can create a non-equilibrium situation, where one particle can feed energy to the other particle. We show that this situation leads to the breaking of detailed balance that can be visualized as finite flux in a coarse-grained phase space spanned by the displacements of the two particles. We test if the slight temperature difference caused by different laser powers drives the flux or if it is due to energy dissipation associated with scattered light, a second-order effect for non-absorbing particles.

**3:06PM H34.00004 Collective motion in populations of colloidal bots** , DENIS BARTOLO, ENS Lyon — One of the origins of active matter physics was the idea that flocks, herds, swarms and shoals could be quantitatively described as emergent ordered phases in self-driven materials. From a somehow dual perspective, I will show how to engineer active materials out of colloidal flocks. I will show how to motorize colloidal particles capable of sensing the orientation of their neighbors and how to handle them in microfluidic chips. These populations of colloidal bots display a non-equilibrium transition toward collective motion. A special attention will be paid to the robustness of the resulting colloidal flocks with respect to geometrical frustration and to quenched disorder.

**3:42PM H34.00005 Self-similarity in active colloid motion** , COLIN CONSTANT, SERGEY SUKHOV, ARISTIDE DOGARIU, Univ of Central Florida - CREOL — The self-similarity of displacements among randomly evolving systems has been used to describe the foraging patterns of animals and predict the growth of financial systems. At micron scales, the motion of colloidal particles can be analyzed by sampling their spatial displacement in time. For self-similar systems in equilibrium, the mean squared displacement increases linearly in time. However, external forces can take the system out of equilibrium, creating active colloidal systems, and making this evolution more complex. A moment scaling spectrum of the distribution of particle displacements quantifies the degree of self-similarity in the colloid motion. We will demonstrate that, by varying the temporal and spatial characteristics of the external forces, one can control the degree of self-similarity in active colloid motion.

**3:54PM H34.00006 Paramagnetic colloids in rotating fields: from chains through chaos to clusters.<sup>1</sup>** , HAMED ABDI, RASAM SOHEILIAN, RANDALL ERB, CRAIG MALONEY, Northeastern — We present computer simulations and experiments on dilute suspensions of superparamagnetic particles subject to rotating magnetic fields. We focus on short chains of particles and their decay routes to stable structures. At low rate, the chains track the external field. At intermediate rate, the short chains break up but perform a periodic (albeit complex) motion. At sufficiently high rates, the chains generally undergo chaotic motion at short times and decay to either close-packed clusters or more dispersed colloidal “molecules” at long times. We show that the transition out of the chaotic states follows a first order reaction kinetics.

<sup>1</sup>NSF

#### **4:06PM H34.00007 Hydrodynamic self-organization and mixing in suspensions of micro-rotors<sup>1</sup>**

, KYONGMIN YEO, IBM Research, ENKELEIDA LUSHI, PETIA VLAHOVSKA, Brown University — Self-organization of active objects has attracted considerable attention recently, especially in the context of living systems. Hydrodynamic interactions can play a crucial role in the emerging behavior when the objects are immersed in fluid, especially in the low Reynolds number regime. While self-propelled active objects have been extensively investigated, the collective behavior of rotating active particle has received limited attention. To elucidate the transition to collective behavior and especially the role of multi-body hydrodynamic interactions, we numerically study systems of co- and counter-rotating spheres by varying the mixture ratio as well as the total volume fraction. With increasing volume fraction, we observe the emergence of intriguing patterns such as lanes, vortices of same-spin rotors as well as dynamic crystals composed of both types of rotors. We consider how the motion of the rotating particles and fluid they collectively generate affects the dispersion or clustering of passive sphere particles or mixing of passive scalar fields in the system.

<sup>1</sup>We acknowledge support from NSF CBET 1437545 and NSF CBET 1544196.

#### **4:18PM H34.00008 Collective dynamics of rotating colloidal particles**

, SOFIA MAGKIRIADOU, VISHAL SONI, University of Chicago, BENNY VAN ZUIDEN, Leiden University, DENIS BARTOLO, Ecole Normale Supérieure de Lyon, VINCENZO VITELLI, Leiden University, WILLIAM T.M. IRVINE, University of Chicago — We study magnetic colloidal particles in suspension under the influence of a rotating magnetic field. When in aggregates, these particles show rich dynamics that are governed by magnetic and hydrodynamic interactions. By tuning these interactions, we probe the phase diagram of this system and study the emergent collective dynamics. Finally, we begin to investigate whether we can control this phase diagram with geometry.

#### **4:30PM H34.00009 Helical motion of chiral liquid crystal droplets<sup>1</sup>**

, TAKAKI YAMAMOTO, MASAKI SANO, Department of Physics, Graduate School of Science, the University of Tokyo — Artificial swimmers have been intensively studied to understand the mechanism of the locomotion and collective behaviors of cells and microorganisms. Among them, most of the artificial swimmers are designed to move along the straight path. However, in biological systems, chiral dynamics such as circular and helical motion are quite common because of the chirality of their bodies, which are made of chiral biomolecules. To understand the role of the chirality in the physics of microswimmers, we designed chiral artificial swimmers and the theoretical model for the chiral motion. We found that chiral liquid crystal droplets, when dispersed in surfactant solutions, swim in the helical path induced by the Marangoni effect. We will discuss the mechanism of the helical motion with our phenomenological model.

<sup>1</sup>This work is supported by Grant-in-Aid for JSPS Fellows (Grant No. 269814), and MEXT KAKENHI Grant No. 25103004.

#### **4:42PM H34.00010 Rolling and spinning swimmers**

, MICHELLE DRISCOLL, MELISSA FERRARI, MENA YOUSSEF, PAUL CHAIKIN, STEFANO SACANNA, New York Univ NYU — We study the dynamics and collective interactions that occur in a system of rotating active matter: an oscillating, externally applied magnetic field is used to drive motion in a system of confined, magnetic colloids. By adjusting the orientation, frequency, and amplitude of the applied field we can drive a wide range of particle motions, from rolling to spinning. These rotations lead to a large variety of collective behaviors, which are driven both by particle-particle magnetic interactions as well as long-range hydrodynamic flows. We observe that the clustering which results from in-plane spinning can be strongly modulated by changing inter-particle magnetic interactions. We explore the strength of this clustering as a function of particle interaction, and can isolate the effect of magnetic and hydrodynamic interactions. We also observe that particle rotation can lead to complex and large-scale flows for both the case of rolling and spinning particles.

#### **4:54PM H34.00011 Emergent order in ensembles of active spinners**

, BENJAMIN C. VAN ZUIDEN, JAYSON PAULOSE, Lorentz Institute, Leiden University, WILLIAM T. M. IRVINE, James Franck Institute, University of Chicago, DENIS BARTOLO, Ecole Normale Supérieure de Lyon, VINCENZO VITELLI, Lorentz Institute, Leiden University — Interacting self-propelled particles is proxy to model many living systems from cytoskeletal motors to bird flocks, while also providing a framework to investigate fundamental questions in non equilibrium statistical mechanics. A surge of recent studies have shown that self-propulsion significantly modifies the phase behavior of particles interacting via potential interactions. A prototypical example is the so-called Motility Induced Phase Separation occurring in ensembles of self-propelled hard spheres. In stark contrast, our understanding of active spinning, as opposed to self-propulsion, remains very scarce. Here, we study a system of self-spinning dimers, interacting via soft repulsive forces. Upon varying the density and activity, we observe a range of emergent phases characterized by different degrees of spatiotemporal order in the position and orientation of the dimers. Changes in bulk properties, including crystallization, melting, and freezing, are reflected in the collective motion of the particles. We rationalize our numerical findings theoretically and demonstrate some of these concepts in a active granular experiment.

#### **5:06PM H34.00012 Emergent collective dynamics in ensembles of magnetic colloidal rollers**

, ALEXEY SNEZHKO, Argonne National Laboratory — Strongly interacting colloids driven out-of-equilibrium by an external periodic forcing often develop nontrivial collective dynamics. Ferromagnetic micro-particles immersed in water and sediment on the bottom surface of the flat cell are energized by a single-axis homogeneous alternating magnetic field applied perpendicular to the surface supporting the particles. Upon application of the alternating magnetic field the magnetic torque on each particle is transferred to the mechanical torque giving rise to a rolling motion of the particle. Experiments reveal a rich collective dynamics of magnetic rollers in a certain range of excitation parameters. Flocking and spontaneous formation of steady vortex motion have been observed. The effects are fine-tuned and controlled by the parameters of the driving magnetic field. Formation of the self-organized collective states spontaneously breaking the symmetry of the underlying interactions has been attributed to the interplay of inelastic inter-particle collisions and self-induced hydrodynamic flows in the system. The research was supported by the U.S. DOE, Office of Basic Energy Sciences, Division of Materials Science and Engineering.

## **Tuesday, March 15, 2016 2:30PM - 5:30PM –**

**Session H35 DBIO GSNP: Population and Evolutionary Dynamics III** 338 - Robert Austin, Princeton University

#### **2:30PM H35.00001 Standing variation in spatially growing populations**

, DIANA FUSCO, MATTI GRALKA, JONA KAYSER, OSKAR HALLATSCHEK, Univ of California - Berkeley — Patterns of genetic diversity not only reflect the evolutionary history of a species but they can also determine the evolutionary response to environmental change. For instance, the standing genetic diversity of a microbial population can be key to rescue in the face of an antibiotic attack. While genetic diversity is in general shaped by both demography and evolution, very little is understood when both factors matter, as e.g. for biofilms with pronounced spatial organization. Here, we quantitatively explore patterns of genetic diversity by using microbial colonies and well-mixed test tube populations as antipodal model systems with extreme and very little spatial structure, respectively. We find that Eden model simulations and KPZ theory can remarkably reproduce the genetic diversity in microbial colonies obtained via population sequencing. The excellent agreement allows to draw conclusions on the resilience of spatially-organized populations and to uncover new strategies to contain antibiotic resistance.

**2:42PM H35.00002 Crowds as an Excitable Medium for Spiral Wave Dynamics<sup>1</sup>**, ANDREA WELSH, EDWIN GRECO, FLAVIO FENTON, Georgia Institute of Technology — Spiral wave (SW) patterns are studied in many physical, biological, and chemical excitable systems. Of particular importance are SW of electrical activity that develop in the heart and give rise to arrhythmias such as tachycardia (single SW) and fibrillation (multiple SWs). We investigate if a crowd of people given simple rules for activation and deactivation, modeled on cardiac cells, can act as a living simulation for SW dynamics. For group sizes ranging from 50 to 650 people we demonstrate, experimentally, the existence of stable spiral waves and of spiral wave breakup leading to chaotic dynamics. Numerical simulation predicts the simple rules lead to well defined wave fronts. People, however, respond with various degrees of anticipation and misinformation. This human behavior can lead to smoothed fronts or even lead to spiral wave breakup and chaos. We present a new cell model that includes variations in reaction to account for the observed behavior in crowds. This model may be useful in the study of coupling and decoupling of cardiac cells that lead to arrhythmic behavior.

<sup>1</sup>Supported by NSF

**2:54PM H35.00003 Adapting populations in space: clonal interference and genetic diversity**, DANIEL WEISSMAN, Emory University, NICK BARTON, IST Austria — Most species inhabit ranges much larger than the scales over which individuals interact. How does this spatial structure interact with adaptive evolution? We consider a simple model of a spatially-extended, adapting population and show that, while clonal interference severely limits the adaptation of purely asexual populations, even rare recombination is enough to allow adaptation at rates approaching those of well-mixed populations. We also find that the genetic hitchhiking produced by the adaptive alleles sweeping through the population has strange effects on the patterns of genetic diversity. In large spatial ranges, even low rates of adaptation cause all individuals in the population to rapidly trace their ancestry back to individuals living in a small region in the center of the range. The probability of fixation of an allele is thus strongly dependent on the alleles spatial location, with alleles from the center favored. Surprisingly, these effects are seen genome-wide (instead of being localized to the regions of the genome undergoing the sweeps). The spatial concentration of ancestry produces a power-law dependence of relatedness on distance, so that even individuals sampled far apart are likely to be fairly closely related, masking the underlying spatial structure.

**3:06PM H35.00004 3-D Technology Approaches for Biological Ecologies<sup>1</sup>**, LIYU LIU, Chongqing University/Institute of Physics, Chinese Academy of Sciences, ROBERT AUSTIN, Princeton University, U.S-CHINA PHYSICAL-ONCOLOGY SCIENCES ALLIANCE (PS-OA) TEAM — Constructing three dimensional (3-D) landscapes is an inevitable issue in deep study of biological ecologies, because in whatever scales in nature, all of the ecosystems are composed by complex 3-D environments and biological behaviors. Just imagine if a 3-D technology could help complex ecosystems be built easily and mimic in vivo microenvironment realistically with flexible environmental controls, it will be a fantastic and powerful thrust to assist researchers for explorations. For years, we have been utilizing and developing different technologies for constructing 3-D micro landscapes for biophysics studies in vitro. Here, I will review our past efforts, including probing cancer cell invasiveness with 3-D silicon based Trepis, constructing 3-D microenvironment for cell invasion and metastasis through polydimethylsiloxane (PDMS) soft lithography, as well as explorations of optimized stenting positions for coronary bifurcation disease with 3-D wax printing and the latest home designed 3-D bio-printer. Although 3-D technologies is currently considered not mature enough for arbitrary 3-D micro-ecological models with easy design and fabrication, I hope through my talk, the audiences will be able to sense its significance and predictable breakthroughs in the near future.

<sup>1</sup>This work was supported by the State Key Development Program for Basic Research of China (Grant No 2013CB837200), the National Natural Science Foundation of China (Grant No 11474345) and the Beijing Natural Science Foundation (Grant No 7154221).

**3:42PM H35.00005 Population Dynamics of Viral Inactivation<sup>1</sup>**, KRISTA FREEMAN, DONG LI, Carnegie Mellon University, MANJA BEHRENS, Lund University, KIRIL STRELETZKY, Cleveland State University, ULF OLSSON, Lund University, ALEX EVILEVITCH, Carnegie Mellon University — We have investigated the population dynamics of viral inactivation *in vitro* using time-resolved cryo electron microscopy combined with light and X-ray scattering techniques. Using bacteriophage  $\lambda$  as a model system for pressurized double-stranded DNA viruses, we found that virions incubated with their cell receptor eject their genome in a stochastic triggering process. The triggering of DNA ejection occurs in a non synchronized manner after the receptor addition, resulting in an exponential decay of the number of genome-filled viruses with time. We have explored the characteristic time constant of this triggering process at different temperatures, salt conditions, and packaged genome lengths. Furthermore, using the temperature dependence we determined an activation energy for DNA ejections. The dependences of the time constant and activation energy on internal DNA pressure, affected by salt conditions and encapsidated genome length, suggest that the triggering process is directly dependent on the conformational state of the encapsidated DNA. The results of this work provide insight into how the *in vivo* kinetics of the spread of viral infection are influenced by intra- and extra cellular environmental conditions.

<sup>1</sup>This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. DGE-1252522

**3:54PM H35.00006 Coalescent Theory Analysis of Population Collapse and Recovery in a Neutral Evolution Model<sup>1</sup>**, DAWN KING, SONYA BAHAR, University of Missouri at Saint Louis — As we move through the Anthropocene Epoch, human-driven climate change is predicted to accelerate extinction risk in the near future. Therefore, understanding basic underlying mechanisms of population loss and recovery could be paramount to saving key species in changing ecosystems. Here, we present an evolutionary model that investigates the dynamics of population collapse and recovery following a simulated mass extinction. Previously, we have shown that nonequilibrium, continuous phase transitions of the directed percolation universality class occur as a function of two different control parameters: the mutability,  $\mu$ , which dictates how phenotypically different an offspring can be from its parent, and the death probability,  $\delta$ , which probabilistically removes organisms within each generation. Here, we characterize the phylogenetic tree structures at two levels of biological organization—the organism and species level. Using methods from coalescent theory, we examine the phylogenetic tree structures at, and above, criticality, by considering common descent. The times to most recent common ancestor show phase transition behavior, as well as scale-free branching behavior at both levels of organization. We further examine these genealogical structures pre- and post-extinction.

<sup>1</sup>This research was supported by funding from the James S. McDonnell Foundation

**4:06PM H35.00007 Confirming Time-reversal Symmetry of a Directed Percolation Phase Transition in a Model of Neutral Evolutionary Dynamics<sup>1</sup>**, STEPHEN ORDWAY, DAWN KING, SONYA BAHAR, University of Missouri at Saint Louis — Reaction-diffusion processes, such as branching-coalescing random walks, can be used to describe the underlying dynamics of nonequilibrium phase transitions. In an agent-based, neutral model of evolutionary dynamics, we have previously shown that our system undergoes a continuous, nonequilibrium phase transition, from extinction to survival, as various system parameters were tuned. This model was shown to belong to the directed percolation (DP) universality class, by measuring the critical exponents corresponding to correlation length  $\xi_{\perp}$ , correlation time  $\xi_{\parallel}$ , and particle density  $\beta$ . The fourth critical exponent that defines the DP universality class is  $\beta'$ , which measures the survival probability of growth from a single seed organism. Since DP universality is theorized to have time-reversal symmetry, it is assumed that  $\beta = \beta'$ . In order to confirm the existence of time-reversal symmetry in our model, we evaluate the system growth from a single asexually reproducing organism. Importantly, the critical exponent  $\beta'$  could be useful for comparison to experimental studies of phase transitions in biological systems, since observing growth of microbial populations is significantly easier than observing death.

<sup>1</sup>This research was supported by funding from the James S. McDonnell Foundation

**4:18PM H35.00008 Holes influence the mutation spectrum of human mitochondrial DNA.** , MARTHA VILLAGRAN, JOHN MILLER, University of Houston, Dept. of Physics & Texas Ctr. for Superconductivity — Mutations drive evolution and disease, showing highly non-random patterns of variant frequency vs. nucleotide position. We use computational DNA hole spectroscopy [M.Y. Suarez-Villagran & J.H. Miller, *Sci. Rep.* 5, 13571 (2015)] to reveal sites of enhanced hole probability in selected regions of human mitochondrial DNA. A hole is a mobile site of positive charge created when an electron is removed, for example by radiation or contact with a mutagenic agent. The hole spectra are quantum mechanically computed using a two-stranded tight binding model of DNA. We observe significant correlation between spectra of hole probabilities and of genetic variation frequencies from the MITOMAP database. These results suggest that hole-enhanced mutation mechanisms exert a substantial, perhaps dominant, influence on mutation patterns in DNA. One example is where a trapped hole induces a hydrogen bond shift, known as tautomerization, which then triggers a base-pair mismatch during replication. Our results deepen overall understanding of sequence specific mutation rates, encompassing both hotspots and cold spots, which drive molecular evolution.

**4:30PM H35.00009 A kinetic theory for age-structured stochastic birth-death processes<sup>1</sup>** , TOM CHOU, Univ of California - Los Angeles, CHRIS GREENMAN, University of East Anglia — Classical age-structured mass-action models such as the McKendrick-von Foerster equation have been extensively studied but they are structurally unable to describe stochastic fluctuations or population-size-dependent birth and death rates. Conversely, current theories that include size-dependent population dynamics (e.g., carrying capacity) cannot be easily extended to take into account age-dependent birth and death rates. In this paper, we present a systematic derivation of a new fully stochastic kinetic theory for interacting age-structured populations. By defining multiparticle probability density functions, we derive a hierarchy of kinetic equations for the stochastic evolution of an aging population undergoing birth and death. We show that the fully stochastic age-dependent birth-death process precludes factorization of the corresponding probability densities, which then must be solved by using a BBGKY-like hierarchy. Our results generalize both deterministic models and existing master equation approaches by providing an intuitive and efficient way to simultaneously model age- and population-dependent stochastic dynamics applicable to the study of demography, stem cell dynamics, and disease evolution.

<sup>1</sup>NSF

**4:42PM H35.00010 Theoretical ecology without species** , MIKHAIL TIKHONOV<sup>1</sup>, Harvard University — The sequencing-driven revolution in microbial ecology demonstrated that discrete “species” are an inadequate description of the vast majority of life on our planet. Developing a novel theoretical language that, unlike classical ecology, would not require postulating the existence of species, is a challenge of tremendous medical and environmental significance, and an exciting direction for theoretical physics. Here, it is proposed that community dynamics can be described in a naturally hierarchical way in terms of population fluctuation eigenmodes. The approach is applied to a simple model of division of labor in a multi-species community. In one regime, effective species with a core and accessory genome are shown to naturally appear as emergent concepts. However, the same model allows a transition into a regime where the species formalism becomes inadequate, but the eigenmode description remains well-defined. Treating a community as a black box that expresses enzymes in response to resources reveals mathematically exact parallels between a community and a single coherent organism with its own fitness function. This coherence is a generic consequence of division of labor, requires no cooperative interactions, and can be expected to be widespread in microbial ecosystems.

<sup>1</sup>Harvard Center of Mathematical Sciences and Applications;  
John A. Paulson School of Engineering and Applied Sciences

**4:54PM H35.00011 A new model for biological effects of radiation and the driven force of molecular evolution.** , TAKAHIRO WADA, Department of Pure and Applied Physics, Kansai University, YUICHIRO MANABE, Division of Sustainable Energy and Environmental Engineering, Osaka University, HIROO NAKAJIMA, Department of Radiation Biology and Medical Genetics, Osaka University, YUICHI TSUNOYAMA, Radioisotope Research Center, Kyoto University, MASAKO BANDO, RCNP, Osaka University — We proposed a new mathematical model to estimate biological effects of radiation, which we call Whack-A-Mole (WAM) model. A special feature of WAM model is that it involves the dose rate of radiation as a key ingredient. We succeeded to reproduce the experimental data of various species concerning the radiation induced mutation frequencies. From the analysis of the mega-mouse experiments, we obtained the mutation rate per base-pair per year for mice which is consistent with the so-called molecular clock in evolution genetics,  $10^{-9}$  mutation/base-pair/year. Another important quantity is the equivalent dose rate for the whole spontaneous mutation,  $d_{\text{eff}}$ . The value of  $d_{\text{eff}}$  for mice is  $1.1 \times 10^{-3}$  Gy/hour which is much larger than the dose rate of natural radiation ( $10^{-(6-7)}$  Gy/hour) by several orders of magnitude. We also analyzed *Drosophila* data and obtained essentially the same numbers. This clearly indicates that the natural radiation is not the dominant driving force of the molecular evolution, but we should look for other factors, such as miscopy of DNA in duplication process. We believe this is the first quantitative proof of the small contribution of the natural radiation in the molecular evolution.

**5:06PM H35.00012 Scaling of expected survival time in a stochastic harvesting model** , HAROLD HASTINGS, Hofstra University and Bard College at Simon's Rock, MICHAEL RADIN, TAMAS WIANDT, Rochester Institute of Technology — We explore the dynamics of modified version of a standard fishery model (Gordon-Schaefer-Munro [1]), with additive and multiplicative noise, under a quota-based harvest. A harvest quota induces an effective strong Allee effect (a positive unstable steady state population level, below which populations die out), with expected survival time following generalized Ornstein-Uhlenbeck dynamics [2]. In particular, for additive noise, the expected survival time is exponential in  $s^3/\sigma^2$ , where  $s$  is the difference between stable and unstable steady state populations and  $\sigma$  the noise level. Thus survival time depends sensitively upon harvest quota (which determines steady state population), perhaps a warning to avoid future collapses such as that of the Atlantic cod fishery [3]. 1. Gordon HS. *J Fisheries Board Canada* 10, 442 (1953); Schaefer MB. *ibid* 14, 669 (1957); Clark, CW, Munro GR. *J Environ Econ and Management* 2, 92 (1975). 2. Beale PD. *Phys Rev A* 40, 3998 (1989). 3. c.f. [www.millenniumassessment.org/](http://www.millenniumassessment.org/)

**5:18PM H35.00013 Computational design of hepatitis C vaccines using maximum entropy models and population dynamics** , GREGORY HART, ANDREW FERGUSON, Univ of Illinois - Urbana — Hepatitis C virus (HCV) afflicts 170 million people and kills 350,000 annually. Vaccination offers the most realistic and cost effective hope of controlling this epidemic. Despite 20 years of research, no vaccine is available. A major obstacle is the virus' extreme genetic variability and rapid mutational escape from immune pressure. Improvements in the vaccine design process are urgently needed. Coupling data mining with spin glass models and maximum entropy inference, we have developed a computational approach to translate sequence databases into empirical fitness landscapes. These landscapes explicitly connect viral genotype to phenotypic fitness and reveal vulnerable targets that can be exploited to rationally design immunogens. Viewing these landscapes as the mutational “playing field” over which the virus is constrained to evolve, we have integrated them with agent-based models of the viral mutational and host immune response dynamics, establishing a data-driven immune simulator of HCV infection. We have employed this simulator to perform in silico screening of HCV immunogens. By systematically identifying a small number of promising vaccine candidates, these models can accelerate the search for a vaccine by massively reducing the experimental search space.

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**  
**Session H36 GSOFT: Soft Matter at Interfaces (Surfactants)** 339 - Jonathan Whitmer, Notre Dame

**2:30PM H36.00001 Stretching and ordering of amyloid fibrils at liquid interfaces** , EMANUELA DEL GADO, Georgetown University, KONRAD SCHWENKE, SOPHIA JORDENS, IVAN USOV, RAFFAELE MEZZENGA, ETH Zurich, GEORGETOWN UNIVERSITY TEAM, ETH ZURICH TEAM — We investigate the formation of nematic domains, which might be precursor of plaque formation, in the adsorption of amyloid fibrils at liquid interfaces. Combining experiments and computer simulations we analyse spatial correlations in the nematic order and in apparent persistence length. Non-equilibrium numerical simulations provide new insight into the coupling between those quantities. The emerging scenario is that the out-of-equilibrium adsorption favors the formation of spatial heterogeneities due to the presence of local nematic order that tend to persist upon increasing the surface coverage. Such structural heterogeneities are directly coupled to the apparent straightening of the fibrils and might affect the density and the mechanical properties of the final self-assembled material.

**2:42PM H36.00002 Effect of headgroup-substrate interactions on the thermal behavior of long-chain amphiphiles** , SARANSHU SINGLA, HE ZHU, Graduate Student, ALI DHINOJWALA, Professor — The structure of amphiphilic molecules at liquid/solid and solid/solid interfaces is relevant in understanding lubrication, colloid stabilization, chromatography, and nucleation. Here, we characterize the interfacial structures of long chain amphiphilic molecules with different head groups (OH, COOH, NH<sub>2</sub>) using interface-sensitive sum frequency generation (SFG) spectroscopy. The behavior of these self-assembled monolayers (SAMs) on sapphire substrate is recorded in situ as a function of temperature (above and below bulk  $T_m$ ) using SFG. Previous studies using synchrotron X-ray reflectivity and SFG show that the melting point of an ordered hexadecanol monolayer is around 30C above its bulk  $T_m$ . The thermal stability of the monolayer is explained due to strong hydrogen bonding interactions between the head-group and the sapphire substrate. The strength of these hydrogen-bonding interactions between substrate and different head groups is calculated using the Badger-Bauer equation. Below  $T_m$ , the ordered monolayer influenced the structure of the interfacial crystalline layer, and the transition from monolayer to the bulk crystalline phases. The results with different head groups will be presented.

**2:54PM H36.00003 The role of hydrophobic mismatch in tuning lipid membrane dynamics** , ELIZABETH KELLEY, National Institute of Standards and Technology, RANA ASHKAR, Oak Ridge National Laboratory, ROBERT BRADBURY, National Institute of Standards and Technology, ANDREA WOODKA, United States Military Academy, MICHIOHITO NAGAO, PAUL BUTLER, National Institute of Standards and Technology — Lipid membranes undergo an array of conformational and dynamic transitions, ranging from individual lipid motions to undulations of micron-sized patches of the membrane. However, the collective dynamics at intermediate length scales are largely unexplored due to experimental challenges in accessing the appropriate length and time scales. Here we use neutron spin echo spectroscopy (NSE) to provide unique insights into these elusive dynamics and measure membrane mechanical properties by probing both bending and thickness fluctuations in model lipid bilayers. We show that hydrophobic mismatch between lipids with different acyl chain lengths tunes the dynamics in a way not achievable in single component systems. For example, the thickness fluctuation amplitude is enhanced in the fluid phase of mixed lipid bilayers, reaching approximately 20% of the bilayer thickness. Combining these experimental results with deformation free energy calculations suggests the mixed bilayers are more compressible than single component bilayers and provides new insights into the role of lipid diversity in controlling the rich dynamics of biomembranes.

**3:06PM H36.00004 Interplay Between Hydrophobic Effect and Dipole Interactions in Peptide Aggregation** , SAI GANESAN, SILVINA MATYSIAK, Univ of Maryland-College Park — In the past decade, the development of various coarse-grained models for proteins have provided key insights into the driving forces in folding and aggregation. We recently developed a low resolution Water Explicit Polarizable PROtein coarse-grained Model by adding oppositely charged dummy particles inside protein backbone beads. With this model, we were able to achieve significant  $\alpha/\beta$  secondary structure content, without any added bias. We now extend the model to study peptide aggregation at hydrophobic-hydrophilic interface using elastin-like octapeptides (GV)<sub>4</sub> as a model system. A condensation-ordering mechanism of aggregation is observed in water. Our results suggest that backbone interpeptide dipolar interactions, not hydrophobicity, plays a more significant role in fibril-like peptide aggregation. We observe a cooperative effect in hydrogen bonding or dipolar interactions, with increase in aggregate size in water and interface. Based on this cooperative effect, we provide a potential explanation for the observed nucleus size in peptide aggregation pathways. Without dipolar particles, peptide aggregation is not observed at the hydrophilic-hydrophobic interface. Thus, the presence of dipoles, not hydrophobicity plays a key role in aggregation observed at hydrophobic interfaces.

**3:18PM H36.00005 Theory of Kinetics of Registration and Anti-Registration in Lipid Bilayers** , PETER OLMSTED, JOHN WILLIAMSON, Georgetown University — Lipid bilayer leaflets are often treated as if they are coupled; i.e., that the two leaflets undergo simultaneous transitions between phases, and that domains involve both leaflets together in a registered fashion. We present theory and simulation showing how interleaflet couplings and hydrophobic mismatch can lead to a complex phase diagram with multiple metastable two-phase and three-phase states. Many of these states can be discerned in the experimental literature, and are expected in the early stages of coarsening when domains are sub-micron (and thus perhaps of significance to lipid rafts). We present different kinetic scenarios for transitions between these state, and show how lipid flip flop can surprisingly lead to non-symmetric anti-registered patterns.

**3:30PM H36.00006 The activity of MscL in asymmetric droplet interface bilayers.**<sup>1</sup> , JOSEPH NAJEM, Virginia Polytechnic Institute and State University , SERGEI SUKHAREV, University of Maryland, DONALD LEO, University of Georgia — The ability to host and activate MscL, a large-conductance channel and osmolyte release valve, in a droplet interface bilayer (DIB) has been demonstrated. In previous work, the V23T mutant of MscL produced a reliable activation when axial compression is applied to the droplets supporting the lipid bilayer. Near maximal compression, the aqueous droplets deform and the resulting increase in surface area leads to an increase in tension in the water-lipid-oil interface. This increase in tension is the product of the relative change in the droplet surface area and the elastic modulus of the DPhPC monolayer (120 mN/m). However, a relatively high potential (~100 mV) is also needed to be applied in order to activate the channels. Here, we use two different types of lipids to form asymmetric DIBs. As a result of an asymmetric interface, a transmembrane potential is created across the membrane (~130 mV) due to the difference in the dipole potentials of both lipids. When MscL channels are incorporated in the bilayer, they are activated upon mechanical stimulation, without the need to apply a high external potential. We also observed that the channels became more susceptible to gating upon the application of a negative potential, compared to when a positive potential is applied, proving their sensitivity to voltage polarity.

<sup>1</sup>We would like to acknowledge the financial support provided by the Air Force Office of Scientific Research Basic Research Initiative Grant FA9550-12-1-0464.

**3:42PM H36.00007 Dynamic surface tension measurements with maximum bubble pressure tensiometry** , NORMAN MORENO, THEODORE WALKER, ADAM BURSHAN, VIVEK SHARMA, Chemical Engineering, University of Illinois at Chicago — Dynamic surface tension refers to the time dependent variation in surface tension, and is intimately linked with the rate of mass transfer of a surfactant from liquid sub-phase to the interface. The diffusion- or adsorption-limited kinetics of mass transfer to interfaces is said to impact the so-called foamability and the Gibbs-Marangoni elasticity of surfaces. Dynamic surface tension measurements carried out with conventional methods like pendant drop analysis, Wilhelmy plate, etc are limited in their temporal resolution (>50 ms). In this study, we describe design and application of maximum bubble pressure tensiometry for the measurement of dynamic surface tension effects at extremely short (1-50 ms) timescales. Using experiments and theory, we discuss the challenges and experimental constraints related with the maximum bubble pressure tensiometry measurement.

**3:54PM H36.00008 Compression-Induced Fusion of Glassy Core Polymer Micelles at the Air-Water Interface**, HYUN CHANG KIM, YOU-YEON WON, Purdue Univ — The surface mechanical and morphological properties of glassy core polymer micelles at the air-water interface were investigated. Asymmetric PS-PEG and PtBMA-PEG block copolymers with PEG weight fractions larger than 0.5 were formulated in the form of aqueous micelles and spread onto water. Compressed films of PS-PEG and PtBMA-PEG micelles reach high dynamic surface pressures. On the detailed level, however, PS-PEG and PtBMA-PEG micelles exhibit different surface pressure-area profiles. The PtBMA-PEG isotherm shows a transition to a plateau around a surface pressure of 24 mN/m, which is attributed to the PtBMA block as it forms a continuous film; this interpretation is supported by the fact that the surface pressure at the plateau transition is identical to the value of the spreading coefficient for PtBMA. This presents evidence that the core domains of PtBMA-PEG micelles melt and merge into a film when the micellar monolayer is laterally compressed. Such behavior was not observed with PS-PEG micelles. We suspect that under lateral compression, PtBMA-PEG micelles undergo fusion into a continuous film because PtBMA has the natural tendency to spread on the water surface, whereas PS-PEG micelles does not because the dewetting tendency of PS preventing formation of a uniform layer.

**4:06PM H36.00009 Temperature Dependent Rotational Correlation in Lipids**, CHRISTINA OTHON, NEDA DADASHVAND, EDUARDO VEGA LOZADA, Wesleyan University — The lateral heterogeneity of lipid dynamics is explored in free standing lipid monolayers. As the temperature is lowered the lipids exhibit increasingly broad and heterogeneous rotational correlation. This increase in heterogeneity appears to exhibit a critical onset, similar to those observed for glass forming fluids. We explore this heterogeneous relaxation by measuring the rotational diffusion of a fluorescent probe (NBD-PC) using wide-field time-resolved fluorescence anisotropy microscopy, in single constituent lipid monolayer of DMPC. The observed relaxation exhibits a narrow, liquid-like distribution at high temperatures ( $\tau \sim 2.4$  ns), consistent with previous experimental measures by different methods. However, as the temperature is quenched, the distribution broadens, and we observe the appearance of a long relaxation population (16.5 ns). This demonstrates that the nanoscale diffusion and reorganization in lipid structures can be significantly complex, even in the simplest unstructured architectures. This result can have a significant impact on the organization, permeability and energetics of natural membrane structures.

**4:18PM H36.00010 Interfacial microrheology study of layer formation by staphylococcal nuclease protein and its disordered variant**, BILYANA TZOLOVA, Johns Hopkins University, DANIEL ALLAN, Brookhaven National Lab, DANIEL FIRESTER, BERTRAND GARCIA-MORENO, DANIEL REICH, ROBERT LEHENY, Johns Hopkins University — We study the formation of layers of staphylococcal nuclease protein adsorbing at the air-water interface. In a series of experiments, we follow the evolution of the rheological response of the layer using an active microrheology technique that involves tracking the rotational motion of magnetic nanowires at the interface in response to time-dependent external magnetic fields. At early stages of layer formation, the wire mobility can be interpreted using a model for viscous drag with an interfacial viscosity that increases rapidly with layer age; however, at later ages deviations from a simple viscous response indicating non-Newtonian behavior are observed. We compare the evolution in microrheology of layers forming from wild-type protein that assumes a folded conformation in solution with a variant that is disordered due to substitution of a single amino acid, thereby gaining a perspective on the impact of initial protein state on the layer formation and rheology.

**4:30PM H36.00011 Interaction of water with melittin inserted in a single-supported lipid bilayer<sup>1</sup>**, ZACHARY BUCK, MENGJUN BAI, JAMES TORRES, HELMUT KAISER, HASKELL TAUB, Univ. of Missouri - Columbia, FLEMMING Y. HANSEN, Technical University of Denmark, ANDREW MISKOWIEC, Oak Ridge National Lab, MADHUSUDAN TYAGI, NIST Center for Neutron Research — The insertion mechanism, conformation, and the function of transmembrane proteins are strongly influenced by both the lipid molecules and the hydration water of a cell membrane. Previously, we have fabricated samples of single-supported lipid bilayers of zwitterionic DMPC and studied extensively their influence on the freezing behavior and diffusion of water in their vicinity [2]. We have recently extended these studies to a more biologically relevant system by depositing melittin proteins onto single-supported DMPC bilayers. By monitoring the elastically-scattered neutron intensity as a function of temperature from such samples, we observe an abrupt freezing transition of the associated water not seen in the bare membrane case. Moreover, the change in elastic intensity of this freezing step increases proportionally with melittin concentration. For a particular peptide concentration, a small increase of the elastically-scattered neutron intensity is measured while annealing the sample at 328 K. We tentatively interpret this increase of the elastic intensity to anchoring and/or insertion of the melittin peptides within the membrane. <sup>2</sup>M. Bai *et al.*, Europhys. Lett. **98**, 48006 (2012).

<sup>1</sup>Supported by NSF Grant Nos. DMR-0944772 and DGE-1069091

**4:42PM H36.00012 Formation, disruption and mechanical properties of a rigid hydrophobin film at an air-water interface<sup>1</sup>**, LYNN WALKER, STEPHANIE KIRBY, SHELLEY ANNA, Carnegie Mellon Univ, CMU TEAM — Hydrophobins are small, globular proteins with distinct hydrophilic and hydrophobic regions that make them extremely surface active. The behavior of hydrophobins at surfaces has raised interest in their potential industrial applications, including use in surface coatings, food foams and emulsions, and as dispersants. Practical use of hydrophobins requires an improved understanding of the interfacial behavior of these proteins, both individually and in the presence of surfactants. Cerato-ulmin (CU) is a hydrophobin that has been shown to strongly stabilize air bubbles and oil droplets through the formation of a persistent protein film at the interface. In this work, we characterize the adsorption behavior of CU at air/water interfaces by measuring the surface tension and interfacial rheology as a function of adsorption time. CU is found to strongly, irreversibly adsorb at air/water interfaces; the magnitude of the dilatational modulus increases with adsorption time and surface pressure, until the CU eventually forms a rigid film. The persistence of this film is tested through the addition of SDS, a strong surfactant, to the bulk. SDS is found to co-adsorb to interfaces pre-coated with a CU film. At high concentrations, the addition of SDS significantly decreases the dilatational modulus, indicating disruption and displacement of CU. These results lend insight into the complex interfacial interactions between hydrophobins and surfactants.

<sup>1</sup>Funding from GoMRI

**4:54PM H36.00013 Boundary condition in liquid thin films revealed through the thermal fluctuations of their free surfaces**, BASILE POTTIER<sup>1</sup>, LAURENCE TALINI, CHRISTIAN FRTIGNY, SIMM — We investigate the properties of liquids confined at nanometric scales from a solid wall with a new noninvasive technique. The optical technique used consists of measuring the height of fluctuations of the free surface, using the reflection of a laser beam on that surface. We hence measure the spontaneous thermal fluctuations of the free surfaces of liquids to probe their hydrodynamic boundary condition at a solid wall. The surface fluctuations of a silicon oil film could be described with a no-slip boundary condition for film thicknesses down to 20 nm. Oppositely, a 4 nm negative slip length had to be introduced to describe the behavior of n-hexadecane, consistently with previous surface force apparatus data on the same system. Our results demonstrate that at vanishing flow, a nanometric solid-like layer close to the wall may exist according to the nature of the liquid.

<sup>1</sup>currently at Laboratoire de Physique ENS Lyon

**5:06PM H36.00014 Charge Effects on Surfactant Membrane Thickness Fluctuations**, ROBERT BRADBURY, MICHIOHRO NAGAO, Indiana University — The mechanical properties of surfactant bilayer membranes have been measured over a range of surface charge densities using small-angle neutron scattering and neutron spin echo spectroscopy. An increase in the surface charge density leads to a stiffening of the membrane, which is consistent with classical theory of charge effects on membranes. The fluctuations in the membrane thickness, however, become slower with increasing charge density, which can be explained by an increase in the membrane viscosity as predicted by Bingham *et al.* We suggest that an increase in the repulsive interactions between the charged headgroups is responsible for this increased membrane viscosity. Furthermore, the amplitude of the thickness fluctuations is observed to remain almost constant with variation in surface charge density which suggests almost constant values for the total compressibility modulus of the bilayer and the optimum fluctuation wavelength. This indicates that the time scale and amplitude of membrane thickness fluctuations are controlled by different membrane effects. This work demonstrates that charge stabilization of lamellar bilayers is not merely affected by inter-membrane interactions but that intra-membrane dynamics also have a significant contribution.

**5:18PM H36.00015 Branching mechanisms in surfactant micelles.**<sup>1</sup>, SUBAS DHAKAL, Department of Biomedical and Chemical Engineering, Syracuse University, Syracuse, NY, RADHAKRISHNA SURESHKUMAR, Department of Biomedical and Chemical Engineering and Department of Physics, Syracuse University, Syracuse, NY — The mechanisms of branch formation in surfactant micelles of cetyltrimethylammonium chloride (CTAC) in presence of sodium salicylate (NaSal) counter ions in water are studied using molecular dynamics simulations. The curvature energy associated with the formation of micelle branches and the effect of branching on the solution viscosity are quantified. Highly curved surfaces are energetically stabilized by a higher density of binding counter ions near the branch points. Simulations show that micellar branches result in a significant reduction in the solution viscosity as observed in experiments [Dhakal & Sureshkumar, J. Chem. Phys. 143, 024905 (2015)]. This reduction in viscosity has long been attributed to the sliding motion of micelle branches across the main chain. However, to date, such dynamics of micelle branches have never been visualized in either experiments or simulations. Here, we explicitly illustrate and quantify, for the first time, how branches slide along the micelle contour to facilitate stress relaxation.

<sup>1</sup>We acknowledged the computational resources provided by XSEDE which is supported by NSF grant number OCI-1053575 and the financial support by National Science Foundation under Grants 1049489 and 1049454.

## **Tuesday, March 15, 2016 2:30PM - 5:30PM – Session H37 GSOFT: Clustering and Gelation with Competing Interactions II 340 - Yun Liu, NIST**

**2:30PM H37.00001 Implicit depletion of anisotropic particles**, JENS GLASER, ANDREW KARAS, SHARON GLOTZER, Univ of Michigan - Ann Arbor — Entropy mediates depletion interactions between particles with excluded volume. We implement a novel algorithm [1] to simulate this emergent attraction between hard anisotropic particles in the presence of penetrable hard spheres. Our algorithm is efficient because it integrates out the degrees of freedom of the ideal depletant gas in parallel, which makes it well suited for high-performance computing. The algorithm can achieve several orders of magnitude speed-up over explicit algorithms. As an application we study the interplay between phase separation and kinetic arrest in the anisotropic clustering of colloidal discoids [2]. We also discuss applications of the algorithm for the assembly of hemispheres [1] and of cuboctahedra [3]. [1] J. Glaser, A. S. Karas, and S. C. Glotzer, arXiv:1508.07077. [2] L. C. Hsiao, B. A. Schultz, J. Glaser, M. Engel, M. E. Szakasits, S. C. Glotzer, and M. J. Solomon, Nat. Commun. 6, 8507 (2015). [3] A. S. Karas, J. Glaser, and S. C. Glotzer, arXiv:1510.04236.

**2:42PM H37.00002 Interplay of directional and isotropic interactions in self-assembly**, DEBRA AUDUS, National Institute of Standards and Technology, FRANCIS STARR, Wesleyan University, JACK DOUGLAS, National Institute of Standards and Technology — Patchy particle models, composed of hard spheres with decorated with attractive patches, have been introduced as models of micron-sized particles with anisotropic interactions, as well as solutions of globular proteins. Here, we extend the canonical model of the patchy particles to include a short-ranged isotropic interaction in order to probe of the coupling of the directional and isotropic interactions on the self-assembly process. In particular, we evaluate basic properties characterizing self-assembly including average cluster mass and the fraction of particles in the clustered state using both Monte Carlo simulation and analytic Wertheim theory. This combination allows for validation of the theory and for insight into analyzing experimental data. We also find that Flory-Stockmayer theory describes the cluster size distribution data found in our simulations remarkably well, despite its erroneous mass-scaling exponent. This result, coupled with Wertheim theory, predicts both a master curve for the average cluster mass and a method to parameterize patchy particle models using experimental data.

**2:54PM H37.00003 Effective potentials in concentrated colloid-polymer mixtures with competing interactions**, MARCO LAURATI, NESTOR VALADEZ PEREZ, Universidad de Guanajuato, RONJA CAPELLMANN, STEFAN EGELHAAF, University of Düsseldorf, RAMON CASTAÑEDA-PRIEGO, Universidad de Guanajuato — We determine the effective potentials describing the interactions between colloidal particles in concentrated colloid-polymer mixtures in which depletion attraction competes with electrostatic repulsion. To obtain the potentials, the method of Monte-Carlo inversion is applied to experimental pair distribution functions obtained by confocal microscopy. Both fluid and gel states are investigated. We compare the results of the inversion method with those obtained by describing the interactions using a combination of a square well potential for the attractive component and a Yukawa potential for the repulsive component. This allows us to test the validity range of the one-component pair-potential.

**3:06PM H37.00004 Short-time dynamics in dispersions with competing short-range attraction and long-range repulsion**, RIEST JONAS, GERHARD NAEGELE, Institute of Complex Systems (ICS-3), Forschungszentrum Juelich GmbH, 52425 Juelich, Germany — The dynamic clustering of globular particles in suspensions exhibiting competing short-range attraction and long-range repulsion such as in protein solutions has gained a lot of interest over the past years. We investigate theoretically the influence of clustering on the dynamics of globular particle dispersions [1]. To this end, we systematically explore various pair potential models by a combination of state-of-the-art analytic methods in conjunction with computer simulations where the solvent-mediated hydrodynamic interactions are likewise included. Our theoretical results show that the cluster peak (intermediate-range-order peak) is present also in the hydrodynamic function characterizing the short-time dynamics, in accord with new experimental data [2]. Enhanced short-range attraction leads to a smaller self-diffusion coefficient and a larger dispersion viscosity. The behavior of the (generalized) sedimentation coefficient is more intricate, e.g. showing a non-monotonic interaction strength dependence.

[1] J. Riest & G. Nägele, *Soft Matter* (2015). doi:10.1039/C5SM02099A

[2] Collaboration with D. Godfrin (NIST & MIT), Y. Liu (NIST) and N. Wagner (UDEL), work in progress

**3:18PM H37.00005 Rheology of clustering protein solutions**, STEVEN HUDSON, NIST, VISHNU DHARMARAJ, Montgomery Blair High School, P. DOUGLAS GODFRIN, MIT, YUN LIU, NIST — Here we explore the rheology of low-salt lysozyme solutions, with special interest in the extremes of high concentration and low temperature. Under these conditions, reversible clustering of protein governed by their competing short-range attraction and long-range repulsion markedly enhances viscosity. Even in these conditions, the solutions exhibit Newtonian behavior over a wide range of shear rates. To test for departures from Newtonian behavior, we examined still higher shear rates. At shear rates in excess of 10,000 /s, we find reversible shear thinning at 40 % mass fraction. These results reveal dynamics of the protein clusters and are compared with other measurements of solution dynamics by neutron spin echo scattering and dynamic light scattering.

**3:30PM H37.00006 Monte Carlo simulation studies of diffusion in crowded environments**, PRITHVIRAJ NANDIGRAMI, Kent State University, BRANDY GROVE, Case Western Reserve University, ANDREW KONYA, ROBIN SELINGER, Kent State University — Anomalous diffusion has been observed in protein solutions and other multi-component systems due to macromolecular crowding. Using Monte Carlo simulations, we investigate mechanisms that govern anomalous diffusive transport and pattern formation in a crowded mixture. We consider a multi-component lattice gas model with “tracer” molecules diffusing across a density gradient in a solution containing sticky “crowder” molecules that cluster to form dynamically evolving obstacles. The dependence of tracer flux on crowder density shows an intriguing re-entrant behavior as a function of temperature with three distinct temperature regimes. At high temperature, crowders segregate near the tracer sink but, for low enough overall crowder density, remain sufficiently disordered to allow continuous tracer flux. At intermediate temperature, crowders segregate and block tracer flux entirely, giving rise to complex pattern formation. At low temperature, crowders aggregate to form small, slowly diffusing obstacles. The resulting tracer flux shows scaling behavior near the percolation threshold, analogous to the scenario when the obstacles are fixed and randomly distributed. Our simulations predict distinct quantitative dependence of tracer flux on crowder density in these temperature limits.

**3:42PM H37.00007 On shape and charges in colloidal dispersions**, EMMANUEL TRIZAC, Univ. Paris-Sud — Coulomb interactions are paramount in determining structural and dynamical properties for a wealth of anisotropic soft matter systems (clays, mineral crystallites, exfoliated nanosheets, patchy colloids, cement etc). The interplay between screening effects and anisotropy leads to distinctive yet often overlooked features, that will be discussed. In turn, the competition between the resulting effective potential and hard core constraints will be addressed. This competition can lead to non trivial structures, or impose strong dynamical slowing down. A distinction will be operated between weak and strong Coulomb coupling regimes.

**4:18PM H37.00008 Wetting-induced clustering and phoretic motions of colloidal particles**, THEYENCHERI NARAYANAN, ENRICO SEMERARO, RAJIV DATTANI, ESRF The European Synchrotron, F-38043, Grenoble — In recent years, self-propelled colloidal systems have received considerable attention as models for active matter. Most commonly used synthetic self-propelled systems involve Janus particles with asymmetric chemical composition in a catalytic medium. An analogous behavior can be obtained when particles are suspended in a phase separating binary liquid mixture due to preferential adsorption of one of the liquid species on the colloidal particles. Above an aggregation temperature ( $T_A$ ), particles become attractive and aggregate to form compact colloidal clusters. In the two phase region of the binary mixture, particles partition into the phase rich in adsorbed component. We have used silica colloids suspended in a binary mixture of 3-methyl pyridine and heavy water to probe this adsorption-induced phoretic motion of particles. Using ultra small-angle X-ray scattering and photon correlation spectroscopy, we investigated the static and dynamic behavior of this system. In the one phase region below  $T_A$ , particles display a repulsive structure factor with diffusive dynamics. In the two-phase region of the host liquid, the static structure is similar but the dynamics is strongly enhanced with the onset of phase separation reminiscent of self-propelled motion.

**4:30PM H37.00009 Multiscale simulations of nanoribbon structures from chromophore amphiphile self-assemblies**, DONGXU HUANG, ZHENWEI YAO, MONICA OLVERA, SAMUEL STUPP, Northwestern University — Finite-width self-assembled one-dimensional nanostructures have many potential applications as electronically or biologically active materials. Understanding the driving forces for supramolecular self-assembly is essential for the molecular design of new highly functional structures. Here we use multi-scale molecular dynamics simulations to study the self-assembly of chromophore amphiphiles into a nanoribbon previously shown to be useful in photocatalysis [1]. We demonstrate that the nanoribbon structure is a result of the competition between electrostatics and the hydrophobic effect. We incorporate a scaling analysis that correlates the electrostatic strength with the finite width of the ribbon. These results with additional numerical calculations show that anisotropy of the short-range intermolecular interactions and long-range electrostatics can be used to control the dimensionality of these systems. [1] Adam S. Weingarten, Roman V. Kazantsev, Liam C. Palmer, et al. & Samuel I. Stupp, Nature Chemistry, 2014

**4:42PM H37.00010 Self-assembly of Ionic Chromonic Liquid Crystals**, HYTHEM SIDKY, JONATHAN K. WHITMER, University of Notre Dame — Chromonic liquid crystals exhibit a unique self-assembly process which is of both theoretical and practical interest. A characteristic feature of chromonics is the occurrence of molecular association through stacking at extremely low concentrations. Experimental evidence has suggested that this process is approximately isodesmic across a broad concentration range. To date, only a handful of computational studies have managed to reproduce crucial aspects of chromonic phases, using expensive atomistic simulations. Here, we present a minimal model capable of capturing key features of the lyotropic chromonic phase. Molecular simulations of coarse-grained mesogens are used to map out the phase behavior and explore how structural and energetic anisotropies influence their ordering and response.

**4:54PM H37.00011 Lipid domains in zwitterionic-anionic lipid mixtures induced by combined effect of monovalent and divalent ions**, HONGCHENG XU, Biophysics Program, University of Maryland, College Park, SAI GANESAN, Fischell Department of Engineering, University of Maryland, College Park, SILVINA MATYSIAK, Biophysics Program, Fischell Department of Engineering, University of Maryland, College Park — Lipid domain formation is an important process for many cellular processes. In experiment, the effects of  $\text{Ba}^{2+}$ ,  $\text{Sr}^{2+}$ ,  $\text{Ca}^{2+}$  and  $\text{Mg}^{2+}$  in inducing lateral phase separation in the binary phosphatidylcholine-phosphatidylserine (PC-PS) bilayer are quite different, of which the molecular mechanism remains to be understood. We have explored the effect of monovalent (MI) and divalent (MII) cationic radii on lipid domain formation in mixed zwitterionic-anionic lipid bilayers. We propose a mechanism for the formation of divalent-cation-induced lipid domains based on MD simulations with our Water-Explicit Polarizable MEMbrane (WEPMEM) coarse-grained model, which uses PC as the model for zwitterionic and PS for anionic lipids. Lipid aggregation only occurs with limited range of monovalent and divalent ion sizes in agreement with experimental observations. More ordering and closer packing of the lipids are noted within the domains, which correlate with bilayer thickness, curvature and lipid asymmetry. The results of the simulations reveal that the lipid domain consists of MII-mediated anionic lipid dimer/trimer complexes bridged by monovalent ions MI and provide a stereochemical insight in understanding the experimentally observed calcium-induced phase separation.

**5:06PM H37.00012 The morphology of small sized clusters in a system with the competing interactions**, YUN LIU, NIST Center for Neutron Research, Gaithersburg, MD, USA, NSTOR VALADEZ-PREZ, RAMON CASTAEDA-PRIEGO, Department of Physical Engineering, University of Guanajuato, Mexico — We have systematically investigated the morphological changes of clusters in a system with both a short-ranged attraction and long-ranged repulsion, which is ubiquitous for protein solutions. Interestingly, even though the delicate balance between the attraction and repulsion controls the fractal dimension of the large clusters, the overall sizes of small clusters seem to be sensitive only to the short-ranged attraction. This microscopic structure change is thus consistent with and provides a microscopic physical picture of the recently proposed general phase diagram where the attractive interaction controls the formation of clustered fluid in the one phase region.

**5:18PM H37.00013 Viscoelastic properties of DNA coated colloid suspensions**, CHRISTINE MIDDLETON, DAVID PINE, New York University — DNA coated colloids are a unique gel forming system because of their tunable short range attraction. The interparticle potential can be varied through the chosen DNA sticky end, the particle coating density, and the temperature. We present studies of how these parameters affect the viscoelastic properties of suspensions of DNA coated colloids around the gel transition.

**Tuesday, March 15, 2016 2:30PM - 5:30PM —**

**Session H38 DPOLY FIAP: Polymer Nanocomposites: Dynamics** 341 - Laura Clarke, NC State University

**2:30PM H38.00001 Dynamics in Polymer Melts and Nanocomposites**, GERALD SCHNEIDER, Louisiana State Univ - Baton Rouge — Intense research has led to substantial progress in the field of polymer melts and nanocomposites, both regarding the fundamental understanding and the relationship to applications. From a fundamental point of view, knowing the microscopic single chain dynamics is important. It may even lead to optimized materials ranging from the classical car tire to battery or fuel cell applications. In polymer melts, different processes, such as diffusion, reptation, contour length fluctuations, etc. occur and determine the macroscopic results, e.g. obtained by rheology. In nanocomposites confinement effects and interactions of chains with surfaces play an important role. High resolution techniques, such as small-angle neutron scattering or neutron spin echo spectroscopy are suited to explore the structure and dynamics of chains. The presentation illuminates the fundamental relationship between the microscopic dynamics and the mesoscopic properties, exploiting different experimental techniques, such as dielectric spectroscopy, rheology, neutron scattering and neutron spin echo spectroscopy.

**2:42PM H38.00002 Phase Stability and Dynamics of nanoparticles in Polymer Nanocomposites**, RAHUL MANGAL, Cornell University, SAMANVAYA SRIVASTAVA, The University of Chicago, LYNDEN ARCHER, Cornell University — In polymer nanocomposites, polymer grafted nanoparticles, where the tethered polymer chains are chemically identical to the host chains, have been reported to irreversibly aggregate if the length of host chains (P) become 5 or more times larger than the length tethered chains (N) due to the autophobic dewetting of the polymer brush. Utilizing Small Angle X-ray scattering as a tool, here we show that by choosing appropriate chemistry one can utilize the enthalpic attractions between the tethered chains and host chains to facilitate uniform nanoparticle dispersion in very large  $M_w$  hosts ( $P/N \sim 140$ ). A generic phase diagram has also been proposed. X-ray Photon Correlation Spectroscopy (XPCS) is employed as a sensitive probe of nanoparticle relaxation dynamics to investigate particle dynamics in these model PNCs. Remarkably, we find that for nanoparticle size  $D$ , slightly larger than the tube diameter of the host polymer ( $a$ ), particles undergo a transition from normal diffusion to hyperdiffusive relaxation dynamics. In contrast, for unentangled hosts, diffusive particle relaxation are observed. Our experimental observations are rationalized by finding that nanoparticle motion in entangled melts only disturb sub-chain entangled segments of size comparable to the particle diameter.

**2:54PM H38.00003 Nanoparticle effect on polymer chain dynamics and entanglement network<sup>1</sup>**, YING LI<sup>2</sup>, University of Connecticut, MARTIN KROGER, ETH Zurich — We investigated structure and dynamics of polymer nanocomposites through molecular modeling, by considering different molecular weights of polymers chains, and volume fractions of fillers. The dynamics of unentangled chains can be separated into two phases, a bulk polymer phase and a confined polymer phase between fillers. The dynamics of a confined polymer is slower than that of a bulk polymer, while still exhibiting high mobility. The amount of the bulk polymer phase is found to exponentially decay with increasing volume fraction of fillers. When highly entangled polymer chains are confined between fillers, their conformation and entanglement network are dramatically changed, in district with their unentangled counterparts. The entangled polymer chains are found to be significantly disentangled and flattened during increment of the volume fractions of spherical nonattractive fillers. A critical volume fraction is found to control the crossover from polymer chain entanglements to 'nanoparticle entanglements', below which the polymer chain relaxation accelerates upon filling. These results provide a microscopic understanding of the dynamics of entangled polymer chains inside their composites, and offer an explanation for the unusual rheological properties of polymer composites.

<sup>1</sup>Supported by Department of Mechanical Engineering, University of Connecticut

<sup>2</sup>Membership Pending

**3:06PM H38.00004 Thermally induced infiltration of polymer into nanoparticle packings**, JYO LYN HOR, University of Pennsylvania, Department of Chemical and Biomolecular Engineering, YIJIE JIANG, KEVIN T. TURNER, University of Pennsylvania, Department of Mechanical Engineering and Applied Mechanics, DAEYEON LEE, University of Pennsylvania, Department of Chemical and Biomolecular Engineering — We present a novel approach in generating three-phase polymer nanocomposites via capillary rise infiltration (CaRI) of polymer into a dense nanoparticle packing, which we have previously utilized to generate dense nanocomposites with extremely high filler fraction. The CaRI process involves first generating a bilayer film of porous nanoparticle layer on a polymer layer, followed by annealing of the bilayer above the  $T_g$  of the polymer to induce polymer infiltration into the voids of the nanoparticle layer. By tuning the amount of polymer to be less than the void volume of the nanoparticle layer, we demonstrate that CaRI is capable of generating spatially homogeneous porous composite. We utilize spectroscopic ellipsometry to characterize and monitor the polystyrene infiltration process into the titania nanoparticle packing in-situ. The infiltration process occurs in two stages. Upon annealing, we observe that the polymer layer is depleted rapidly via capillary-induced infiltration to form a dense composite at the base of the nanoparticle packing. Eventually, the front of this composite layer propagates throughout the nanoparticle packing, just as the composite refractive index decreases, indicating the redistribution of polymer throughout the nanoparticle matrix.

**3:18PM H38.00005 The effect of chain rigidity on the interfacial layer thickness and dynamics of polymer nanocomposites.**, SHIWANG CHENG, JAN-MICHAEL Y. CARRILLO, Oak Ridge National Laboratory, BOBBY CARROLL, Department of Physics and Astronomy, University of Tennessee, BOBBY G. SUMPTER, Oak Ridge National Laboratory, ALEXEI P. SOKOLOV, Department of Chemistry, University of Tennessee — There are growing experimental evidences showing the existence of an interfacial layer that has a finite thickness with slowing down dynamics in polymer nanocomposites (PNCs). Moreover, it is believed that the interfacial layer plays a significant role on various macroscopic properties of PNCs. A thicker interfacial layer is found to have more pronounced effect on the macroscopic properties such as the mechanical enhancement. However, it is not clear what molecular parameter controls the interfacial layer thickness. Inspired by our recent computer simulations that showed the chain rigidity correlated well with the interfacial layer thickness,[1] we performed systematic experimental studies on different polymer nanocomposites by varying the chain stiffness. Combining small-angle X-ray scattering, broadband dielectric spectroscopy and temperature modulated differential scanning calorimetry, we find a good correlation between the polymer Kuhn length and the thickness of the interfacial layer, confirming the earlier computer simulations results. Our findings provide a direct guidance for the design of new PNCs with desired properties. [1] Carrillo, J.-M. Y. *et al*; *Macromolecules* **2015**, *48*, (12), 4207-4219.

**3:30PM H38.00006 Fragility-Controllable Polymer Grafted Nanoparticles.**<sup>1</sup> , MAKOTO ASAI, SANAT KUMAR, ANGELO CACCIUTO, Columbia Univ — 20 years ago, the concept of 'Fragility' has been suggested to categorize glass-forming liquids. Currently, we know there are two kinds of glass-forming liquids group. One is Arrhenius type liquids called as Strong glass (large Fragility). Another one is non-Arrhenius liquid called as Fragile glass (small Fragility). The physical meaning of Fragility is unknown yet, but people believe that to understand the physical meaning of Fragility leads to understand glass transition. Recently we found Polymer Grafted Nanoparticles (PGNPs) could behave like glass-forming liquids depending on their grafting density in MD simulations. Surprisingly, their Fragility can be controlled by grafting density and we can obtain both 'Strong' and 'Fragile' glass using this system.

<sup>1</sup>The authors thank the National Science Foundation for financial support of this work. AC acknowledges financial supported from the National Science Foundation under CAREER Grant No. DMR-0846426

**3:42PM H38.00007 Activated Dynamics in Dense Model Nanocomposites** , SHIJIE XIE, KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — The nonlinear Langevin equation approach is applied to investigate the ensemble-averaged activated dynamics of small molecule liquids (or disconnected segments in a polymer melt) in dense nanocomposites under model isobaric conditions where the spherical nanoparticles are dynamically fixed. Fully thermalized and quenched-replica integral equation theory methods are employed to investigate the influence on matrix dynamics of the equilibrium and nonequilibrium nanocomposite structure, respectively. In equilibrium, the miscibility window can be narrow due to depletion and bridging attraction induced phase separation which limits the study of activated dynamics to regimes where the barriers are relatively low. In contrast, by using replica integral equation theory, macroscopic demixing is suppressed, and the addition of nanoparticles can induce much slower activated matrix dynamics which can be studied over a wide range of pure liquid alpha relaxation times, interfacial attraction strengths and ranges, particle sizes and loadings, and mixture microstructures. Numerical results for the mean activated relaxation time, transient localization length, matrix elasticity and kinetic vitrification in the nanocomposite will be presented.

**3:54PM H38.00008 Effect of polymer-nanoparticle interactions on the capillary rise infiltration of polymers into nanoporous media**<sup>1</sup> , DAVID RING, AMIT SHAVIT<sup>2</sup>, ROB RIGGLEMAN, DAEYEON LEE, Univ of Pennsylvania — By wicking a polymer into a porous packing of nanoparticles, it is possible to generate polymer nanocomposites with extremely high filler fractions. Although capillary rise of simple fluids in porous media is fairly well understood based on the Lucas-Washburn model, there remain many unanswered questions related to the infiltration of high molecular weight polymer melts in nanoporous media. In this work, we probe the thermally induced infiltration of polymers into packings of nanoparticles using molecular dynamics (MD) simulations. In particular, we investigate the effect of polymer-nanoparticle interactions on the three phase contact angle of the polymer on the nanoparticle surface, and probe how the infiltration process is affected by changes in these interactions. We also study the effect of molecular weight on the capillary rise behavior of polymers in nanoparticle packings.

<sup>1</sup>XSEDE, MRSEC

<sup>2</sup>Graduated

**4:06PM H38.00009 Effects of Attractive Interactions on Nanoparticle Diffusion in Entangled Polymer Melts** , PHILIP GRIFFIN, University of Pennsylvania, NIGEL CLARKE, University of Sheffield, RUSSELL COMPOSTO, KAREN WINEY, University of Pennsylvania — Developing a complete picture for the mechanism of nanoparticle diffusion in model polymer nanocomposites remains a great challenge, especially experimentally. Using Rutherford backscattering spectroscopy, we have measured the translational diffusion coefficient of spherical nanoparticles (diameter = 20 nm) infiltrated into poly(2-vinylpyridine) melts across a range of molecular weights (35-300 kg/mol). Our results reveal that the diffusion coefficient of nanoparticles in attractive nanocomposites is several times slower than what is predicted from the melt viscosity according to the Stokes-Einstein (SE) relation. This runs contrary to recent theoretical studies of non-attractive systems, where it is predicted that nanoparticle diffusion can be many orders of magnitude faster than SE predictions. Potential explanations for this unusual slowing of nanoparticle diffusion are discussed.

**4:18PM H38.00010 Understanding the interfacial layer dynamics of polymer nanocomposites from broadband dielectric spectroscopy** , ROBERT CARROLL, SHIWANG CHENG, ALEXEI SOKOLOV, Univ of Tennessee, Knoxville — Polymer nanocomposites show many advanced mechanical, thermal, optical, and transport properties mainly due to the vast interfacial area between the polymer matrix and nanoparticles. Recent studies show that there is an interfacial polymer layer with structure and dynamics that are different from the bulk polymer, and that contributes to the advanced macroscopic properties. It has been shown that broadband dielectric spectroscopy provides good method to study the interfacial dynamics in nanocomposites. However, current dielectric spectroscopy studies ignore the heterogeneous nature of polymer nanocomposites. Models based on a simple superposition of bulk polymer and interfacial layer spectra, or those that assume the interfacial layer is dynamically dead are inaccurate. In this talk, the prevailing methods in the literature will be compared with an accurate method accounting for the heterogeneity of the nanocomposites. Different nanocomposites with well-dispersed nanoparticles will be used as examples. The analysis clearly shows that the width and the amplitude of the relaxation peaks are affected by the data analysis. Thus accurate quantitative conclusions on properties and thickness of the interfacial layer can be achieved only using heterogeneous models.

**4:30PM H38.00011 Interfacial Effect on Confined Crystallization of Poly(ethylene oxide)/Silica Composites**<sup>1</sup> , YUNLAN SU, WEIWEI ZHAO, XIA GAO, Institute of Chemistry, Chinese Academy of Sciences, JIANJUN XU, 2DSM Resolve, P.O. Box 18, the Netherlands , DUJIN WANG, Institute of Chemistry, Chinese Academy of Sciences — The impact of nanoconfinement introduced by nanoparticles on polymer crystallization has attracted extensive attention because it plays the decisive role in the ultimate properties of polymer nanocomposites. In this study, interfacial and spatial confinement effects of silica (SiO<sub>2</sub>) nanoparticles on the crystallization behaviors of poly(ethylene oxide) (PEO)/SiO<sub>2</sub> composites were systematically investigated by changing the size and concentration of SiO<sub>2</sub> in PEO matrix. The composites with high silica loadings exhibit two crystallization peaks of PEO as determined by differential scanning calorimetry (DSC). The first peak at 7–43 C is related to the bulk PEO, while the second peak at –20 to –30 C is attributed to the restricted PEO segments. Three-layer (amorphous, interfacial and bulk) model is proposed to interpret the confined crystallization of PEO/SiO<sub>2</sub> composites, which is supported by the results of thermogravimetric analysis (TGA) and solid-state <sup>1</sup>H nuclear magnetic resonance (NMR). In amorphous layer, most PEO segments are directly adsorbed on SiO<sub>2</sub> surface via hydrogen bonding. The interfacial PEO layer, which is nonuniform, is composed of crystallizable loops and tails extending from amorphous layer.

<sup>1</sup>National Natural Science Foundation of China (NSFC) under contract 21274156

**4:42PM H38.00012 Molecular Dynamics Simulations of Silica-Filled Copolymers with Variable Sequence for Applications in Tire Treads**, ALEX J. TRAZKOVICH, The Ohio State University and The Cooper Tire and Rubber Company, LISA M. HALL, The Ohio State University — We simulate a simple nanocomposite relevant to tire tread compounds consisting of a single spherical nanoparticle surrounded by coarse-grained polymer chains. The polymers are composed of two different monomer types, which have different interaction strengths with the nanoparticle. The monomer sequence can be varied to model different copolymer configurations. We study the polymer end-to-end vector autocorrelation functions to obtain relaxation times of adsorbed and bulk polymer, showing how the interphase is affected by the polymer type and the monomer-nanoparticle interaction strengths. An understanding of the effect of copolymer sequence on the range of the polymer interphase and the magnitude of the effect on chain dynamics is critical to tire tread material design since the primary polymer component of modern tire tread is styrene-butadiene rubber (SBR) copolymer, which may be synthesized in primarily random or in various blocky copolymer configurations. Macromolecular adsorption to and desorption from filler surfaces has a significant effect on hysteresis, and in tire treads, hysteresis must be controlled to optimize the tradeoff between traction and rolling resistance. Superior tire tread materials must have high hysteresis under the operating conditions of traction while maintaining low hysteresis under the operating conditions of rolling resistance. An opportunity exists to control hysteresis through the use of SBR with specific monomer sequences.

**4:54PM H38.00013 Distortion of chain conformation and reduced entanglement in polymer-graphene oxide nanocomposites**, MICHAEL WEIR, Department of Physics and Astronomy, University of Sheffield, STEPHEN BOOTHROYD, DAVID JOHNSON, RICHARD THOMPSON, KARL COLEMAN, Durham University, NIGEL CLARKE, University of Sheffield — Graphene and related two-dimensional materials are excellent candidates as filler materials in polymer nanocomposites due to their extraordinary physical properties and high aspect ratio. To explore the mechanism by which the filler affects the bulk properties of these unique systems, and to build understanding from the macromolecular level upwards, we use a combination of small-angle neutron scattering (SANS) and oscillatory rheology. Where a good dispersion is achieved in poly(methyl methacrylate)-graphene oxide (PMMA-GO) nanocomposites, we observe a reduction in the polymer radius of gyration with increasing GO concentration that is consistent with the predicted behavior of polymer melt chains at a solid interface. We use concepts from thin-film polymer physics to formulate a scaling relation for the reduction in entanglements caused by the GO interfaces. Using these scaling arguments, we utilize SANS results to directly estimate the changes to the elastic plateau modulus of the network of entangled polymer chains, and find a correlation with the measured bulk rheology. We present a direct link between interfacial confinement effects and the bulk polymer nanocomposite properties, whilst demonstrating a model system for measuring thin film polymer physics in the bulk.

**5:06PM H38.00014 Thin Film Deformation Behavior of Polystyrene Grafted Nanoparticle Assemblies**, YANG JIAO, MING-SIAO HSIAO, LAWRENCE DRUMMY, RICHARD VAIA, Air Force Research Laboratory, WPAFB — Assemblies of polymer-grafted “hairy” nanoparticles (HNPs) are of current interest for a wide array of mechanical, photonic and electrical applications. In contrast to nanoparticles dispersed in a free polymer matrix, the grafted polymer determines particle spacing and circumvents nanoparticle agglomeration. The extent to which these grafted polymers are entangled determines the robustness and strength of the HNP assembly. Here in, we investigate the correlations between grafted polymer conformation, entanglements and deformation mechanisms of thin film assemblies of polystyrene-grafted HNPs by controlling the HNP architecture (grafting density and molecular weight). HNPs with varied corona structures are synthesized with surface-initiated controlled/living radical polymerization. Thin films with controlled thickness are prepared by flow coating. Plastic deformation of thin films are examined using static (bright field, HAADF-STEM, tomography) and AFM techniques. Results show a decrease of void density in craze as grafted polymer length increases for semi-dilute polymer brushes. These correlations between HNP architecture and assembly deformation and failure modes refine the HNP design space for the synthesis and fabrication of assemblies with excellent mechanical properties.

**5:18PM H38.00015 Tuning mechanical properties of polymer-grafted nanoparticle networks by using biomimetic catch bonds**, BADEL L. MBANGA, BALAJI V. S. IYER, VICTOR V. YASHIN, ANNA C. BALAZS, Chemical Engineering Department, University of Pittsburgh, Pennsylvania 15261, USA — Cross-linked networks of polymer-grafted nanoparticles (PGNs) constitute a class of composites with tunable mechanical properties that exhibit a self-healing behavior. A PGN network consists of nanoparticles that are decorated with end-grafted polymer chains. Reactive groups on the free ends of these grafted chains can form bonds with the chain ends on the nearby particles. We study these materials using a 3D computational model that encompasses the particle-particle interactions, the kinetics of bond formation and rupture, and the external forces applied to the network. In our model, a fraction of cross-links is formed through biomimetic catch bonds. In contrast to conventional slip bonds, catch bonds can effectively become stronger under a deformation. We show that by varying the fraction of these catch bonds in the network, the toughness, ductility, and tensile strength of the material could be tuned to desired levels.

**Tuesday, March 15, 2016 2:30PM - 5:06PM —**

**Session H39 DBIO GSOF: Cell Motility: From Single Cell to Collective Dynamics III** 342 - Thomas Gregor, Princeton University

**2:30PM H39.00001 Expulsion of swimming bacteria by a circular flow.**<sup>1</sup>, ANDREY SOKOLOV, IGOR ARONSON, Argonne National Laboratory — Macroscopic shear flow alters swimming trajectories in a highly nontrivial way and results in dramatic reduction of viscosity and heterogeneous bacterial distributions. We report on experimental and theoretical studies of rapid expulsion of microswimmers, such as motile bacteria, by a circular flow created by a rotating microparticle. We observed a formation of a macroscopic depletion area in a high-shear region, in the vicinity of a microparticle. The rapid migration of bacteria from the shear-rich area is caused by a circular structure of the flow rather than intrinsic random fluctuations of bacteria orientations, in stark contrast to planar shear flow. Our mathematical model revealed that expulsion is a combined effect of motility and alignment by a vortical flow. Our findings offer a novel approach for manipulation of motile microorganisms and shed new light on bacteria-flow interactions.

<sup>1</sup>was supported by the US DOE, Office of Basic Energy Sciences, Division of Materials Science And Engineering, under contract No. DE AC02-06CH11357

**2:42PM H39.00002 Bacterial haptotaxis: Effect of auto-attraction and bacterial motility on microcolony formation**, BERNARD BECKERMAN, Northwestern University, KUN ZHAO, Tianjin University, GERARD C. L. WONG, University of California, Los Angeles, ERIK LUIJTEN, Northwestern University — Recent work<sup>1</sup> has demonstrated that surface-adhered *Pseudomonas aeruginosa* tend to self-organize into microcolonies using a positive-feedback mechanism mediated by the exopolysaccharide Psl, which the bacteria secrete as they traverse the surface. We elucidate this colony-nucleation process and explore how it is influenced by the deposition rate of Psl and by bacterial motility. A detailed analysis of the data presented in our earlier study, in combination with additional simulations, provides further insight into the exploratory strategy of *P. aeruginosa*. Specifically, the isogenic bacterial population is found to exhibit polyphenic motility. As a result, the bacterial population splits into two distinct subpopulations when depositing Psl, those that become trapped in their self-deposited Psl and those that move sufficiently quickly to escape their Psl beds and explore the surface. We perform computer simulations in which we adjust the relative prevalence of these subpopulations by varying the Psl deposition rate and find that there is a trade-off between surface exploration, microcolony diversity and microcolony fortification.

<sup>1</sup>K. Zhao *et al.*, Nature **497**, 388 (2013)

**2:54PM H39.00003 Invariant manifolds as barriers to the motion of bacteria in vortex flows<sup>1</sup>**, MINH DOAN, KATIE LILIENTHAL, TOM SOLOMON, Bucknell University — We present experiments that study the motion of swimming bacteria (*Bacillus subtilis*) in a time-independent flow in a microfluidic T-channel. Experiments are done with both wild-type and a genetically-mutated “smooth swimming” <sup>2</sup> *Bacillus subtilis*. We analyze the behavior of these bacteria in terms of invisible barriers, based on a theory of “burning invariant manifolds” <sup>3</sup> that act as one-way barriers that impede the motion of reaction fronts in a fluid flow. We explore whether similar one-way barriers impede the motion of bacteria.

<sup>1</sup>Supported by NSF Grants DMR-1361881 and PHY-1156964.

<sup>2</sup>R. Rusconi, J.S. Guasto and R. Stocker, *Nature Physics* **10**, 212 (2014).

<sup>3</sup>J. Mahoney, D. Bargteil, M. Kingsbury, K. Mitchell and T. Solomon, *Europhys. Lett.* **98**, 44005 (2012).

**3:06PM H39.00004 Tethered motion of unflagellated bacteria at the liquid-solid surface**, JORDAN BELL, JAY TANG, Brown University — Direct evidence of the bacterial flagellar motors rotation was first noted when multiflagellated bacterial cells were observed (under the optical microscope) to rotate when tethered to glass by a single flagellum. The tethered cell assay has continued to play a significant role throughout the subsequent studies of motor characteristics and behavior. Such studies have expanded to include unflagellated bacteria, such as *Vibrio alginolyticus*, *Pseudomonas aeruginosa*, and *Caulobacter crescentus*. Here we show that such cells are not necessarily tethered by their flagellum, but rather elsewhere on the cell body. The observed cell body rotation is actually due to the flagellum either rolling against the glass surface, or pushing the cell body at the flagellar base. These motions are directly observed for *Vibrio alginolyticus* with darkfield microscopy. Additionally, our recently measured distributions of intervals between motor switches for tethered *Caulobacter crescentus* also confirm this more complicated mode of tethering. Therefore, the rotational speed of tethered unflagellated bacteria may not equate to that of the motor itself, as is commonly assumed.

Phone: +852-3943-6354. Fax: +852-2603-5204.

**3:18PM H39.00005 Two-dimensional swimming behavior of bacteria**, YE L

The Chinese University of Hong Kong, SANDRA SANCHEZ, DANIEL KEARNS, Department of Biology, Indiana University, The Chinese University of Hong Kong; Department of Physics, The Chinese University of Hong Kong — Many motile bacteria use flagella, which is essential for bacterial dispersal, chemotaxis, and pathogenesis. Here we combined single-cell tracking, theoretical analysis, and experiments to investigate two-dimensional swimming behavior of a well-characterized flagellated bacterium *Bacillus subtilis* at the single-cell motion pattern of *B. subtilis* in confined space and studied how cells interact with each other. Our findings shed light on bacterial collective motion environments, and will serve as the ground for building more accurate models to understand bacterial collective motion.

E-mail: ylwu@phy.cuhk.edu.hk

**3:30PM H39.00006 Swimming of bacteria under dielectrophoresis**, NGOC PHU TRAN, MARCOS MARCOS<sup>1</sup>, School of Mechanical and Aerospace Engineering, Nanyang Technological University, Singapore — In this work, we present a model to predict the response of a swimming helically flagellated bacterium to a unidirectional dielectrophoretic (DEP) force with its strength varying linearly in space. We employ resistive force theory to compute the hydrodynamic force on the flagellar bundle, and the effects of DEP force and rotational diffusion are examined using the Fokker-Planck equation. The DEP force greatly contributes to the reorientation of the bacterium such that the bacterium's primary axis is aligned with the direction of the force. Interestingly, when the DEP strength varies perpendicularly to the direction of the force, the bacterium's primary axis is no longer aligned with the DEP force, which results in a translation of the bacterium perpendicular to its primary axis. Finally, we show the feasibility to utilize this phenomenon to achieve bacterial focusing.

<sup>1</sup>The full name of the second author is MARCOS.

**3:42PM H39.00007 The bacterial gliding machinery**, ABHISHEK SHRIVASTAVA, Department of Molecular and Cellular Biology, Harvard University, Cambridge, MA — Cells of *Flavobacterium johnsoniae*, a rod-shaped bacterium, glide over surfaces with speeds reaching up to 2 micrometer's. Gliding is powered by a protonmotive force. The adhesin SprB forms filaments about 160 nm long that move on the cell-surface along a looped track. Interaction of SprB filaments with a surface produces gliding. We tethered *F. johnsoniae* cells to glass by adding anti-SprB antibody. Tethered cells spun about fixed points, rotating at speeds of about 1 Hz. The torques required to sustain such speeds were large, comparable to those generated by the flagellar rotary motor. Using a flow cell apparatus, we changed load on the gliding motor by adding the viscous agent Ficoll to tethered cells. We found that a gliding motor runs at constant speed rather than constant torque. We attached gold nanoparticles to the SprB filament and tracked its motion. We fluorescently tagged a bacterial Type IX secretion system (T9SS) protein and imaged its dynamics. Fluorescently tagged T9SS protein localized near the point of tether, indicating that T9SS localizes with the gliding motor. Based on our results, we propose a model to explain bacterial gliding.

**4:18PM H39.00008 Coordinated Beating of Algal Flagella is Mediated by Basal Coupling**, KIRSTY WAN, RAYMOND GOLDSTEIN, Univ of Cambridge — Cilia or flagella often exhibit synchronized behavior. This includes phase-locking, as seen in *Chlamydomonas*, and metachronal wave formation in the respiratory cilia of higher organisms. Since the observations by Gray and Rothschild of phase synchrony of nearby swimming spermatozoa, it has been a working hypothesis that synchrony arises from hydrodynamic interactions between beating filaments. Recent work on the dynamics of physically separated pairs of flagella isolated from the multicellular alga *Volvox* has shown that hydrodynamic coupling alone is sufficient for synchrony. However, the situation is more complex when considering multiple flagella on a single cell. We suggest that a mechanism, internal to the cell, provides an additional flagellar coupling. For instance, flagella of *Chlamydomonas* mutants deficient in filamentary connections between basal bodies are found to display markedly different synchronization from the wildtype. Diverse flagellar coordination strategies found in quadri-, octo- and hexadecaflagellates reveal further evidence that intracellular couplings between flagellar basal bodies compete with hydrodynamic interactions to determine the precise form of flagellar synchronization in unicellular algae.

**4:30PM H39.00009 Non-Poissonian run-and-turn motions**, FRANCOIS DETCHEVERRY, University of Lyon, CNRS — Swimming bacteria exhibit a variety of motion patterns (run-and-tumble, run-reverse, run-reverse-flick), in which persistent runs are punctuated by sudden turning events. What are the properties of such random motions? If a complete answer has been given when the turning events follow a Poisson process, it has remained elusive outside this particular case. We present a generic framework for such non-Poissonian run-and-turn random motions. We obtain the generating function of moments by building on the framework of continuous time random walks and using non-commutative calculus. The approach is applied to a bimodal model of persistent motion that is directly applicable to swimming patterns and cell motility.

**4:42PM H39.00010 Directionality Time - New Analytical Treatment of Directionally Biased, Crawling Motility** , JAY TANG, ALEXANDER LOOSLEY, Brown University — Insights on crucial biological functions often emerge from measuring how animal cells crawl on surfaces, particularly in response to gradients of external cues that cause directionally biased motion. Most existing metrics commonly used to characterize directional migration, such as straightness index (or chemotactic index), persistence time, and turning angle distribution, tend to be sensitive to relatively large errors at short sampling times. In contrast, we recently introduced a new metric, called directionality time, to define the onset time by which a seemingly random motion becomes directionally biased (OBrien et al., J Leukocyte Biol, 2014, 95:9931004; Loosley et al., PLOS ONE, 2015, 10.1371). Directionality time is obtained by fitting the mean squared displacement as a function of time interval, in log-log coordinates, to a fit function based on biased and persistent random walk processes. We show that the fit function is approximately model invariant and is applicable to a variety of directionally biased motions. Simulations are performed to show the robustness of the directionality time model and its decoupling from measurement errors. Finally, we demonstrate as an example how to usefully apply the directionality time fit to trajectories of chemotactic neutrophils.

**4:54PM H39.00011 Paramagnetic ellipsoidal microswimmer in a magnetic field** , MARIO SANDOVAL, Metropolitan Autonomous University, LOUIS FAN, University of Wisconsin, Madison, ON SHUN PAK, University of Santa Clara — We study the two-dimensional Brownian dynamics of an ellipsoidal paramagnetic microswimmer moving at low-Reynolds-number and subject to a magnetic field. Its corresponding mean-square displacement tensor showing the effect of particles's shape, activity and magnetic field, on the microswimmer's diffusion is analytically obtained. A comparison among analytical and computational results is also made and we obtain excellent agreement.

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**  
**Session H40 GSNP GSOFT: Mechanical Metamaterials and Origami I** 343 - Chris Santangelo, University of Massachusetts Amherst

**2:30PM H40.00001 Wave Manipulation in Metamaterials: A LEGO® Bricks Enabled Platform<sup>1</sup>** , PAOLO CELLI, STEFANO GONELLA, University of Minnesota — In this work, we show how simple, reconfigurable arrangements of LEGO® bricks can be turned into the building blocks of an experimental platform for the investigation of wave phenomena in metamaterial architectures. The approach involves the assembly of reconfigurable specimens consisting of patterns of bricks on a baseplate and the use of a 3D laser vibrometer to reconstruct global and local wave features. The ability to seamlessly transition between different topologies makes this an effective approach for rapid experimental verification and proof of concept in the arena of mechanical metamaterials engineering. The intuitive nature of the brick-and-baseplate assembly paradigm can also be leveraged to implement families of intuitive lab demonstrations with significant didactic and scientific outreach potential. The versatility of the platform is tested through a series of experiments that illustrate a variety of wave manipulation effects, such as waveguiding and seismic isolation, both in periodic and disordered topologies.

<sup>1</sup>We acknowledge the support of the National Science Foundation (grant CMMI-1266089)

**2:42PM H40.00002 Transformable topological mechanical metamaterials<sup>1</sup>** , D. ZEB ROCKLIN, SHANGNAN ZHOU, KAI SUN, XIAOMING MAO, University of Michigan, Department of Physics — We present a class of mechanical metamaterials characterized by a *uniform soft deformation*—a large, zero-energy homogeneous elastic deformation mode of the structure—that may be used to induce topological transitions and dramatically change mechanical and acoustic properties of the structure. We show that the *existence* of such a mode determines certain exotic mechanical and acoustic properties of the structure and its *activation* can reversibly alter and tune these properties. This serves as the basis for a design principle for mechanical metamaterials with tunable properties. When the structure's uniform mode is primarily dilational (shearing) its surface (bulk) possesses phonon modes with vanishing speed of sound. Maxwell lattices comprise a subclass of such material which, owing to their critical coordination number (four, in 2D), necessarily possess such a uniform zero mode, often termed a Guest mode, and which may be *topologically polarized*, such that zero modes are moved from one edge to another. We show that activating the deformation can alter the shear/dilational character of the mode and topologically polarize the structure, thereby altering the bulk and surface properties at no significant energy cost. arXiv:1510.06389 [cond-mat.soft]

<sup>1</sup>NWO, Delta Institute of Physics, ICAM fellowship (DZR) and NSF grant PHY-1402971 at University of Michigan (KS)

**2:54PM H40.00003 Tuning the Response in Disordered Networks** , NIDHI PASHINE, Department of Physics, The University of Chicago, Chicago, IL, JASON W. ROCKS, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA, IRMGARD BISCHOFBERGER, Department of Physics, The University of Chicago, Chicago, IL, CARL P. GOODRICH, School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, SIDNEY R. NAGEL, Department of Physics, The University of Chicago, Chicago, IL, ANDREA J. LIU, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA — The fact that amorphous materials are structurally different from crystals has important consequences for how the properties of a disordered structure can be tuned. We have used jamming as a method to create spring networks in both two and three dimensions. By selectively removing a small percentage of bonds, we can tune the network to have a desired response. For example, we can tune the network's Poisson ratio anywhere between the auxetic and incompressible limits. We can also produce a targeted response at a local scale; by perturbing the positions of pair of particles at one point we can tune in a desired response a large distance away. This response is similar to the allosteric regulation in proteins where a reaction at one site activates another site of the protein molecule. Experimentally, we have successfully demonstrated such mechanical networks in 2D (by laser cutting) or in 3D (3D printing).

**3:06PM H40.00004 The breakdown of breathers in the Fermi-Pasta-Ulam-Tsingou system<sup>1</sup>** , ALEXANDRA WESTLEY, RAHUL KASHYAP, SURAJIT SEN, State Univ of NY - Buffalo — It is well known that in many nonlinear lattices, remarkably stable and localized disturbances known as breathers may form. Here we discuss in short the properties of these objects in the context of the Fermi-Pasta-Ulam-Tsingou (FPUT) system which consists of a mass-spring chain, with spring potentials containing both quadratic and quartic terms. These breathers, though long-lasting, inevitably decay and eventually break apart with sudden violence. This talk in particular will focus on recent numerical work studying the lead-up to the breakdown in which the breather emits at (seemingly) random intervals solitary and anti-solitary waves in the highly nonlinear limit. Furthermore, a possible method to predict the times at which these waves are emitted by examining the frequency structure of the breather will be discussed.

<sup>1</sup>Partially supported by US Army Research Office

**3:18PM H40.00005 Multifunctional Lattices with Low Thermal Expansion and Low Thermal Conductivity** , HANG XU, LU LIU, DAMIANO PASINI<sup>1</sup>, Mechanical Engineering, McGill University — Systems in space are vulnerable to large temperature changes when travelling into and out of the Earth's shadow. Variations in temperature can lead to undesired geometric changes in susceptible applications requiring very fine precision. In addition, temperature-sensitive electronic equipment hosted in a satellite needs adequate thermal-control to guarantee a moderate ambient temperature. To address these specifications, materials with low coefficient of thermal expansion (CTE) and low coefficient of thermal conductivity (CTC) over a wide range of temperatures are often sought, especially for bearing components in satellites. Besides low CTE and low CTC, these materials should also provide desirable stiffness, strength and extraordinarily low mass. This work presents ultralightweight bi-material lattices with tunable CTE and CTC, besides high stiffness and strength. We show that the compensation of the thermal expansion and joint rotation at the lattice joints can be used as an effective strategy to tailor thermomechanical performance. Proof-of-concept lattices are fabricated from Al and Ti alloy sheets via a simple snap-fit technique and vacuum brazing, and their CTE and CTC are assessed via a combination of experiments and theory.

<sup>1</sup>Corresponding Author

**3:30PM H40.00006 Finite-temperature twisted-untwisted transition of the kagome lattice** , DESHPREET BEDI, D. ZEB ROCKLIN, XIAOMING MAO, University of Michigan — Mechanical instability governs many fascinating phenomena in nature, including jamming, glass transitions, and structural phase transitions. Although mechanical instability in athermal systems is well understood, how thermal fluctuations modify such transitions remains largely unexplored. Recent studies reveal that, due to the large number of floppy modes that emerge at mechanical instability, intriguing new phenomena occur, such as fluctuation-driven first-order transitions and order-by-disorder. In this talk, we present an analytic study of the finite-temperature rigidity transition for the kagome lattice. Our model exhibits a zero-temperature continuous twisted-untwisted transition as the sign of the next-nearest-neighbor spring constant changes. At finite temperature, we show that the divergent contribution of floppy modes to the vibrational entropy renormalizes this spring constant, resulting in a first-order transition. We also propose an experimental manifestation of this transition in the system of self-assembling triblock Janus particles.

**3:42PM H40.00007 Topological design of torsional metamaterials** , VINCENZO VITELLI, JAYSON PAULOSE, ANNE MEEUSSEN, Institute Lorentz for Theoretical Physics, Leiden, TOPOLOGICAL MECHANICS LAB TEAM — Frameworks – stiff elements with freely hinged joints – model the mechanics of a wide range of natural and artificial structures, including mechanical metamaterials with auxetic and topological properties. The unusual properties of the structure depend crucially on the balance between degrees of freedom associated with the nodes, and the constraints imposed upon them by the connecting elements. Whereas networks of featureless nodes connected by central-force springs have been well-studied, many real-world systems such as frictional granular packings, gear assemblies, and flexible beam meshes incorporate torsional degrees of freedom on the nodes, coupled together with transverse shear forces exerted by the connecting elements. We study the consequences of such torsional constraints on the mechanics of periodic isostatic networks as a foundation for mechanical metamaterials. We demonstrate the existence of soft modes of topological origin, that are protected against disorder or small perturbations of the structure analogously to their counterparts in electronic topological insulators. We have built a lattice of gears connected by rigid beams that provides a real-world demonstration of a torsional metamaterial with topological edge modes and mechanical Weyl modes.

**3:54PM H40.00008 Surface morphology of pre-stressed bilayer shells for tunable optical transmittance** , RASHED AL-RASHED, FRANCISCO LPEZ JIMNEZ, JOEL MARTHELOT, ANNA LEE, PEDRO REIS, Massachusetts Institute of Technology — We introduce a new class of pre-stressed bilayer shells, whose surface morphology can be used to smoothly tune their optical transmittance by pneumatic actuation. Each sample is fabricated by pressurizing a disk made out of an optically clear silicone-based rubber to bulge it into a nearly hemispherical pre-strained shell. The surface of this shell is then taken as a substrate and coated with a thin layer of a polymer suspension with black micron-sized dye particles, which, upon curing, can make the samples opaque. The sample becomes planar when it is depressurized to remove the pre-strain, and its surface develops a complex topography that significantly affects its optical transmittance (i.e. the amount of light that passes through the sample). Re-pressurization of the samples allow for their transmittance to be smoothly tuned in a reversible manner. We explore the parameter space of the system by systematically varying its geometric and material properties. A phase diagram is then constructed where we characterize the transmittance of each of the surface patterns at varying levels of pre-strain.

**4:06PM H40.00009 Elastic theory of origami-based metamaterials<sup>1</sup>** , FREDERIC LECHENAULT, Laboratoire de Physique Statistique, ENS, Paris, V. BRUNCK, Lab. de Physique Statistique, Ecole Normale Supérieure, UPMC, Univ. Paris 06, Univ. Paris-Diderot, CNRS, Paris, France, A. REID, Lab. de Physique Statistique, Ecole Normale Supérieure, UPMC, Univ. Paris 06, Univ. Paris-Diderot, CNRS, Paris, France & NC State Univ, M. ADDA-BEDIA, Lab. de Physique Statistique, Ecole Normale Supérieure, UPMC, Univ. Paris 06, Univ. Paris-Diderot, CNRS, Paris, France — Origami offers the possibility for new metamaterials whose overall mechanical properties can be programmed by acting locally on each crease. Starting from a thin plate and having knowledge about the properties of the material and the folding procedure, one would aim to determine the shape taken by the structure at rest and its mechanical response. We introduce a vector deformation field acting on the imprinted network of creases, that allows to express the geometrical constraints of rigid origami structures in a simple and systematic way. This formalism is then used to write a general covariant expression of the elastic energy of  $n$ -creases meeting at a single vertex, and then extended to origami tessellations. The generalized waterbomb base and the Miura-Ori are treated within this formalism. For the Miura folding, we uncover a phase transition from monostable to two metastable states, that explains the efficient deployability of this structure for a given range of geometrical and mechanical parameters.

<sup>1</sup>This research was supported by the ANR grant 14-CE07-0031 METAMAT

**4:18PM H40.00010 Self-Folding With Graphene Bimorphs** , MARC MISKIN, KYLE DORSEY, PETER ROSE, ITAI COHEN, PAUL MCEUEN, Cornell University — We have developed a new technique that let us program two layer stacks, or bimorphs, made of graphene and ultra-thin films to self-fold via differential stress. Our approach works in the extreme regime of bimorph folding: we construct bimorphs that optimize folding efficiency when one layer is atomically thin. The resulting devices controllably fold to micron sized radii of curvature. By applying this technique in concert with lithographic patterning, we have produced a powerful platform to build three dimensional structures at the nanoscale. We demonstrate that this this approach is intrinsically scalable and facilitates the construction of both fixed 3d structures and actuation.

**4:30PM H40.00011 The role of geometry in 4-vertex origami mechanics** , SCOTT WAITUKAITIS, PETER DIELEMAN, MARTIN VAN HECKE, Leiden University, AMOLF — Origami offers an interesting design platform metamaterials because it strongly couples mechanics with geometry. Even so, most research carried out so far has been limited to one or two particular patterns. I will discuss the full geometrical space of the most common origami building block, the 4-vertex, and show how exotic geometries can have dramatic effects on the mechanics.

**4:42PM H40.00012 Generalized Bistability in Origami Cylinders** , AUSTIN REID, North Carolina State University, MOKHTAR ADDA-BEDIA, FREDERIC LECHENAULT, Laboratoire de Physique Statistique de l'ENS — Origami folded cylinders (origami bellows) have found increasingly sophisticated applications in space flight, medicine, and even experimental nuclear physics. In spite of this interest, a general understanding of the dynamics of an origami folded cylinder has been elusive. By solving the fully constrained behavior of a periodic fundamental origami cell defined by unit vectors, we have found an analytic solution for all possible rigid-face states accessible from a cylindrical Miura-ori pattern. Although an idealized bellows has two rigid-face configurations over a well-defined region, a physical device, limited by nonzero material thickness and forced to balance hinge with plate-bending energy, often cannot stably maintain a stowed configuration. We have identified and measured the parameters which control this emergent bistability, and have demonstrated the ability to fabricate bellows with tunable deployability.

**4:54PM H40.00013 Origami Optimization: Role of Symmetry in Accelerating Design<sup>1</sup>**, PHILIP BUSKOHL, Air Force Research Laboratory, KAZUKO FUCHI, Wright State Research Institute, GIORGIO BAZZAN, UES, Inc, MICHAEL DURSTOCK, GREGORY REICH, JAMES JOO, RICHARD VAIA, Air Force Research Laboratory — Origami structures morph between 2D and 3D conformations along predetermined fold lines that efficiently program the form, function and mobility of the structure. Design optimization tools have recently been developed to predict optimal fold patterns with mechanics-based metrics, such as the maximal energy storage, auxetic response and actuation. Origami actuator design problems possess inherent symmetries associated with the grid, mechanical boundary conditions and the objective function, which are often exploited to reduce the design space and computational cost of optimization. However, enforcing symmetry eliminates the prediction of potentially better performing asymmetric designs, which are more likely to exist given the discrete nature of fold line optimization. To better understand this effect, actuator design problems with different combinations of rotation and reflection symmetries were optimized while varying the number of folds allowed in the final design. In each case, the optimal origami patterns transitioned between symmetric and asymmetric solutions depended on the number of folds available for the design, with fewer symmetries present with more fold lines allowed. This study investigates the interplay of symmetry and discrete vs continuous optimization in origami actuators and provides insight into how the symmetries of the reference grid regulate the performance landscape.

<sup>1</sup>This work was supported by the Air Force Office of Scientific Research.

**5:06PM H40.00014 How do bendy straws bend? A study of re-configurability of multi-stable corrugated shells<sup>1</sup>**, NAKUL BENDE, SARAH SELDEN, Univ of Mass - Amherst, ARTHUR EVANS, University of Wisconsin–Madison, CHRISTIAN SANTANGELO, RYAN HAYWARD, Univ of Mass - Amherst — Shape programmable systems have evolved to allow for reconfiguration of structures through a variety of mechanisms including swelling, stress-relaxation, and thermal expansion. Particularly, there has been a recent interest in systems that exhibit bi-stability or multi-stability to achieve transformation between two or more pre-programmed states. Here, we study the ubiquitous architecture of corrugated shells, such as drinking straws or bellows, which has been well known for centuries. Some of these structures exhibit almost continuous stability amongst a wide range of reconfigurable shapes, but the underlying mechanisms are not well understood. To understand multi-stability in 'bendy-straw' structures, we study the unit bi-conical segment using experiments and finite element modeling to elucidate the key geometrical and mechanical factors responsible for its multi-stability. The simple transformations of a unit segment – a change in length or angle can impart complex re-configurability of a structure containing many of these units. The fundamental understanding provided of this simple multi-stable building block could yield improvements in shape re-configurability for a wide array of applications such as corrugated medical tubing, robotics, and deployable structures.

<sup>1</sup>NSF EFRI ODISSEI-1240441

**5:18PM H40.00015 Q: How many folded angels can we fit on the head of pin? A: 22+/-5**, ITAI COHEN, Cornell University, TOM HULL, Western New England University, ROBERT LANG, Lang Origami, CHRISTIAN SANTANGELO, University of Massachusetts, Amherst, MARC MISKIN, KYLE DORSEY, PAUL MCEUEN, Cornell University — For centuries, origami, the Japanese art of paper folding, has been a powerful technique for transforming two dimensional sheets into beautiful three dimensional sculptures. Recently, origami has made its foray into a new realm, that of physics, where it has been revolutionizing our concept of materials design. Arguably the greatest strength of this new paradigm is the fact that origami is intrinsically scalable. Thus sculptures built at one size can be shrunk down smaller and smaller. This begs the question: what is the smallest fold one can make? Or in other words how many folded angels can we fit on the head of a pin? This talk takes a deep dive into how origami has been marching smaller and smaller in size. From folding by hand, to self-folding through shape memory alloys and even folding via polymer layers, I will argue that the ultimate limit for scaling down origami is set by folding asheet of atomic dimensions. I will conclude by showing this vision realized in the folds of a single sheet of graphene.

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**

**Session H41 DBIO DPOLY: Biopolymers in Confinement II** 344 - Kevin Dorfman, University of Minnesota  
- Minneapolis

**2:30PM H41.00001 Zero-Mode Waveguide detection of biomolecules transport through artificial nanopores and nuclear pore complexes**, THOMAS AUGER, LOIC AUVRAY, FABIEN MONTEL, Universit Paris Diderot — We have developed a novel single molecule optical observation method using a custom Zero-Mode Waveguide setup to study the translocation of biopolymers through artificial and biological nanopores. Our work focuses on two aspects. First we monitored the flow driven injection of DNA molecules through solid state nanopores and showed that DNA starts translocating over a flow threshold independent of the pore radius, the DNA concentration and length. We demonstrate that the translocation is controlled by an energy barrier as proposed by the de Gennes - Brochard suction model. The height of the energy barrier can be modulated by functionalizing the nanopores with PEG-Thiols. More recently we adapted our setup to the study of transport through the nuclear pore complex (NPC) using extracted nuclear membranes from *Xenopus Laevis* oocytes. We aim at probing the conformation of unstructured proteins – the FG-Nucleoporins – crowding the central channel of the NPC by monitoring the free diffusion of small Dextran molecules (3kDa). We have been able to estimate the radius of the central pore of the NPC. We want to study the effects of transporter molecules, which have a high affinity for the FG-Nups, on the central pore size and correlate it to the conformation of FG-Nups.

**2:42PM H41.00002 A Nanopore with an Internal Cavity to Selectively Translocate Polymers of a Specific Length<sup>1</sup>**, HENDRICK W. DE HAAN, MARTIN MAGILL, University of Ontario Institute of Technology — In the majority of experimental and simulation studies of polymer translocation through a nanopore, the scaling of the translocation time,  $\tau$ , with polymer length,  $N$ , is well described by a single exponent:  $\tau \sim N^\alpha$ . Hence, an increase in  $N$  always yields an increase in  $\tau$ . I will present a nanopore geometry in which there is a large central cavity between narrow nanopores at both the *cis* entrance and the *trans* exit. Results from simulations of this system reveal a complex dependence of  $\tau$  on  $N$ . Most notably, the translocation time is now non-monotonic in polymer length such that  $\tau$  is a minimum for polymers of an intermediate length with both longer and shorter polymers taking a longer time to cross across the membrane. A simple yet effective model for predicting this critical length as a function of the size of the cavity and the magnitude of the external field will be presented. The pore thus can be designed to be optimized for particular lengths with some dynamic tuning being possible by varying the strength of the external field. These results suggest new applications for nanopore-based devices such as the ability to select DNA strands of a specific length from a sample containing both shorter and longer strands.

<sup>1</sup>Funding provided by NSERC

**2:54PM H41.00003 Effect of excluded volume on the force-extension of wormlike chains in slit confinement**, XIAOLAN LI, KEVIN DORFMAN, University of Minnesota - Twin cities — We will present a quantitative phase diagram for the stretching of a wormlike chain confined in a slit with excluded volume interactions. Using pruned-enriched Rosenbluth method (PERM) simulations, we demonstrate the existence of a “confined Pincus” regime in slit confinement. This regime is similar to the Pincus regime in free solution, where excluded volume effects are sensible. The lower bound for the confined Pincus regime in the force-contour length plane and the dependence of the extension with force and slit size are in agreement with scaling theory. The upper bound of the confined Pincus regime depends on the confinement strength; it ends in strong confinement when the Pincus blobs do not have excluded volume, while it ends in weak confinement when the Pincus blobs do not fit in the slit. We also show the existence of a free-solution Pincus regime in weak confinement that exists before ideal chain behavior sets in under strong forces. We will discuss the implication of our results on the analysis of experiments on the “tug-of-war” stretching of DNA partially confined to a slit.

**3:06PM H41.00004 Visualizing Chemical Interaction Dynamics of Confined DNA Molecules**, GILEAD HENKIN, DANIEL BERARD, FRANK STABILE, SABRINA LESLIE, McGill Univ — We present a novel nanofluidic approach to controllably introducing reagent molecules to interact with confined biopolymers and visualizing the reaction dynamics in real time. By dynamically deforming a flow cell using CLIC (Convex Lens-induced Confinement) microscopy, we are able to tune reaction chamber dimensions from micrometer to nanometer scales. We apply this gentle deformation to load and extend DNA polymers within embedded nanotopographies and visualize their interactions with other molecules in solution. Quantifying the change in configuration of polymers within embedded nanotopographies in response to binding/unbinding of reagent molecules provides new insights into their consequent change in physical properties. CLIC technology enables an ultra sensitive, massively parallel biochemical analysis platform which can access a broader range of interaction parameters than existing devices.

**3:18PM H41.00005 Relaxation dynamics of internal segments of DNA chains in nanochannels**, AASHISH JAIN, ABHIRAM MURALIDHAR, KEVIN DORFMAN, Department of Chemical Engineering and Materials Science, University of Minnesota, DORFMAN GROUP TEAM — We will present relaxation dynamics of internal segments of a DNA chain confined in nanochannel. The results have direct application in genome mapping technology, where long DNA molecules containing sequence-specific fluorescent probes are passed through an array of nanochannels to linearize them, and then the distances between these probes (the so-called DNA barcode) are measured. The relaxation dynamics of internal segments set the experimental error due to dynamic fluctuations. We developed a multi-scale simulation algorithm, combining a Pruned-Enriched Rosenbluth Method (PERM) simulation of a discrete wormlike chain model with hard spheres with Brownian dynamics (BD) simulations of a bead-spring chain. Realistic parameters such as the bead friction coefficient and spring force law parameters are obtained from PERM simulations and then mapped onto the bead-spring model. The BD simulations are carried out to obtain the extension autocorrelation functions of various segments, which furnish their relaxation times. Interestingly, we find that (i) corner segments relax faster than the center segments and (ii) relaxation times of corner segments do not depend on the contour length of DNA chain, whereas the relaxation times of center segments increase linearly with DNA chain size.

**3:30PM H41.00006 Controlling the Motion of Knotted Polymers through Nanopores**, VIVEK NARSIMHAN, C. BENJAMIN RENNER<sup>1</sup>, PATRICK DOYLE, Massachusetts Inst of Tech-MIT — Nanopore sequencing is a technique where DNA moves through a pore and base-pair information is read along the chain as an electric signal. One hurdle facing this technique is that DNA passes too quickly through the pore, rendering the signal to be too noisy. In this talk, we discuss one strategy to control the speed by which polymers move through pores. By tying a knot on a polymer chain, we find that we can jam the polymer at the pore's entrance and halt translocation completely. This idea by itself may not seem useful, but by cycling the field on and off at the relaxation time scale of the knot, we can control the swelling dynamics of the knot at the pore's entrance, and hence ratchet the polymer through the pore. This talk focuses on two parts. First, we will discuss the dynamics of a knot jamming at the pore entrance and determine what sets the critical tension to halt translocation. We will determine how knot topology affects these results and discuss what regimes lead to large fluctuations in the translocation speed. We will then discuss the dynamics of a knot under a time-dependent, periodic force. Lastly, we develop a model to describe the knot's swelling dynamics during relaxation, and use this to explain some of the trends observed in our simulations.

<sup>1</sup>Now at Liquiglide

**3:42PM H41.00007 Confined polymers in the extended de Gennes regime**, BERNHARD MEHLIG, University of Gothenburg — In the “extended de Gennes regime” the problem of describing the conformations of a semiflexible polymer confined to a channel can be mapped onto the weakly self-avoiding random-walk model. For large contour lengths the asymptotically exact solution of this model predicts how the conformational fluctuations of the confined polymer depend upon the channel dimensions and upon the physical properties of the polymer, its effective width and persistence length. The extended de Gennes regime (where the polymer is neither weakly nor strongly confined) has recently been studied intensively experimentally and by means of computer simulations of worm-like chain models. In this talk I explain the mapping, summarise the predictions derived from the exact solution, and compare the predictions to results of computer simulations [Dorfman *et al.*] and experiments [Westerlund *et al.*] of DNA molecules confined to nanochannels. I conclude by summarising open questions. This talk is mainly based on joint work with E. Werner [Phys. Rev. E 90 (2014) 062602].

**4:18PM H41.00008 From stripe to slab confinement for DNA linearization in nanochannels<sup>1</sup>**, PETER CIFRA, ZUZANA BENKOVA, PAVOL NAMER, Polymer Institute, Slovak Academy of Sciences, Bratislava, Slovakia — We investigate suggested advantageous analysis in the linearization experiments with macromolecules confined in a stripe-like channel using Monte Carlo simulations. The enhanced chain extension in a stripe that is due to significant excluded volume interactions between monomers in two dimensions weakens on transition to experimentally feasible slit-like channel. Based on the chain extension-confinement strength dependence and the structure factor behavior for the chain in stripe we infer the excluded volume regime typical for two-dimensional systems. On transition to the slab geometry, the advantageous chain extension decreases and the Gaussian regime is observed for not very long semiflexible chains. The evidence for pseudo-ideality in confined chains is based on indicators such as the extension curves, variation of the extension with the persistence length or the structure factor. The slab behavior is observed when the stripe (originally of monomer thickness) reaches the thickness larger than cca 10nm in the third dimension. This maximum height of the slab to retain the advantage of the stripe is very low and this has implication for DNA linearization experiments. The presented analysis, however, has a broader relevance for confined polymers.

<sup>1</sup>Support from Slovak RD Agency (SRDA-0451-11) is acknowledged.

**4:30PM H41.00009 Knotted DNA in Nanofluidic Confinement**, ALEXANDER KLOTZ, PATRICK DOYLE, MIT — The behavior of topologically simple semiflexible polymers such as DNA has become well-understood in the last several years. Recently, several computational analyses have predicted that certain topological features of a polymer, such as the average size of pseudo-knots and the probability of knot formation, are enhanced by confinement. Here, we extend recent work on the stretching of knotted DNA and examine diffusion, relaxation, and chain statistics of topologically complex linear DNA molecules. Topological phenomena are studied both in the bulk and under nanofluidic confinement to examine the interplay between knotting and confinement in semiflexible polymers, as well as to provide a controlled experimental interrogation of the knotted region of the polymer.

**4:42PM H41.00010 DNA Partitioning in Confining Nanofluidic Slits**, MADELINE GREENIER, STEPHEN LEVY, Physics Department, Binghamton University — We measure the partitioning of double stranded DNA molecules in moderately and strongly confining nanofluidic slit-like structures. Using fluorescent microscopy, the free energy penalty of confinement is inferred by comparing the concentration of DNA molecules in adjoining slits of different depths. These depths range in size from several persistence lengths to the DNA molecule's radius of gyration. The partition coefficient is determined as a function of the slit depth, DNA contour length, and DNA topology. We compare our results to theory and Monte Carlo simulations that predict the loss of free energy for ideal and semiflexible excluded volume polymers confined between parallel plates.

**4:54PM H41.00011 To Knot or Not-That is the Question: A Nanofluidic Knot Factory based on Compression of Single DNA Molecules against Slit Barriers in Nanochannels**, SUSAN AMIN, AHMED KHORSHID, LILI ZENG, Department of Physics- McGill University, PHILIP ZIMNY, Department of Biomedical Engineering- McGill University, WALTER REISNER, Department of Physics- McGill University — Knots can form during DNA packaging in chromosome and obstruct mapping of DNA in nanochannels. Studies have focused on theoretical and numerical studies of knots, but an efficient and fully controlled means of knotting has not yet been explored. Here, we introduce a knot factory on chip based on pneumatic compression of single T4 DNA against a slit barrier in a nanochannel. The DNA are compressed to a well-defined fraction of their initial equilibrium extension. The pressure is then released and the DNA molecules relax back to their equilibrium extension; knots are present along the relaxed DNA, visualized as sharply localized regions of high intensity. Via repeated compression and relaxation, we can measure the probabilities of forming single and multiple knot states and the distribution of knot sizes as a function of fractional compression and waiting time in the compressed state. We show that the total probability of knot formation increases with greater compression and waiting time. These findings are well described via a knot formation free energy derived from scaling arguments, suggesting that the enhanced knotting probability at high compression arises from avoiding the free energy cost due to self-exclusion interactions that would arise from contour stored in the knot.

**5:06PM H41.00012 Polymer translocation from a confining tube: the effect of a finite tube length**, DAVID SEAN, GARY W SLATER, Univ of Ottawa — Coarsed-grained Langevin Dynamics simulations of driven polymer translocation are used to study situations where the polymer is initialized inside a confining cylindrical cavity. The latter limits the number of conformations at the onset of translocation, which (in the highly driven limit) should lead to a net reduction in the variance of the mean translocation time. We vary both the confinement volume and the cavity aspect ratio to minimize the coefficient of variation of the translocation time. We also use a tension-propagation model and find that its predictions are in good agreement with our simulation results: both yield a minimum in the coefficient of variation for a tube having an aspect ratio corresponding to a diameter which is roughly twice the tube length. Moreover, fluctuations in the translocation coordinate  $s(t)$  do not generally follow a power law with time  $\langle \Delta s^2 \rangle \sim t^\beta$ ; for some of the geometries we actually observed non-monotonic fluctuations. We attribute this result to conformations containing hairpins, which are an outcome of having a polymer initially confined in a tube with a finite volume.

**5:18PM H41.00013 Experimental Evidence of Weak Excluded Volume Effects for Nanochannel Confined DNA**, DAMINI GUPTA, JEREMY J. MILLER, ABHIRAM MURALIDHAR, Chemical Engineering and Materials Science, University of Minnesota, Minneapolis MN, USA, SARA MAHSHID, WALTER REISNER, Physics Department, McGill University, Montreal QC, Canada, KEVIN D. DORFMAN, Chemical Engineering and Materials Science, University of Minnesota, Minneapolis MN, USA — In the classical de Gennes picture of weak polymer nanochannel confinement, the polymer contour is envisioned as divided into a series of isometric blobs. Strong excluded volume interactions are present both within a blob and between blobs. In contrast, for semiflexible polymers like DNA, excluded volume interactions are of borderline strength within a blob but appreciable between blobs, giving rise to a chain description consisting of a string of anisometric blobs. We present experimental validation of this subtle effect of excluded volume for DNA nanochannel confinement by performing measurements of variance in chain extension of T4 DNA molecules as a function of effective nanochannel size (305-453 nm).<sup>1</sup> Additionally, we show an approach to systematically reduce the effect of molecular weight dispersity of DNA samples, a typical experimental artifact, by combining confinement spectroscopy with simulations.

<sup>1</sup> Gupta et al., ACS MacroLett. 4, 759 (2015)

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**  
**Session H42 DPOLY: Polymer Assembly II** 345 - Boualem Hammouda, NIST

**2:30PM H42.00001 Phase Behavior and Micellar Packing of Impurity-Free Pluronic Block Copolymers in Water**<sup>1</sup>, CHANG YEOL RYU, HANJIN PARK, Rensselaer Polytechnic Institute — We have investigated the impacts of the non-micellizable polymeric impurities on the micellar packing and solution phase behavior of Pluronic block copolymers in water. In particular, small angle x-ray scattering, rheology and dynamic light scattering techniques have been employed to elucidate how the low MW impurities affect the micellar packing and solution phase diagram in water, when ordered cubic structures of spherical micelles are formed. A silica slurry method has been developed using the competitive adsorption of the PEO-PPO-PEO triblock copolymers over the low MW polymeric impurities for a large scale purification of Pluronics and its purity of Pluronics has been assessed by interaction chromatography. Based on the comparative studies on micellar packing between As-Received (AR) and Purified (Pure) Pluronic F108 solutions, we found experimental evidence to support the hypothesis that the inter-micellar distance of Pluronic cubic structures in aqueous solution is governed by the effective polymer concentration in terms of PEO-PPO-PEO triblock copolymers. Removal of the impurities in AR F108 offers an important clue on window into the onset of BCC ordering via hydrodynamic contact between micelles in solution.

<sup>1</sup> NSF DMR Polymers

**2:42PM H42.00002 Controlled Solution Self-Assembly of a Midblock-Sulfonated Pentablock Copolymer**<sup>1</sup>, KENNETH MINEART, North Carolina State University, MICHAEL GRADZIELSKI, Technische Universität Berlin, RICHARD SPONTAK, North Carolina State University — The solution self-assembly of midblock-sulfonated block ionomers (SBIs) has been shown to translate to their bulk, solution-cast morphology, which can further impact their function in applications such as desalination, fuel cell, and photovoltaic membranes. Previous studies have identified that increasing the degree of sulfonation (DOS) in SBIs dispersed in a nonpolar solvent results in the growth of micellar aggregates due to increased interfacial energy. However, these works have not attempted to control the assembly at a given DOS by tuning the solvent environment. The current study probes the tunability of SBI aggregation behavior using a nonpolar/polar solvent mixture varying in composition. A combination of light scattering (SLS and DLS) and small angle X-ray scattering (SAXS) independently confirm that SBI micelles grow larger, both in core and corona, as the solvent environment becomes more nonpolar. The increases in both core and corona size will be explained using polymer thermodynamics and further supported through presentation of small angle neutron scattering (SANS) data. In addition, these results will be compared with SBI self-assembly in a single solvent, which is expected to distribute between the micelle cores and bulk solvent environment.

<sup>1</sup> We would like to acknowledge funding from NSF IRES (App 1065466) and MANN+HUMMEL GmbH.

**2:54PM H42.00003 Self-Assembly of Soft Colloids with Multi-scale Phase-Separated Structures<sup>1</sup>**, CHRIS SOSA, ROBERT K. PRUD'HOMME, RODNEY D. PRIESTLEY, Princeton Univ — The ability of polymers and block co-polymers to self-assemble into highly-ordered structures in bulk two-dimensional films under specific environmental conditions has allowed in recent years for the fabrication of nano-porous membranes, nano-structured surfaces, and sacrificial templates for the preparation of inorganic nanomaterials with well-defined geometries. Extending these fairly specific fabrication techniques to the creation of similar three-dimensional colloidal structures in bulk solutions, however, has proven quite challenging despite the significant need for heterogeneously-structured colloidal materials in medicine and industry. Here we present a strategy for controlling the structural heterogeneity of soft polymer particles along multiple length scales by inducing the rapid phase-separation of polymer mixtures through a continuous nanoprecipitation process.

<sup>1</sup>DOE SCGF Fellowship Program

**3:06PM H42.00004 Solution assembly behaviors of 3-hexylthiophene polymer based rod-coil graft copolymer**, YOUNGKWON KIM, JIN-SUNG KIM, HYEONG JUN KIM, BUMJOON KIM, KAIST — Solution assembly of conjugated polymer based block copolymers (BCPs) is an attractive approach for achieving conducting nanowires (NWs) with nanometer-scale cross-sectional dimensions. In particular, conjugated block offers one-dimensional self-growth of crystalline NWs, and secondary block gives rise to stable dispersion of NWs and additional tuning parameter for the structures of NWs. Herein, we developed a series of poly(3-hexylthiophene)-graft-poly(2-vinylpyridine) (P3HT-g-P2VP) rod-coil copolymers with systematically controlled crystallinity by modifying both grafting density and molecular weight (Mn) of coil block, and their solution assembly behaviors were carefully examined. As increasing the volume fraction and grafting density of the secondary blocks, melting temperatures, crystallization temperatures, and the crystallinity were gradually decreased by hindering rod-rod interaction between P3HT backbones, resulting in the formation of short NWs. Furthermore, the length of NMs was relatively shorter for the densely grafted copolymer despite same volume fraction of secondary block. These results suggested that controlling Mn and the number of branched coil block was critical to regulate the crystalline properties and new approach for determining the NWs growth.

**3:18PM H42.00005 Tuning nanoscale viscoelasticity of polyelectrolyte complexes with multiple types of cross-links**, TIANZHU MA, BIAO HAN, Drexel University, School of Biomedical Eng, Sci and Health Systems, DAEYEON LEE, University of Pennsylvania, School of Engineering and Applied Science, LIN HAN, Drexel University, School of Biomedical Engineering, Science, and Health Systems — Mechanical properties of hydrogels are manifestation of cross-link type and density, fixed charges and water-polymer interactions. In this study, we revealed how different types of cross-links regulate the nanoscale viscoelasticity of polyelectrolyte networks. Ionically cross-linked PAH/PAA layer-by-layer complexes were modified to include covalent cross-links using EDC. AFM-nanoindentation and force relaxation were performed at various ionic strength (0.01-1M) and pH (1.5-5.5). As-assembled networks, held only by ionic cross-links, underwent >95% relaxation, dominated by cross-link breaking and re-formation. Addition of covalent cross-links increased the instantaneous modulus by 1.6-fold and attenuated relaxation to ≈80% of net neutral states (pH≥3.5), as covalent cross-links provide additional elastic components. The network remained stabilized when all ionic cross-links were dissociated at pH≤1.5, whereby further attenuation to 31% in relaxation could be due to viscoelastic polymer conformational changes and fluid flow-induced poroelasticity. Taken together, this study demonstrates the potential of using multiple cross-linking types to tune the viscoelastic mechanisms in polyelectrolyte complexes.

**3:30PM H42.00006 Coarse-grained Simulation of Complexation between Small Interfering RNA and Polycations**, ZONGHUI WEI, Northwestern University, YONG REN, JOHN-MICHAEL WILLIFORD, HAI-QUAN MAO, Johns Hopkins University, ERIK LUIJTEN, Northwestern University, NORTHWESTERN UNIVERSITY COLLABORATION, JOHNS HOPKINS UNIVERSITY COLLABORATION — Nanoparticles formed through self-assembly of polycations and nucleic acids are promising systems for gene delivery. A full understanding of the behavior of these particles in physiological context requires detailed knowledge of their physical properties. All-atom molecular dynamics simulations can provide insight into the interaction of polymeric carriers with genomic material, but only at limited time and length scales. To overcome these limitations and explore the full complexation process, a reliable coarse-grained model is needed. Here, we systematically develop such a model for a system comprised of small interfering RNA (siRNA) and polyethyleneimine-based carriers, and evaluate the quality of the coarse-grained model through comparison with all-atom simulations. We show that our coarse-grained model provides a reliable description of detailed binding pictures, charge characteristics, and water dynamics, while accelerating the simulations by two orders of magnitude. This makes it possible to quantitatively investigate nanoparticle formation involving multiple siRNA molecules and cationic copolymers.

**3:42PM H42.00007 Mesoscale Lattices Assembled from Charge-Tunable Block Copolymer Blends in Selective Solvents**, SEYOUNG KIM, JEWON CHOI, Seoul Natl Univ, SOO-HYUNG CHOI, Hongik Univ, KOOKHEON CHAR, Seoul Natl Univ — Recent studies revealed that block copolymer (BCP) microdomains are capable of being organized into unusual symmetries such as the Frank-Casper phases. These unique structures result from a compromise between domain geometry and space-filling constraint; in other words, the deformability of soft matter. Our mesoscale micellar lattices co-assembled from the blends of oppositely charged BCPs demonstrate the nature of deformable soft materials in a distinctive way. The micellar structures and interactions of BCPs in selective solvents can be finely tuned by controlling the charge density such that the spherical micelles further assemble into hexagonal arrays. The micellar lattices show unconventional symmetry and sub-10 nm clean facet formation compared to hard-sphere counterparts reported so far. We attribute these novel phenomena to multi-compartment intrastructure of the micelles assembled and their strong interactions, since the crystalline symmetry disappears with a subtle control of solvency, mixing ratio of BCP blends, and micellar interactions. Analysis on the nucleation condition reveals that such deviation in the micellar lattices arises from the soft nature of BCP assemblies which can be readily deformed upon swelling.

**3:54PM H42.00008 The Sheet Trapped in a Plumber's Nightmare**, CHRISTOPHER O'BRYAN, TAPOMOY BHATTACHARJEE, W. GREGORY SAWYER, THOMAS ANGELINI, Univ of Florida - Gainesville — Block co-polymer systems offer exquisite control in the molecular-level design of self-assembled structures. The application of block copolymer phases has been generally limited to their use as bulk stabilizing agents in mass produced commodity chemicals and plastics. Recently, we have found the complex phase structures of self-assembled styrene ethylene/propylene diblock and styrene ethylene/butylene triblock co-polymers useful in 3D printing of other soft materials; the co-polymer structure yields around a writing nozzle as it moves through space while leaving material (polymers or colloids) trapped in the form of programmed structures. However, the relationship between the structural phase of the co-polymer self-assembly and its ability to support printed soft matter materials is not understood. In this study, we explore how different block co-polymer assemblies interact with and support soft matter materials once localized yielding has occurred.

**4:06PM H42.00009 Structural transformation of peptide amphiphile self-assembly induced by headgroup charge and size regulation**, CHANGRUI GAO, Northwestern University, MICHAEL BEDZYK, MONICA OLVERA, SUMIT KEWALRAMANI, Northwestern University, Materials Science and Engineering, LIAM PALMER, Northwestern University, Chemistry — The ability to control the nano and the meso-scale architecture of molecular assemblies is one of the major challenges in nanoscience. Significantly, structural transformations of amphiphilic aggregates induced by variations in environmental conditions have attracted attention due to their biotechnological relevance. Here, we study the assembly in aqueous solution for a modular series of peptide amphiphiles with 3, 2 or 1 lysine groups conjugated to a C<sub>16</sub> carbon tail (C<sub>16</sub>K<sub>3</sub>, C<sub>16</sub>K<sub>2</sub>, and C<sub>16</sub>K<sub>1</sub>). This system design allow us to probe how the equilibrium structure of the self-assembly can be tuned by controlling the coupling between steric (via choice of headgroup: K<sub>3</sub>, K<sub>2</sub>, or K<sub>1</sub>) and electrostatic (via solution pH) interactions. Solution small- and wide-angle X-ray scattering (SAXS/WAXS) and transmission electron microscopy (TEM) studies reveal that depending on pH and number of lysines in the lipid headgroup, amphiphiles can assemble into a range of structures: spherical micelles, bilayer ribbons and vesicles. We also perform detailed phase space mapping of pH-and headgroup size dependency of the structures of assembly over 0.1-100 nm length scales via SAXS/WAXS. The experimental results in conjunction with molecular dynamics (MD) simulations deduce quantitative relations between pH-dependent molecular charges, steric constraints and self-assembly morphologies, which is significant for developing experimental routes to obtain assembly structures with specific nano- and meso-scale features through controlled external stimuli.

**4:18PM H42.00010 Multibody Interactions, Phase Behavior and Clustering in Nanoparticle-Polyelectrolyte Mixtures**, VENKATRAGHAVAN GANESAN, GUNJA PANDAV, VICTOR PRYAMITSYN, Univ of Texas, Austin, JEFFREY ERRINGTON, SUNY Buffalo — We present the results of a computational study of the interactions, phase-behavior and aggregation characteristics of charged nanoparticles (CNPs) suspended in solution of oppositely charged polyelectrolytes (PEs). We used an extension of the mean-field polymer self-consistent field theory (SCFT) model to explicitly characterize the multibody interactions in such systems. For dilute-moderate particle volume fractions, the magnitudes of three and higher multibody interactions were seen to be weak relative to the contributions from pair interactions. We embedded the pair-interaction potentials within a thermodynamic perturbation theory approach to identify the phase behavior of such systems. The results of such a framework suggested that the gas and FCC crystal phases were thermodynamically stable, whereas the fluid-like phase was metastable in such systems. To complement the parameters studied, we used a recently developed simulation approach to study the aggregation and cluster morphologies in CNP-PE mixtures. For low particle charges, such systems mainly exhibited clusters arising from direct contact aggregation between CNPs. However, for higher particle and PE charges and low PE concentrations, large regions of PE-bridged clusters were seen to form.

**4:30PM H42.00011 Early Stage Kinetics in Polyelectrolyte Complexation Studied in a Stopped-Flow Configuration**, XIAOQING LIU, MARIE HADDOU, JOANNA GIERMANSKA, Centre de Recherche Paul Pascal (CRPP), UPR CNRS 8641, Universit Bordeaux, 33600 Pessac, France, CHRISTOPHE SCHATZ, Laboratoire de Chimie des Polymres Organiques, Ecole Nationale Suprieure de Chimie de Biologie et de Physique, 33600 Pessac, France, JEAN-PAUL CHAPEL, Centre de Recherche Paul Pascal (CRPP), UPR CNRS 8641, Universit Bordeaux, 33600 Pessac, France — Polyelectrolyte complexes (PECs) are the association complexes formed between oppositely charged macromolecules. A large body of work has been devoted to the preparation and morphology characterizations of PECs. Much less attention was paid on formation kinetics of PECs, which often occurs under non-equilibrium conditions. Stopped-flow technique combined with light scattering was used to investigate the early stage complexation kinetics in the poly(acrylic acid) and poly(diallyldimethylammonium chloride) system. It was found that initial complexes form within a few ms. Depending on the PEs molar charge ratio  $z$ , initial complexes followed different evolution pathways. For  $z > 0.7$ , a large complex aggregation ascribed to the onset of coacervation was identified by an increase of the scattered intensity while an unexpected decay was observed for  $z < 0.7$  where small PECs are formed. The appearance of characteristic bell-shaped curves in the presence of different ionic strengths ( $I$ ) highlighted the strong influence of the interaction intensity on the complexation/reorganization kinetics. The results revealed distinct assembly and ageing mechanisms as a function of  $z$ ,  $I$  and molecular weights.

**4:42PM H42.00012 Supramolecular Assemblies of Poly(propyleneimine) Dendrimers Driven by Simple Monovalent Counterions**, SEYED ALI EGHTESADI, FADI HASO, MARJAN ALSADAT KASHFIPOUR, DR. ROBERT LILLARD, DR. TIANBO LIU, University of Akron, DR. TIANBO LIU'S GROUP TEAM, DR. LILLARD'S GROUP COLLABORATION — Polyelectrolytes (PE) are fascinating class of polymers carrying dissociative ionic groups which give them unique properties in solutions and at charged surfaces. The properties of these polymers in solution are mainly depending on the fraction of dissociated ionic groups, the quality of solvent and salt concentration. Describing the solution properties of polyelectrolytes have always been an obstacle for polymer scientists due to their different behavior as a result of their dual character of being highly charged electrolytes and at macromolecular size. The question we tried to address was what happens to solution behavior of charged polyelectrolytes when they reach to the nano-scale size which can neither be considered as point charges nor colloids. Second generation of poly(propyleneimine) dendrimer in different solvent qualities, salt concentrations, pH and temperatures were studied using techniques such as LLS, TEM, AFM and zeta-potential, and dominant controlling factors over their self-assembly into hollow spherical "Blackberry" like nanoparticles was investigated.

**4:54PM H42.00013 Self-Assembly of Polyoxometalate and Polyelectrolyte Macroions into Mechanically Strong Supramolecular Hydrogels**, BENXIN JING, Y. ELAINE ZHU, Department of Chemical Engineering and Materials Science, Wayne State University, Detroit, MI 48202 — Polyoxometalate (POM) macroions are the nanoclusters of transition metal oxide with size 1-10 nm and well-defined structure at the atom level. Because of their stoichiometric surface groups and high solubility in polar solvents to form thermodynamically stable solution, POMs are studied as excellent model macroions at nanoscale. In this work, we explore the electrostatic controlled self-assembly of anionic POMs and cationic or zwitterionic polyelectrolytes (PEs) in aqueous solution. Specifically we examine the complex formation of zwitterionic poly(3-(methacryloylamino)propyl]dimethyl(3-sulfopropyl)ammonium hydroxide) (PSBMA) and cationic poly(diallyldimethylammonium chloride) (PDADMAC) with tungstate based POMs of varied valence. The phase diagram of POM/polyelectrolyte complexes is determined with varied POM/PE charge ratios. It is interesting to observe the coacervation of POMs with PSBMA. With cationic PDADMAC, hybrid POM-PDADMAC hydrogels can be formed. Nevertheless, POM-PDADMAC complexes exhibit much enhanced mechanical properties in comparison to polymer hydrogel. The viscoelastic properties of hybrid macroion complexes strongly depend on PDADMAC concentration, POM-to-PDADMAC molar ratio, the size and valence of POMs. At the intermediate range of POM-to-PDADMAC concentration ratio, shear thickening and strain hardening are observed with soft supramolecular hydrogels, which is resulted from the non-Gaussian stretching of polymer chains.

**5:06PM H42.00014 Polyelectrolyte Complex Hydrogels: Self-assembly and the Influence of Charged and Neutral Blocks**, SAMANVAYA SRIVASTAVA, DAVID GOLDFELD, ADAM LEVI, JUN MAO, Univ of Chicago, WEI CHEN, Argonne National Laboratory, MATTHEW TIRRELL, Univ of Chicago — Polyelectrolyte complexes (PEC) form when oppositely charged polyelectrolyte chains spontaneously associate and phase separate in aqueous mediums. Bulk phase separation of the PECs can be evaded by combining one or both of the polyelectrolytes with a neutral polymer, thus engineering pathways for self-assembled PEC micelles and hydrogels. The PEC domains in these assemblies can encapsulate therapeutics as well as genetic materials and thus have tremendous potential in drug delivery and tissue engineering applications. We will present insights on the equilibrium structure and self-assembly kinetics of PEC hydrogels with large-scale ordering of the nanoscale PEC domains through detailed structure characterization and rheology studies of self-assembled materials comprising of functionalized polyallyl glycidyl ethers (PAGE) connected to either single poly(ethylene glycol) (PEG) chain to form diblock copolymers or as functionalized end-groups on a triblock copolymer with a PEG midblock. The effect of key parameters such as polymer concentration, polymer block lengths, salt, ionic strength, and degree of charge mismatch on the equilibrium materials properties will be discussed, with a special emphasis on the structure-defining role of the charged blocks and the structure-directing role of neutral blocks. Additionally, interesting similarities, and differences between structures and dynamics of hydrogels comprising diblock and corresponding triblock polyelectrolytes, respectively, will be discussed.

**5:18PM H42.00015 Thermo-reversible morphology and conductivity of a conjugated polymer network embedded in polymeric self-assembly.**<sup>1</sup>, YOUNGKYU HAN, JAN-MICHAEL Y. CARRILLO, ZHE ZHANG, YUNCHAO LI, KUNLUN HONG, BOBBY G. SUMPTER, Oak Ridge National Laboratory, MICHAEL OHL, Jlich Center for Neutron Science, MARIAPPAN PARANS PARANTHAMAN, GREGORY S. SMITH, CHANGWOO DO, Oak Ridge National Laboratory — Self-assembly of block copolymers provides opportunities to create nano hybrid materials, utilizing self-assembled micro-domains with a variety of morphology and periodic architectures as templates for functional nano-fillers. Here we report new progress towards the fabrication of a thermally responsive conducting polymer self-assembly made from a water-soluble poly(thiophene) derivative with short PEO side chains and Pluronic L62 solution in water. The structural and electrical properties of conjugated polymer-embedded nanostructures were investigated by combining SANS, SAXS, CGMD simulations, and impedance spectroscopy. The L62 solution template organizes the conjugated polymers by stably incorporating them into the hydrophilic domains thus inhibiting aggregation. The changing morphology of L62 during the micellar-to-lamellar phase transition defines the embedded conjugated polymer network. The conductivity is strongly coupled to the structural change of the templating L62 phase and exhibits thermally reversible behavior with no signs of quenching of the conductivity at high temperature.

<sup>1</sup>The research was sponsored by the Scientific User Facilities Division, Office of BES, U.S. DOE and Laboratory Directed Research and Development Program of ORNL, managed by UT-Battelle, LLC.

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**  
**Session H43 GSNP GSOF: Aging in the Jammed State** 346 - Stefan Boettcher, Emory University

**2:30PM H43.00001 A Time-Temperature Transistor - An Application of Aging Dynamics**, GREGORY KENNING, Indiana University of Pennsylvania — Aging dynamics occur as systems far from thermodynamic equilibrium evolve towards equilibrium. We have produced a magnetic nanoparticle system composed of Co nanoparticles, which self-assemble during Co deposition on Sb. At a particular time in the formation of the nanoparticles, they are encased in a layer of Sb producing a system far from equilibrium. Magnetization vs. temperature measurements as well as Magnetic Force Microscopy (MFM) indicates that the nanoparticles initially have a large magnetic moment. We observe, as a function of time, an approximately 80% decay in the sample magnetization and an approximately 50% decay in the DC electrical resistivity. MFM suggests that the magnetization decay proceeds from the magnetic nanoparticles losing their net moments possibly due to spin rearrangement. Evidence also suggests that the initial magnetic moments, drive the Sb layer semiconducting. As the net moments of the magnetic nanoparticles decrease, the Sb reverts back to its semi-metal behavior with the accompanying decrease in the electrical resistivity. The magnetization and resistance decays follow the same Arrhenius type behavior. By varying the Co layer thickness, the Arrhenius parameters can be tuned. We have been able to tune the parameters making these materials excellent candidates for sensors for electronically monitoring the age and lifetime of perishable foods.

**2:42PM H43.00002 Density variations of plastic carriers in metallic glasses during aging.**, YUE FAN, Oak Ridge National Lab, TAKUYA IWASHITA, University of Tennessee, TAKESHI EGAMI, University of Tennessee; Oak Ridge National Lab — Thermally induced deformation in metallic glasses was investigated by sampling the potential energy landscape (PEL) and probing the changes in the atomic properties (e.g. energy, displacement, stress). We demonstrate that there exists a universal plastic carrier in amorphous materials, which corresponds to the hopping between local minima on PEL. However very interestingly, the density of plastic carrier is largely affected by the aging history of the glasses. The higher fictive temperature (*i.e.* fast cooling rate), the larger density of plastic carrier is contained in the system. In particular, we observe a scaling of  $\rho \sim \exp(-\alpha/T_{fic})$ , which is consistent with the prediction of shear transformation zone theory. The work is supported by U.S. Department of Energy.

**2:54PM H43.00003 Aging and memory effects in the spin jam states of densely populated frustrated magnets**, ANJANA SAMARAKOON, SEUNG-HUN LEE, University of Virginia, TAKU SATO, Tohoku University, Katahira, Sendai, Japan, HAIDONG ZHOU, RYAN SINCLAIR, University of Tennessee, JUNJIE YANG, TIANRAN CHEN, GIA-WEI CHERN, ISRAEL KLICH, University of Virginia — Defects and randomness has been largely studied as the key mechanism of glassiness find in a dilute magnetic system. Even though the same argument has also been made to explain the spin glass like properties in dense frustrated magnets, the existence of a glassy state arise intrinsically from a defect free spin system, far from the conventional dilute limit with different mechanisms such as quantum fluctuations and topological features, has been theoretically proposed recently. We have studied field effects on zero-field cooled and field cooled susceptibility bifurcation and memory effects below freezing transition, of three different densely populated frustrated magnets which glassy states we call spin jam, and a conventional dilute spin glass. Our data show common behaviors among the spin jam states, which is distinct from that of the conventional spin glass. We have also performed Monte Carlo simulations to understand the nature of their energy landscapes.

**3:06PM H43.00004 Time Dependence of the freezing temperature for thin film spin glasses**<sup>1</sup>, RAYMOND ORBACH, The University of Texas at Austin — There have been many measurements of the dependence of the “freezing temperature”,  $T_f$ , on the thickness  $\mathcal{L}$  of thin film spin glasses.  $T_f$  decreases with decreasing  $\mathcal{L}$ , but never vanishes. This contribution suggests that the dependence of  $T_f$  on  $\mathcal{L}$  is a time dependent relationship. Because the lower critical dimension of a spin glass,  $d_\ell \approx 2.5$ , when the spin glass correlation length  $\xi(t, T)$  grows to  $\mathcal{L}$ , the spin glass dimensionality crosses over from  $d = 3$  to  $d = 2$ . What remains are spin glass correlations for length scales  $\leq \mathcal{L}$ . The time dependence of the magnetization dynamics are then activated, with activation energy equal to a largest barrier  $\Delta_{max}(\mathcal{L})$ , and an associated activation time  $\tau$ . For measurements at time scales such that  $\xi(t, T) < \mathcal{L}$ , the effective dimension  $d = 3$ , and the characteristic cusp and knee of a spin glass is observed. For experimental time scales greater than  $\tau$ , with  $\xi(t, T) \approx \mathcal{L}$ , the zero-field cooled magnetization has grown to the field-cooled value of the magnetization, leading to the identification of  $T_f$ . Quantitative agreement with experiment is exhibited.

<sup>1</sup>Supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering under Award DE-SC0013599

**3:18PM H43.00005 Intermittent Aging Dynamics in a Metallic Glass Studied by X-ray Photon Correlation Spectroscopy**, ZACH EVENSON, Technical University Munich / Maier-Leibnitz Zentrum (MLZ), BEATRICE RUTA, ESRF - The European Synchrotron, SIMON HECHLER, MORITZ STOLPE, Saarland University, ELOI PINEDA, Universitat Politècnica de Catalunya-BarcelonaTech, ISABELLA GALLINO, RALF BUSCH, Saarland University — Although physical aging is a universal feature of glasses and other non-equilibrium matter, the atomic-level processes involved still remain a puzzling mystery. Here we study the microscopic aging dynamics of a metallic glass using coherent X-rays. Contrary to the common assumption of a steady slowing down of the dynamics usually observed in macroscopic studies, we show that the structural relaxation processes underlying aging in this metallic glass are intermittent and highly heterogeneous at the atomic scale. Moreover, physical aging is triggered by cooperative atomic rearrangements, driven by the relaxation of internal stresses. These results strengthen the similarities between metallic glasses and non-equilibrium soft materials and suggest a common microscopic origin stemming from a complex energy landscape.

**3:30PM H43.00006 Record Dynamics and the Parking Lot Model for granular dynamics<sup>1</sup>**, PAOLO SIBANI, University of Southern Denmark, STEFAN BOETTCHER, Emory University — Also known for its application to granular compaction (E. Ben-Naim et al., *Physica D*, 1998), the Parking Lot Model (PLM) describes the random parking of identical cars in a strip with no marked bays. In the thermally activated version considered, cars can be removed at an energy cost and, in thermal equilibrium, their average density increases as temperature decreases. However, equilibration at high density becomes exceedingly slow and the system enters an aging regime induced by a kinematic constraint, the fact that parked cars may not overlap. As parking an extra car reduces the available free space, the next parking event is even harder to achieve. Records in the number of parked cars mark the salient features of the dynamics and are shown to be well described by the log-Poisson statistics known from other glassy systems with record dynamics. Clusters of cars whose positions must be rearranged to make the next insertion possible have a length scale which grows logarithmically with age, while their life-time grows exponentially with size. The implications for a recent cluster model of colloidal dynamics, (S. Boettcher and P. Sibani, *J. Phys.: Cond. Matter*, 2011 N. Becker et al., *J. Phys.: Cond. Matter*, 2014) are discussed.

<sup>1</sup>Support from the Villum Foundation is gratefully acknowledged

**3:42PM H43.00007 Non-equilibrium phenomena in disordered colloidal solids**, PETER YUNKER, Georgia Institute of Technology — Colloidal particles are a convenient tool for studying a variety of non-equilibrium phenomena. I will discuss experiments that investigate the aging and non-equilibrium growth of disordered solids. In the first set of experiments, colloidal glasses are rapidly formed to study aging in jammed packings. A colloidal fluid, composed of micron-sized temperature-sensitive pNIPAM particles, is rapidly quenched into a colloidal glass. After the glass is formed, collective rearrangements occur as the glass ages. Particles that undergo irreversible rearrangements, which break nearest-neighbor pairings and allow the glass to relax, are identified. These irreversible rearrangements are accompanied by large clusters of fast moving particles; the number of particles involved in these clusters increases as the glass ages, leading to the slowing of dynamics that is characteristic of aging. In the second set of experiments, we study the role particle shape, and thus, interparticle interaction, plays in the formation of disordered solids with different structural and mechanical properties. Aqueous suspensions of colloidal particles with different shapes evaporate on glass slides. Convective flows during evaporation carry particles from drop center to drop edge, where they accumulate. The resulting particle deposits grow heterogeneously from the edge on the air-water interface. Three distinct growth processes were discovered in the evaporating colloidal suspensions by tuning particle shape-dependent capillary interactions and thus varying the microscopic rules of deposition. Mechanical testing of these particulate deposits reveals that the deposit bending rigidity increases as particles become more anisotropic in shape.

**4:18PM H43.00008 Correlated Clusters in Aging Colloidal Glass<sup>1</sup>**, DOMINIC ROBE, STEFAN BOETTCHER<sup>2</sup>, Emory University, PETER YUNKER<sup>3</sup>, Georgia Tech — A numerical model of correlated domains in glassy colloids is recreated, following its development by Becker, et. al.<sup>4</sup>. The model is a coarse grained representation of 2D colloidal systems inspired by record dynamics, and produces emergent dynamic heterogeneity and aging. Results from the original development are reproduced, and compared to the same observables in an experimental system of bidisperse microgel spheres studied by Yunker, et. al.<sup>5</sup>. Basic observables such as particle persistence and mean square displacement are measured at different waiting times to observe aging. Four-point correlation lengths are also examined for signs of dynamic heterogeneity. Results from both the numerical and experimental systems are consistent with the predictions of record dynamics, that aging systems evolve on a logarithmic time scale.

<sup>1</sup>This work is supported by NSF grant DMR-1207431

<sup>2</sup>Website: <http://www.physics.emory.edu/faculty/boettcher/>

<sup>3</sup>Website: <https://www.physics.gatech.edu/user/peter-yunker>

<sup>4</sup>N Becker, et. al. Mesoscopic model of temporal and spatial heterogeneity in aging colloids 2014 *J. Phys.: Condens. Matt.* <http://arxiv.org/abs/1401.6521v1>

<sup>5</sup>P Yunker, et. al. Irreversible rearrangements, correlated domains, and local structure in aging glasses 2009 *Phys. Rev. Lett.* <http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.103.115701>

**4:30PM H43.00009 Universal Scaling in the Aging of the Strong Glass Former SiO<sub>2</sub><sup>1</sup>**, KATHARINA VOLLMAIR-LEE, Bucknell University, HORACIO CASTILLO, Department of Physics and Astronomy and Nanoscale and Quantum Phenomena Institute, CHRISTOPHER GORMAN, University of California, Santa Barbara — We show that the aging dynamics of a strong glass former displays a strikingly simple scaling behavior. Using molecular dynamics simulations, we quench the system from high temperature to 2500 K, below the glass transition and investigate dynamic heterogeneities as function of waiting time, the time elapsed since the quench. We find that both the dynamic susceptibility and the probability distribution of the local incoherent intermediate scattering function can be described by simple scaling forms in terms of the global incoherent intermediate scattering function. The scaling forms are the same that have been found to describe the aging of several fragile glass formers. Furthermore we find that the aging dynamics is controlled by a unique aging clock which is the same for Si and O atoms.

<sup>1</sup>We acknowledge the support via NSF REU Grant PHY-1156964, DFG via SFB 602 and FOR1394, and DOE under grant DE-FG02-06ER46300 and NSF Grant PHY-1066293.

**4:42PM H43.00010 Aging near the wall in colloidal glasses**, CONG CAO, XINRU HUANG, ERIC WEEKS, Emory University — In a colloidal glass system, particles move slower as sample ages. In addition, their motions may be affected by their local structure, and this structure will be different near a wall. We examine how the aging process near a wall differs from that in the bulk of the sample. In particular, we use a confocal microscope to observe 3D motion in a bidisperse colloidal glass sample. We find that flat walls induce the particles to organize into layers. The aging process behaves differently near the boundary, especially within the first three layers. Particle motion near the wall is noticeably slower but also changes less dramatically with age. We compare and contrast aging seen in samples with flat and rough walls.

**4:54PM H43.00011 Thermal fluctuations and elastic relaxation in the compressed exponential dynamics of colloidal gels**, MEHDI BOUZID, JADER COLOMBO, EMANUELA DEL GADO, Georgetown University — Colloidal gels belong to the class of amorphous systems, they are disordered elastic solids that can form at very low volume fraction, via aggregation into a rich variety of networks. They exhibit a slow relaxation process in the aging regime similar to the glassy dynamics. A wide range of experiments on colloidal gels show unusual compressed exponential of the relaxation dynamical properties. We use molecular dynamics simulation to investigate how the dynamic change with the age of the system. Upon breaking and reorganization of the network structure, the system may display stretched or compressed exponential relaxation. We show that the transition between these two regimes is associated to the interplay between thermally activated rearrangements and the elastic relaxation of internal stresses. In particular, ballistic-like displacements emerge from the non local relaxation of internal stresses mediated by a series of "micro-collapses". When thermal fluctuations dominate, the gel restructuring involves instead more homogeneous displacements across the heterogeneous gel network, leading to a stretched exponential type of relaxation.

**5:06PM H43.00012 Power-law creep and residual stresses in carbopol microgels** , PIERRE LIDON, SEBASTIEN MANNEVILLE, Physics Laboratory - Ecole Normale Supérieure de Lyon - France — We report on the interplay between creep and residual stresses in carbopol microgels. When a constant shear stress  $\sigma$  is applied below the yield stress  $\sigma_c$ , the strain is shown to increase as a power law of time,  $\gamma(t) = \gamma_0 + (t/\tau)^\alpha$ , with an exponent  $\alpha \simeq 0.38$  that is strongly reminiscent of Andrade creep in hard solids. For applied shear stresses lower than some characteristic value of about  $\sigma_c/10$ , the microgels experience a more complex creep behavior that we link to the existence of residual stresses and to weak aging of the system after preshear. The influence of the preshear protocol, of boundary conditions and of microgel concentration on residual stresses is investigated. We discuss our results in light of previous works on colloidal glasses and other soft glassy systems.

**5:18PM H43.00013 Creep and aging in jammed granular materials** , ISHAN SRIVASTAVA, TIMOTHY FISHER, Purdue Univ — Granular materials flow (or unjam) when stressed above the Coulomb yield stress, but a slow creep is observed when the applied stresses are low. In this work, using a recently introduced enthalpy-based variable-cell simulation method, we will present results on the creep and slow aging dynamics in granular systems comprised of soft particles of varying shape that are hydrostatically jammed and subjected to an external stress. We observe a two-stage creep with an initial fast exponential evolution followed by a slow logarithmic evolution over long time scales. We correlate the slow creeping dynamics with micromechanical evolution at the grain scale, such as increasing dynamical heterogeneity and force-chain rearrangements. Results will also be presented on the effect of grain shape (faceted vs. spherical) on the creep and aging dynamics. Finally, a continuum granular fluidity model is developed to rationalize these observations.

## Tuesday, March 15, 2016 2:30PM - 5:30PM –

Session H44 GQI: Quantum Algorithms 347 - Kenneth Rudinger, Sandia National Labs

**2:30PM H44.00001 Quantum linear systems algorithm with exponentially improved dependence on precision**<sup>1</sup> , ROLANDO SOMMA, Los Alamos National Laboratory, ANDREW CHILDS, University of Maryland, ROBIN KOTHARI, Massachusetts Institute of Technology — Harrow, Hassidim, and Lloyd showed that for a suitably specified  $N \times N$  matrix  $A$  and  $N$ -dimensional vector  $\vec{b}$ , there is a quantum algorithm that outputs a quantum state proportional to the solution of the linear system of equations  $A\vec{x} = \vec{b}$ . If  $A$  is sparse and well-conditioned, their algorithm runs in time polynomial in  $\log N$  and  $1/\epsilon$ , where  $\epsilon$  is the desired precision in the output state. We improve this to an algorithm whose running time is polynomial in  $\log(1/\epsilon)$ , exponentially improving the dependence on precision while keeping essentially the same dependence on other parameters. Our algorithm is based on a general technique for implementing any operator with a suitable Fourier or Chebyshev series representation. This allows us to bypass the quantum phase estimation algorithm, whose dependence on  $\epsilon$  is prohibitive.

<sup>1</sup>The authors acknowledge support from AFOSR, ARO, CIFAR, IARPA, NRO, and NSF

**2:42PM H44.00002 QUANTUM ALGORITHM FOR LINEAR PROGRAMMING PROBLEMS** , PRAMOD JOAG, Professor, DHANANJAY MEHENDALE, Associate Professor — The quantum algorithm (PRL 103, 150502, 2009) solves a system of linear equations with exponential speedup over existing classical algorithms. We show that the above algorithm can be readily adopted in the iterative algorithms for solving linear programming (LP) problems. The first iterative algorithm that we suggest for LP problem follows from duality theory. It consists of finding nonnegative solution of the equation for duality condition; for constraints imposed by the given primal problem and for constraints imposed by its corresponding dual problem. This problem is called the problem of nonnegative least squares, or simply the NNLS problem. We use a well known method for solving the problem of NNLS due to Lawson and Hanson. This algorithm essentially consists of solving in each iterative step a new system of linear equations. The other iterative algorithms that can be used are those based on interior point methods. The same technique can be adopted for solving network flow problems as these problems can be readily formulated as LP problems. The suggested quantum algorithm can solve LP problems and Network Flow problems of very large size involving millions of variables.

**2:54PM H44.00003 A quantum Algorithm for the Moebius Function** , PETER LOVE, Tufts Univ — We give an efficient quantum algorithm for the Moebius function from the natural numbers to  $-1, 0, 1$ . The cost of the algorithm is asymptotically quadratic in  $\log n$  and does not require the computation of the prime factorization of  $n$  as an intermediate step.

**3:06PM H44.00004 The Deutsch-Jozsa algorithm as a suitable framework for MapReduce in a quantum computer** , SAMIR LIPOVACA, None — The essence of the MapReduce paradigm [1] is a parallel, distributed algorithm across hundreds or thousands of machines. In crude fashion this parallelism reminds us of the method of computation by quantum parallelism which is possible only with quantum computers. Deutsch and Jozsa [2] showed that there is a class of problems which can be solved more efficiently by quantum computer than by any classical or stochastic method. The method of computation by quantum parallelism solves the problem with certainty in exponentially less time than any classical computation. This leads to the question: would it be possible to implement the MapReduce paradigm in a quantum computer and harness this incredible speedup over the classical computation performed by the current computers. Although present quantum computers are not robust enough for code writing and execution, it is worth exploring this question from a theoretical point of view. We will show from a theoretical point of view that the Deutsch-Jozsa algorithm is a suitable framework to implement the MapReduce paradigm in a quantum computer. References: [1] Chuck Lam, *Hadoop in Action*, (Manning Publications Co. Greenwich, CT, USA ©2010). [2] Deutsch, D., Jozsa, R. 1992 *Proc. R. Soc. Lond. A* 439, 553-558.

**3:18PM H44.00005 Optimizing Qubit Resources for Quantum Chemistry Simulations in Second Quantization on a Quantum Computer** , NIKOLAJ MOLL, ANDREAS FUHRER, PETER STAAR, IVANO TAVERNELLI, IBM Research - Zurich — Quantum chemistry simulations on a quantum computer suffer from the overhead needed for encoding the fermionic problem in a bosonic system of qubits. By exploiting the block diagonality of a fermionic Hamiltonian, we show that the number of required qubits can be reduced by a factor of two or more. There is no need to go into the basis of the Hilbert space for this reduction because all operations can be performed in the operator space. The scheme is conceived as a pre-computational step that would be performed on a classical computer prior to the actual quantum simulation. We apply this scheme to reduce the number of qubits necessary to simulate both the Hamiltonian of the two-site Fermi-Hubbard model and the hydrogen molecule. Both quantum systems can then be simulated with a two-qubit quantum computer.

**3:30PM H44.00006 Modelling Quantum Subsystem Dynamics<sup>1</sup>**, JASON DOMINY, University of Southern California, ALIREZA SHABANI, Google Research, DANIEL LIDAR, University of Southern California — We describe a general and consistent mathematical model for linear subsystem quantum dynamical maps, developed from a minimal set of postulates, primary among which is a relaxation of the usual, restrictive assumption of uncorrelated initial system-bath states. The resulting space of physically realizable dynamical maps, far from being limited to only completely positive (CP) maps, comprises essentially all  $C$ -linear, Hermiticity-preserving, trace-preserving subsystem maps. We will discuss some implications for the standard theory of open quantum systems and the search for necessary and sufficient conditions for complete positivity. See [1], [2] for additional details. [1] Jason M. Dominy, Alireza Shabani, and Daniel A. Lidar. A general framework for complete positivity. *Quantum Inf. Proc.*, 2015. (To appear). URL: <http://dx.doi.org/10.1007/s11128-015-1148-0>. [2] Jason M. Dominy and Daniel A. Lidar. Beyond complete positivity. [arXiv:1503.05342](https://arxiv.org/abs/1503.05342).

<sup>1</sup>This research was supported by the ARO MURI grant W911NF-11-1-0268 and by NSF grant numbers PHY-969969 and PHY-803304.

**3:42PM H44.00007 Hybrid quantum-classical approach to correlated materials**, BELA BAUER, DAVE WECKER, Microsoft Research, ANDREW J. MILLIS, Columbia University, MATTHEW B. HASTINGS, Microsoft Research, MATTHIAS TROYER, ETH Zurich — Recent improvements in control of quantum systems make it seem feasible to finally build a programmable general-purpose quantum computer within a decade. While it has been shown that such a quantum computer can in principle solve certain small electronic structure problems and idealized model Hamiltonians, the highly relevant problem of directly solving a complex correlated material appears to require a prohibitive amount of resources. Here, we show that by using a hybrid quantum-classical algorithm that incorporates the power of a small quantum computer into a framework of classical embedding algorithms, the electronic structure of complex correlated materials can be efficiently tackled using a quantum computer. In our approach, the quantum computer solves a small effective quantum impurity problem that is self-consistently determined via a feedback loop between the quantum and classical computation. Use of a quantum computer enables much larger and more accurate simulations than with any known classical algorithm, and will allow many open questions in quantum materials to be resolved once a small quantum computer with around one hundred logical qubits becomes available.

**3:54PM H44.00008 A method to efficiently simulate the thermodynamic properties of the Fermi-Hubbard model on a quantum computer**, PIERRE-LUC DALLAIRE-DEMERS, FRANK WILHELM-MAUCH, Saarland University — Many phenomena of strongly correlated materials are encapsulated in the Fermi-Hubbard model whose thermodynamic properties can be computed from its grand canonical potential. In general, there is no closed form expression of the grand canonical potential for lattices of more than one spatial dimension, but solutions can be approximated with cluster perturbation theory. To model long-range effects such as order parameters, a powerful method to compute the cluster's Green's function consists in finding its self-energy through a variational principle. This opens the possibility of studying various phase transitions at finite temperature in the Fermi-Hubbard model. However, a classical cluster solver quickly hits an exponential wall in the memory (or computation time) required to store the computation variables. Here it is shown theoretically that the cluster solver can be mapped to a subroutine on a quantum computer whose quantum memory scales as the number of orbitals in the simulated cluster. A quantum computer with a few tens of qubits could therefore simulate the thermodynamic properties of complex fermionic lattices inaccessible to classical supercomputers.

**4:06PM H44.00009 Efficient Simulation of Dissipative Dynamics**, KYUNGJOO NOH, VICTOR V. ALBERT, CHAO SHEN, LIANG JIANG, Yale University — Open quantum systems with engineered dissipations may have more than one steady states. These steady states may form a non-trivial decoherence free subspace (DFS) that can store quantum information against major decoherences. Besides unitary operations within DFS, it is also useful to have dissipative/cooling operations within the DFS. We investigate the possibility of using Hamiltonian perturbation to the engineered dissipation to induce an effective dissipative dynamics within the DFS in a controlled manner. The major challenge is to simulate all the Lindblad jump operators in the master equation. By designing the dissipation within the subspace complementary to the DFS, we can simply use the Hamiltonian perturbation to the designed dissipation with a *single* jump operator to produce an effective dissipation with *multiple* Lindblad jump operators.

**4:18PM H44.00010 Racing in parallel: Quantum versus Classical**, DAMIAN S. STEIGER, MATTHIAS TROYER, ETH Zurich — In a fair comparison of the performance of a quantum algorithm to a classical one it is important to treat them on equal footing, both regarding resource usage and parallelism. We show how one may otherwise mistakenly attribute speedup due to parallelism as quantum speedup. We apply such an analysis both to analog quantum devices (quantum annealers) and gate model algorithms and give several examples where a careful analysis of parallelism makes a significant difference in the comparison between classical and quantum algorithms.

**4:30PM H44.00011 How far can we push quantum variational algorithms without error correction?**, RYAN BABBUSH, Google — Recent work has shown that parameterized short quantum circuits can generate powerful variational ansatzes for ground states of classically intractable fermionic models. This talk will present numerical and experimental evidence that quantum variational algorithms are also robust to certain errors which plague the gate model. As the number of qubits in superconducting devices keeps increasing, their dynamics are becoming prohibitively expensive to simulate classically. Accordingly, our observations should inspire hope that quantum computers could provide useful insight into important problems in the near future. This talk will conclude by discussing future research directions which could elucidate the viability of executing quantum variational algorithms on classically intractable problems without error correction.

**4:42PM H44.00012 A Quantum Algorithm for Estimating Hitting Times of Markov Chains<sup>1</sup>**, ANIRBAN NARAYAN CHOWDHURY, University of New Mexico, ROLANDO SOMMA, Los Alamos National Laboratory — We present a quantum algorithm to estimate the hitting time of a reversible Markov chain faster than classically possible. To this end, we show that the hitting time is given by an expected value of the inverse of a Hermitian matrix. To obtain this expected value, our algorithm combines three important techniques developed in the literature. One such a technique is called spectral gap amplification and we use it to amplify the gap of the Hermitian matrix or reduce its condition number. We then use a new algorithm by Childs, Kothari, and Somma to implement the inverse of a matrix, and finally use methods developed in the context of quantum metrology to reduce the complexity of expected-value estimation for a given precision.

<sup>1</sup>The authors acknowledge support from AFOSR grant number FA9550-12-1-0057 and the Google Research Award.

**4:54PM H44.00013 Continuous Time Quantum Walks in finite Dimensions<sup>1</sup>**, SHANSHAN LI, STEFAN BOETTCHER, Emory University — Continuous time quantum walk (CTQW) provides optimal quadratic speedup for spatial search on complete graphs, hypercubes, and connected random graphs compared to classical algorithms. Instead of these high dimensional graphs, we consider the performance of CTQW on the finite dimensional Migdal-Kadanoff lattices. We relate the critical point for the walk Hamiltonian to the lattice Laplacian. Using renormalization group analysis<sup>2</sup>, we calculate the critical point and derive the search performance on instances of different spectral dimension. For those with integer dimension, we reproduce the known algorithmic efficiency on regular lattices. In particular, we show that on these finite dimensional graphs, the algorithmic efficiency of quantum walk is entirely determined by the spectral dimension of the Laplacian. Quadratic speedup can only be achieved when the spectral dimension is larger than four.

<sup>1</sup>NSF grant DMR-1207431

<sup>2</sup>Boettcher, Stefan, and Shanshan Li, *Journal of Physics A* 48, 415001 (2015)

**5:06PM H44.00014 Spatial search by quantum walk is optimal for almost all graphs**, SHANTANAV CHAKRABORTY, LEONARDO NOVO, University of Lisbon, ANDRIS AMBAINIS, University of Latvia, YASSER OMAR, Instituto de Telecomunicaes, Lisbon — The problem of finding a marked node in a graph can be solved by the spatial search algorithm based on continuous-time quantum walks (CTQW). However, this algorithm is known to run in optimal time only for a handful of graphs. In this work, we prove that for Erds-Renyi random graphs, i.e. graphs of  $n$  vertices where each edge exists with probability  $p$ , search by CTQW is almost surely optimal as long as  $p \geq \log^{3/2}(n)/n$ . Consequently, we show that quantum spatial search is in fact optimal for almost all graphs, meaning that the fraction of graphs of  $n$  vertices for which this optimality holds tends to one in the asymptotic limit. We obtain this result by proving that search is optimal on graphs where the ratio between the second largest and the largest eigenvalue is bounded by a constant smaller than 1. Finally, we show that we can extend our results on search to establish high fidelity quantum communication between two arbitrary nodes of a random network of interacting qubits, namely to perform quantum state transfer, as well as entanglement generation. Our work shows that quantum information tasks typically designed for structured systems retain performance in very disordered structures.

**5:18PM H44.00015 Connecting the Discrete-time and Continuous-time Quantum Walks**, ALBERT SCHMITZ, University of North Dakota — Much work has gone into connecting the discrete-time and continuous-time versions of the quantum walk. This talk will demonstrate a method for finding an appropriate coin operator to simulate the continuous-time dynamics generated by a graph Hamiltonian for any arbitrary bigraph. This method draws a connection between a continuous-time model on the standard 1D and 2D lattice and the Hadamard walk. Furthermore, some extensions will be discussed with applications to algorithm design.

**Tuesday, March 15, 2016 2:30PM - 5:18PM –**  
**Session H45 GQI DAMOP: Quantum Information with Ions, Photons and Spins** 348 - Philipp Schindler, Innsbruck University

**2:30PM H45.00001 Parallel transport gates in a mixed-species ion trap processor<sup>1</sup>**, JONATHAN HOME, ETH Zurich — Scaled up quantum information processors will require large numbers of parallel gate operations. For ion trap quantum processing, a promising approach is to perform these operations in separated regions of a multi-zone processing chip between which quantum information is transported either by distributed photonic entanglement or by deterministic shuttling of the ions through the array. However scaling the technology for controlling pulsed laser beams which address each of multiple regions appears challenging. I will describe recent work on the control of both beryllium and calcium ions by transporting ions through static laser beams <sup>2, 3</sup>. We have demonstrated both parallel individually addressed operations as well as sequences of operations. Work is in progress towards multi-qubit gates, which requires good control of the ion transport velocity. We have developed a number of techniques for measuring and optimizing velocities in our trap, enabling significant improvements in performance <sup>4</sup>. In addition to direct results, I will give an overview of our multi-species apparatus, including recent results on high fidelity multi-qubit gates.

<sup>1</sup>We are grateful for funding from the Swiss National Science Foundation and the ETH Zurich.

<sup>2</sup>Leibfried et al. PRA 76:032324 (2007)

<sup>3</sup>deClercq et al. arXiv:1509.06624 (2015)

<sup>4</sup>deClercq et al. arXiv:1509.07083 (2015)

**3:06PM H45.00002 Quantum information processing with long-wavelength radiation**, DAVID MURGIA, Imperial College London, SEBASTIAN WEIDT, University of Sussex, JOSEPH RANDALL, Imperial College London, BJOERN LEKITSCH, SIMON WEBSTER, TOMAS NAVICKAS, ANTON GROUNDS, ANDREA RODRIGUEZ, ANNA WEBB, EAMON STANDING, University of Sussex, STUART PEARCE, IBRAHIM SARI, KIAN KIANG, HWANJIT RATTANASONTI, MICHAEL KRAFT, University of Southampton, WINFRIED HENSINGER, University of Sussex — To this point, the entanglement of ions has predominantly been performed using lasers. Using long wavelength radiation with static magnetic field gradients provides an architecture to simplify construction of a large scale quantum computer. The use of microwave-dressed states protects against decoherence from fluctuating magnetic fields, with radio-frequency fields used for qubit manipulation. I will report the realisation of spin-motion entanglement using long-wavelength radiation, and a new method to efficiently prepare dressed-state qubits and qutrits, reducing experimental complexity of gate operations. I will also report demonstration of ground state cooling using long wavelength radiation, which may increase two-qubit entanglement fidelity. I will then report demonstration of a high-fidelity long-wavelength two-ion quantum gate using dressed states. Combining these results with microfabricated ion traps allows for scaling towards a large scale ion trap quantum computer, and provides a platform for quantum simulations of fundamental physics. I will report progress towards the operation of microchip ion traps with extremely high magnetic field gradients for multi-ion quantum gates.

**3:18PM H45.00003 Controlled-phase gate for photons based on stationary light**, IVAN IAKOUPOV, Niels Bohr Institute, JOHANNES BORREGAARD, Harvard University, ANDERS S. SØRENSEN, Niels Bohr Institute — We propose a controlled-phase gate for optical photons based on an atomic ensemble coupled to a one-dimensional waveguide. When an ensemble of  $\Lambda$ -type atoms is subject to a standing wave control field, it creates a *stationary light* [1] effect where the ensemble develops a band gap for light propagation. For frequencies close to the band gap, the light-matter interactions are enhanced due to the reduced group velocity of the light pulses. Changing the internal state of one of the atoms, such that it behaves as an absorbing two-level atom instead of a transparent  $\Lambda$ -type atom, can change the scattering properties of the whole ensemble, switching it from being completely transmissive to being completely reflective. To realize a controlled-phase gate between photons, we store one of the photons inside the atomic ensemble (thereby changing the internal state of one of the atoms), scatter a second photon off the ensemble, and retrieve the first photon. Finally, we consider an application of the proposed controlled-phase gate – a quantum repeater.

## References

[1] M. Bajcsy, A. S. Zibrov, M. D. Lukin, *Nature* **426**, 638-641 (2003).

### 3:30PM H45.00004 Photonic Quantum Logic with Narrowband Light from Single Atoms

ALLISON RUBENOK, University of Bristol, ANNEMARIE HOLLECZEK, OLIVER BARTER, JEROME DILLEY, PETER B. R. NISBET-JONES<sup>1</sup>, GUNNAR LANGFAHL-KLABES, AXEL KUHN, University of Oxford, CHRIS SPARROW, University of Bristol, Imperial College London, GRAHAM D. MARSHALL, JEREMY L. O'BRIEN, KONSTANTINOS POULIOS<sup>2</sup>, JONATHAN C. F. MATTHEWS, University of Bristol — Atom-cavity sources of narrowband photons are a promising candidate for the future development of quantum technologies. Likewise, integrated photonic circuits have established themselves as a fore-running contender in quantum computing, security, and communication. Here we report on recent achievements to interface these two technologies: Atom-cavity sources coupled to integrated photonic circuits. Using narrow linewidth photons emitted from a single <sup>87</sup>Rb atom strongly coupled to a high-finesse cavity we demonstrate the successful operation of an integrated control-not gate. Furthermore, we are able to verify the generation of post-selected entanglement upon successful operation of the gate. We are able to see non-classical correlations in detection events that are up to three orders of magnitude farther apart than the time needed for light to travel across the chip. Our hybrid approach will facilitate the future development of technologies that benefit from the advantages of both integrated quantum circuits and atom-cavity photon sources.

<sup>1</sup>Now at: National Physics Laboratory

<sup>2</sup>Now at: IESL-FORTH

### 3:42PM H45.00005 Scalable Boson Sampling with Noisy Components

TYLER KEATING, University of New Mexico, JOSEPH SLOTE, Carleton College, GOPIKRISHNAN MURALEEDHARAN, EZEQUIEL CARRASCO, IVAN DEUTSCH, University of New Mexico — The goal of a Boson Sampler is to efficiently and scalably sample from a probability distribution that cannot be simulated efficiently on a classical computer, thus violating the Extended Church-Turing Thesis (ECTT). To properly falsify the ECTT, the physical device must do so even in the face of realistic noise. Scaling a Boson Sampler requires increasing quantities of a set of fixed-size components (beamsplitters, detectors, etc.), so it is natural to consider noise models that act on each component independently. We show that for any such model, the per-component noise need only decrease polynomially to keep the sampling problem hard. In this sense, Boson Sampling with noise is scalable. However, the same result applies to a number of other quantum information systems, including universal circuit-model quantum computers. Such devices are widely believed to require error correction in order to be truly scalable, even though polynomial reduction of per-component errors would allow them to work without error correction. This belief is consistent with the stricter requirement that error rates should be not just polynomially small, but constant in problem size. We conclude that a more precise definition of scalability with noise is needed to properly evaluate Boson Samplers.

### 3:54PM H45.00006 Spin models and boson sampling<sup>1</sup>

JUAN JOSE GARCIA RIPOLL, Institute of Fundamental Physics, IFF-CSIC, Spain, BORJA PEROPADRE, ALAN ASPURU-GUZI, Department of Chemistry and Chemical Biology, Harvard University — Aaronson & Arkhipov showed that predicting the measurement statistics of random linear optics circuits (i.e. boson sampling) is a classically hard problem for highly non-classical input states [1]. A typical boson-sampling circuit requires N single photon emitters and M photodetectors, and it is a natural idea to rely on few-level systems for both tasks. Indeed, we show that 2M two-level emitters at the input and output ports of a general M-port interferometer interact via an XY-model with collective dissipation and a large number of dark states that could be used for quantum information storage. More important is the fact that, when we neglect dissipation, the resulting long-range XY spin-spin interaction is equivalent [2] to boson sampling under the same conditions that make boson sampling efficient. This allows efficient implementations of boson sampling using quantum simulators & quantum computers. [1] S. Aaronson, A. Arkhipov, Proc. of the 43rd annual ACM symposium on Theory of computing (ACM, 2011) 333-342 [2] arXiv:1509.02703

<sup>1</sup>We acknowledge support from Spanish Mineco Project FIS2012-33022, CAM Research Network QITEMAD+ and EU FP7 FET-Open project PROMISCE

### 4:06PM H45.00007 Experimental fault tolerant universal quantum gates with solid-state spins under ambient conditions.<sup>1</sup>

XING RONG, University of Science and Technology of China — Quantum computation provides great speedup over classical counterpart for certain problems, such as quantum simulations, prime factoring and database searching. One of the challenges for realizing quantum computation is to execute precise control of the quantum system in the presence of noise. Recently, high fidelity control of spin-qubits has been achieved in several quantum systems. However, control of the spin-qubits with the accuracy required by the fault tolerant quantum computation under ambient conditions remains exclusive. Here we demonstrate a universal set of logic gates in nitrogen-vacancy centers with an average single-qubit gate fidelity of 0.99995 and two qubit gate fidelity of 0.992. These high control fidelities have been achieved in the C naturally abundant diamonds at room temperature via composite pulses and optimal control method. This experimental implementation of quantum gates with fault tolerant control fidelity sets an important step towards the fault-tolerant quantum computation under ambient conditions.

<sup>1</sup>National Key Basic Research Program of China (Grant No. 2013CB921800)

### 4:18PM H45.00008 Universal Superadiabatic Geometric Quantum Gates in Nitrogen-Vacancy Centers

HUI YAN, ZHENGTAO LIANG, South China Normal University, SHILIANG ZHU, Nan Jing University — We propose a scheme to implement a universal set of quantum gates based on geometric phases and superadiabatic quantum control. The proposed quantum gates consolidate the advantages of both strategies for robust and fast. The diamond nitrogen-vacancy center system is adopted as a typical example to illustrate the scheme. We show those gates can be realized in a simple two-level configuration by appropriately controlling the amplitude, phase and frequency of just one microwave field. The robust and fast features are confirmed by comparing the fidelities of the proposed superadiabatic geometric phase gate with three other kinds of phase gates.

replacing MAR16-2015-000077.

### 4:30PM H45.00009 Nonlinear opti- tum electrodynamics

IMRAN M. MIRZA, D. Center for Optics, Department of Physics, University of Oregon — We propose a scheme to perform linear optics quantum computation (LOQC). The Heisenberg-Wigner (HW) [18], 2044-2046 (1987)] i.e. complete destructive interference of two 50/50 beam splitter, is a well-known example in this context. In particular and by applying quantum jump/trajectory formalism, we show that the HW is produced by two-level emitter and spectral filtering due to the HW [18], 2044-2046 (1987)]. Along with LOQC, this work [18], 2044-2046 (1987)] (without altering their temporal and spectral traits) [Imran M.

And this abstract can also go in the sorting categories 6.9 and 6.11.

**4:42PM H45.00010 Saving entangled photons from sudden death in a single-mode fiber — Interplay of decoherence and dynamical decoupling.** , MANISH K. GUPTA, CHENGLONG YOU, HWANG LEE, JONATHAN P. DOWLING, Hearne Institute of Theoretical Physics, Louisiana State Univ - Baton Rouge — We study the dynamics of decoherence in an optical fiber for the case of entangled photons. Such a study will allow us to increase the physical length of fiber for the transmission of entangled photon from the sources such as SPDC. We analytically derive the model for decoherence of entangled state photons in a single-mode fiber. We also show that entanglement lifetime can be increased with open loop control technique called dynamical decoupling.

**4:54PM H45.00011 Restoring photon indistinguishability via pulse and continuous-wave control of solid-state quantum emitters.**<sup>1</sup> , HERBERT F. FOTSO, Ames Laboratory, ADRIAN E. FEIGUIN, Northeastern University, DAVID D. AWSCHALOM, University of Chicago, VIATCHESLAV V. DOBROVITSKI, Ames Laboratory — Interference of indistinguishable photons is a central element of many protocols for entangling distant qubits in quantum networks. In spite of great progress [1,2,3] in development and applications of solid-state quantum emitters, the entanglement rate remains severely limited. One of the major obstacles is the photon indistinguishability which is greatly reduced by the uncontrollable slow drift of the qubit emission frequency. We investigate several pulse-based and continuous-wave control protocols which suppress the spectral diffusion. We confirm, using both analytics and direct numerical simulations, that these protocols effectively keep the emission at a set target frequency, and explicitly show that the indistinguishability of the emitted photons is restored by the control. We also compare several pulse-based protocols with different pulse timings, and discuss how they affect the emission line and the photon properties. Considering the nitrogen-vacancy centers in diamonds as a convenient example, we demonstrate that both pulse-based and continuous-wave controls can boost the success rate of the long-range entanglement. [1]B. Hensen et al., Nature 526, 682 (2015). [2]B. B. Buckley et al., Science 330, 1212 (2010). [3]W. B. Gao et al., Nature Comm. 4, 2744 (2013).

<sup>1</sup>This work was supported by AFOSR MURI program and The US Department of Energy - Basic Energy Sciences (contract no. DE-AC02-07CH11358).

**5:06PM H45.00012 Optimizing Adiabaticity in NMR** , JONATHAN VANDERMAUSE, CHANDRASEKHAR RAMANATHAN, Dartmouth College — We demonstrate the utility of Berry's superadiabatic formalism for numerically finding control sequences that implement quasi-adiabatic unitary transformations. Using an iterative interaction picture, we design a shortcut to adiabaticity that reduces the time required to perform an adiabatic inversion pulse in liquid state NMR. We also show that it is possible to extend our scheme to two or more qubits to find adiabatic quantum transformations that are allowed by the control algebra, and demonstrate a two-qubit entangling operation in liquid state NMR. We examine the pulse lengths at which the fidelity of these adiabatic transitions break down and compare with the quantum speed limit.

## Tuesday, March 15, 2016 2:30PM - 5:30PM – Session H46 DCMP: Metals I 311 - Duane Johnson, Ames Laboratory

**2:30PM H46.00001 Multiscale modelling of gallium induced embrittlement in aluminium** , VENKATA SAI PAVAN KUMAR BHOGIREDDY, MIRA TODOROVA, Max Planck Inst für Eisenforschung GmbH, ROBERT SPATSCHEK, Research Center Jülich and Max Planck Inst für Eisenforschung GmbH, JÖRG NEUGEBAUER, Max Planck Inst für Eisenforschung GmbH — Liquid metal embrittlement is a degradation phenomenon in which a solid metal undergoes brittle failure when it is stressed while in contact with a liquid metal. The transition from ductile to brittle metal failure manifests itself by rapid crack propagations which reduces the elongation to failure ratio. Combining density functional theory calculations with continuum methods, we study the liquid metal embrittlement of aluminium in contact with gallium. Comparing ab initio calculated energies for a  $\Sigma 3$  and a  $\Sigma 5$  Al grain boundary and their corresponding surface energies in the presence and absence of Ga, we identify critical Ga concentrations which result in a weakening of the mechanical strength of aluminium. Parametrising the DFT results in continuum model we obtain the concentration as a function of the strain in the system. In a final step we extend this approach and compute the stress field induced by cracks in bulk and at grain boundaries. The stress field explains the large segregation of gallium atoms at the crack tip and the crack tips subsequent propagation.

**2:42PM H46.00002 Corrosion Thermodynamics of Magnesium and Alloys from First Principles as a Function of Solvation** , KRISTA LIMMER, US Army Rsch Lab - Aberdeen, KRISTEN WILLIAMS, Boeing, JAN ANDZELM, US Army Rsch Lab - Aberdeen — Thermodynamics of corrosion processes occurring on magnesium surfaces, such as hydrogen evolution and water dissociation, have been examined with density functional theory (DFT) to evaluate the effect of impurities and dilute alloying additions. The modeling of corrosion thermodynamics requires examination of species in a variety of chemical and electronic states in order to accurately represent the complex electrochemical corrosion process. In this study, DFT calculations for magnesium corrosion thermodynamics were performed with two DFT codes (VASP and DMol3), with multiple exchange-correlation functionals for chemical accuracy, as well as with various levels of implicit and explicit solvation for surfaces and solvated ions. The accuracy of the first principles calculations has been validated against Pourbaix diagrams constructed from solid, gas and solvated charged ion calculations. For aqueous corrosion, it is shown that a well parameterized implicit solvent is capable of accurately representing all but the first coordinating layer of explicit water for charged ions.

**2:54PM H46.00003 Role of defect coordination environment on point defects formation energies in Ni–Al intermetallic alloys** , EMRYS TENNESSEN, JAMES RONDINELLI, Northwestern Univ — We present a relationship among the point defect formation energies and the bond strengths, lengths, and local coordination environment for Ni–Al intermetallic alloys based on density functional calculations, including  $\text{Ni}_3\text{Al}$ ,  $\text{Ni}_5\text{Al}_3$ ,  $\text{NiAl}$ ,  $\text{Ni}_3\text{Al}_4$ ,  $\text{Ni}_2\text{Al}_3$  and  $\text{NiAl}_3$ . We find the energetic stability of vacancy and anti-site defects for the entire family can be attributed primarily to changes in interactions among first nearest neighbors, owing to spatially localized charge density reconstructions in the vicinity of the defect site. We also compare our interpretation of the local coordination environment with a DFT-based cluster expansion and discuss the performance of each approach in predicting defect stability in the Ni–Al system.

**3:06PM H46.00004 A high-throughput search for new ternary superalloys**<sup>1</sup> , CHANDRAMOULI NYSHADHAM, JACOB HANSEN, Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84602, USA., COREY OSES, Center for Materials Genomics, Duke University, Durham, North Carolina 27708, USA., STEFANO CURTAROLO, Center for Materials Genomics, Department of Mechanical Engineering and Materials Science and Department of Physics, Duke University, Durham, North Ca, GUS HART, Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84602, USA. — In 2006 an unexpected new superalloy,  $\text{Co}_3[\text{Al,W}]$ , was discovered[1]. This new alloy is cobalt-based, in contrast to conventional superalloys, which are nickel-based. Inspired by this new discovery, we performed first-principles calculations, searching through 2224 ternary metallic systems of the form  $\text{A}_3[\text{B}_{0.5}\text{C}_{0.5}]$ , where  $\text{A} = \text{Ni/Co/Fe}$  and  $[\text{B}, \text{C}] = \text{all binary combinations of 40 different elements chosen from the periodic table}$ . We found 175 new systems that are better than the  $\text{Co}_3[\text{Al}, \text{W}]$  superalloy. 75 of these systems are brand new—they have never been reported in experimental literature. These 75 new potential superalloys are good candidates for further experiments. Our calculations are consistent with current experimental literature where data exists.

[1] Sato *et. al.*, “Cobalt-base high temperature alloys. Science 2006; 312 (5770):90-1.”

<sup>1</sup>Work supported under: ONR (MURI N00014-13-1-0635)

**3:18PM H46.00005 High-throughput study of crystal structures and stability of strengthening precipitates in Mg alloys**, DONGSHU WANG, MAXMILIAN AMSLER, VINAY HEGDE, JAMES SAAL, AHMED ISSA, Northwestern University, XIAOQIN ZENG, Shanghai Jiao Tong University, CHRISTOPHER WOLVERTON, Northwestern University — Age hardening, in which precipitates form and impede the movement of dislocations, can be applied to magnesium alloys in order to increase their limited strengthening behavior. To help clarify the energetics of precipitation hardening of Mg alloys, we employed first principles density functional theory calculations to elucidate both crystal structures and energetics of a very large set of precipitates in Mg alloys. We find the enthalpy changes of (stable and metastable) observed precipitates during the age hardening process are consistent with the experimental sequence of formation for many Mg binary alloys (Mg- {Nd, Gd, Y, Sn, Al, Zn}). For cases where the metastable precipitate crystal structure is unavailable, we search over several prototypes and predict structures/stoichiometries for several ternary precipitates. In addition, high-throughput calculations are performed to construct hcp-based based convex hulls, which assist the identification of coherent GP zones and new metastable phases in age-hardened hcp systems.

**3:30PM H46.00006 High hardness and superlative oxidation resistance in a pseudo-icosahedral Cr-Al binary**, J. W. SIMONSON, R. ROSA, A. K. ANTONACCI, Department of Physics, Farmingdale State College, H. HE, Department of Physics and Astronomy, Stony Brook University, A. D. BENDER, J. PABLA, W. ADRIAP, Department of Physics, Farmingdale State College, D. E. MCNALLY, A. ZEBRO, P. KAMENOV, G. GESCHWIND, Department of Physics and Astronomy, Stony Brook University, S. GHOSE, E. DOORYHEE, National Synchrotron Light Source II, Brookhaven National Laboratory, A. IBRAHIM, Department of Mechanical Engineering Technology, Farmingdale State College, M. C. ARONSON, Department of Physics and Astronomy, Stony Brook University — Improving the efficiency of fossil fuel plants is a practical option for decreasing carbon dioxide emissions from electrical power generation. Present limits on the operating temperatures of exposed steel components, however, restrict steam temperatures and therefore energy efficiency. Even as a new generation of creep-resistant, high strength steels retain long term structural stability to temperatures as high as  $\sim 973$  K, the low Cr-content of these alloys hinders their oxidation resistance, necessitating the development of new corrosion resistant coatings. We report here the nearly ideal properties of potential coating material  $\text{Cr}_{55}\text{Al}_{229}$ , which exhibits high hardness at room temperature as well as low thermal conductivity and superlative oxidation resistance at 973 K, with an oxidation rate at least three times smaller than those of benchmark materials. These properties originate from a pseudo-icosahedral crystal structure, suggesting new criteria for future research.

**3:42PM H46.00007 Ordering Transformations in High-Entropy Alloys<sup>1</sup>**, PRASHANT SINGH, Ames Laboratory, DUANE D. JOHNSON, Ames Laboratory and Iowa State University — The high-temperature disordered phase of multi-component alloys, including high-entropy alloys (HEA), generally must experience segregation or else passes through partially-ordered phases to reach the low-temperature, fully-ordered phase. Our first-principles KKR-CPA-based atomic short-range ordering (SRO) calculations (analyzed as concentration-waves) reveal the competing partially and fully ordered phases in HEA, and these phases can be then directly assessed from KKR-CPA results in larger unit cells [Phys. Rev. B 91, 224204 (2015)]. For  $\text{Al}_x\text{CrFeNiTi}_{0.25}$ , Liu et al. [J Alloys Compd 619, 610 (2015)] experimentally find FCC+BCC coexistence that changes to BCC with increasing Al ( $x$  from 0-to-1), which then exhibits a partially-ordered B2 at low temperatures. CALPHAD (Calculation of Phase Diagrams) predicts a region with  $\text{L}_{21}+\text{B}_2$  coexistence. From KKR-CPA calculations, we find crossover versus Al from FCC+BCC coexistence to BCC, as observed, and regions for partially-order  $\text{B}_2+\text{L}_{21}$  coexistence, as suggest by CALPHAD. Our combined first-principles KKR-CPA method provides a powerful approach in predicting SRO and completing long-range order in HEA and other complex alloys.

<sup>1</sup>Supported by the U.S. DOE, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division. Work was performed at Ames Laboratory, which is operated by Iowa State University for the U.S. DOE under contract #DE-AC02-07CH11358.

**3:54PM H46.00008 KKR-DCA Thermodynamics for Cluster Short-Range Order with Full Charge Self-Consistency**, DOMINIC A. BIAVA, University of Illinois - Urbana, DUANE D. JOHNSON, Ames Laboratory, Ames, Iowa — The Dynamical Cluster Approximation (DCA) implemented in the Korringa-Kohn-Rostoker (KKR) electronic-structure method gives a systematically exact, *course-grained* theory of the electronic states of substitutionally disordered alloys, including the effects of chemical short-ranged order (SRO). We implement the KKR-DCA within density functional theory (DFT) to calculate directly the charge self-consistent electronic contributions to the alloy grand potential. The KKR-DCA is combined with the chemical entropy from the Cluster Variation Method (CVM), which when minimized predicts the SRO directly. The calculated SRO has been tested in several metallic systems with agreement to measured values. For very large clusters, the KKR-DCA can be sampled, as done within Quantum Monte Carlo, and provides the charge self-consistent thermodynamic grand potential in complex alloys with SRO at finite temperature, at the same level as done for perfect ordered alloys in other electronic-structure methods at zero Kelvin.

**4:06PM H46.00009 The Effect of Disorder on Lattice Thermal Transport in Solid Solution Alloys**, RAINA OLSEN, Oak Ridge National Laboratory, BISWANATH DUTTA, Max-Planck-Institut für Eisenforschung GmbH, GERMAN SAMOLYUK, BRIAN SALES, BEN LARSON, HONGBIN BEI, ELIOT SPECHT, MALCOLM STOCKS, Oak Ridge National Laboratory, THE ENERGY DISSIPATION TO DEFECT EVOLUTION ENERGY FRONTIER RESEARCH CENTER COLLABORATION — Dramatic decreases in radiation damage for 3- and 4-component equiatomic single phase solid solution Ni-based alloys have been recently observed. The strongly decreased damage retention in these highly disordered materials is attributed to severe disruption of the pathways of energy dissipation away from atomic displacement cascades. Because the energy of an irradiating ion is primarily deposited into the lattice degrees of freedom, it is the lattice thermal conductivity that is most important to the dissipation of heat from damage events. Here we report measurements of phonon linewidths in NiCo, NiFe, and NiFeCoCr using inelastic neutron and X-ray scattering, showing a dramatic increase in phonon linewidth by a factor of 4 with increasing disorder. Measured phonon linewidths are shown in comparison to theoretical phonon linewidths originating from disorder calculated using the itinerant coherent potential approximation (I-CPA). Lattice thermal conductivity is calculated from the phonon properties, and compared to measurements of bulk thermal and electrical properties. The impact of the observed decrease in lattice thermal conductivity on damage resistance is discussed.

**4:18PM H46.00010 Extreme Chemical Disorder and the Electrical Transport Properties of Concentrated Solid Solution Alloys: From Binaries to High Entropy Alloys Replace this text with your abstract title**, G. MALCOLM STOCKS, GERMAN SAMOLYUK, SUFFIAN KHAN, Materials Science & Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830, USA, MARKUS DAENE, Physical and Life Sciences, Lawrence Livermore National Laboratory, Livermore CA 94551, USA, SEBASTIAN WIMMER, Department Chemie, Ludwig-Maximilians-Universität München, 81377 München, Germany, BRIAN SALES, HONGBIN BEI, KE JIN, Materials Science & Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830, USA — We present the results of experimental and theoretical studies of electrical transport properties of a family of 2, 3, 4 and 5-component concentrated solid solution alloys (CSA) comprising subsets of the 3d- and 4d-transition metal elements Cr, Mn, Fe, Co, Ni and Pd. Many of this family of CSA show unusual mechanical, magnetic and transport properties as well as indications of increased radiation resistance that are clearly related to the underlying chemical disorder. Here we show the results of calculations of the electrical transport properties that are based on the *ab initio* Korringa-Kohn-Rostoker coherent-potential-approximation (KKR-CPA) method for treating the effect of substitutional disorder, and necessary configurational averaging, on the underlying electronic structure. We compare calculated residual ( $T=0\text{K}$ ) resistivities to corresponding experimental measurements and relate the variations in residual resistivity, which span almost two orders of magnitude, to the underlying electron structure.

**4:30PM H46.00011 Electronic origin of atomic-level stresses in High-Entropy Alloys**, KHOR-GOLKHUU ODBADRAKH, JICS at ORNL, University of Tennessee, TAKESHI EGAMI, MADHU OJHA, UTK, DON NICHOLSON, UNCA, MALCOLM STOCKS, ORNL — High-entropy alloys are multi-component solid solutions in which four or more elements occupy the same crystallographic lattice sites with roughly equal compositions. The underlying chemical disorder gives rise to small local lattice distortions and atomic-level stresses, which are also disorders on their own. These disorders lead to radiation resistance and mechanical strength in high temperature environment, making HEAs alloys attractive candidates as nuclear materials. We report electronic origin of the atomic-level stresses based upon first-principles calculations using Locally Self-consistent Multiple Scattering theory method. Strong atomic-level stresses are present in HEAs due not only to the differences in the intrinsic atomic sizes but due to charge transfer among the elements. We suggest that the improved properties of HEAs originate mainly from the high magnitudes of atomic-level stresses in these complex disordered alloys.

**4:42PM H46.00012 ABSTRACT WITHDRAWN —**

**4:54PM H46.00013 Ab Initio Investigation of He Bubbles at the  $Y_2Ti_2O_7$ -Fe Interface in Nanostructured Ferritic Alloys**, THOMAS DANIELSON, ERIC TEA, CELINE HIN, Virginia Tech — Nanostructured ferritic alloys are promising materials candidates for the next generation of nuclear reactors due to their ability to withstand high temperatures, high pressures, high neutron flux and especially, the presence of high concentrations of transmutation product helium. As helium diffuses through the matrix, large number densities of complex oxide nanoclusters, namely  $Y_2Ti_2O_7$ ,  $Y_2O_3$  and  $Y_2TiO_5$ , act as trapping sites for individual helium atoms and helium clusters. Consequently, there is a significant decrease in the amount of helium that reaches grain boundaries, mitigating the threat of pressurized bubble formation and embrittlement. In order to understand the helium trapping mechanisms of the oxides at a fundamental level, the interface between the nanoclusters and the iron matrix must be modeled. We present results obtained using density functional theory on the  $Y_2Ti_2O_7$ -Fe interface where the structure has been modeled based on experimental observations. Helium has been added along the interface in order to investigate the influence of helium on the structure and to obtain thermodynamic and kinetic parameters of helium along the interface.

**5:06PM H46.00014 The impact of short-range forces on high-energy atom collisions in displacement cascades.**<sup>1</sup>, GERMAN SAMOLYUK, ROGER STOLLER, Oak Ridge National Lab, USA, ARTUR TAMM, Institute of Technology, University of Tartu, Estonia, LAURENT BELAND, G. MALCOLM STOCKS, Oak Ridge National Lab, USA, ALFREDO CARO, Los Alamos National Laboratory, USA, LYUDMILA SLIPCHENKO4, Purdue University, USA, YURY OSETSKIY, Oak Ridge National Lab, USA, ALVO AABLOO, Institute of Technology, University of Tartu, Estonia, MATTIAS KLINTENBERG, Uppsala University, Sweden, YANG WANG, Pittsburgh Supercomputer Center, Carnegie-Mellon University, US — Simulation of primary radiation damage formation in solid materials involves collisions between atoms with a few hundred keV of kinetic energy. As a result, during these collisions, the distance between two colliding atoms can approach 0.05 nm. For such small atomic separations, interatomic potentials significantly underestimate the potential energy. The common practice involves using a screened Coulomb pair potential to describe the high-energy interactions and to smoothly join this to the equilibrium potential. However, there is no standard method for choosing the joining parameters and defect production during cascade evolution has been shown to be sensitive to how the joining is done. We developed a new procedure, which includes the use of ab initio, calculations to determine the pair interactions at intermediate distances, together with systematic criteria for choosing the joining parameters. Results are presented for the case of nickel.

<sup>1</sup>Research at the Oak Ridge National Laboratory and Los Alamos National Laboratory sponsored by the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, Center for Energy Dissipation to Defect Evolution

**5:18PM H46.00015 ABSTRACT WITHDRAWN —**

**Tuesday, March 15, 2016 2:30PM - 5:30PM —**

**Session H47 DCP: Chemical Physics of Graphene and Carbon** 312 - Masuro Kuno, University of Notre Dame

**2:30PM H47.00001 Adsorption Characteristics of Binary Mixtures of Two Halomethanes on Graphite Surface**<sup>1</sup>, KIRAN KHANAL, Department of Polymer Science, The University of Akron, Akron, Ohio, GARY LEUTY, Air Force Research Lab, Dayton, Ohio, MESFIN TSIGE, Department of Polymer Science, The University of Akron, Akron, Ohio — Understanding the physisorption mechanism of mixtures of small molecules on graphite substrate has been a growing interest in materials science in order to investigate the changes in adsorption behavior of mixtures near interfaces vs. the individual components. Using atomic-scale molecular dynamics simulations, we have studied the structure and dynamics of multilayer adsorption of binary mixtures of two halomethanes (CF<sub>4</sub> and CF<sub>3</sub>Cl) on graphite substrates for different bulk compositions of CF<sub>4</sub>. Simulations were performed in the temperature range 60-120K. The goal of this study is to explore how the compositions of individual components as well as temperature, affect the structure of films near the interface, the mobility of molecules, the molecular orientation and the substrate affinity. Preliminary results suggest a strong influence of the concentration of CF<sub>4</sub> and temperature on the structure and mobility of molecules in first adsorbed layer on the graphite surface. In agreement with the recent experimental results, CF<sub>4</sub> displaces CF<sub>3</sub>Cl from the first adsorbed layer at all temperatures in our range and becomes the leading component in the mixture at high temperature for large CF<sub>4</sub> concentrations in the mixture.

<sup>1</sup>This work is supported by NSF grant CHE 1506275.

**2:42PM H47.00002 Exfoliation and Dispersion of 2-Dimensional Materials by Elevating Temperature**<sup>1</sup>, SANGHYUK KWON, School of Mechanical Engineering, Sungkyunkwan University, 2066 Seobu-ro, Jangan-gu, Suwon 440-746, Korea, JINSEON KIM, Mechanical Test & Analysis Section, Korea Electric Power Corporation Nuclear Fuel, Daedeok-daero 989 beon-gil, Yuseong-gu, Daejeon 305-353, Korea, HYUKJOON KWON, SKKU Advanced Institute of Nanotechnology, Sungkyunkwan University, 2066 Seobu-ro, Jangan-gu, Suwon 440-746, Korea, CHANGGU LEE, School of Mechanical Engineering, Sungkyunkwan University, 2066 Seobu-ro, Jangan-gu, Suwon 440-746, Korea, GRAPHENE ENGINEERING LAB TEAM — It is known that graphene and other 2-dimensional materials are hard to dissolve in water without using chemicals or surfactants. Here, we present a facile method to exfoliate and disperse those materials in water by simply controlling temperature. Graphene, when sonicated in water at high temperature (60C), was edge-functionalized due to the extremely high temperature and pressure locally induced by ultrasonic cavitation, and dissolved in water stably even for longer than 1 month. However, it was not dispersed at low temperature(30C) because of less cavitation and reduced sonochemical reaction. Other 2-dimensional materials, such as h-BN, MoS<sub>2</sub>, and other layered metal chalcogenides, were also well dissolved in water as graphene, but even at low temperature. Their stable solution is from the electric double layer because their relatively high insulating property. Also elevated storage temperature (60C) improved the long-term dispersion stability compared to lower storage temperature (20C)

<sup>1</sup>Exfoliation and Dispersion of 2-Dimensional Materials by Elevating Temperature

## 2:54PM H47.00003 ABSTRACT WITHDRAWN —

**3:06PM H47.00004 Role of edge dehydrogenation in magnetization and spin transport of zigzag graphene nanoribbons with line defects<sup>1</sup>**, BIN CUI, DESHENG LIU, School of Physics, Shandong University, Jinan 250100, China — We investigate the effects of edge dehydrogenation on magnetism and spin transport of zigzag graphene nanoribbons (ZGNRs) with line defects (558defect and 57defect) by the first-principles calculations. Results show that magnetization can be induced or strengthened obviously in 558defect-ZGNRs underterminated by hydrogen, but not for 57defect-ZGNRs. This is because a spin-polarized  $\sigma$  edge state appears near the Fermi level and strengthens spin-splitting of energy bands at bare edges of the 558defect-ZGNRs. Moreover, compared with pristine ZGNRs, the 558defect-ZGNRs with bare edges can realize a transition from antiferromagnetic coupling to ferromagnetic coupling between both edges. In addition, the spin-filter efficiency can be effectively improved in our proposed devices by edge dehydrogenation. Our results demonstrate that the presence of  $\sigma$  edge state near the Fermi level plays an important role in controlling spin transport of the graphene-based spintronic devices.

<sup>1</sup>This work was supported by the Natural Science Foundation of China (Grant No. 11374183 and 11404188).

**3:18PM H47.00005 New insights into the opening band gap of graphene oxides**, NGOC THANH THUY TRAN, SHIH-YANG LIN, MING-FA LIN, National Cheng Kung University — Electronic properties of oxygen absorbed few-layer graphenes are investigated using first-principle calculations. They are very sensitive to the changes in the oxygen concentration, number of graphene layer, and stacking configuration. The feature-rich band structures exhibit the destruction or distortion of the Dirac cone, opening of band gap, anisotropic energy dispersions, O- and (C,O)-dominated energy dispersions, and extra critical points. The band decomposed charge distributions reveal the  $\pi$ -bonding dominated energy gap. The orbital-projected density of states (DOS) have many special structures mainly coming from a composite energy band, the parabolic and partially flat ones. The DOS and spatial charge distributions clearly indicate the critical orbital hybridizations in O-O, C-O and C-C bonds, being responsible for the diversified properties. All of the few-layer graphene oxides are semi-metals except for the semiconducting monolayer ones.

**3:30PM H47.00006 Raman Spectra Study and the Corresponding Strain Dependence of Graphyne and Graphdiyne**, SHUQING ZHANG, Peking University, COLLEGE OF CHEMISTRY AND MOLECULAR ENGINEERING TEAM — Graphynes, composed of  $sp$ - $sp^2$  carbon atoms, have attracted increasing interest of research due to particular optical, electrical and mechanical properties they might have. According to recent theoretical studies prediction, the synthesis of graphyne and graphdiyne are difficult but offer more possible compared to other graphynes, and they have been tried to form and got initial achievement<sup>1</sup>. For new materials, their widespread application is impossible without a convenient, fast, non-destructive characterization tool. Raman spectroscopy has performed remarkable ability for studying the properties of  $sp^2$  and  $sp^3$  carbon materials, such as diamond, graphite, carbon fibers and nanotubes. Naturally, we may expect it is also work in  $sp$ - $sp^2$  carbon materials<sup>2</sup>. In our work, the Raman features of graphyne and graphdiyne are studied systematically and their variations versus mechanical strain are also investigated by group theory and first-principles calculations. 1. Guoxing Li, et al. *Chem. Commun.* 2010, 46: 3256 2. Jinying Wang\*, Shuqing Zhang\*, et al. *Phys. Chem. Chem. Phys.* 2014, 16 (23): 11303

**3:42PM H47.00007 Complete Wetting of Graphene by Biological Membrane**, BINQUAN LUAN, RUHONG ZHOU, IBM T J Watson Research Center — In a very recent study, we found that surprisingly graphene nanosheets can extract large amount of lipid molecules directly out of cell membranes thus causing serious damage in cell's integrity (Nat. Nanotechnol. 8, 594, 2013). Here through extensive molecular dynamics simulations and theoretical analyses, we show that this novel phenomenon can be categorized as a complete wetting of graphene by membrane lipids in the medium of water. A wetting-based theory was developed to associate the free energy change during the extraction with the macroscopic spreading parameter. With a customer-designed thermodynamic cycle for detailed energetics, we demonstrated that the dispersive adhesion between graphene and lipids plays a dominant role during this extraction as manifested by the curved graphene.

**3:54PM H47.00008 Electrical conductivity of graphite oxide nanoplatelets obtained from bamboo: Effect of the deoxidation degree.**, K. GROSS, CENM, Universidad del Valle, Cali, Colombia, J. J. PRIAS-BARRAGAN, IS Institute and Electronic IT Program, Universidad del Quindío, Armenia, Colombia, S. SANGIAO, LMA, INA and DFMC, Universidad de Zaragoza, 50009 Zaragoza, Spain, J. M. DE TERESA, DFMC and ICMA, CSIC, Universidad de Zaragoza, 50009 Zaragoza, Spain, L. LAJAUNIE, R. ARENAL, LMA, Instituto de Nanociencia de Aragon (INA), Universidad de Zaragoza, Spain, H. ARIZA-CALDERN, IS Institute, Universidad del Quindío, Armenia, Colombia, P. PRIETO, CENM, Universidad del Valle, Cali, Colombia — Given the high interest in the fabrication and application of carbon-based materials, we present a new and cost-effective method for the synthesis of graphite oxide nanoplatelets (GONP) using bamboo pyrolytic acid (BPA) as source. GONP-BPA present lateral dimensions of 5-100 micro-meter and thickness less than 80 nm, as confirmed by TEM. EEL spectra show that locally the carbon is mainly in  $sp^2$  bonding configuration and confirm a short/medium range crystalline order. Elemental analysis by EDX confirms the presence of oxygen in an atomic percentage ranging from 17 to 5%. For electrical characterization, single platelets were contacted by focused-ion-beam-induced deposition of Pt nanowires. The four-point probe electrical conductivity shows a direct correlation with the oxygen percentage. Three orders of magnitude conductivity rise is observed by the oxygen reduction, reaching a value of  $2.3 \times 10^3$  S/m at the final deoxidation degree. The results suggest that GONP-BPA could be used in the development of advanced devices and sensors.

**4:06PM H47.00009 Simulation of Adsorption of Carbon Dioxide and Methane on Graphene Sheet.**<sup>1</sup>, SIDI MAIGA, Student, SILVINA GATICA<sup>2</sup>, None — Carbon dioxide (CO<sub>2</sub>) and Methane (CH<sub>4</sub>) constitute 90% of the annual greenhouse emission. These gases are emitted from multitude of sources such as: power station, transportation fuels, industrial processes, and agricultural byproducts. Scientists around the globe are looking for materials capable of capturing, separating, and storing these gases. Graphene with its high specific surface area provides a great platform for gas adsorption and separation. Adsorption is defined as the attachment of atoms, or molecules of a gas, liquid or dissolved solid onto a surface, creating a film or monolayer of material onto the adsorbing surface. Using the Method of Grand Canonical Monte Carlo, we computed the adsorption of carbon dioxide (CO<sub>2</sub>) and methane (CH<sub>4</sub>) on a monolayer graphene sheet, at various temperatures for each gas. For each temperature, we compute the adsorption isotherm, Energy gas-surface and Energy gas-gas. We compare the uptake pressures of CO<sub>2</sub> and CH<sub>4</sub>. Using the Ideal Adsorbed Solution Theory (IAST), we predict the selectivity of a mixture CO<sub>2</sub>/CH<sub>4</sub>.

<sup>1</sup>Center for Integrated Quantum Materials (CIQM), NSF Grant No. DMR-1231319.

<sup>2</sup>Advisor

**4:18PM H47.00010 Structural and Compositional Study of Graphene grown on SrTiO<sub>3</sub> by Chemical Vapour Deposition**, SHUMAILA KARAMAT, Middle East Technical University (ODTU), Ankara, Turkey, UMIT CELIK, 3Nano-magnetics Instruments, Ankara Turkey, AHMET ORAL, Middle East Technical University (ODTU), Ankara, Turkey — Graphene, a monolayer of sp<sup>2</sup> bonded carbon atom, is considered as one of the most promising candidate materials for future electronics. The most critical step in graphene research is its transfer from the growth catalyst to the dielectric substrate, many unavoidable issues in the transfer process are: contamination from etchants, photoresist residues, wrinkles, and mechanical breakage. The direct growth of graphene on the substrates without using catalyst offer new opportunities in device fabrication without any transfer process. But till now, the field of direct graphene growth on dielectrics or insulating substrates is not mature like growth on metallic catalysts using CVD. We used chemical vapour deposition to grow graphene on SrTiO<sub>3</sub> (110) substrates. The growth was carried out in presence of methane, argon and hydrogen. Raman Spectrum clearly showed the D and G peaks which were absent in bare substrate. XPS was used to get information about the presence of necessary elements, their bonding with STO substrates. AFM imaging clearly showed graphene island formation on substrates.

**4:30PM H47.00011 Surface and Compositional Study of Graphene grown on Lithium Niobate (LiNbO<sub>3</sub>) substrates by Chemical Vapour Deposition**, SHUMAILA KARAMAT, Middle East Technical University (ODTU), Ankara, Turkey, UMIT CELIK, Nanomagnetics Instruments, Ankara Turkey, AHMET ORAL, Middle East Technical University (ODTU), Ankara, Turkey — The diversity required in the designing of electronic devices motivated the community to always attempt for new functional materials and device structures. Graphene is considered as one of the most promising candidate materials for future electronics and carbon based devices. It is very exciting to combine graphene with new dielectric materials which exhibit multifunctional properties. Lithium Niobate exhibits ferro-, pyro-, and piezoelectric properties with large electro-optic, acousto-optic, and photoelastic coefficients as well as strong photorefractive and photovoltaic effects which made it one of the most extensively studied materials over the last 50 years. We used ambient pressure chemical vapour deposition to grow graphene on LiNbO<sub>3</sub> substrates without any catalyst. The growth was carried out in presence of methane, argon and hydrogen. AFM imaging showed very unique structures on the surface which contains triangular domains. X-ray photoelectron spectroscopy (XPS) was used to get information about the presence of necessary elements, their bonding with LiNbO<sub>3</sub> substrates. Detailed characterization is under process which will be presented later.

**4:42PM H47.00012 Atomically precise nitrogen-doped graphene nanoribbons<sup>1</sup>**, ALEXANDER SINITSKII, University of Nebraska - Lincoln — There is a considerable interest in graphene nanoribbons (GNRs), few-nm-wide strips of graphene with high aspect ratios, because of their intriguing physical properties. For example, GNRs with zigzag edges are predicted to exhibit low-dimensional magnetism, while GNRs with armchair edges can possess large energy band gaps, making them promising materials for future electronics and photovoltaics. The ability to control structural parameters of GNRs, such as their width, edge structure and termination, with atomic precision is the key for practical realization of these intriguing nanoscale properties. Physical properties of GNRs can also be modified by their doping with heteroatoms, such nitrogen, resulting in nitrogen-doped GNRs or N-GNRs. In this talk I will discuss several types of N-GNRs with different doping levels that have been synthesized and systematically studied by spectroscopic, microscopic and transport methods. Incorporation of nitrogen atoms in graphene lattice is shown to be an effective route to affect GNRs' band gap, doping level as well as aggregation behavior.

<sup>1</sup>The support from NSF CHE-1455330 is gratefully acknowledged.

**4:54PM H47.00013 CVD films of narrow atomically precise graphene nanoribbons**, MIKHAIL SHEKHIREV, ALEXEY LIPATOV, University of Nebraska-Lincoln, ASHLEY HARKLERoad, University of Missouri - Kansas City, ALEXANDER SINITSKII, University of Nebraska-Lincoln — Atomically precise graphene nanoribbons (GNRs) is a promising material for the next-generation electronics and optoelectronics. So far, solution-based and surface-assisted approaches have been the two main routes to synthesize GNRs with atomically smooth armchair edges. However, efficient processing of the resulting GNRs into uniform thin films to fabricate GNR-based functional devices remains a formidable challenge. In this presentation we will report the synthesis of narrow armchair GNRs using an alternative approach – a radical polymerization of rationally designed molecular precursors. The technique allows fabrication of thin, transparent and conductive films of GNRs on almost any substrate. Microscopic structure and electrical properties of the fabricated GNR films will also be discussed.

**5:06PM H47.00014 Analysis of vibrational response in graphite oxide nanoplatelets.**, JHON JAIRO PRIAS BARRAGAN, IS Institute and Electronic IT Program of the Universidad del Quindío, KATHERINE GROSS, CENM of the Universidad del Valle, LUC LAJAUNIE, RAUL ARENAL, LMA, Instituto de Nanociencia de Aragón (INA), Universidad de Zaragoza, Spain, HERNANDO ARIZA CALDERON, PEDRO PRIETO, CENM of the Universidad del Valle, Colombia — In this work, we present a new low-cost fabrication process to obtain graphite oxide nanoplatelets from bamboo pyrolytic acid (GO-BPA) by thermal decomposition method using a pyrolysis system for different carbonization temperatures from 673 to 973 K. The GO-BPA samples were characterized by using Raman, FTIR, XRD, SEM and TEM techniques, whose results suggest that increased carbonization temperature increases graphite conversion, boundary defects, desorption of some organic compounds and phonon response, respectively. We discuss potential applications of the GO-BPA samples involving phonon response that would benefit from a fully scaled technology, advanced electronic sensors and devices.

**5:18PM H47.00015 Surface aging phenomena in multidimensional *sp*<sup>2</sup> carbon allotropes**, YUN-HSIANG CHANG, SERGIO SANTOS, MATTEO CHIESA, Laboratory for Energy and NanoScience, Masdar Institute — Despite the current interest in the scientific community in exploiting divergent surface properties of graphitic carbon allotropes, conclusive differentiation remains elusive even when dealing with parameters as fundamental as adhesion. Here we set out to provide conclusive experimental evidence on the time evolution of the surface properties of highly oriented pyrolytic graphite (HOPG), graphene monolayer (GML) and multiwalled carbon nanotubes (MWCNTs) as we expose these materials to airborne contaminants, by providing 1) statistically significant results based on large data-sets, i.e. thousands of force measurements, and 2) errors sufficiently self-consistent to treat the comparison between data-sets in atomic force microscopy measurements. We first consider HOPG as a model system and then employ our results to draw conclusions from the GML and MWCNT samples. We find that, in terms of surface properties and thus regarding surface functionality, aged HOPG and GML are more similar than aged HOPG and cleaved HOPG. The state of the HOPG samples is also as relevant for the comparison between HOPG and MWCNTs.

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**

**Session H48 GQI: Entanglement in Superconducting Circuits** 349 - Konrad Lehnert, JILA, University of Colorado, NIST-Boulder

## 2:30PM H48.00001 Entanglement of remote transmon qubits by concurrent photon detection

**- Part 1<sup>1</sup>**, S. SHANKAR, A. NARLA, M. HATRIDGE, W. PFAFF, Z. LEGHTAS, K.M. SLIWA, E. ZALYS-GELLER, L. FRUNZIO, M.H. DEVORET, Department of Applied Physics, Yale University — One proposed realization for a quantum computer is the modular architecture, which consists of error-corrected quantum memories that are connected via a quantum router. A fundamental requirement for this modular quantum computer is the ability to entangle arbitrary, distant qubits on demand. This can be realized in circuit QED using a protocol inspired by recent experiments based on trapped ions and nitrogen-vacancy centers. First, each qubit is entangled with a single cavity photon (Fock state  $n=1$ ) using sideband pulses. On their way out of the cavity, the now flying photons interfere on a beam-splitter and are concurrently detected by a novel microwave photo-multiplier that employs a third qubit-cavity system. In this protocol, the presence of losses in the photon flight path only affect the success probability of creating an entangled state but not its fidelity. In this talk, we present the experimental realization of this protocol for entangling two transmon qubits, focusing on the implementation and optimization of the microwave photo-multiplier.

<sup>1</sup>Work supported by ARO, AFOSR and YINQE

## 2:42PM H48.00002 Entanglement of remote transmon qubits by concurrent photon detection

**- Part 2<sup>1</sup>**, A. NARLA, S. SHANKAR, M. HATRIDGE, W. PFAFF, Z. LEGHTAS, K.M. SLIWA, E. ZALYS-GELLER, L. FRUNZIO, M.H. DEVORET, Department of Applied Physics, Yale University — One proposed realization for a quantum computer is the modular architecture, which consists of error-corrected quantum memories that are connected via a quantum router. A fundamental requirement for this modular quantum computer is the ability to entangle arbitrary, distant qubits on demand. This can be realized in circuit QED using a protocol inspired by recent experiments based on trapped ions and nitrogen-vacancy centers. First, each qubit is entangled with a single cavity photon (Fock state  $n=1$ ) using sideband pulses. On their way out of the cavity, the now flying photons interfere on a beam-splitter and are concurrently detected by a novel microwave photo-multiplier that employs a third qubit-cavity system. In this protocol, the presence of losses in the photon flight path only affect the success probability of creating an entangled state but not its fidelity. In this talk, we present experimental results for this protocol and discuss the factors influencing the success probability and the fidelity of the generated entangled states.

<sup>1</sup>Work supported by ARO, AFOSR and YINQE

## 2:54PM H48.00003 Using a Superconducting Resonator with Frequency-Compensated Tunable Coupling to Transfer a Quantum State Deterministically and Directly

, JAMES WENNER, C. NEILL, C. QUINTANA, B. CAMPBELL, Z. CHEN, B. CHIARO, A. DUNSWORTH, P. O'MALLEY, A. VAINSENER, University of California, Santa Barbara, T. WHITE, R. BARENDT, Y. CHEN, A. FOWLER, E. JEFFREY, J. KELLY, E. LUCERO, A. MEGRANT, J. MUTUS, M. NEELEY, P. ROUSHAN, D. SANK, Google, Santa Barbara, JOHN M. MARTINIS, University of California and Google, Santa Barbara — Deterministic direct quantum state transfer between devices on different chips requires the ability to transfer quantum states between traveling qubits and fixed logic qubits. Reflections must be minimized to avoid energy loss and phase interference; this requires tunable coupling to an inter-chip line while the two devices are at equal frequencies. To achieve this, we use a 6GHz superconducting coplanar resonator with tunable coupling to a 50 Ohm transmission line. We compensate for the resulting shift in resonator frequency by simultaneously tuning a second SQUID. We measure the device coherence and demonstrate the ability to release a single-frequency shaped pulse into the transmission line, efficiently capture a shaped pulse, and deterministically and directly transfer a quantum state.

## 3:06PM H48.00004 Controlled release of cavity states into propagating modes induced via a single qubit

, WOLFGANG PFAFF, MARIUS CONSTANTIN, MATTHEW REAGOR, CHRISTOPHER AXLINE, JACOB BLUMOFF, KEVIN CHOU, ZAKI LEGHTAS, STEVEN TOUZARD, REINIER HEERES, PHILIP REINHOLD, NISSIM OFEK, KATRINA SLIWA, LUIGI FRUNZIO, Yale University, MAZYAR MIRRAHIMI, Yale University & INRIA, KONRAD LEHNERT, University of Colorado, LIANG JIANG, MICHEL DEVORET, ROBERT SCHOELKOPF, Yale University — Photonic states stored in long-lived cavities are a promising platform for scalable quantum computing and for the realization of quantum networks. An important aspect in such a cavity-based architecture will be the controlled conversion of stored photonic states into propagating ones. This will allow, for instance, quantum state transfer between remote cavities. We demonstrate the controlled release of quantum states from a microwave resonator with millisecond lifetime in a 3D circuit QED system. Dispersive coupling of the cavity to a transmon qubit allows us to enable a four-wave mixing process that transfers the stored state into a second resonator from which it can leave the system through a transmission line. This permits us to evacuate the cavity on time scales that are orders of magnitude faster than the intrinsic lifetime. This Q-switching process can in principle be fully coherent, making our system highly promising for quantum state transfer between nodes in a quantum network of high-Q cavities.

## 3:18PM H48.00005 Concurrent remote entanglement with continuous variables<sup>1</sup>

, E. ZALYS-GELLER, A. NARLA, S. SHANKAR, M. HATRIDGE, M. SILVERI, K.M. SLIWA, S.O. MUNDHADA, S.M. GIRVIN, M.H. DEVORET, Department of Applied Physics, Yale University — A necessary ingredient for large scale quantum information processing is the ability to entangle distant qubits on demand. In the field of superconducting quantum information, this process can be achieved by entangling stationary superconducting qubits with flying coherent states of microwave light, which are then co-amplified by a Josephson Parametric Converter (JPC). The JPC also serves as a which-path information eraser, causing the probabilistic continuous measurement process to concurrently entangle the qubits. We discuss the sensitivity of the experiment to the loss of quantum information during the flight of the coherent states, as well as strategies to improve which-path information erasure and reduce information loss to the degree required for entanglement generation.

<sup>1</sup>Work supported by ARO, AFOSR, NSF, and YINQE

## 3:30PM H48.00006 Preparation of a narrowband, itinerant microwave qubit for quantum information transfer<sup>1</sup>

, XIZHENG MA, ADAM REED, LUCAS SLETTEN, Department of Physics, University of Colorado, Boulder, Colorado, USA, MATTHEW REAGOR, LUKE BURKHART, WOLFGANG PFAFF, R.J. SCHOELKOPF, Departments of Applied Physics and Physics, Yale University, New Haven, Connecticut, USA., K.W. LEHNERT, JILA, University of Colorado and NIST, Boulder, Colorado, USA; Department of Physics, University of Colorado, Boulder, Colorado, USA — Narrowband microwave-frequency signals are compatible with many quantum information processing technologies and can coherently transfer quantum information between devices. The creation of itinerant, microwave single photon states has been successfully demonstrated. Here, we show progress towards generating a narrowband, itinerant microwave qubit in a coherent superposition of zero and one Fock states. Specifically, we use the red-sideband transition of a transmon to map a superposition of qubit states onto a propagating microwave signal. This signal should have a bandwidth sufficiently narrow to be absorbed by a quantum-enabled electro-optic converter [1], potentially enabling the transfer of quantum information from a transmon qubit to the optical domain.

<sup>1</sup>[1] R.W. Andrews, *et al.*, Nature Phys. **10**, 321–326 (2014).

**3:42PM H48.00007 Characterizing an itinerant microwave Fock state compatible with transfer to a macroscopic mechanical oscillator<sup>1</sup>**, L.R. SLETTEN, A.P. REED, XIZHENG MA, JILA, University of Colorado, Boulder, Colorado, L.D. BURKHART, M. REAGOR, W. PFAFF, R.J. SCHEOLKOPF, Department of Physics and Applied Physics, Yale University, New Haven, Connecticut, K.W. LEHNERT, JILA and National Institute of Standards and Technology, Boulder, Colorado — Transferring propagating single-photon signals generated by a qubit to a mechanical oscillator offers a way to prepare non-classical motional states of a macroscopic object. In this concept, a highly coherent transmon qubit in a cavity is used to create single itinerant microwave photons. These photons can then be directed towards a tunable electromechanical circuit where they can be converted into single phonons. In this talk, we present measurements of itinerant single photons engineered to realize this concept. In particular, we characterize their quantum state tomographically, demonstrate that they have sufficiently narrow bandwidth for capture by an electromechanical circuit, and measure the efficiency with which they travel between microwave cavities.

<sup>1</sup>This work was supported by the Gordon and Betty Moore Foundation

**3:54PM H48.00008 Entangled Schrodinger cats in circuit QED: Experimental Architecture**, CHEN WANG, YVONNE Y. GAO, PHILIP REINHOLD, REINIER W. HEERES, NISSIM OFEK, KEVIN CHOU, CHRISTOPHER AXLINE, LUIGI FRUNZIO, MICHEL H. DEVORET, ROBERT J. SCHEOLKOPF, Yale University — The development of quantum information technology relies on creating and controlling entanglement over an increasingly large Hilbert space. Superconducting cavities offer high-dimensional spaces for quantum states in a low-loss and hardware-efficient fashion, making it an ideal memory of quantum information and an important element towards fault-tolerant quantum computation. In this talk we present a cQED architecture that allows quantum control over the coherent state basis of two superconducting cavities with millisecond coherence. In particular, we show deterministic entanglement of coherent-state microwave fields in two superconducting cavities of the form:  $\frac{1}{\sqrt{2}}(|\beta_a\rangle|\beta_a\rangle \pm |-\beta_a\rangle|-\beta_a\rangle)$ . We engineer the capability to measure the joint photon number parity to achieve complete state tomography of the two-cavity state. Following widespread efforts of realizing “Schrodinger’s cat”-like mesoscopic superposition in various physical systems, this experiment demonstrates mesoscopic entanglement between two “Schrodinger’s cats”.

**4:06PM H48.00009 Entangled Schrodinger cats in circuit QED: Joint Wigner Tomography**, YVONNE Y. GAO, CHEN WANG, PHILIP REINHOLD, REINIER W. HEERES, NISSIM OFEK, KEVIN CHOU, CHRISTOPHER AXLINE, LUIGI FRUNZIO, MICHEL H. DEVORET, ROBERT J. SCHEOLKOPF, Yale University — Creating and controlling entanglement of quantum states over large Hilbert space is an important element of quantum information processing. Using the cQED architecture consisting of two long-lived superconducting cavities dispersively coupled to a transmon qubit, we successfully created an entangled coherent-state microwave fields in two superconducting cavities. In this talk, we will present the full joint Wigner tomography of the state, measured using the method of joint photon number parity measurement introduced in the previous talk. Furthermore, we will show the redundant encoding and efficient read-out of two logical bits of information in such entangled state and hence demonstrating that the entangled “Schrodinger cats” is a viable candidate as an error-correctable quantum memory as well as a valuable platform for implementation of two-qubit logical operations.

**4:18PM H48.00010 Generating entanglement via symmetry-selective bath engineering in superconducting qubits<sup>1</sup>**, IRFAN SIDDIQI, MOLLIE SCHWARTZ, LEIGH MARTIN, EMMANUEL FLURIN, Quantum Nanoelectronics Laboratory, UC Berkeley, CAMILLE ARON, Laboratoire de Physique Thorique, cole Normale Suprieure; Instituut voor Theoretische Fysica, KU Leven, MANAS KULKARNI, Department of Physics, New York City College of Technology, City University of New York, HAKAN TURECI, Department of Electrical Engineering, Princeton University — Bath engineering, which utilizes coupling to lossy modes in a quantum system to generate non-trivial steady states, is a potential alternative to gate- and measurement-based quantum science. In this talk, we discuss autonomous stabilization of entanglement between two superconducting transmon qubits in a symmetry-selective manner. Our experiments are implemented using two 3D transmons housed in separate copper cavities. The cavities are coupled via an aperture, and hybridize into nondegenerate symmetric and antisymmetric bath modes. We utilize the engineered symmetries of the dissipative environment to stabilize a target Bell state  $\frac{1}{\sqrt{2}}(|ge\rangle \pm |eg\rangle)$  in the qubit sector; we further demonstrate suppression of the Bell state of opposite symmetry due to parity selection rules. This implementation is resource-efficient, achieves a steady-state fidelity  $\mathcal{F} = 0.70$ , and is scalable to multiple qubits. <http://arxiv.org/abs/1511.00702>

<sup>1</sup>This research was supported by the ARO.

**4:30PM H48.00011 Multimode Entanglement Generation in a Parametric Superconducting Cavity**, C.W.S. CHANG, University of Waterloo, M. SIMOEN, Chalmers University of Technolog, A.M. VADIRAJ, University of Waterloo, P. DELSING, Chalmers University of Technolog, C.M. WILSON, University of Waterloo — Parametric microwave resonators implemented with superconducting circuits have become increasingly important in various application within quantum information processing. For example, quantum-limited parametric amplifiers based on these devices have now become commonplace as first-stage amplifiers for qubit experiments. Here we study the generation of multimode entangled states of propagating microwave photons, which can be used a resource in quantum computing and communication applications. We use a CPW resonator with a low fundamental resonance frequency that than has a number of modes in the common frequency band of 4-12 GHz. These modes are all parametrically coupled by a single SQUID that terminates the resonator. When parametrically pumping the system at the sum of two mode frequencies, we observe parametric downconversion and two-mode squeezing. By pumping at the difference frequency, we observe a beamsplitter-like mode conversion. By using multiple pump tones that combine these different processes, theory predicts we can construct multimode entangled states with a well-controlled entanglement structure, e.g., cluster states. Preliminary measurements will be presented.

**4:42PM H48.00012 Simultaneous measurement of non-commuting observables in circuit QED: Theory<sup>1</sup>**, LEIGH MARTIN, SHAY HACOEN-GOURGY, EMMANUEL FLURIN, Quantum Nanoelectronics Laboratory, UC Berkeley, BIRGITTA WHALEY, Berkeley Quantum Information and Computation Center, UC Berkeley, IRFAN SIDDIQI, Quantum Nanoelectronics Laboratory, UC Berkeley — We describe the theory of a novel technique for simultaneously and continuously measuring a pair of non-commuting qubit observables, which has until now not been realized experimentally. Our proposed experimental platform consists of a qubit dispersively coupled to two linear cavity modes. Driving the qubit on resonance realizes an effective two-level system with energy splitting given by the Rabi frequency. Non-commuting measurements are performed on this system by application of sideband tones detuned from the cavity resonance frequencies by the Rabi frequency. We show that this realizes cooling and back-action free measurements constituting destructive and QND measurements, respectively, along an arbitrary axis of the Bloch sphere. Simultaneous application of a distinct pair of measurements may then be achieved by choosing a different axis for each cavity mode. We show that existing high quantum efficiency homodyne measurement techniques will enable the reconstruction of quantum trajectories of the qubit. Finally, we describe methods for characterizing the system’s dynamics and verifying that the scheme does enable access to incommensurate, competing degrees of freedom.

<sup>1</sup>This research is supported by the ARO.

**4:54PM H48.00013 Simultaneous measurement of non-commuting observables in circuit QED: Experiment<sup>1</sup>**, SHAY HACOEN-GOURGY, LEIGH MARTIN, EMMANUEL FLURIN, Quantum Nanoelectronics Laboratory, UC Berkeley, BRIGITTA WHALEY, Berkeley Quantum Information Center, UC Berkeley, IRFAN SIDDIQI, Quantum Nanoelectronics Laboratory, UC Berkeley — The existence of incompatible measurements lies at the heart of numerous fundamental concepts in quantum mechanics, such as entanglement, contextuality and measurement-disturbance tradeoffs. We implement a novel technique for simultaneously and continuously measuring a pair of non-commuting observables in a circuit-QED architecture, which features a transmon qubit coupled to two modes of an electromagnetic cavity. By driving the transmon on resonance, we form an effective, low-frequency two-level system on which we perform the non-commuting measurements. To this end, we use microwave tones near the cavity's resonances to implement cooling and backaction-evading measurements familiar from optomechanics. Control of the relative amplitude and phase of these sideband tones enables qubit state measurement along an arbitrary axis of the Bloch sphere. We apply this technique to both modes of the cavity simultaneously, with distinct axes chosen for each mode. This realizes a continuous and simultaneous measurement of two non-commuting observables. We use high quantum-efficiency parametric amplifiers to track the resulting quantum trajectories of the qubit, enabling a measurement of the mutual disturbance of the two observables.

<sup>1</sup>This research is supported by the ARO

**5:06PM H48.00014 Optimized entanglement purification schemes for modular based quantum computers**, STEFAN KRASTANOV, LIANG JIANG, Yale University — The choice of entanglement purification scheme strongly depends on the fidelities of quantum gates and measurements, as well as the imperfection of initial entanglement. For instance, the purification scheme optimal at low gate fidelities may not necessarily be the optimal scheme at higher gate fidelities. We employ an evolutionary algorithm that efficiently optimizes the entanglement purification circuit for given system parameters. Such optimized purification schemes will boost the performance of entanglement purification, and consequently enhance the fidelity of teleportation-based non-local coupling gates, which is an indispensable building block for modular-based quantum computers. In addition, we study how these optimized purification schemes affect the resource overhead caused by error correction in modular based quantum computers.

**5:18PM H48.00015 Entanglement distillation in circuit quantum electrodynamics**, MARKUS OPPLIGER, JOHANNES HEINSOO, YVES SALATHE, ANTON POTOCNIK, MINTU MONDAL, ANDREAS WALLRAFF, ETH Zurich, GHEORGHE SORIN PAROANU, Aalto University School of Science — Entanglement is an essential resource for quantum information processing, such as quantum error correction, quantum teleportation and quantum communication. Such algorithms perform optimally with maximally entangled states. In practice entangled quantum states are very fragile due to a wide range of decoherence mechanisms. When two parties share degraded entangled states they are still able to generate an entangled state with higher fidelity using local operations and classical communication. This process is commonly referred to as entanglement distillation. Here we demonstrate distillation of highly entangled Bell states from two copies of less entangled states on a four transmon qubit device realized in the circuit-QED architecture. We characterize the output state for different degrees of entanglement at the input with quantum state tomography. A clear improvement of the entanglement measures is observed at the output.

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**

**Session H50 DAMOP: Many-Body Localization in Atomic Systems II** Hilton Baltimore Holiday Ballroom

1 -

**2:30PM H50.00001 Characterizing eigenstate thermalization via measures in the Fock space of operators**, XIAO-LIANG QI, PAVAN HOSUR, Stanford Univ — The eigenstate thermalization hypothesis (ETH) attempts to bridge the gap between quantum mechanical and statistical mechanical descriptions of isolated quantum systems. Here, we define unbiased measures for how well the ETH works in various regimes, by mapping general interacting quantum systems on regular lattices onto a single particle living on a high-dimensional graph. By numerically analyzing deviations from ETH behavior in the non-integrable Ising model, we propose quantities that we call the "n-weight" and the "n-distinguishability" to democratically characterize the average and the maximum deviations, respectively, for all operators residing on  $n$  sites. Along the way, we discover that complicated operators on average are worse than simple ones at distinguishing between neighboring eigenstates, contrary to the naive intuition created by the usual statements of the ETH that few-body (many-body) operators acquire the same (different) expectation values in nearby eigenstates at finite energy density.

**2:42PM H50.00002 Dynamical Many-Body Localization in a System of Coupled Relativistic Kicked Rotors**, EFIM ROZENBAUM, VICTOR GALITSKI, University of Maryland, College Park — A periodically-driven rotor is a prototypical model that exhibits a transition to chaos in the classical regime and dynamical localization (related to Anderson localization) in the quantum regime. In a recent preprint, arXiv:1506.05455, Keser *et al.* considered a many-body generalization of coupled quantum kicked rotors, and showed that in the special integrable linear case, the dynamical localization survives interactions. By analogy with many-body localization, the phenomenon was dubbed dynamical many-body localization (DMBL). In the present work, we study a non-integrable model of coupled quantum relativistic kicked rotors. Our analysis of such coupled "kicked" Dirac equations indicates that DMBL can exist for generic, non-integrable systems. We also analyze quantum dynamics of the model, which for certain select values of model's parameters exhibits highly unusual behavior – e.g., superballistic transport and peculiar spin dynamics.

**2:54PM H50.00003 A renormalization group approach to identifying the local quantum numbers in a many-body localized system<sup>1</sup>**, DAVID PEKKER, University of Pittsburgh, BRYAN K. CLARK, UIUC, VADIM OGANESYAN, College of Staten Island and the Graduate Center, CUNY, GIL REFAEL, Caltech, BINBIN TIAN, University of Pittsburgh — Many-body localization is a dynamical phase of matter that is characterized by the absence of thermalization. One of the key characteristics of many-body localized systems is the emergence of a large (possibly maximal) number of local integrals of motion (local quantum numbers) and corresponding conserved quantities. We formulate a robust algorithm for identifying these conserved quantities, based on Wegner's flow equations – a form of the renormalization group that works by disentangling the degrees of freedom of the system as opposed to integrating them out. We test our algorithm by explicit numerical comparison with more engineering based algorithms – Jacobi rotations and bi-partite matching. We find that the Wegner flow algorithm indeed produces the more local conserved quantities and is therefore more optimal. A preliminary analysis of the conserved quantities produced by the Wegner flow algorithm reveals the existence of at least two different localization lengthscales.

<sup>1</sup>Work was supported by AFOSR FA9550-10-1-0524 and FA9550-12-1-0057, the Kaufmann foundation, and SciDAC FG02-12ER46875.

### 3:06PM H50.00004 Many-body localization and thermalization in disordered Hubbard chains

, RUBEN MONDAINI, MARCOS RIGOL, The Pennsylvania State University — Recently, a lot of attention has been given to the aspects that lead isolated interacting quantum systems to thermalize. In the presence of disorder, however, the thermalization process fails resulting in a phenomena where transport is suppressed known as many-body localization. Unlike the standard Anderson localization for non-interacting systems, the delocalized (ergodic) phase is very robust against disorder even for moderate values of interaction. Another interesting aspect of the many-body localization phase is that under the time evolution of the quenched disorder, information present in the initial state may survive for arbitrarily long times. This was recently used as a probe of many-body localization of ultracold fermions in optical lattices with quasi-periodic disorder<sup>1</sup>. Here, we will use numerical results in one-dimensional Hubbard chains to show that this analysis may suffer from substantial finite-size effects. We will also compare different types of disorder to see how the ergodicity is affected.<sup>2</sup>

<sup>1</sup>M. Schreiber *et al.*, Science, **349** 842 (2015)

<sup>2</sup>R. Mondaini and M. Rigol, Phys. Rev. A **92**, 041601(R) (2015)

### 3:18PM H50.00005 Particle-hole symmetry, many-body localization, and topological edge

**modes**<sup>1</sup>, ROMAIN VASSEUR, UC Berkeley and Lawrence Berkeley National Laboratory, AARON J. FRIEDMAN, S.A. PARAMESWARAN, University of California, Irvine, ANDREW C. POTTER, UC Berkeley — We study the excited states of interacting fermions in one dimension with particle-hole symmetric disorder (equivalently, random-bond XXZ chains) using a combination of renormalization group methods and exact diagonalization. Absent interactions, the entire many-body spectrum exhibits infinite-randomness quantum critical behavior with highly degenerate excited states. We show that though interactions are an irrelevant perturbation in the ground state, they drastically affect the structure of excited states: even arbitrarily weak interactions split the degeneracies in favor of thermalization (weak disorder) or spontaneously broken particle-hole symmetry, driving the system into a many-body localized spin glass phase (strong disorder). In both cases, the quantum critical properties of the non-interacting model are destroyed, either by thermal decoherence or spontaneous symmetry breaking. This system then has the interesting and counterintuitive property that edges of the many-body spectrum are less localized than the center of the spectrum. We argue that our results rule out the existence of certain excited state symmetry-protected topological orders.

<sup>1</sup>Supported by the Gordon and Betty Moore Foundation's EPIQS Initiative (Grant GBMF4307 (ACP), the Quantum Materials Program at LBNL (RV), NSF Grant DMR-1455366 and UCOP Research Catalyst Award No. CA-15-327861 (SAP).

### 3:30PM H50.00006 Dynamical many-body localization in an integrable model

, AYIN C. KESER, Condensed Matter Theory Center, University of Maryland, College Park, SRIRAM GANESHAN, Simon Center for Geometry and Physics, GIL REFAEL, Institute of Quantum Information and Matter, Caltech, VICTOR GALITSKI, Condensed Matter Theory Center and Joint Quantum Institute, University of Maryland, College Park — We investigate dynamical many-body localization and delocalization in an integrable system of periodically-kicked, interacting linear rotors. The linear-in-momentum Hamiltonian makes the Floquet evolution operator analytically tractable for arbitrary interactions. One of the hallmarks of this model is that depending on certain parameters, it manifest both localization and delocalization in momentum space. We explicitly show that, for this model, the energy being bounded at long times is neither a necessary nor a sufficient condition for dynamical localization. We present a set of integrals of motion, which can serve as a fundamental diagnostic of dynamical localization. We also propose an experimental scheme, involving voltage-biased Josephson junctions, to realize such many-body kicked models.

### 3:42PM H50.00007 Dynamics of Hubbard-Band Quasiparticles in Disordered Optical Lattices<sup>1</sup>

, VITO SCAROLA, Virginia Tech, BRIAN DEMARCO, University of Illinois, Urbana-Champaign — Recent experiments use transport of degenerate Fermi gases in optical lattices (Kondov et al. Phys. Rev. Lett. **114**, 083002 (2015)) to probe the interplay of disorder and strong interactions. These experiments find evidence for an intriguing insulating phase where quantum diffusion is completely suppressed by strong disorder. Quantitative interpretation of these experiments remains an open problem that requires inclusion of non-zero entropy, strong interaction, and trapping in an Anderson-Hubbard model. We construct a theory of dynamics of Hubbard-band quasiparticles tailored to trapped optical lattice experiments. We compare the theory directly with center-of-mass transport experiments of Kondov et al. with no fitting parameters. The close agreement between theory and experiments shows that the suppression of transport is only partly due to finite entropy effects. We argue that the complete suppression of transport is consistent with short-time, finite size precursors of Anderson localization of Hubbard-band quasiparticles. The combination of our theoretical framework and optical lattice experiments offers an important platform for studying localization in isolated many-body quantum systems.

<sup>1</sup>V.W.S. acknowledges support from AFOSR under grant FA9550-11-1-0313

### 3:54PM H50.00008 Many-body localization and symmetry protected topology with ultracold

**Rydberg atoms**, IONUT-DRAGOS POTIRNICHE, Univ of California - Berkeley, MONIKA SCHLEIER-SMITH, Stanford University, ASHVIN VISHWANATH, NORMAN YAO, Univ of California - Berkeley — The interplay between quantum entanglement and symmetry-protected topological order has led to the classification of gapped, interacting, one dimensional quantum phases. A consequence of this classification is the existence of a diverse set of exactly solvable models, which serve as paradigmatic examples of various SPT orders. The experimental realization of such models has been hampered by the challenge of implementing tunable multi-body interactions. Recently, an alternate strategy has arisen: periodic driving. Indeed, it has been shown that the dynamics of a simple Floquet transverse-field Ising model can mirror that of the celebrated Haldane chain. However, as SPT order is expected only in the ground state while a driven system is expected to heat to infinite temperature, the ability to observe such Floquet SPT phases remains an open question. Here, we demonstrate that strong disorder, leading to many-body localization, stabilizes SPT order at finite energy densities while also preventing arbitrary heating of the system. Moreover, we propose a natural experimental implementation in a 1D optical lattice of ultracold Rydberg atoms.

### 4:06PM H50.00009 Probing Anderson localization of light via decay rate statistics in aperiodic

**Vogel spirals**<sup>1</sup>, ARISTI CHRISTOFI, Department of Electrical and Computer Engineering, Boston University, 8 Saint Marys street, Boston, MA 02215 USA, FELIPE A. PINHEIRO, Universidade Federal do Rio de Janeiro, Rio de Janeiro-RJ, 21941-972, Brazil & University of Southampton, Highfield, Southampton SO17 1BJ, UK, LUCA DAL NEGRO, Department of Electrical and Computer Engineering & Photonics Center, Boston University, 8 Saint Marys street, Boston, MA 02215 USA — We systematically investigate the spectral properties of different types of two-dimensional aperiodic Vogel spiral arrays of pointlike scatterers and three-dimensional metamaterials with Vogel spiral chirality using rigorous Greens function spectral method. We considered an efficient T-matrix approach to analyze multiple-scattering effects, including all scattering orders, and to understand localization properties through the statistics of the Greens matrix eigenvalues. The knowledge of the spectrum of the Green matrix of multi-particle scattering systems provides important information on the character of light propagation and localization in chiral media with deterministic aperiodic geometry. In particular, we analyze for the first time the statistics of the eigenvalues and eigenvectors of the Green matrix and extract the decay rates of the eigenmodes, their inverse participation ratio (IPR), the Wigner delay times and their quality factors. We emphasize the unique properties of aperiodic Vogel spirals with respect to random scattering media, which have been investigated so far.

<sup>1</sup>This work was supported by the Army Research Laboratory under Cooperative Agreement Number W911NF-12-2-0023

**4:18PM H50.00010 Anomalous transport in ergodic lattice systems<sup>1</sup>** , YEVGENY BAR LEV, DAVID R. REICHMAN, Columbia University — Many-body localization transition is a peculiar dynamical transition between ergodic and non-ergodic phases, which may occur at any temperature and in any dimension. For temperatures below the transition the system is nonergodic and localized, such that conductivity strictly vanishes at the thermodynamic limit, while for temperatures above the transition the system is thermal and conductive. In this talk I will present a comprehensive study of the dynamical properties of the ergodic phase in one and two dimensional generic disordered and interacting systems, conducted using a combination of nonequilibrium diagrammatic techniques and numerically exact methods. I will show that the ergodic phase, which was expected to be diffusive, exhibits anomalous transport regime for nontrivial times and explain how our findings settle with phenomenological theoretical models.

<sup>1</sup>NSF-CHE-1644802

**4:30PM H50.00011 Eigenstate Order in Floquet Systems** , CURT VON KEYSERLINGK, SHIVAJI SONDHAI, Princeton Univ — Recent work has introduced the notion of eigenstate order for many body systems and extended it to periodically driven, or Floquet, systems. I will discuss a set of results on possible phases in Floquet systems. These involve generalisations of topological insulators and superconductors as well as generalisations of interacting symmetry protected and topological phases of matter. Many body localisation plays an essential role in their realisation.

**4:42PM H50.00012 Localization in systems with long-range interactions<sup>1</sup>** , LEA SANTOS, Yeshiva University, USA, FRANCISCO PEREZ-BERNAL, Universidad de Huelva, Spain, FAUSTO BROGONÓVI, GIUSEPPE CELARDO, Università Cattolica del Sacro Cuore, Italy — In recent experiments with ion traps, long-range interactions were associated with the very fast propagation of excitations. Here, we show that, depending on the initial state, the evolution of these systems may actually be exceedingly slow. This is justified with the analysis of the density of states and structures of the eigenstates, and confirmed with numerical simulations of quench dynamics. The two sources of restricted dynamics that we discuss are: the presence of an excited state quantum phase transition and the onset of subspaces shielded from the effects of long-range interactions. Both scenarios can be tested experimentally.

<sup>1</sup>NSF Grant No. DMR-1147430.

**4:54PM H50.00013 Dynamics of a Many-Body-Localized System Coupled to a Bath** , MARK FISCHER, MYKOLA MAKSYMENKO, EHUD ALTMAN, Weizmann Institute of Science — Coupling a many-body localized system to a dissipative bath necessarily leads to delocalization. Here we investigate the nature of the ensuing relaxation dynamics and the information it holds on the many-body localized state. To solve for the time evolution, we formulate the relevant Lindblad equation in terms of the local integrals of motion of the underlying localized Hamiltonian. This allows to map the quantum evolution deep in the localized state to tractable classical rate equations. We consider two different types of dissipation relevant to systems of ultra-cold atoms: particle loss and dephasing due to inelastic scattering on the lattice lasers. Only the first mechanism shows a pronounced effect of interactions on the relaxation of observables.

**5:06PM H50.00014 Extended slow dynamical regime near the many-body localization transition** , DAVID J. LUITZ, University of Illinois at Urbana-Champaign, NICOLAS LAFLORENCIE, FABIEN ALET, Laboratoire de Physique Théorique, IRSAMC, Université de Toulouse, CNRS — Many-body localization is characterized by a slow logarithmic growth of entanglement entropy after a global quantum quench while the local memory of an initial spin imbalance remains at infinite time. We address the dynamics in the delocalized ergodic regime, where thermalization is expected. Using an exact Krylov space technique, the out-of-equilibrium dynamics of the random-field Heisenberg chain is studied up to  $L = 28$  sites, starting from an initially unentangled high-energy product state. With such a global quench protocol, we study the time evolution of the entanglement entropy, as well as the spin density imbalance in order to make contact with recent cold atom experiments. Within most of the delocalized phase, we unambiguously find a sub-ballistic entanglement growth  $S(t) \propto t^{1/z}$  with a disorder-dependent exponent  $z \geq 1$ , in contrast with the pure ballistic growth  $z = 1$  of clean systems. At the same time, anomalous relaxation is also observed for the spin imbalance  $I(t) \propto t^{-\zeta}$  with a continuously varying disorder-dependent exponent  $\zeta$ , vanishing at the transition. This provides a clear experimental signature for detecting this non-conventional metallic state where transport is sub-diffusive.

**5:18PM H50.00015 Effective localization potential of quantum states in disordered media<sup>1</sup>** , FILOCHE MARCEL, Ecole Polytechnique, DOUGLAS N. ARNOLD, University of Minnesota, GUY DAVID, Université Paris-Sud, DAVID JERISON, Massachusetts Institute of Technology, SVITLANA MAYBORODA, University of Minnesota — The amplitude of localized quantum states in random or disordered media may exhibit long range exponential decay. We present here a theory that unveils the existence of a localization landscape that controls the amplitude of the eigenstates in any quantum system. For second order operators such as the Schrödinger operator, this localization landscape is simply the solution of a Dirichlet problem with uniform right-hand side [1]. Moreover, we show that the reciprocal of this landscape plays the role of an effective potential which finely governs the confinement of the quantum states. In this picture, the boundaries of the localization subregions for low energy eigenfunctions correspond to the barriers of this effective potential, and the long range exponential decay characteristic of Anderson localization is explained as the consequence of multiple tunneling in the dense network of barriers created by this effective potential. Finally, we show that the Weyl's formula based on this potential turns out to be a remarkable approximation of the density of states for a large variety of systems, periodic or random, 1D, 2D, or 3D. [1] M. Filoche and S. Mayboroda, Proceedings of the National Academy of Sciences of the USA 109, 14761 (2012).

<sup>1</sup>NSF grant DMS-1418805, ANR Grant GEOMETRYA ANR-12-BS01-0014, NSF Grant DMS-1069225, NSF CAREER Award DMS-1056004, NSF INSPIRE Grant.

## Tuesday, March 15, 2016 2:30PM - 5:18PM –

Session H51 GPC DFD GSNP: Climate as a Non-equilibrium and Stochastic System Hilton Baltimore Holiday Ballroom 2 - Juan Restrepo, Oregon State University

**2:30PM H51.00001 Fluctuations and Response in Geophysical Fluid Dynamics** , VALERIO LUCARINI, University of Hamburg — The climate is a complex, chaotic, non-equilibrium system featuring a limited horizon of predictability, variability on a vast range of temporal and spatial scales, instabilities resulting into energy transformations, and mixing and dissipative processes resulting into entropy production. Despite great progresses, we still do not have a complete theory of climate dynamics able to account for instabilities, equilibration processes, response to changing parameters of the system, and multiscale effects. We will outline some possible applications of the response theory developed by Ruelle for non-equilibrium statistical mechanical systems, showing how it allows for setting on firm ground and on a coherent framework concepts like climate sensitivity, climate response, and climate tipping points, and to construct parametrizations for unresolved processes. We will show results for comprehensive global climate models. The results are promising in terms of suggesting new ways for approaching the problem of climate change prediction and for using more efficiently the enormous amounts of data produced by modeling groups around the world. Ref: V. Lucarini, R. Blender, C. Herbert, F. Ragone, S. Pascale, J. Wouters, Mathematical and Physical Ideas for Climate Science, Reviews of Geophysics 52, 809-859 (2014)

**3:06PM H51.00002 Balanced Dynamics in the Madden-Julian Oscillation<sup>1</sup>**, SHARON SESSIONS, STIPO SENTIC, New Mexico Tech, ZELJKA FUCHS, University of Split, Croatia, and New Mexico Tech, DAVID RAYMOND, New Mexico Tech — Balanced dynamics describes the response of the tropical thermodynamic environment to changes in the atmospheric vorticity patterns. Observations and numerical simulations have demonstrated that positive mid-tropospheric vorticity anomalies produce a more stable thermodynamic environment with cool anomalies at low levels and warm anomalies aloft. The increase in atmospheric stability creates more bottom-heavy convective profiles which are highly conducive for developing tropical cyclones. Balanced dynamics may also play a role in other varieties of tropical convection, including the most significant source of intraseasonal variability: the Madden-Julian Oscillation (MJO). Using data from DYNAMO—a field program aimed to investigate the dynamics of the MJO—we investigate the role of balanced dynamics in the Madden-Julian Oscillation.

<sup>1</sup>This work supported by the NSF

**3:18PM H51.00003 Stochastic dynamics of melt ponds and sea ice-albedo climate feedback**, IVAN SUDAKOV, Department of Physics, University of Dayton — Evolution of melt ponds on the Arctic sea surface is a complicated stochastic process. We suggest a low-order model with ice-albedo feedback which describes stochastic dynamics of melt ponds geometrical characteristics. The model is a stochastic dynamical system model of energy balance in the climate system. We describe the equilibria in this model. We conclude the transition in fractal dimension of melt ponds affects the shape of the sea ice albedo curve.

**3:30PM H51.00004 A Novel Method to Unravelling Energy Pathways in the Ocean**, HUSSEIN ALUIE, University of Rochester — Large-scale currents and eddies pervade the ocean and play a prime role in the general circulation and climate. The coupling between scales ranging from  $10^4$  km down to  $10^1$  mm presents a major difficulty in understanding, modeling, and predicting oceanic circulation and mixing, where the energy budget is uncertain within a factor possibly as large as ten. Identifying the energy sources and sinks at various scales can reduce such uncertainty and yield insight into new parameterizations. To this end, we refine a novel coarse-graining framework, which accounts for the spherical geometry of the problem, to directly analyze the coupling between scales. We apply these tools to strongly eddying high-resolution simulations using LANL's Parallel Ocean Program (POP).

**4:06PM H51.00005 The impact of the diurnal insolation cycle on the tropical cyclone heat engine**, MORGAN E. O'NEILL, Department of Earth and Planetary Sciences, Weizmann Institute of Science, DIAMILET PEREZ-BETANCOURT, Program in Atmospheres, Oceans and Climate, Massachusetts Institute of Technology, ALLISON A. WING, Lamont-Doherty Earth Observatory, Columbia University — A hurricane, or tropical cyclone, is understood as a heat engine that moves heat from the warm sea surface to the cold tropopause. The efficiency of this engine depends in part on the strength and duration of solar heating. Over land, peak rainfall associated with individual thunderstorms occurs in the late afternoon. Over ocean, with its markedly higher surface heat capacity, deep convection responds more to radiational cooling than daytime surface heating. However, the role of daily varying solar forcing on the dynamics of tropical cyclones is poorly understood. Recently, Dunion et al. (2014) reported significant, repeating diurnal behavior propagating outward from tropical cyclone centers, using infrared imagery from nine years of North Atlantic tropical cyclones. We study the impact of the diurnal cycle on tropical cyclones using a high resolution 3D numerical model, the System for Atmospheric Modeling (Khairoutdinov and Randall 2003). Simulations are run with and without variable sunlight. We are able to reproduce the observational finding of Dunion et al. (2014), and further identify a diurnally-varying residual circulation in the tropical cyclone at midlevels. The impact of the diurnal cycle on the equilibrium dynamics of tropical cyclones is also discussed.

**4:18PM H51.00006 Towards a General Turbulence Model for Planetary Boundary Layers Based on Direct Statistical Simulation<sup>1</sup>**, BRAD MARSTON, BAYLOR FOX-KEMPER, JOE SKITKA, Brown University — Sub-grid turbulence models for planetary boundary layers are typically constructed additively, starting with local flow properties and including non-local (KPP) or higher order (Mellor-Yamada) parameters until a desired level of predictive capacity is achieved or a manageable threshold of complexity is surpassed. Such approaches are necessarily limited in general circumstances, like global circulation models, by their being optimized for particular flow phenomena. By using direct statistical simulation (DSS) that is based upon expansion in equal-time cumulants we offer the prospect of a turbulence model and an investigative tool that is equally applicable to all flow types and able to take advantage of the wealth of nonlocal information in any flow. We investigate the feasibility of a second-order closure (CE2) by performing simulations of the ocean boundary layer in a quasi-linear approximation for which CE2 is exact. As oceanographic examples, wind-driven Langmuir turbulence and thermal convection are studied by comparison of the statistics of quasi-linear and fully nonlinear simulations. We also characterize the computational advantages and physical uncertainties of CE2 defined on a reduced basis determined via proper orthogonal decomposition (POD) of the flow fields.

<sup>1</sup>Supported in part by NSF DMR-1306806

**4:30PM H51.00007 Non-equilibrium Statistical Mechanics and the Sea Ice Thickness Distribution<sup>1</sup>**, JOHN WETTLAUER, SRIKANTH TOPPALADODDI, Yale University — We use concepts from non-equilibrium statistical physics to transform the original evolution equation for the sea ice thickness distribution  $g(h)$  due to Thorndike et al., (1975) into a Fokker-Planck like conservation law. The steady solution is  $g(h) = \mathcal{N}(q)h^q e^{-h/H}$ , where  $q$  and  $H$  are expressible in terms of moments over the transition probabilities between thickness categories. The solution exhibits the functional form used in observational fits and shows that for  $h \ll 1$ ,  $g(h)$  is controlled by both thermodynamics and mechanics, whereas for  $h \gg 1$  only mechanics controls  $g(h)$ . Finally, we derive the underlying Langevin equation governing the dynamics of the ice thickness  $h$ , from which we predict the observed  $g(h)$ . This allows us to demonstrate that the ice thickness field is ergodic. The genericity of our approach provides a framework for studying the geophysical scale structure of the ice pack using methods of broad relevance in statistical mechanics.

<sup>1</sup>Swedish Research Council Grant No. 638-2013-9243, NASA Grant NNH13ZDA001N-CRYO and the National Science Foundation and the Office of Naval Research under OCE-1332750 for support.

**4:42PM H51.00008 Large-eddy simulation of the transient and near-equilibrium behavior of precipitating shallow convection**, THIJS HEUS, Cleveland State University, AXEL SEIFERT, Deutscher Wetter Dienst, Offenbach, Germany, ROBERT PINCUS, University of Colorado, BJORN STEVENS, Max Planck Institute for Meteorology, Hamburg, Germany — Cloud-aerosol remain one of the largest uncertainties in climate modeling. Many of the postulated cloud-aerosol interactions involve precipitation to limit cloud size and life time, in particular for barely precipitating shallow cumulus clouds. If the precipitation exceeds a certain threshold, it will create feedback on the cloud field through cold pools and mesoscale organization. Such mesoscale responses have mostly been ignored so far in the discussion of aerosol indirect effects. We study the sensitivity of trade wind cumulus clouds to perturbations in cloud droplet number concentrations. Over time, the cloud system approaches a radiative-convective equilibrium state. The transient behavior and the properties of the near-equilibrium cloud field depend on the microphysical state and therefore on the cloud droplet number density. The primary response of the cloud field to changes in the cloud droplet number density is deepening of the cloud layer, and results in a shorter cloud life time. If the atmospheric time scales are long enough compared to the microphysical time scales, the cloud field may reach a near-equilibrium regime. In this regime, the decrease in cloud cover compensates much of the brightening of the clouds, and the overall effect on the albedo is small.

#### **4:54PM H51.00009 Statistical state dynamics of jet/wave coexistence in beta-plane turbulence**

, NAVID CONSTANTINOU, Scripps Inst. of Oceanography, Univ of California - San Diego, BRIAN FARRELL, Department of Earth and Planetary Sciences, Harvard University, PETROS IOANNOU, Physics Department, National and Kapodistrian University of Athens — Jets are commonly observed to coexist in the turbulence of planetary atmospheres with planetary scale waves and embedded vortices. These large-scale coherent structures arise and are maintained in the turbulence on time scales long compared to dissipation or advective time scales. The emergence, equilibration at finite amplitude, maintenance and stability of these structures pose fundamental theoretical problems. The emergence of jets and vortices from turbulence is not associated with an instability of the mean flow and their equilibration and stability at finite amplitude does not arise solely from the linear or nonlinear dynamics of these structures in isolation from the turbulence surrounding them. Rather the dynamics of these large-scale structures arises essentially from their cooperative interaction with the small-scale turbulence in which they are embedded. It follows that fundamental theoretical understanding of the dynamics of jets and vortices in turbulence requires adopting the perspective of the statistical state dynamics (SSD) of the entire turbulent state. In this work a theory for the jet/wave coexistence regime is developed using the SSD perspective.

#### **5:06PM H51.00010 A stochastic shallow cumulus ensemble model as a scale-aware parameterization of convective fluctuations<sup>1</sup>**

, MIRIANA SAKRADZIJIA, Max Planck Institute for Meteorology, AXEL SEIFERT, Deutscher Wetterdienst, THIJS HEUS, Cleveland State University, ANURAG DIPANKAR, Max Planck Institute for Meteorology — Numerical models are approaching the high-resolution limit where some aspects of deep convection and mesoscale convective systems can be explicitly modeled, while shallow cumuli are still a subgrid process that requires a parameterization. The classical assumption of a sufficiently large cloud sample within a model grid column breaks down in this regime, so it is crucial to develop scale-aware parameterizations. Therefore, we propose an approach to represent the variability of subgrid shallow cumuli about the ensemble average convective response. The shallow clouds are studied using Large Eddy Simulation (LES), where the original cloud field modeled on the grid of 25 m resolution is coarse-grained to mimic resolutions from 1 to 50 km. A canonical statistical ensemble is developed based on theoretical and LES findings and fluctuations of shallow convection are modeled by random subsampling of microstates from the convective ensemble distribution. The resulting distribution of subgrid convective states is scale-aware, and it represents stochastic fluctuations that increase with grid resolution and become substantial on the kilometre-scale grids. We find that the local cloud memory plays an important role in defining the convective ensemble statistics in a steady cumulus regime.

<sup>1</sup>Hans Ertel Centre for Weather Research

## **Tuesday, March 15, 2016 2:30PM - 5:30PM –**

### **Session H52 DAMOP: Optomechanics and Hybrid Systems II: Metrology and Other Topics**

Hilton Baltimore Holiday Ballroom 3 - Mukund Vengalatorre, Cornell University

#### **2:30PM H52.00001 Hybrid atom-membrane optomechanics**

, PHILIPP TREUTLEIN, University of Basel, Department of Physics — We have realized a hybrid mechanical system in which ultracold atoms and a micromechanical membrane are coupled by radiation pressure forces. The atoms are trapped in an optical lattice, formed by retro-reflection of a laser beam from an optical cavity that contains the membrane as mechanical element. When we laser cool the atoms, we observe that the membrane is sympathetically cooled from ambient to millikelvin temperatures through its interaction with the atoms. Sympathetic cooling with ultracold atoms or ions has previously been used to cool other microscopic systems such as atoms of a different species or molecular ions up to the size of proteins. Here we use it to efficiently cool the fundamental vibrational mode of a macroscopic solid-state system, whose mass exceeds that of the atomic ensemble by ten orders of magnitude. Our hybrid system operates in a regime of large atom-membrane cooperativity. With technical improvements such as cryogenic pre-cooling of the membrane, it enables ground-state cooling and quantum control of mechanical oscillators in a regime where purely optomechanical techniques cannot reach the ground state. References: A. Jöckel, A. Faber, T. Kampschulte, M. Korppi, M. T. Rakher, and P. Treutlein, Sympathetic cooling of a membrane oscillator in a hybrid mechanical-atomic system, *Nature Nanotechnology* 10, 55 (2015). B. Vogell, T. Kampschulte, M. T. Rakher, A. Faber, P. Treutlein, K. Hammerer, and P. Zoller, Long distance coupling of a quantum mechanical oscillator to the internal states of an atomic ensemble, *New J. Phys.* 17, 043044 (2015). B. Vogell, K. Stannigel, P. Zoller, K. Hammerer, M. T. Rakher, M. Korppi, A. Jöckel, and P. Treutlein, Cavity-enhanced long-distance coupling of an atomic ensemble to a micromechanical membrane, *Phys. Rev. A* 87, 023816 (2013).

#### **3:06PM H52.00002 Detecting continuous gravitational waves with a jug of superfluid**

, SWATI SINGH, University of Arizona, LAURA DELORENZO, ADAM PEARLMAN, Caltech, IGOR PIKOVSKI, ITAMP, MILES BLENCOWE, Dartmouth College, KEITH SCHWAB, Caltech — We investigate the sensitivity to narrow band, continuous-wave strain fields of a kg-scale optomechanical system formed by the acoustic motion of superfluid helium-4 parametrically coupled to a super-conducting microwave cavity. This narrowband detection scheme is tunable through pressurization of the helium, thereby making both doppler tracking of astrophysical sources and tuning the detector on/off from the source possible. For reasonable experimental parameters, we find that gravitational metric strain fields from nearby pulsars could be detected with a few weeks of integration time.

#### **3:18PM H52.00003 Measurement and Applications of Radiation Pressure<sup>1</sup>**

, DAKANG MA, JOSEPH GARRETT, JOSEPH MURRAY, JEREMY MUNDAY, University of Maryland, College Park, MUNDAY LAB TEAM — Light reflected off a material or absorbed within it exerts radiation pressure through the transfer of momentum. Measuring and utilizing radiation pressure have aroused growing interest in a wide spectrum of research fields. Micromechanical transducers and oscillators are good candidates for measuring radiation pressure, but accompanying photothermal effects often obscure the measurement. In this work, we investigate the accurate measurement of the radiation force on microcantilevers in ambient conditions and ways to separate radiation pressure and photothermal effects. Further, we investigate an optically broadband switchable device based on polymer dispersed liquid crystal which has potential applications in solar sails and maneuvering spacecraft without moving parts.

<sup>1</sup>The authors would like to thank NASA Early Career Faculty Award and NASA Smallsat Technology Partnership Award for their funding support.

#### **3:30PM H52.00004 Real-time Measurement of Mechanical Fluctuations in Carbon Nanotube Resonators**

, IOANNIS TSIOUTSIOS, ALEXANDROS TAVERNARAKIS, JOHANN OSMOND, ICFO, Institut de Cincies Fotniques, Mediterranean Technology Park, 08860 Castelldefels, Barcelona, Spain, PIERRE VERLOT<sup>1</sup>, Universit Claude Bernard Lyon 1, UCBL, Domaine Scientifique de La Doua, 69622 Villeurbanne, France, ADRIAN BACHTOLD, ICFO, Institut de Cincies Fotniques, Mediterranean Technology Park, 08860 Castelldefels, Barcelona, Spain — Carbon nanotube resonators have been recently shown to hold an exceptional sensing potential, relying on their extremely low mass. As a consequence, they are also expected to transduce the fundamental thermal force into very large motion fluctuations. Recently, an increasing number of theoretical proposals have suggested that this property may strongly affect the vibrational behaviour of carbon nanotube resonators, which has so far remained unobserved. Here we report the first, real-time detection of the thermally-induced vibrations in carbon nanotube resonators with masses in the 10 *ag* range. We show that coupling singly-clamped carbon nanotubes to a focused electron beam enables the full access to their mechanical trajectories. Our detailed analysis demonstrates that our devices behave as linear harmonic oscillators undergoing thermally-driven Brownian motion. Our result establishes the viability of carbon nanotube resonator technology at room temperature and paves the way towards the observing novel thermodynamics regimes in nanomechanics.

<sup>1</sup>ICFO, Institut de Cincies Fotniques, Mediterranean Technology Park, 08860 Castelldefels, Barcelona, Spain

**3:42PM H52.00005 Testing quantum mechanics and quantum gravity with cavity optomechanics**, DAVID VITALI, Physics Division, School of Science and Technology, University of Camerino — Cavity optomechanical setups represents a promising platform for testing quantum mechanics and its validity at a macroscopic scale. Here we present two different examples. We first show the result of an experiment which, by a high sensitive measurement of the free evolution of the nanomechanical resonator probed by an optical field, has improved by many orders of magnitude the bounds on commutator deformation parameters which characterize a wide class of approaches to quantum gravity. In the second case we propose an experiment able to discriminate unambiguously collapse models, postulating the existence of intrinsic noise which modifies quantum mechanics and is responsible for the emergence of macroscopic classicality, from standard environmental sources of decoherence. In particular, we show that the stationary state of a trapped nanosphere is particularly sensitive, under specific experimental conditions, to the interplay between the cavity size, the trapping frequency and the momentum diffusion induced by the collapse models, allowing to detect them even in the presence of standard environmental noises.

**3:54PM H52.00006 Torque Magnetometry and Susceptometry using Split-Beam Optomechanical Nanocavities**, TAYYABA FIRDOUS, Department of Physics and National Institute for Nanotechnology, University of Alberta, Canada, NATHANAEL WU, MARCELO WU, Department of Physics and Astronomy and Institute for Quantum Science and Technology, University of Calgary, Canada, FATEMEH FANI SANI, JOSEPH LOSBY, Department of Physics and National Institute for Nanotechnology, University of Alberta, Canada, PAUL BARCLAY, Department of Physics and Astronomy and Institute for Quantum Science and Technology, University of Calgary, Canada, MARK FREEMAN, Department of Physics and National Institute for Nanotechnology, University of Alberta, Canada — A large number of sensitive magnetometry methods are limited to cryogenic operation. We present a highly sensitive torque magnetometer using a photonic crystal optomechanical split-beam nanocavity operating in air at room temperature. The chip-based magnetometer is proficient for probing both the net magnetization and AC susceptibility of individual magnetic microstructures. This is demonstrated through the observation of nanoscale Barkhausen transitions in the magnetic hysteresis of a permalloy thin-film element. Control of the vector direction of the radio frequency drive allows detection of accompanying AC susceptibility terms.

**4:06PM H52.00007 Appearance and disappearance of motional sideband asymmetry in measurement-based control of a mechanical oscillator**, VIVISHEK SUDHIR, DALZIEL WILSON, RYAN SCHILLING, HENDRIK SCHUETZ, Ecole Polytechnique Federale de Lausanne, ANDREAS NUNNENKAMP, University of Cambridge, TOBIAS KIPPENBERG, Ecole Polytechnique Federale de Lausanne — Measurement-based feedback provides an avenue to study the delicate interplay between the quantum correlations established during the process of measurement, and their progressive obfuscation when exposed to uncorrelated noise in the form of fundamental quantum fluctuations in the feedback path. Here we demonstrate this tradeoff using a feedback strategy whose objective is to cool a nano-mechanical oscillator close to its ground state. The correlations established due to the measurement are revealed in the appearance of motional sideband asymmetry. The latter, faithfully measured using an optical heterodyne interferometer with an imprecision  $\sim 17$  dB below that at the standard quantum limit, increases to 6% as the oscillator is feedback cooled to an occupation of 15 phonons. Further increase in the gain of the feedback loop leads to a decrease in the asymmetry. This is due to the addition of unavoidable quantum fluctuations in a feedback amplifier – photon shot-noise amplified by a homodyne detector in our case.

**4:18PM H52.00008 Enhanced nonlinear interactions in quantum optomechanics via mechanical amplification**, NICOLAS DIDIER, Quantic team, INRIA Paris, MARC-ANTOINE LEMONDE, Atominstut, Vienna University of Technology, AASHISH A. CLERK, Department of Physics, McGill University — A key challenge limiting truly quantum behaviour in optomechanical systems is the typically small value of the optomechanical coupling at the single-photon, single-phonon level. We present an approach for exponentially enhancing the single-photon coupling strength in an optomechanical system using only additional linear resources. It allows one to reach the quantum nonlinear regime of optomechanics, where nonlinear effects are observed at the single photon level, even if the bare coupling strength is much smaller than the mechanical frequency and cavity damping rate. Our method is based on using a large amplitude, strongly detuned mechanical parametric drive to amplify mechanical zero-point fluctuations and hence enhance the radiation pressure interaction. It has the further benefit of allowing time-dependent control, enabling pulsed schemes. For a two-cavity optomechanical setup, we show that our scheme generates photon blockade for experimentally accessible parameters, and even makes the production of photonic states with negative Wigner functions possible. We discuss how our method is an example of a more general strategy for enhancing boson-mediated two-particle interactions and nonlinearities. Preprint: arXiv:1509.09238.

**4:30PM H52.00009 Quantum squeezing of a mechanical resonator**, CHAN U LEI, AARON WEINSTEIN, California Institute of Technology, JUNHO SUH, Korea Research Institute of Standards and Science, EMMA WOLLMAN, KEITH SCHWAB, California Institute of Technology — Generating nonclassical states of a macroscopic object has been a subject of considerable interest. It offers a route toward fundamental test of quantum mechanics in an unexplored regime. However, a macroscopic quantum state is very susceptible to decoherence due to the environment. One way to generate robust quantum states is quantum reservoir engineering. In this work, we utilize the reservoir engineering scheme developed by Kronwald et al. [1] to generate a steady quantum squeezed state of a micron-scale mechanical oscillator in an electromechanical system. Together with the backaction evading measurement technique [2], we demonstrate a quantum nondemolition measurement of the mechanical quadratures to characterize the quantum squeezed state. By measuring the quadrature variances of the mechanical motion, more than 3dB squeezing below the zero-point level has been achieved. [1] A. Kronwald, F. Marquardt, and A. A. Clerk, Phys. Rev. A 88, 063833 (2013). [2] J. Suh, A. J. Weinstein, C. U. Lei, E. E. Wollman, S. K. Steinke, P. Meystre, A. A. Clerk, and K. C. Schwab, Science 344, 1262 (2014).

**4:42PM H52.00010 Quantum nondemolition measurement of a nonclassical state of a massive object**, FLORENT LECOCQ, JEREMY CLARK, RAYMOND SIMMONDS, JOSE AUMENTADO, JOHN TEUFEL, NIST - Boulder — By coupling a macroscopic mechanical oscillator to two microwave cavities, we simultaneously prepare and monitor a nonclassical steady state of mechanical motion [1]. In each cavity, correlated radiation pressure forces induced by two coherent drives engineer the coupling between the quadratures of light and motion. We first demonstrate the ability to perform a continuous quantum nondemolition measurement of a single mechanical quadrature at a rate that exceeds the mechanical decoherence rate, while avoiding measurement backaction by more than 13dB. Second, we apply this measurement technique to independently verify the preparation of a squeezed state in the mechanical oscillator, resolving quadrature fluctuations 20% below the quantum noise. [1] F.Lecocq, et al, ArXiv 1509.01629 (2015)

**4:54PM H52.00011 Observation of Nonclassical Radiation Pressure Forces on a Mechanical Oscillator<sup>1</sup>**, JEREMY CLARK, FLORENT LECOCQ, RAYMOND SIMMONDS, JOSE AUMENTADO, JOHN TEUFEL, NIST Boulder — Squeezed states of light are known to be useful for enhancing mechanical displacement sensing since they can be tailored to reduce the “photon counting noise” that limits the measurement’s noise floor. On the other hand, recent experiments in cavity optomechanics have reached measurement regimes where an interrogating light field exerts radiation pressure noise on a mechanical oscillator. One outstanding challenge has been to explore the intersection between such experiments. I will present data obtained using a superconducting cavity optomechanical system wherein a mechanical oscillator is driven by nonclassical radiation pressure imparted by squeezed microwave fields.

<sup>1</sup>JBC acknowledges the NRC for financial support

**5:06PM H52.00012 Complex squeezing for force measurement beyond the standard quantum limit**, SYDNEY SCHREPLER, University of California, Berkeley, LUKAS BUCHMANN, Aarhus Universitet, JONATHAN KOHLER, University of California, Berkeley, NICOLAS SPETHMANN, University of California, Berkeley, Technische Universitt Kaiserslautern, DAN STAMPER-KURN, University of California, Berkeley, Lawrence Berkeley National Laboratory — Squeezed quantum states are popular theoretical and experimental means of overcoming precision limits set by quantum mechanics. We identify "complex squeezing" as time delayed correlations that can in general not be measured using homodyne or heterodyne detection schemes, but nonetheless arise naturally in measurement devices such as optomechanical systems. In this case, the dispersive coupling between a mechanical element and an electromagnetic resonator causes real ponderomotive squeezing at frequencies away from mechanical resonance, but that squeezing becomes complex closer to resonance, where the system can be operated more sensitively for force detection. We describe a measurement protocol sensitive to complex squeezing and show how it can lead to enhanced sensitivity of force measurements using optomechanical oscillators.

**5:18PM H52.00013 Frequency stabilization of single layer graphene oscillators through optical injection locking**, SAMER HOURI<sup>1</sup>, SANTIAGO CARTAMIL BUENO, Delft University of Technology, WARNER VENSTRA<sup>2</sup>, Quantified Air — Single layer graphene (SLG) drum resonators offer exciting prospects as experimental testbeds for nonlinear dynamics. Recently, photo-thermal induced feedback effects leading to self-oscillations in graphene have been demonstrated [1]. In this paper we examine the phase jitter of self-oscillating SLG, and the means to improve the frequency stability through optical injection locking. The resonator consists of an SLG on top of a 10 micron diameter circular cavity with a cavity depth of 750 nm. By shining a 10 mW He-Ne laser the drum enters a regime of photo-thermally induced self-oscillation. The oscillating SLG suffers from a significant phase noise that can be directly observed in the time domain as random walk of the oscillation period. By applying a lock tone to the oscillator through the application of a modulated blue laser (405 nm), the SLG motion is then phase locked to the applied tone with more than an order of magnitude improvement in its coherence time. The injection locking is also studied as a function of lock signal detuning and power. [1] Barton, Robert A., et al. "Photothermal self-oscillation and laser cooling of graphene optomechanical systems." *Nano letters* 12.9 (2012): 4681-4686.

<sup>1</sup>Presenting author

<sup>2</sup>Quantified Air, Lorentzweg 1, 2628 CJ Delft, The Netherlands

**Tuesday, March 15, 2016 2:30PM - 5:30PM –**  
**Session H53 COM: Explore the Expertise and Facilities at the DOE Nanocenters: Come Work With Us!** Hilton Baltimore Holiday Ballroom 4 - Fernando Camino, Brookhaven National Laboratory

**2:30PM H53.00001 Pushing the lipid envelope: using bio-inspired nanocomposites to understand and exploit lipid membrane limitations**, GABRIEL MONTANO, Los Alamos National Laboratory — Lipids serve as the organizing matrix material for biological membranes, the site of interaction of cells with the external environment. . As such, lipids play a critical role in structure/function relationships of an extraordinary number of critical biological processes. In this talk, we will look at bio-inspired membrane assemblies to better understand the roles of lipids in biological systems as well as attempt to generate materials that can mimic and potentially advance upon biological membrane processes. First, we will investigate the response of lipids to adverse conditions. In particular, I will present data that demonstrates the response of lipids to harsh conditions and how such responses can be exploited to generate nanocomposite rearrangements. I will also show the effect of adding the endotoxin lipopolysaccharide (LPS) to lipid bilayer assemblies and describe implications on our understanding of LPS organization in biological systems as well as describe induced lipid modifications that can be exploited to organize membrane composites with precise, two-dimensional geometric control. Lastly, I will describe the use of amphiphilic block copolymers to create membrane nanocomposites capable of mimicking biological systems. In particular, I will describe the use of our polymer-based membranes in creating artificial photosynthetic assemblies that rival biological systems in function in a more flexible, dynamic matrix.

**3:06PM H53.00002 Expanding the versatility of silicon carbide thin films and nanowires<sup>1</sup>**, LUNET LUNA, Univ of California - Berkeley — Silicon carbide (SiC) based electronics and sensors hold promise for pushing past the limits of current technology to achieve small, durable devices that can function in high-temperature, high-voltage, corrosive, and biological environments. SiC is an ideal material for such conditions due to its high mechanical strength, excellent chemical stability, and its biocompatibility. Consequently, SiC thin films and nanowires have attracted interest in applications such as micro- and nano-electromechanical systems, biological sensors, field emission cathodes, and energy storage devices. However to fully realize SiC in such technologies, the reliability of metal contacts to SiC at high temperatures must be improved and the nanowire growth mechanism must be understood to enable strict control of nanowire crystal structure and orientation. Here, we present a novel metallization scheme, utilizing solid-state graphitization of SiC, to improve the long-term reliability of Pt/Ti contacts to polycrystalline n-type SiC films at high temperature. The metallization scheme includes an alumina protection layer and exhibits low, stable contact resistivity even after long-term (500 hr) testing in air at 450 °C. We also report the crystal structure and growth mechanism of Ni-assisted silicon carbide nanowires using single-source precursor, methyltrichlorosilane. The effects of growth parameters, such as substrate and temperature, on the structure and morphology of the resulting nanowires will also be presented. Overall, this study provides new insights towards the realization of novel SiC technologies, enabled by advanced electron microscopy techniques located in the user facilities at the Molecular Foundry in Berkeley, California.

<sup>1</sup>This work was performed in part at the Molecular Foundry, supported by the Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

**3:42PM H53.00003 Graphene Oxide/ Ruthenium Oxide Composites for Supercapacitors Electrodes<sup>1</sup>**, FATIMA AMIR, Winthrop University — Supercapacitors are electrical energy storage devices with high power density, high rate capability, low maintenance cost, and long life cycle. They complement or replace batteries in harvesting applications when high power delivery is needed. An important improvement in performance of supercapacitors has been achieved through recent advances in the development of new nanostructured materials. Here we will discuss the fabrication of graphene oxide/ ruthenium oxide supercapacitors electrodes including electrophoretic deposition. The morphology and structure of the fabricated electrodes were investigated and will be discussed. The electrochemical properties were determined using cyclic voltammetry and galvanostatic charge/discharge techniques and the experiments that demonstrate the excellent capacitive properties of the obtained supercapacitors will also be discussed. The fabrication and characterization of the samples were performed at the Center of Functional Nanomaterials at Brookhaven National Lab. The developed approaches in our study represent an exciting direction for designing the next generation of energy storage devices.

<sup>1</sup>This work was supported in part by the U.S. Department of Energy through the Visiting Faculty Program and the research used resources of the Center for Functional Nanomaterials at Brookhaven National Laboratory

**4:18PM H53.00004 Pushing the limits of nanolithography outside the box<sup>1</sup>**, LEONIDAS OCOLA, Argonne Natl Lab — The Center for Nanoscale Materials (CNM) at Argonne National Laboratory was constructed in 2006, and opened its doors to serve the user community in 2007 with the objective to provide research opportunities in Nanoscience for the scientific community worldwide. Currently, the CNM hosts over 400 user proposals a year. There are six research groups at the CNM that do work in nanophotonics, electronic and magnetic materials and devices, nanobio interfaces, nanofabrication and devices, x-ray nanoscale microscopy and theory and modeling. At the CNM Nanofabrication and Devices Group we have been able to push the limits of electron beam lithography to make plasmonic nanostructures obtain sharp corners with less than 6 nm radius of curvature and expand the use of ion beams to 3D large area nanofabrication in microfluidics by novel design methodologies, among other accomplishments. None of these accomplishments are possible without detailed understanding of the physics and chemistry mechanisms involved during fabrication. During my talk I will discuss a few clear cases where lithography and fabrication are used in ways not commonly found in current nanofabrication facilities and what make our facility unique.

<sup>1</sup>This work was supported by the Department of Energy under Contract No. DE-AC02-06CH11357. Use of the Center for Nanoscale Materials was supported by the U. S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

**4:54PM H53.00005 The USER: Utilizing Scientific Environments for Research<sup>1</sup>**, LAKEISHA WALKER, Oak Ridge National Lab — A lot of hard work goes into submitting a proposal for access to equipment in our nation's top science research facilities. It seems the biggest focus for a facility USER should be on the acceptance of the proposal, however, the job of a facility USER actually begins after the acceptance letter arrives. In order to make the most of the awarded experiment time and cultivate collaborations for the future, facility USERS need to look beyond the proposal. From experiment scheduling to arrival to data analysis the entire USER experience is valuable and worth doing well. This presentation will discuss best practices for facility USERS and highlight successful USER collaborations at ORNL's High Flux Isotope Reactor.

<sup>1</sup>Funded by the Office of Basic Energy Sciences, U.S. DOE. ORNL is managed by UT-Battelle, LLC for US DOE.

**Tuesday, March 15, 2016 2:30PM - 5:06PM –**  
**Session H54 DCMP GERA FIAP: Materials for Energy Storage Devices I** Hilton Baltimore Holiday Ballroom 5 - Marina Leite, Univ. of Maryland - College Park

**2:30PM H54.00001 Dual Electrospray Pyrolysis for Mixed Metal Oxide (and Carbon) Composite Nanoparticle Synthesis with Applications in Energy Storage**, JUSTIN TANG, WEN LIU, HAILIANG WANG, ALESSANDRO GOMEZ, Yale University — We present a novel approach to synthesizing mixed metal oxide nanoparticles with a continuous, scalable aerosol flow process using the electrospray. The electrospray is a liquid atomization technique that generates a monodisperse population of highly charged liquid droplets over a broad size range (nanometric to tens of microns). Each liquid droplet serves as a micro-reactor, containing a payload of suitable precursors (such as metal nitrides), allowing for precise control over particle composition and size. By using two electrosprays of opposite polarities, the two highly charged droplets plumes are electrostatically mixed to produce a charge-neutral aerosol. Electrostatically driven droplet-droplet collisions can also be used to control morphology to some degree. This aerosol is passed through a tubular furnace via carrier gas, pyrolyzing the precursors to synthesize nanomaterials. We apply this approach to manganese oxide, cobalt oxide, and carbon composite nanoparticles for use in energy storage applications.

**2:42PM H54.00002 The Basic Understanding of Lithium Superoxide in Li-O<sub>2</sub> Battery<sup>1</sup>**, KAH CHUN LAU, Argonne National Lab, DENG YUN ZHAI, Graduate School at Shenzhen, Tsinghua University, China, HSIEN-HAU WANG, XIANGYI LUO, JIANGUO WEN, DEAN MILLER, PAUL REDFERN, JUN LU, LARRY CURTISS, KHALIL AMINE, Argonne National Lab — The electrochemical and chemical processes that involved in Li-O<sub>2</sub> battery are complex, and depend heavily on electrode materials, electrolytes, interfaces, and cell operating conditions. In non-aqueous Li-O<sub>2</sub> battery, the main discharge products are commonly known to be lithium peroxide (Li<sub>2</sub>O<sub>2</sub>), and possibly some other parasitic components (i.e. Li<sub>2</sub>CO<sub>3</sub>, LiOH, Li<sub>2</sub>O). However, the superoxide intermediates and lithium superoxide (O<sub>2</sub><sup>-</sup>, LiO<sub>2</sub>) which are commonly known to be metastable can also be found as reported [1, 2]. Relative to these compounds (i.e. Li<sub>2</sub>CO<sub>3</sub>, Li<sub>2</sub>O, LiOH, Li<sub>2</sub>O<sub>2</sub>) in discharge products, little is known about LiO<sub>2</sub>. To have a basic understanding of lithium superoxide, both theoretical studies and experimental characterizations are important. In this presentation, the recent developments, studies and findings of this exotic species will be discussed. References: 1. D. Zhai<sup>+</sup>, K.C. Lau<sup>+</sup>, H. Wang, J. Wen, D. Miller, J. Lu, F. Kang, B. Li, W. Yang, J. Gao, E. Indacochea, L.A. Curtiss, K.A. Amine, Nano Lett. 15 (2), 1041-1046 (2015). 2. J. Lu<sup>+</sup>, Y.J. Lee<sup>+</sup>, X. Luo<sup>+</sup>, K.C. Lau<sup>+</sup>, M. Asadi<sup>+</sup>, et. al. Nature (accepted).

<sup>1</sup>This work was primarily supported by the U.S. Department of Energy under Contract DE-AC02-06CH11357 from the Vehicle Technologies Office, Department of Energy, Office of Energy Efficiency and Renewable Energy.

**2:54PM H54.00003 3D strain engineered self-rolled thin-film architecture for high-energy density lithium-ion batteries**, GRIFFIN GODBEY, CHEN GONG, CYNTHIA YU, CLAYTON BLYTHE, MARINA LEITE, Depart. of Materials Science and Eng. & Institute for Research in Electronics and Applied Physics, Univ. of Maryland, College Park, MD — Recently, multiple 3D geometries have been implemented into energy storage devices (e.g. nanowire anodes and arrays of interdigitated rods) in order to better accommodate the large volume expansion experienced by the anode during lithiation and to increase the structure energy density. However, most approached structures are difficult to scale up. Here we show how self-rolled thin-films can maintain a high energy density and can potentially accommodate the volume expansion suffered by the anode. The self-rolled tubes are fabricated by physical deposition of the active layers, creating a stress gradient between thin-film stack due to differences in coefficient of thermal expansion. Upon a sacrificial layer removal, the thin-film rolls to relieve this built-in stress. We predict the final dimension of self-rolled battery tubes using known elastic properties of materials commonly used as the active layers of the device. We will discuss an appropriate figure-of-merit that defines how the winding process can ultimately affect the volumetric capacity of 3D self-rolled batteries.

**3:06PM H54.00004 Electrochemical properties of Li<sub>2</sub>FeSiO<sub>4</sub>/C nanocomposites prepared by sol-gel and hydrothermal methods**, AJAY KUMAR, Wayne State University, O.D. JAYAKUMAR, Bhabha atomic research centre, VAMAN M. NAIK, University of Michigan Dearborn, GHOLAM A. NAZRI, RATNA NAIK, Wayne State University — Li<sub>2</sub>FeSiO<sub>4</sub> is considered as potential cathode material for next generation lithium ion batteries because of its high specific theoretical capacity, low cost, and safety. However, it suffers from poor electronic conductivity and slow lithium ion diffusion in the solid phase. To address these issues, we have studied mesoporous Li<sub>2</sub>FeSiO<sub>4</sub>/C composites synthesized by sol-gel (SG) and hydrothermal (HT) methods using tri-block copolymer (P123) as carbon source and structure directing agent. The structure and morphology of the composites were characterized by XRD, SEM and TEM and the surface area and pore size distribution were measured by using N<sub>2</sub> adsorption/desorption. Galvanostatic cycling, electrochemical impedance spectroscopy, and cyclic voltammetry were used to evaluate the electrochemical performance of the Li<sub>2</sub>FeSiO<sub>4</sub>/C composites. The Li<sub>2</sub>FeSiO<sub>4</sub>/C (HT) composites show a superior electrochemical performance compared to Li<sub>2</sub>FeSiO<sub>4</sub>/C (SG). At C/30 rate, the discharge capacity of Li<sub>2</sub>FeSiO<sub>4</sub>/C (HT) reached ~276 mAh/g in the 1.5-4.6 V window and shows better rate capability and stability at high rates. We attribute the improved electrochemical performance of Li<sub>2</sub>FeSiO<sub>4</sub>/C (HT) to its large surface area and reduced particle size. The details of the study will be presented.

**3:18PM H54.00005 Transmission Electron Microscopy and First Principle Studies Investigating Intercalation Phenomenon Of Vanadium Pentoxide( $V_2O_5$ ) nanowire cathode<sup>1</sup>**, ARIJITA MUKHERJEE, UIC, HASTI ASAYESH ARDAKANI, MTU, TANGHONG YI, CHEON JUNG KIM, UIC, JUSTIN ANDREWS, SARBAJIT BANERJEE, Texas AM, JORDI CABANA, REZA S YASSAR, ROBERT F KLIIE, UIC, JCESR COLLABORATION — Vanadium Pentoxide( $V_2O_5$ ) is an attractive intercalation compound due to its characteristic layered structure from weak vanadium-oxygen bonding which enables the intercalation of ions between the layers. Here, we will discuss an in-situ transmission electron microscopy and electron energy-loss spectroscopy approach investigating lithiation of orthorhombic  $\alpha$ - $V_2O_5$  nanowires where the center of the nanowire undergoes a transformation to  $\gamma$ - $Li_2V_2O_5$  phase. Since  $V_2O_5$  has also been predicted as a potential cathode host for magnesium ion intercalation, we also investigate Mg intercalation in  $\alpha$ - $V_2O_5$  nanowire and determine if our reaction pathway leads to the formation of  $\varepsilon$ - $Mg_{0.5}V_2O_5$  phase, as predicted by density functional theory calculations. In-situ Li and Mg intercalation experiments into the new tunnel structured  $\zeta$ - $V_2O_5$  nanowires will also be presented and the resulting phases will be compared with theoretical predictions.

<sup>1</sup>This work is supported by Joint Center for Energy Storage Research(JCESR)

**3:30PM H54.00006 Dry Pressed Holey Graphene Composites for Li-air Battery Cathodes<sup>1</sup>**, STEVEN LACEY, University of Maryland, College Park, YI LIN, National Institute of Aerospace, LIANGBING HU, University of Maryland, College Park — Graphene is considered an “omnipotent” material due to its unique structural characteristics and chemical properties. By heating graphene powder in an open-ended tube furnace, a novel compressible carbon material, holey graphene (hG), can be created with controlled porosity and be further decorated with nanosized catalysts to increase electrocatalytic activity. All hG-based materials were characterized using various microscopic and spectroscopic techniques to obtain morphological, topographical, and chemical information as well as to identify any disordered/crystalline phases. In this work, an additive-free dry press method was employed to press the hG composite materials into high mass loading mixed, sandwich, and double-decker Li-air cathode architectures using a hydraulic press. The sandwich and double-decker (i.e. Big Mac) cathode architectures are the first of its kind and can be discharged for more than 200 hours at a current density of 0.2 mA/cm<sup>2</sup>. The scalable, binderless, and solventless dry press method and unique Li-air cathode architectures presented here greatly advance electrode fabrication possibilities and could promote future energy storage advancements.

<sup>1</sup>Support appreciated from the NASA Internships Fellowships Scholarships (NIFS) Program

**3:42PM H54.00007 Importance of liquid fragility for energy applications of ionic liquids<sup>1</sup>**, PIT SIPPEL, PETER LUNKENHEIMER, STEPHAN KROHNS, ERIK THOMS, ALOIS LOIDL, Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany — Ionic liquids (ILs) are salts that are liquid at ambient temperatures. The strong electrostatic forces between their molecular ions result, e.g., in low volatility and high stability for many members of this huge material class [1]. For this reason they bear a high potential for new advancements in applications, e.g., as electrolytes in energy-storage devices such as supercapacitors or batteries, where the ionic conductivity is an essential figure of merit.

Most ILs show dynamic properties typical for glassy matter, which dominate many of their physical properties. An important method to study these dynamical glass-properties is dielectric spectroscopy that can access relaxation times of dynamic processes and the conductivity in a broad frequency and temperature range. In the present contribution, we present results on a large variety of ionic liquids showing that the conductivity of ILs depends in a systematic way not only on their glass temperature but also on the so-called fragility, characterizing the non-canonical super-Arrhenius temperature dependence of their ionic mobility [2].

[1] D. R. MacFarlane, *et al.*, Energy Environ. Sci. **7**, 232250 (2014).

[2] P. Sippel *et al.*, Sci. Rep. **5**, 13922 (2015).

<sup>1</sup>This work was supported by the Deutsche Forschungsgemeinschaft via Research Unit FOR1394 and by the BMBF via ENREKON 03EK3015.

**3:54PM H54.00008 A joint *first principles* and ATR-IR study of the vibrational properties of interfacial water at semiconductor-water solid-liquid interfaces**, LEI YANG, STEFANIE TECKLENBURG, FANG NIU, ANDREAS ERBE, STEFAN WIPPERMANN, Max-Planck-Institut für Eisenforschung, FRANCOIS GYGI, University of California, Davis, GIULIA GALLI, University of Chicago — Despite the importance of understanding the structural and bonding properties of solid-liquid interfaces for a wide range of (photo-)electrochemical applications, there are presently no experimental techniques available to directly probe the microscopic structure of solid-liquid interfaces. We carried out joint ATR-IR spectroscopy measurements and *ab initio* molecular dynamics simulations of the vibrational properties of interfaces between liquid water and prototypical semiconductor substrates. In particular, the Ge(100)/H<sub>2</sub>O interface is shown to feature a reversible bias potential dependent surface phase transition. Our study highlights the key role of coupled theory-experimental investigations on well controlled and characterized interfaces, in order to develop robust strategies to interpret experiments and validate theory. The authors wish to thank T. A. Pham for helpful discussions. G. G. and F. G. acknowledge DOE-BES Grant No. DE-SS0008939.

**4:06PM H54.00009 Effect of Metal Ion Intercalation on the Structure of MXenes and its Impact on the Dynamics of Water in MXenes**, NARESH OSTI, MICHEAL NAGUIB, Oak Ridge National Laboratory, Oak Ridge, TN, USA, ALIREZA ÖSTADHOSSEIN, ADRI VAN DUIN, The Pennsylvania State University, PA, USA, YURY GOGOTSI, Drexel University PA, USA, DAVID WESOLOWSKI, EUGENE MAMONTOV, Oak Ridge National Laboratory, Oak Ridge, TN, USA — MXenes are two-dimensional materials of sheet-like morphology invented as an alternative to graphene with a potential for energy applications. Because of the heterogeneous bonding between different species and the presence of surface functionalities, MXenes can be intercalated with different chemical species including metal ions and water. The presence of water in MXenes even at ambient conditions impacts their properties relevant to technical applications. Therefore, it is important to understand how intercalants change the structure of MXene and the behavior of water in these materials. Here, using different scattering techniques (x-ray and neutron), we found that intercalation of MXenes with potassium ion increases the c- lattice parameter, yielding a more homogeneous structure with higher water uptake compared to pristine MXenes. In the latter, inhomogeneous structure was observed, with most water residing between the MXenes stacks rather than in between the layers. We found a two orders of magnitude reduction in the diffusion coefficient of water resulting from potassium intercalation, which is in good agreement with the values predicted from ReaxFF simulation. Consequences of improved homogeneity on the water dynamics following metal ion intercalation will be discussed..

**4:18PM H54.00010 Low Temperature Synthesis of Cubic-phase Fast-ionic Conducting Bismuth-doped Garnet Solid State Electrolytes.**, DEREK K. SCHWANZ, ERNESTO MARINERO, School of Materials Engineering, Purdue University — We report on the synthesis of cubic-phase fast ionic conducting garnet solid state electrolytes based on LiLaZrO (LLZO) at unprecedented low synthesis temperatures. Ionic conductivities around  $1.2 \times 10^{-4}$  S/cm are readily achieved. Bismuth aliovalent substitution into LLZO utilizing the Pechini processing method is successfully employed to synthesize LiLaZrBiO compounds. Cubic phase LiLaZrBiO powders are generated in the temperature range 650C to 900C in air. In contrast, in the absence of Bi and under identical synthesis conditions, the cubic phase of LiLaZrO is not formed below 750C and a transformation to the poor ionically conducting tetragonal phase is observed at 800C for the undoped compound. The critical role of Bi in lowering the formation temperature of the garnet cubic phase and the improvements in ionic conductivity are elucidated in this work through microstructural and electrochemical studies.

**4:30PM H54.00011 Electrophoretic deposition of RuO<sub>2</sub>/HRGO composites for flexible supercapacitor electrodes** , FATIMA AMIR, Winthrop University, VIET PHAM, Brookhaven National Laboratory, DAKODA MULLINAX, Winthrop University, JAMES DICKERSON, Brookhaven National Laboratory — Flexible energy storage devices are essential for the development of wearable electronics, such as bendable displays and wearable multi-media systems. A subset of these energy storage devices, flexible supercapacitors have received increased attention because of their long cycle life, low cost, and easy fabrication. Herein, we report an easy and low cost method to fabricate bendable ruthenium oxide (RuO<sub>2</sub>)/holey reduced graphene oxide (HRGO) electrodes using electrophoretic deposition. Analysis of the surface morphology using scanning electron microscopy (SEM) shows a highly nanoporous structure with pores ranging from 2 to 3 nm. The obtained RuO<sub>2</sub>/HRGO supercapacitor exhibited excellent electrochemical capacitive performance in a PVA-H<sub>2</sub>SO<sub>4</sub> gel electrolyte, with a specific capacitance of 418.5F/g. Additionally, a high rate performance with capacitance retention of 85% was observed when the current was increased by a factor of 20 from 1.0 to 20.0 A/g. The supercapacitor exhibited an exceptional cycling stability of 88.5% after 10,000 cycles, indicating excellent long term electrochemical stability.

**4:42PM H54.00012 Li<sup>+</sup> ion diffusion in nanoscale alumina coatings** , MICHELLE JOHANNES, NOAM BERNSTEIN, Naval Research Lab — Nanoscale coatings of alumina are used to stabilize surfaces for a variety of technologies. Diffusion of ions through these coatings is of primary importance: in some cases, diffusion is unwanted (e.g. corrosion) and in others (e.g. electrode materials), it is necessary. In this work DFT and AIMD calculations are used to investigate Li<sup>+</sup> ion diffusion through a nano-layer of alumina, examining the phase (alpha, gamma, and amorphous), ion concentration, and electron count dependence. We look at the role of the surface itself in promoting diffusion. One of our main findings is that as the number of ions or charge increases, the diffusivity rises. We show how our data can explain electrochemical data from coated LiCoO<sub>2</sub> cathodes and may point toward better and more efficient coatings for stabilizing electrodes.

**4:54PM H54.00013 Finding out the optimal boron concentration in BC<sub>x</sub> sheets for high capacity anode material in Li-ion batteries** , DEYA DAS, RAHUL HARDIKAR, Indian Institute of Science, SANG SOO HAN, KWANG RYEOL LEE, Korea Institute of Science and Technology, ABHISHEK KUMAR SINGH, Indian Institute of Science — Boron doped graphene shows better adsorption of Li compared to pristine graphene and has been investigated as a potential anode material for Li-ion batteries. Using first principles density functional theory calculations, we investigate the effect of increasing boron concentration on the gravimetric capacity of mono-layered boron doped graphene sheets, BC<sub>x</sub> (x = 7, 5, 3, 2 and 1). Li storage capacity increases with the increase in boron concentration giving highest capacity for monolayer BC<sub>2</sub> (~ 1400 mAh/g), and is about 1.6 times higher than previously reported capacity of BC<sub>3</sub>. This is due to the more number of available empty states above the Fermi level in BC<sub>2</sub> compared to other sheets. Moreover, owing to a very low Li diffusion barrier, the Li kinetics in BC<sub>2</sub> is also found to be better among all the layered boron doped carbon sheets. Further enhancement of B concentration, as in BC, leads to strong binding of Li, thereby hindering the delithiation processes. Hence, BC<sub>2</sub> with optimal concentration of B among the BC<sub>x</sub> phases, emerges as a promising choice for anode material in rechargeable Li ion battery.

## Tuesday, March 15, 2016 2:30PM - 5:30PM –

Session H55 DBIO: Theoretical Physics and Networks of Real Neurons Hilton Baltimore Holiday Ballroom 6 - William Bialek, Princeton University

**2:30PM H55.00001 Neural circuit mechanisms of short-term memory<sup>1</sup>** , MARK GOLDMAN, Center for Neuroscience, UC Davis — Memory over time scales of seconds to tens of seconds is thought to be maintained by neural activity that is triggered by a memorized stimulus and persists long after the stimulus is turned off. This presents a challenge to current models of memory-storing mechanisms, because the typical time scales associated with cellular and synaptic dynamics are two orders of magnitude smaller than this. While such long time scales can easily be achieved by bistable processes that toggle like a flip-flop between a baseline and elevated-activity state, many neuronal systems have been observed experimentally to be capable of maintaining a continuum of stable states. For example, in neural integrator networks involved in the accumulation of evidence for decision making and in motor control, individual neurons have been recorded whose activity reflects the mathematical integral of their inputs; in the absence of input, these neurons sustain activity at a level proportional to the running total of their inputs. This represents an analog form of memory whose dynamics can be conceptualized through an energy landscape with a continuum of lowest-energy states. Such continuous attractor landscapes are structurally non-robust, in seeming violation of the relative robustness of biological memory systems. In this talk, I will present and compare different biologically motivated circuit motifs for the accumulation and storage of signals in short-term memory. Challenges to generating robust memory maintenance will be highlighted and potential mechanisms for ameliorating the sensitivity of memory networks to perturbations will be discussed.

<sup>1</sup>Funding for this work was provided by NIH R01 MH065034, NSF IIS-1208218, Simons Foundation 324260, and a UC Davis Ophthalmology Research to Prevent Blindness Grant

**3:06PM H55.00002 Dynamical criticality in the collective activity of a neural population** , THIERRY MORA, CNRS and Ecole normale supérieure, Paris — The past decade has seen a wealth of physiological data suggesting that neural networks may behave like critical branching processes. Concurrently, the collective activity of neurons has been studied using explicit mappings to classic statistical mechanics models such as disordered Ising models, allowing for the study of their thermodynamics, but these efforts have ignored the dynamical nature of neural activity. I will show how to reconcile these two approaches by learning effective statistical mechanics models of the full history of the collective activity of a neuron population directly from physiological data, treating time as an additional dimension. Applying this technique to multi-electrode recordings from retinal ganglion cells, and studying the thermodynamics of the inferred model, reveals a peak in specific heat reminiscent of a second-order phase transition.

**3:42PM H55.00003 Adaptation on multiple time scales** , ADIRENNE FAIRHALL, University of Washington — No abstract available.

**4:18PM H55.00004 A theory of neural dimensionality, dynamics, and measurement.** , SURYA GANGULI<sup>1</sup>, Stanford University — In many experiments, neuroscientists tightly control behavior, record many trials, and obtain trial-averaged firing rates from hundreds of neurons in circuits containing millions of behaviorally relevant neurons. Dimensionality reduction has often shown that such datasets are strikingly simple; they can be described using a much smaller number of dimensions than the number of recorded neurons, and the resulting projections onto these dimensions yield a remarkably insightful dynamical portrait of circuit computation. This ubiquitous simplicity raises several profound and timely conceptual questions. What is the origin of this simplicity and its implications for the complexity of brain dynamics? Would neuronal datasets become more complex if we recorded more neurons? How and when can we trust dynamical portraits obtained from only hundreds of neurons in circuits containing millions of neurons? We present a theory that answers these questions, and test it using neural data recorded from reaching monkeys. Overall, this theory yields a picture of the neural measurement process as a random projection of neural dynamics, conceptual insights into how we can reliably recover dynamical portraits in such under-sampled measurement regimes, and quantitative guidelines for the design of future experiments. Moreover, it reveals the existence of phase transition boundaries in our ability to successfully decode cognition and behavior as a function of the number of recorded neurons, the complexity of the task, and the smoothness of neural dynamics.

<sup>1</sup>membership pending

**4:54PM H55.00005 Understanding vision through the lens of prediction<sup>1</sup>** , STEPHANIE PALMER, Univ of Chicago — Prediction is necessary for long-term planning and decision-making, but prediction is also essential to the short-term calculations necessary to overcome the sensory and motor delays present in all neural systems. In order to interact appropriately with a changing environment, the brain must respond not only to the current state of sensory inputs but to rapid predictions of these inputs' future state. To test whether the visual system performs optimal predictive compression and computation, we compute the past and future stimulus information in populations of retinal ganglion cells, the output cells of the retina, in salamanders and rats. By controlling the motion statistics of the input stimulus presented to the retina, a moving bar with inertia making a random walk in space, we can derive the optimal tradeoff between compressing information about the past stimulus while retaining as much information as possible about the future stimulus. By changing parameters in the equation of motion for the bar, we can explore qualitatively different motion prediction problems. We show that retinal ganglion cells sit near this optimum for some motion types but not others, and compare these results between the two sampled species. Taking the next step towards exploring the predictive capacity of neural systems, we characterize the ensemble of spatiotemporal correlations present in the natural environment. To do so, we construct and analyze a database of natural motion videos. We have made high-speed, high-pixel-depth recordings of natural scenes and have preliminary data quantifying the space-time power spectra and the local motion content of these scenes.

<sup>1</sup> Alfred P. Sloan Foundation, France-Chicago Center FACCTS grant, Chateaubriand Fellowship from the French Embassy (JS)

## **Tuesday, March 15, 2016 4:30PM - 6:00PM —**

**Session J1 Meet the Editors of APS Reception** Ballroom Foyer -

**4:30PM J1.00001 Meet the Editors of APS Reception** — The Editors of the APS journals invite you to join them for conversation on Tuesday, March 15, 4:30-6:00 pm. The Editors will be available to answer questions, hear your ideas, and discuss any comments about the journals. All are welcome. Light refreshments will be served.

## **Tuesday, March 15, 2016 5:30PM - 8:00PM —**

**Session J2 APS: Student Reception & Awards Ceremony** Exhibit Hall C - Crystal Bailey, APS

**5:30PM J2.00001 Student Reception & Awards Ceremony** — Graduate and undergraduate students may mingle with working physicists at the special student reception with light fare from 5:30 until 7:00 p.m. Immediately following, all students who presented at the March Meeting in the Undergraduate Research Sessions will be recognized, and students with outstanding presentations will also receive a special prize.

## **Tuesday, March 15, 2016 5:45PM - 6:45PM —**

**Session J15 GMAG: GMAG Business Meeting** 314 -

**5:45PM J15.00001 GMAG BUSINESS MEETING** —

## **Tuesday, March 15, 2016 5:45PM - 6:45PM —**

**Session J28 FIAP: FIAP Business Meeting** 327 -

**5:45PM J28.00001 FIAP BUSINESS MEETING** —

## **Tuesday, March 15, 2016 5:45PM - 6:45PM —**

**Session J29 GIMS: GIMS Business Meeting** 328 -

**5:45PM J29.00001 GIMS BUSINESS MEETING** —

## **Tuesday, March 15, 2016 5:45PM - 6:45PM —**

**Session J32 DCP: DCP Business Meeting** 332 -

**5:45PM J32.00001 DCP BUSINESS MEETING** —

## **Tuesday, March 15, 2016 5:45PM - 6:45PM —**

**Session J33 DPOLY: DPOLY Business Meeting** 336 -

**5:45PM J33.00001 DPOLY BUSINESS MEETING** —

## **Tuesday, March 15, 2016 6:45PM - 7:30PM —**

**Session JA33 DPOLY: DPOLY NSF Question & Answer Session** 336 -

**6:45PM JA33.00001 DPOLY NSF Question & Answer Session** —

**Tuesday, March 15, 2016 5:45PM - 6:45PM —**

Session J37 GERA: GERA Business Meeting 340 -

5:45PM J37.00001 GERA BUSINESS MEETING —

**Tuesday, March 15, 2016 5:45PM - 6:45PM —**

Session J38 GQI: GQI Business Meeting 341 -

5:45PM J38.00001 GQI BUSINESS MEETING —

**Tuesday, March 15, 2016 5:45PM - 6:45PM —**

Session J39 DBIO: DBIO Business Meeting 342 -

5:45PM J39.00001 DBIO BUSINESS MEETING —

**Tuesday, March 15, 2016 5:45PM - 6:45PM —**

Session J40 GSNP: GSNP Business Meeting 343 -

5:45PM J40.00001 GSNP BUSINESS MEETING —

**Tuesday, March 15, 2016 5:45PM - 6:45PM —**

Session J51 GPC: GPC Business Meeting Holiday Ballroom 2 -

5:45PM J51.00001 GPC BUSINESS MEETING —

**Tuesday, March 15, 2016 5:45PM - 6:45PM —**

Session J52 DCOMP: DCOMP Business Meeting Hilton Baltimore Holiday Ballroom III -

5:45PM J52.00001 DCOMP BUSINESS MEETING —

**Tuesday, March 15, 2016 5:00PM - 6:00PM —**

Session J60 CSWP: CSWP Networking Reception Hilton Baltimore Latrobe -

**5:00PM J60.00001 CSWP Networking Reception** — Unwind after a long day of sessions by networking with women physicists from the APS Committee on the Status of Women in Physics and members of the APS Panel on Public Affairs (POPA). Cocktails and conversation will flow as we learn about the recently approved APS Statement on the Status of Women in Physics; a POPA study underway, designed to evaluate what top universities are doing to address gender disparity in undergraduate physics programs; and initiatives & programs designed to attract, retain, develop, and support the female physicists in our community.

**Tuesday, March 15, 2016 7:00PM - 8:00PM —**

Session JA50 DMP: DMP Business Meeting Hilton Baltimore Holiday Ballroom 1 -

7:00PM JA50.00001 DMP BUSINESS MEETING —

**Tuesday, March 15, 2016 7:00PM - 8:00PM —**

Session JA51 DCMP: DCMP Business Meeting Hilton Baltimore Holiday Ballroom 2 -

7:00PM JA51.00001 DCMP BUSINESS MEETING —

**Wednesday, March 16, 2016 8:00AM - 11:00AM —**

Session K1 DCMP: Visualization of Vorticity in Quantum Fluids Ballroom I - Katepalli Sreenivasan, New York Univ

**8:00AM K1.00001 Three-dimensional nanoparticle dynamics in superfluid helium<sup>1</sup>**, DANIEL LATHROP, University of Maryland — Quantized vortices have been observed in superfluid <sup>4</sup>He and AMO trapped atom systems, and have been inferred in superfluid <sup>3</sup>He and neutron stars. The dynamics of quantum fluids is substantially controlled by the motion of quantized vortices, which are topological phase defects analogous to crystalline dislocations. Long-range quantum order underlies a number of related physical phenomena, including superfluidity, trapped-atom Bose-Einstein condensates, superconductivity, ferromagnetism, antiferromagnetism, lasers, and the Higgs mechanism. While superfluidity in <sup>4</sup>He is one of the first discovered of these, it is one of the least understood, given that the strongly interacting nature of helium makes theory difficult, and that development of local experimental probes is lagging. The advent of three-dimensional flow visualization of particles that trace quantized vortices provides new opportunities to investigate their creation and dynamics. We work to address the following questions using flow visualization in this system: What are field equations that express the coupling of the ordered and disordered parts of the flow? How does vortex reconnection lead to dissipation and breaking of time-reversal invariance? What are the similarities and differences between quantum and classical turbulence at small and large scales? How do quantized vortices form through the lambda transition?

<sup>1</sup>This work is supported by the National Science Foundation DMR CMP 1407472

**8:36AM K1.00002 Imaging of quantum vortices in superfluid helium droplets**, ANDREY VILESOV, University of Southern California — Helium nanodroplets are especially promising for exploring quantum hydrodynamics in self-contained, isolated superfluids. However, until very recently, the dynamic properties of individual droplets, such as vorticity, could not be assessed experimentally. Here we investigate the rotation of single superfluid 4-He droplets ranging from 200 to 2000 nm in diameter at T = 0.4 K via single-shot femtosecond X-ray coherent diffractive imaging. The droplets were produced by free jet expansion of liquid helium into vacuum. The angular velocities of the droplets were estimated from the centrifugal distortion and span a range from vanishing to those close to the disintegration limit. For visualization of vortices, Xe atoms were added to the droplets where they gather in cores forming nm-thin filaments. A newly developed phase retrieval technique enables the reconstruction of the instantaneous positions and shapes of the vortices from the diffraction images with about 20 nm resolution. The vorticity attainable in the nano-droplets was found to be about six orders of magnitude larger than achieved in previous experiments in the bulk. Stationary configurations of vortices are represented by triangular lattice in large (2 μm) droplets and symmetric arrangements of few vortices in smaller (200 nm) droplets. Evidence for non-stationary vortex dynamics comes from observation of asymmetric formations of vortices in some droplets. This collaborative work was performed at Linac Coherent Light Source, the free electron laser within SLAC National Accelerator Laboratory. The experiments and the full list of collaborators are reported in: L. F. Gomez et. al. Science, 345 (2014) 906.

**9:12AM K1.00003 Numerical simulation of quantum turbulence**, MAKOTO TSUBOTA, Osaka City University — Turbulence in quantum fluids has been studied for more than half century, and the recent developments of visualization experiments are so remarkable that they have made significant contributions for understanding the topics. Numerical simulation is also indispensable for this field. Two kinds of formulation are generally available. One is the vortex filament model useful for simulation of dynamics of quantized vortices in superfluid helium. The other is the Gross-Pitaevskii model that addresses the order parameters in Bose-Einstein condensation and is applicable for atomic condensates. We discuss some novel important topics of both simulations. One is inhomogeneous turbulence in superfluid helium, which was recently revealed by the visualization experiments. Another is quantum turbulence in atomic Bose condensates addressing multi-component order parameters.

**9:48AM K1.00004 Turbulent flows of superfluid helium visualized by particle dynamics<sup>1</sup>**, MARCO LA MANTIA, Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic — The motions of relatively small particles in quantum flows of superfluid helium (He II) are visualized in order to reveal the underlying flow-induced physics. It is specifically shown how the derived flow properties - such as the particle velocity distribution - depend on the length scale probed by the particles, for both thermally and mechanically driven flows of He II. Quantum features may indeed appear at small enough length scales, smaller than the quantum scale of the flow, the average distance between quantized vortices, while, at larger length scales, a classical (viscous-like) picture emerges, reinforcing the idea that quantum turbulence is not only interesting in its own right but may also lead to the deeper understanding of fluid turbulence in general, an open problem of classical physics relevant to many research fields, ranging from fluid dynamics to cosmology.

<sup>1</sup>Support from the Czech Science Foundation is acknowledged.

**10:24AM K1.00005 Flow visualization in superfluid helium-4 using He2 molecular tracers<sup>1</sup>**, WEI GUO, Florida State Univ — Flow visualization in superfluid helium is challenging, yet crucial for attaining a detailed understanding of quantum turbulence. Two problems have impeded progress: finding and introducing suitable tracers that are small yet visible; and unambiguous interpretation of the tracer motion. We show that metastable He<sub>2</sub> triplet molecules are outstanding tracers compared with other particles used in helium. These molecular tracers have small size and relatively simple behavior in superfluid helium: they follow the normal fluid motion at above 1 K and will bind to quantized vortex lines below about 0.6 K. A laser-induced fluorescence technique has been developed for imaging the He<sub>2</sub> tracers. We will present our recent experimental work on studying the normal-fluid motion by tracking thin lines of He<sub>2</sub> tracers created via femtosecond laser-field ionization in helium. We will also discuss a newly launched experiment on visualizing vortex lines in a magnetically levitated superfluid helium drop by imaging the He<sub>2</sub> tracers trapped on the vortex cores. This experiment will enable unprecedented insight into the behavior of a rotating superfluid drop and will untangle several key issues in quantum turbulence research.

<sup>1</sup>We acknowledge the support from the National Science Foundation under Grant No. DMR-1507386 and the US Department of Energy under Grant No. DE-FG02 96ER40952.

**Wednesday, March 16, 2016 8:00AM - 11:00AM —**  
**Session K2 DCMP DMP GMAG: Kitaev Spin Liquid Physics in Honeycomb and Related Lattice Materials** Ballroom II - Stephen Nagler, Oak Ridge National Lab

**8:00AM K2.00001 The magnetic ground state and relationship to Kitaev physics in  $\alpha$ -RuCl<sub>3</sub><sup>1</sup>**, ARNAB BANERJEE, Quantum Condensed Matter Div., Oak Ridge Nat. Lab., Oak Ridge, TN - 37830. — The 2D Kitaev candidate  $\alpha$ -RuCl<sub>3</sub> consists of stacked honeycomb layers weakly coupled by Van der Waals interactions. Here we report the measurements of bulk properties and neutron diffraction in both powder and single crystal samples. Our results show that the full three dimensional magnetic ground state is highly pliable with at least two dominant phases corresponding to two different out-of-plane magnetic orders. They have different Neel temperatures dependent on the stacking of the 2D layers, such as a broad magnetic transition at T<sub>N</sub> = 14 K as observed in phase-pure powder samples, or a sharp magnetic transition at a lower T<sub>N</sub> = 7 K as observed in homogeneous single crystals with no evidence for stacking faults. The magnetic refinements of the neutron scattering data [1] will be discussed, which in all cases shows the in-plane magnetic ground state is the zigzag phase common in Kitaev related materials including the honeycomb lattice Iridates. Inelastic neutron scattering in all cases shows that this material consistently exhibit strong two-dimensional magnetic fluctuations leading to a break-down of the classical spin-wave picture [2]. [1] H.B. Cao, A. Banerjee, J-Q. Yan, C.B. Bridges, M. Lumsden, B.C. Chakoumakos, D.G. Mandrus, D.A. Tennant, S.E. Nagler, *Low-temperature crystal and magnetic structure of  $\alpha$ -RuCl<sub>3</sub>*, (manuscript in preparation). [2] A. Banerjee et al., *arxiv:1504.08037* (2015);

<sup>1</sup>Work performed at ORNL is supported by U.S. Dept. of Energy, Office of Basic Energy Sciences and Office of User Facilities Division.

**8:36AM K2.00002 How to identify and resolve beyond-geometrical frustration**, ITAMAR KIMCHI, Massachusetts Institute of Technology — In this talk, we will discuss recent theoretical developments triggered by the experimental discoveries of iridium oxides  $\alpha, \beta, \gamma$ -Li<sub>2</sub>IrO<sub>3</sub>. In these polytypes, spin-orbit-coupled  $J=1/2$  moments form 2D and 3D lattices (honeycomb, hyperhoneycomb and stripyhoneycomb) which generalize the 2D honeycomb lattice. Scattering experiments on these compounds have uncovered a peculiar non-coplanar incommensurate magnetic order, involving spirals which counter-rotate across neighboring sites. We discuss the emergence of this ordering, and the striking similarities visible across the three Li<sub>2</sub>IrO<sub>3</sub> structures. The model Hamiltonians that capture the materials indicate strong magnetic frustration, which arises from spin-orbit coupling. Tuning the frustration, perhaps by just a 10% Hamiltonian perturbation, exposes a fractionalized phase: Kitaev's three-dimensional quantum spin liquid (QSL). What is its range of stability to the competing Hamiltonian terms which occur in the materials, such as antiferromagnetic Heisenberg exchange? The frustration prohibits direct computations. Instead, we demonstrate a viable approach by numerically solving the model in a fully quantum infinite-dimensional approximation, which captures both the magnetically ordered and the QSL phases. Finally, we discuss the phenomenology of the QSL phase, including the role of its emergent magnetic-like field lines in stabilizing its deconfined fermion excitations to finite temperatures. The resulting phase transition is a signature unique to three-dimensional fractionalization.

**9:12AM K2.00003 3D Kitaev spin liquids**, MARIA HERMANNNS, University of Cologne — The Kitaev honeycomb model has become one of the archetypal spin models exhibiting topological phases of matter, where the magnetic moments fractionalize into Majorana fermions interacting with a  $Z_2$  gauge field. In this talk, we discuss generalizations of this model to three-dimensional lattice structures. Our main focus is the metallic state that the emergent Majorana fermions form. In particular, we discuss the relation of the nature of this Majorana metal to the details of the underlying lattice structure. Besides (almost) conventional metals with a Majorana Fermi surface<sup>1</sup>, one also finds various realizations of Dirac semi-metals, where the gapless modes form Fermi lines or even Weyl nodes<sup>2</sup>. We introduce a general classification of these gapless quantum spin liquids using projective symmetry analysis. Furthermore, we briefly outline why these Majorana metals in 3D Kitaev systems provide an even richer variety of Dirac and Weyl phases than possible for electronic matter and comment on possible experimental signatures. Work done in collaboration with Kevin O'Brien and Simon Trebst.

<sup>1</sup>M. Hermanns and S. Trebst, PRB **89**, 235102 (2014).

<sup>2</sup>M. Hermanns, K. O'Brien, and S. Trebst, PRL **114**, 157202 (2015).

**9:48AM K2.00004 Hyperhoneycomb iridate beta-Li<sub>2</sub>IrO<sub>3</sub> as a platform for Kitaev spin liquid**, TOMOHIRO TAKAYAMA, Max Planck Inst — Realization of quantum spin liquid has been a long-sought dream in condensed matter physics, where exotic excitations and unconventional superconductivity upon doping are expected. Honeycomb iridates recently emerged as a possible materialization of Kitaev spin liquid with frustrated "*bond-dependent ferromagnetic interaction*". However, the real materials,  $\alpha$ -Na<sub>2</sub>IrO<sub>3</sub> and  $\alpha$ -Li<sub>2</sub>IrO<sub>3</sub>, undergo antiferromagnetic ordering likely due to the presence of other dominant magnetic interactions and lattice distortion. We discovered a new form of Li<sub>2</sub>IrO<sub>3</sub>,  $\beta$ -Li<sub>2</sub>IrO<sub>3</sub>, which comprises a three-dimensional analogue of honeycomb lattice dubbed as "hyperhoneycomb". Each Ir<sup>4+</sup> ion of the hyperhoneycomb lattice has three neighboring like ions rotated by 120° and thus the local structure is identical with 2D honeycomb, indicating that the hyperhoneycomb lattice is a new platform for Kitaev physics.  $\beta$ -Li<sub>2</sub>IrO<sub>3</sub> displays a spiral magnetic order below 38 K, which likely originates from dominance of ferromagnetic Kitaev interaction. We argue that  $\beta$ -Li<sub>2</sub>IrO<sub>3</sub> locates in a close proximity to Kitaev spin liquid. We also discuss the spin liquid behavior observed in a new honeycomb iridate obtained by chemical modulation.

**10:24AM K2.00005 Magnetic "three states of matter" in two and three dimensions: a quantum Monte Carlo study of the extended toric codes**, YOSHITOMO KAMIYA, RIKEN - Saitama — The possibility of quantum spin liquids, characterized by nontrivial entanglement properties or a topological nonlocal order parameter, has long been debated both theoretically and experimentally. Since candidate systems (e.g., frustrated quantum magnets or 5d transition metal oxides) may host other competing phases including conventional magnetic ordered phases, it is natural to ask what types of global phase diagrams can be anticipated depending on coupling constants, temperature, dimensionality, etc. In this talk, by considering an extension of the Kitaev toric code Hamiltonians by Ising interactions on 2D (square) and 3D (cubic) lattices, I will present thermodynamic phase diagrams featuring magnetic "three states of matter," namely, quantum spin liquid, paramagnetic, and magnetically ordered phases (analogous to liquid, gas, and solid, respectively, in conventional matter) obtained by unbiased quantum Monte Carlo simulations [YK, Y. Kato, J. Nasu, and Y. Motome, PRB **92**, 100403(R) (2015)]. We find that the ordered phase borders on the spin liquid around the exactly solvable point by a discontinuous transition line in 3D, while it grows continuously from the quantum critical point in 2D. In both cases, peculiar *proximity effects* to the nearby spin liquid phases are observed at high temperature even when the ground state is magnetically ordered. Such proximity effects include flux-shrinking and a tricritical behavior in 3D and a "fractionalization" of the order parameter field at the quantum critical point in 2D, both of which can be detected by measuring critical exponents. (\*) Work done in collaboration with Yasuyuki Kato, Joji Nasu, and Yukitoshi Motome

**Wednesday, March 16, 2016 8:00AM - 11:00AM**

**Session K3 DCMP DMP: Weyl Topological Semimetals: Theory and Experiment** Ballroom III - Arun Bansil, Northeastern University

**8:00AM K3.00001 Weyl semimetals and topological phase transitions**, SHUICHI MURAKAMI, Tokyo Inst of Tech - Tokyo — Weyl semimetals are semimetals with nondegenerate 3D Dirac cones in the bulk. We showed that in a transition between different  $Z_2$  topological phases, i.e. between the normal insulator (NI) and topological insulator (TI), the Weyl semimetal phase necessarily appears when inversion symmetry is broken. In the presentation we show that this scenario holds for materials with any space groups without inversion symmetry. Namely, let us take any band insulator without inversion symmetry, and assume that the gap is closed by a change of an external parameter. In such cases we found that the system runs either into (i) a Weyl semimetal or (ii) a nodal-line semimetal, but no insulator-to-insulator transition happens. This is confirmed by classifying the gap closing in terms of the space groups and the wavevector. In the case (i), the number of Weyl nodes produced at the gap closing ranges from 2 to 12 depending on the symmetry. In (ii) the nodal line is protected by mirror symmetry. In the presentation, we explain some Weyl semimetal and nodal-line semimetals which we find by using this classification. As an example, we explain our result on ab initio calculation on tellurium (Te). Tellurium consists of helical chains, and therefore lacks inversion and mirror symmetries. At high pressure the band gap of Te decreases and finally it runs into a Weyl semimetal phase, as confirmed by our ab initio calculation. In such chiral systems as tellurium, we also theoretically propose chiral transport in systems with such helical structures; namely, an orbital magnetization is induced by a current along the chiral axis, in analogy with a solenoid. [1] S. Murakami, New J. Phys. **9**, 356 (2007). [2] S. Murakami and S. Kuga, Phys. Rev. B **78**, 165313 (2008). [3] R. Okugawa, and S. Murakami, Phys. Rev. B **89**, 235315 (2014). [4] M. Hirayama, R. Okugawa, S. Ishibashi, S. Murakami, and T. Miyake, Phys. Rev. Lett. **114**, 206401 (2015). [5] T. Yoda, T. Yokoyama, S. Murakami, Sci. Rep. **5**, 12024 (2015).

**8:36AM K3.00002 Topological insulator route to Weyl fermions**, ANTON BURKOV, University of Waterloo — I will describe one of the possible routes to realizing Weyl fermions in condensed matter, which is based on violating either time reversal or spatial inversion symmetry in a system, tuned near a quantum phase transition between a topological and an ordinary insulator. This route is particularly attractive, since it may lead to the simplest possible realization of a Weyl semimetal, with only two opposite-chirality Weyl nodes in the first Brillouin zone, which is yet to be found experimentally. I will describe some of the most important physical properties of such an elemental Weyl semimetal, in particular a negative longitudinal magnetoresistance due to the chiral anomaly and possible exotic superconducting states.

**9:12AM K3.00003 Discovery of Weyl fermion semimetal and topological Fermi arc quasiparticles in TaAs, NbAs, NbP, TaP and related materials** , M. ZAHID HASAN<sup>1</sup>, Princeton Univ — Topological matter can host Dirac, Majorana and Weyl fermions as quasiparticle modes on their boundaries. First, I briefly mention the basic theoretical concepts defining insulators and superconductors where topological surface state modes are robust only in the presence of a gap (Hasan & Kane; Rev. of Mod. Phys. 82, 3045 (2010)). In these systems topological protection is lost once the gap is closed turning the system into a trivial metal. A Weyl semimetal is the rare exception in this scheme which is a topologically robust metal (semimetal) whose low energy emergent excitations are Weyl fermions. In a Weyl fermion semimetal, the chiralities associated with the Weyl nodes can be understood as topological charges, leading to split monopoles and anti-monopoles of Berry curvature in momentum space. This gives a measure of the topological strength of the system. Due to this topology a Weyl semimetal is expected to exhibit 2D Fermi arc quasiparticles on its surface (Wan et.al., 2011). These arcs ("fractional" Fermi surfaces) are discontinuous or disjoint segments of a two dimensional Fermi contour, which are terminated onto the projections of the Weyl fermion nodes on the surface we have observed experimentally in TaAs, NbAs, NbP class of materials (Xu, Belopolski et.al., Science 349, 613 (2015); Xu, Alidoust et.al., Nature Phys. (2015); Xu, Belopolski et.al., Science Adv. (2015), Belopolski, Xu et.al., arXiv (2015)) following our theoretical predictions (Huang, Xu, Belopolski et.al., Nature Commun. 6:7373 (2015), submitted in November 2014). Our theoretical predictions (Nature Commun. 2015) and experimental demonstrations (Science 2015, Nature Physics 2015, Science Advances 2015) reveal that these Fermi arc quasiparticles can only live on the boundary of a 3D crystal which collectively represents the realization of a new state of quantum matter beyond our earlier work on Fermi arcs in topological materials (Xu, Liu, Kushwaha et.al., Science 347, 294 (2015), adv.online (2014)). This work is in collaboration with Su-Yang Xu, Ilya Belopolski, Nasser Alidoust, Madhab Neupane, Chenglong Zhang, Raman Sankar, Shin-Ming Huang, Chi-Cheng Lee, Guoqing Chang, BaoKai Wang, Guang Bian, Hao Zheng, Daniel S. Sanchez, Fangcheng Chou, Hsin Lin, Shuang Jia, Titus Neupert. This work is supported by GBMF and U.S. DOE.

<sup>1</sup>In collaboration with Su-Yang Xu, I. Belopolski, N. Alidoust, M. Neupane, C. Zhang, R. Sankar, S.-M. Huang, C.-C. Lee, G. Chang, B. Wang, G. Bian, H. Zheng, D. Sanchez, F.-C. Chou, T. Neupert, Hsin Lin, Shuang Jia. Work supported by GBMF(Moore) & DOE.

**9:48AM K3.00004 Observation of Weyl fermions in condensed matter** , HONG DING, Institute of Physics, Chinese Academy of Sciences — In 1929, a German mathematician and physicist Hermann Weyl proposed that a massless solution of the Dirac equation represents a pair of new type of particles, the so-called Weyl fermions. However, their existence in particle physics remains elusive after more than eight decades, e.g., neutrino has been regarded as a Weyl fermion in the Standard Model until it was found to have mass. Recently, significant advances in topological materials have provided an alternative way to realize Weyl fermions in condensed matter as an emergent phenomenon. Weyl semimetals are predicted as a class of topological materials that can be regarded as three-dimensional analogs of graphene breaking time reversal or inversion symmetry. Electrons in a Weyl semimetal behave exactly as Weyl fermions, which have many exotic properties, such as chiral anomaly, magnetic monopoles in the crystal momentum space, and open Fermi arcs on the surface. In this talk I will report our experimental discovery of a Weyl semimetal in TaAs by observing Fermi arcs with a characteristic spin texture in the surface states and Weyl nodes in the bulk states using angle-resolved photoemission spectroscopy.

**10:24AM K3.00005 Two Types of Weyl Semimetals** , ANDREI BERNEVIG, Princeton U — No abstract available.

**Wednesday, March 16, 2016 8:00AM - 11:00AM —**

**Session K4 DPOLY FIAP: From Nano to Meso: Assembly, Structure and Dynamics of Polymers and Polymer Nanocomposite Thin Films I - Industry Day** Ballroom IV - Sanat Kumar, Columbia Univ

**8:00AM K4.00001 Directed Assembly of Nanofilled Polymer Thin Films** , ALAMGIR KARIM, University of Akron — Facile directed self-assembly (DSA) of multicomponent thin films is important for potential technological applications. This requires a fine control of a complex interplay of processing parameters that need to be properly optimized for different organized structures. This talk will discuss some of our recent success towards realizing tunable DSA of soft matter multicomponent systems involving a dispersion of polymer-grafted nanoparticles in block copolymer or homopolymer matrices. DSA methods for such multicomponent films will be discussed. These include the use of zone-annealing with soft-shear to create highly anisotropic nanoparticle arrays, while direct immersion annealing (DIA) has been used to order nanoparticle filled films by dipping the films into controlled solvent quality solvent mixtures. A recently observed phenomena of confinement driven entropic order and phase segregation of polymer grafted nanoparticles in similar and dissimilar polymer matrices in melt state will be discussed. A high density of nano particles of different types ranging from metallic to inorganic to organic were patterned almost exclusively into channels via topographical soft confinement using entropic forces. Enthalpic interactions between the nanoparticle grafted layer and the polymer matrix could be used as a further handle to tune the directed assembly of the nanoparticles. The phenomena will be discussed in terms of confinement parameters, partition coefficient, free energy gain and entropic versus enthalpic interactions.

**8:36AM K4.00002 Photothermal heating at the nano and meso scales within polymer nanocomposites<sup>1</sup>** , LAURA CLARKE<sup>2</sup>, North Carolina State University — Metal nanoparticles strongly absorb specific wavelengths of visible/infrared light with no radiative relaxation by which to release this energy. As a result, the absorbed energy is efficiently converted to local heat (a photothermal effect [1]). With an effective cross-section of up to 10 times its physical size, each particle acts as a "super-sized" absorber even when embedded within a material environment, resulting in dramatic heating [2,3] originating at the particles. Polymer nanocomposites containing metal nanoparticles can then be probed [4] and altered by applying internal heat at nano- and meso- length scales. I'll discuss our recent studies [5] utilizing this effect, including internal annealing to increase crystallinity fraction in both films and nanofibers of poly(ethylene oxide) [6], in-situ curing of epoxy, and intentional degradation of starch-poly(ethyl cyanoacrylate) composites. The talk will highlight the unique features of a photothermal approach, such as the ability to couple energy quickly (as light) into low thermal conductivity environments and possible changes in thermal conductivity at the particle-polymer interface. [1] S. Maity et al., *Polymer* **52**, 1674 (2011). [2] S. Maity et al., *Adv. Funct. Mater.* **22**, 5259 (2012). [3] S. Maity et al., *Part. & Part. Sys. Char.* **30**, 193 (2013). [4] S. Maity et al., *Nanoscale* **6**, 15236 (2014). [5] D. B. Abbott et al., *Macromol. Chem. & Phys.* **215**, 2345 (2014). [6] V. Viswanath et al., *Macromolecules* **46**, 8596 (2013).

<sup>1</sup> Support from National Science Foundation (CMMI-0829379, CMMI-106910, CMMI-1462966)

<sup>2</sup>Department of Physics

**9:12AM K4.00003 Evaporation-induced Nanoparticle Self-Assembly in a Polymer Matrix**, SHENGFENG CHENG, Virginia Polytechnic Institute and State University — A critical challenge in many applications of polymer nanocomposites is to control the dispersion of nanoparticles in a polymer matrix. We employ large-scale molecular dynamics simulations to study the assembly of nanoparticles as the solvent evaporates from a polymer solution containing nanoparticles. Results show that the organization of nanoparticles can be controlled by varying the strength of the polymer-nanoparticle interactions. When the nanoparticles and polymers strongly attract, as the solvent evaporates, a concentrated polymer film forms at the surface and entraps a layer of nanoparticles, which assemble into a close-packed hexagonal lattice. This dense film of polymers and nanoparticles dramatically reduce the rate of evaporation as the solvent has to transverse the film to reach the surface. If the nanoparticle-polymer interactions are weak, then as the solvent evaporates, the surface layer is almost entirely made of polymers. The nanoparticles are largely excluded from the surface and dispersed randomly in the region below the surface layer. In this case the slowing-down of the evaporation by the surface layer is less dramatic. Also of interest is the case of a nanoparticle solution in contact with polymers that are end grafted to a flat surface to form a polymer brush. For a relatively weak nanoparticle-brush attraction, after evaporation of the solvent the nanoparticles straddle the brush surface and form an ordered lattice. For a strong nanoparticle-polymer attraction, however, the nanoparticles are engulfed inside the brush and the packing quality diminishes because the lateral diffusion of the nanoparticles is suppressed. To better understand the nanoparticle-brush interactions, our calculations to quantify the free energy penalty of inserting a nanoparticle into a polymer brush will also be discussed.

**9:48AM K4.00004 Influence of microstructure and environment on nanoparticle membrane and superlattice mechanical properties**, K. MICHAEL SALERNO, Sandia National Laboratories — Assembly of nanoparticles (NPs) offers a means to tailor materials, incorporating unique nanoscale electro-optical behavior with controllable, responsive mechanical properties. Encoding NPs with organic ligands provides a way to simultaneously drive assembly and control assembly properties. Atomistic molecular dynamics simulations of alkanethiol-coated gold nanoparticles are used to examine how coating chemistry, temperature, and assembly history affect the properties of two-dimensional nanoparticle membranes and three-dimensional nanoparticle superlattices. Specifically, NPs were coated with dodecanethiol and octadecanethiol ligands with COOH or CH<sub>3</sub> end groups and assembled into two-dimensional membranes at water vapor interface. Capping ligands with hydrogen-bond forming carboxyl groups rather than methyl groups more than doubles the membrane Young's modulus from 1.5 to 3.6 GPa. The orientational order of the coating oligomers indicates that ligands strongly bundle and orient within the membrane. This effect inhibits ligand interdigitation, decreasing stiffness. Ligand structure is also highly temperature dependent, causing membranes to lose mechanical stability at about 400K. We observe that the interface asymmetry leads to a measurable stress asymmetry. Due to buckling, stresses in 2D membranes are typically quite small, however 3D superlattices can reversibly reach pressures of 8 GPa. Simulations show that at these pressures the ligand-core bond can be an important failure point, and experiments show that core sintering occurs at high pressure, creating novel 3D and quasi-2D structures.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

**10:24AM K4.00005 Polymer Melt Diffusion inside Nanoscale Cylindrical Pores.**, KAREN WINEY, University of Pennsylvania — Polymers in composites and inside porous media are frequently confined to spaces that are comparable to or even smaller than their mean end-to-end distances in the unconfined bulk state. Understanding the impact of nanoscale confinement on both polymer structure and dynamics is critical during processing and in applications. Anodized aluminum oxide (AAO) membranes with uniform cylindrical pores (diameters 18, 35, 55 or 80 nm) were filled with polystyrene (200 kDa) and then a thin layer of deuterated polystyrene was deposited on top. After annealing the concentration profile of the deuterated polymer was measured using elastic recoil detection and the center-of-mass polymer diffusion coefficient was determined. Melt diffusion is faster in AAO membranes with smaller pore diameters. This experimental finding is corroborated by coarse grain simulations with neutral interactions with the pore walls, although the increase is more pronounced in the simulations. Our simulations previously found that chain conformations slightly elongated parallel to the cylinder axis and compressed perpendicular to the cylinder and the number of entanglements per chain decreases as the cylinder diameter decreases. It is primarily the reduction in polymer entanglements that allows polymers to diffuse faster when the pore diameter is smaller in an athermal or weakly interacting system. Segmental dynamics have been measured using quasielastic neutron scattering. Polymer diffusion in cylindrical pores is now being studied at a fixed pore diameter as a function of molecular weight.

## Wednesday, March 16, 2016 8:00AM - 11:00AM – Session K5 GMAG DMP: Frustrated Magnetism: Spinels 301 - Daniel Khomskii, University of Cologne

**8:00AM K5.00001 From Spin Glass to Spin Liquid Ground States in Pyrochlore Molybdates**, LUCY CLARK, University of St Andrews — Magnetic pyrochlores continue to generate intense interest due to the wealth of interesting behaviours that they can display as a result of their highly frustrated nature. Here we will present our study of the molybdate pyrochlore Lu<sub>2</sub>Mo<sub>2</sub>O<sub>7</sub>, which contains non-magnetic Lu<sup>3+</sup> and an antiferromagnetic network of corner-sharing tetrahedra of Mo<sup>4+</sup>  $4d^2$   $S = 1$  ions [1]. Magnetic susceptibility data show that Lu<sub>2</sub>Mo<sub>2</sub>O<sub>7</sub> enters an unconventional spin glass state at  $T_f \sim 16$  K that displays a quadratic dependence of the low temperature magnetic heat capacity, akin to that observed for its well-studied sister compound Y<sub>2</sub>Mo<sub>2</sub>O<sub>7</sub> [2]. This spin glass transition is also clearly marked in our inelastic (CNCS, SNS) and diffuse elastic magnetic (D7, ILL) neutron scattering data. Furthermore, we will show that it is possible to topochemically substitute the oxide, O<sup>2-</sup>, ions within Lu<sub>2</sub>Mo<sub>2</sub>O<sub>7</sub> for nitride, N<sup>3-</sup>, to produce an oxynitride molybdate pyrochlore of composition Lu<sub>2</sub>Mo<sub>2</sub>O<sub>5</sub>N<sub>2</sub>. Magnetic susceptibility measurements confirm that strong antiferromagnetic correlations persist within the oxynitride, which contains Mo<sup>5+</sup>  $4d^1$   $S = \frac{1}{2}$  ions and is thus a prime candidate to host exotic quantum spin liquid behavior. We will discuss how the enhanced quantum spin fluctuations in Lu<sub>2</sub>Mo<sub>2</sub>O<sub>5</sub>N<sub>2</sub> appear to suppress the spin freezing transition observed in its parent oxide and instead support the formation of a gapless spin liquid phase that displays a linear dependence of the low temperature magnetic heat capacity [3]. [1] L. Clark *et al.*, J. Solid State Chem. **203**, 199 (2013), [2] H. J. Silverstein *et al.*, Phys. Rev. B **89**, 054433 (2014), [3] L. Clark *et al.*, Phys. Rev. Lett. **113**, 117201 (2014).

**8:36AM K5.00002 Observation of a new incommensurate phase in the spinel MnV<sub>2</sub>O<sub>4</sub><sup>1</sup>**, GILBERTO DE LA PENA MUNOZ, SANGJUN LEE, SAMUEL GLEASON, TAYLOR BYRUM, XINYUE FANG, Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, SHIH-CHANG WENG, National Synchrotron Radiation Research Center, PETER ABBAMONTE, Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign — Using x-ray scattering, we studied the temperature dependence of a large volume of reciprocal space in a MnV<sub>2</sub>O<sub>4</sub> spinel crystal. In addition to the known cubic to tetragonal phase transition at around 56 K, we observed previously unreported incommensurate modulation peaks at  $\delta q = 0.33$   $0.33$   $-0.16$ . We measured the temperature dependence of these modulations and, while they exhibit a shift or splitting in momentum space analogous to that of the structural phase transition, they do so at higher temperature than the Bragg reflections ( $\sim 100$ K). Our results suggest that MnV<sub>2</sub>O<sub>4</sub> has an additional phase transition that may be a precursor for the V t<sub>2g</sub> orbital ordering, which is closely related to the cubic to tetragonal transition.

<sup>1</sup>This work was supported by the DOE grant no. DE-FG02-06ER46285

**8:48AM K5.00003 Geometric Magnetic Frustration in  $\text{Li}_3\text{Mg}_2\text{OsO}_6$  Studied with Muon Spin Relaxation**<sup>1</sup>, J. P. CARLO, Villanova University, S. DERAKHSHAN, California State University - Long Beach, J. E. GREEDAN, McMaster University — Geometric frustration manifests when the spatial arrangement of ions inhibits magnetic order. Typically associated with antiferromagnetically (AF)-correlated moments on triangular or tetrahedral lattices, frustration occurs in a variety of structures and systems, resulting in rich phase diagrams and exotic ground states. As a window to exotic physics revealed by the cancellation of normally dominant interactions, the research community has taken great interest in frustrated systems. One family of recent interest are the rock-salt ordered oxides  $\text{A}_5\text{BO}_6$ , in which the B sites are occupied by magnetic ions comprising a network of interlocked tetrahedra, and nonmagnetic ions on the A sites control the B oxidation state through charge neutrality. Here we will discuss studies of  $\text{Li}_3\text{Mg}_2\text{OsO}_6$  using muon spin relaxation ( $\mu\text{SR}$ ), a highly sensitive local probe of magnetism. Previous studies of this family included  $\text{Li}_5\text{OsO}_6$ , which exhibits AF order below 50K with minimal evidence for frustration, and  $\text{Li}_4\text{MgReO}_6$ , which exhibits glassy magnetism.  $\text{Li}_3\text{Mg}_2\text{RuO}_6$ , meanwhile, exhibits long-range AF, with the ordering temperature suppressed by frustration. But its isoelectronic twin,  $\text{Li}_3\text{Mg}_2\text{OsO}_6$  ( $5d^3$  vs.  $4d^3$ ) exhibits very different behavior, revealed by  $\mu\text{SR}$  to be a glassy ground state below 12K. Understanding why such similar systems exhibit diverse ground-state behavior is key to understanding the nature of geometric magnetic frustration.

<sup>1</sup>\*Financial support from the Research Corporation for Science Advancement

**9:00AM K5.00004 Effects of Zn doping on the A-Site antiferromagnet spinel  $\text{CuRh}_2\text{O}_4$** <sup>1</sup>, ALEXANDER ZAKJEVSKII, DALMAU REIG-I-PLESSIS, University of Illinois, Urbana, IL, ALEXANDER THALER, ASHFIA HUQ, Oak Ridge National Laboratory, Oak Ridge, TN, GREGORY MACDOUGALL, University of Illinois, Urbana, IL — A major recent focus of the correlated electron community has been the investigation of 4d and 5d transition metal oxides, which are predicted to have novel phases arising from relativistic spin-orbit coupling. We have recently synthesized and characterized several compounds of the doped spinel series  $\text{Cu}_{1-x}\text{Zn}_x\text{Rh}_2\text{O}_4$ . The parent compound is a normal spinel which undergoes a cubic-tetragonal structural phase transition at  $T \sim 850\text{K}$ , and further undergoes a suspected antiferromagnetic transition at  $T_N = 22\text{K}$ . We have performed powder x-ray and neutron diffraction, and bulk magnetization measurements on members of the Zn-doping series. Magnetization measurements clearly indicate a monotonic suppression of the Néel temperature with increasing Zn content, to a quantum critical point at  $x \approx 0.42$ . X-ray results indicate a change in structure occurring near the same doping. We will present these data and discuss the results within the context of exotic predictions in the literature. Lastly, we will discuss our recent neutron powder diffraction measurements and insights gleaned about the local spin state.

<sup>1</sup>This work was sponsored by the National Science Foundation, under grant number DMR14-55264.

**9:12AM K5.00005 Magnetic Ordering in  $\text{FeSc}_2\text{S}_4$** <sup>1</sup>, K.W. PLUMB, J.R. MOREY, Johns Hopkins University, J.P.C. RUFF, CHESS, Cornell University, J.A. RODRIGUEZ-RIVERA, NIST, T.M. MCQUEEN, S.M. KOOHPAYEH, C.L. BROHOLM, Johns Hopkins University —  $\text{FeSc}_2\text{S}_4$  is a cubic spinel where orbitally active  $\text{Fe}^{2+}$  ions occupy the A-site diamond sublattice. Despite a high spin ( $S=2$ ) state and Curie Weiss temperature of 45 K thermodynamic measurements show no indication of a phase transition and the material has been proposed as a unique example of a spin-orbital liquid. This ground state might arise from competition between on site spin-orbit coupling and Kugel-Khomskii exchange. We report neutron scattering measurements on polycrystalline samples of  $\text{FeSc}_2\text{S}_4$  which bring this picture into question. They reveal a previously unreported magnetically ordered state below 11 K. No structural distortions are visible with neutron or x-ray scattering. The effect of hydrostatic pressure on the magnetic excitation spectrum was also explored and found to be minimal.

<sup>1</sup>This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Material Sciences and Engineering, under Grant No. DEFG02-08ER46544.

**9:24AM K5.00006 Quantum phase transitions and anomalous Hall effect in a pyrochlore Kondo lattice**, SARAH GREFE, Rice University, WENXIN DING, University of California Santa Cruz, QIMIAO SI, Rice University — The metallic variant of the pyrochlore iridates  $\text{Pr}_2\text{Ir}_2\text{O}_7$  has shown characteristics of a possible chiral spin liquid state [PRL **96** 087204 (2006), PRL **98**, 057203 (2007), Nature **463**, 210 (2010)] and quantum criticality [Nat. Mater. **13**, 356 (2014)]. An important question surrounding the significant anomalous Hall response observed in  $\text{Pr}_2\text{Ir}_2\text{O}_7$  is the nature of the f-electron local moments, including their Kondo coupling with the conduction d-electrons. The heavy effective mass and related thermodynamic characteristics indicate the involvement of the Kondo effect in this system's electronic properties. In this work, we study the effects of Kondo coupling on candidate time-reversal-symmetry-breaking spin liquid states on the pyrochlore lattice. Representing the f-moments as slave fermions Kondo-coupled to conduction electrons, we study the competition between Kondo-singlet formation and chiral spin correlations and determine the zero-temperature phase diagram. We derive an effective chiral interaction between the local moments and the conduction electrons and calculate the anomalous Hall response across the quantum phase transition from the Kondo destroyed phase to the Kondo screened phase. We discuss our results' implications for  $\text{Pr}_2\text{Ir}_2\text{O}_7$  and related frustrated Kondo-lattice systems.

**9:36AM K5.00007 Chemical insights into the synthesis and properties of polycrystalline and single crystal iron scandium sulfide ( $\text{FeSc}_2\text{S}_4$ )**<sup>1</sup>, JENNIFER R. MOREY, KEMP W. PLUMB, SEYED M. KOOHPAYEH, COLLIN L. BROHOLM, TYREL M. MCQUEEN, Institute for Quantum Matter and Johns Hopkins University — Iron scandium sulfide,  $\text{FeSc}_2\text{S}_4$ , has recently attracted significant theoretical and experimental interest as a candidate spin-orbital liquid. An  $\text{AB}_2\text{X}_4$  spinel,  $\text{FeSc}_2\text{S}_4$  (space group  $\text{Fd-3m}$ , No. 227) features a high degree of frustration associated with the  $\text{Fe}^{2+}$ , which occupies the A-site diamond sublattice and is tetrahedrally coordinated by sulfur. The  $\text{Fe}^{2+}$  ion is in a high spin ( $S=2$ ) state, resulting in orbital degeneracy due to a single hole on the  $e$  orbitals. We report the strides we have made to produce material in powder and single crystal form, and the relationship between the chemistry and the structural, magnetic, and thermodynamic properties of  $\text{FeSc}_2\text{S}_4$ .

<sup>1</sup>This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Material Sciences and Engineering, under Grant No. DEFG02-08ER46544.

**9:48AM K5.00008 Weyl Magnon**, FEI-YE LI, Institute of Theoretical Physics, Chinese Academy of Sciences, YAO-DONG LI, Department of Computer Sciences, Fudan Univ, YUE YU, Physics Department, Fudan Univ, YONG BAEK KIM, Physics Department, Univ of Toronto, Ontario; School of Physics, Korea Institute for Advanced Study, Seoul, LEON BALENTS, Kavli Institute for Theoretical Physics, UCSB, California, GANG CHEN<sup>1</sup>, Physics Department, State Key Laboratory of Surface Physics, Fudan Univ; Perimeter Institute for Theoretical Physics — Conventional magnetic orders in Mott insulators are often believed to be trivial as they are simple product states. In this talk, we argue that this belief is not always right. We study a realistic spin model on the breathing pyrochlore lattice. We find that, although the system has a magnetic ordered ground state, the magnetic excitation is rather nontrivial and supports linear band touchings in its spectrum. This linear band touching is a topological property of the magnon band structure and is thus robust against small perturbation. We thus name this magnon band touching as Weyl magnon. Just like the Weyl fermion, the existence of Weyl magnon suggests the presence of chiral magnon surface states. Unlike the surface Fermi arcs for the Weyl fermions, the chiral surface state for Weyl magnon appears at a finite energy due to the bosonic nature of the magnons. Moreover, the external magnetic field only couples to the spins with a Zeeman term and thus can readily shift the Weyl node position. This provides a way to control the Weyl magnon. Our work will inspire a re-examination of the excitation spectrum of many magnetic ordered systems.

<sup>1</sup>chggst@gmail.com

**10:00AM K5.00009 Spin Glass Behavior and Field Induced Anisotropic Magnetic Ordering in  $S = 2$  Frustrated Spinel  $\text{GeFe}_2\text{O}_4$** , TAO ZOU, Michigan State Univ, ZHILING DUN, University of Tennessee, TAO HONG, HUIBO CAO, CLARINA DELA CRUZ, Oak Ridge National Lab, MICHAEL GOTTSCHALK, MENGZE ZHU, Michigan State Univ, HAIDONG ZHOU, University of Tennessee, XIANGLIN KE, Michigan State Univ — We report comprehensive studies of magnetic properties of spinel  $\text{GeFe}_2\text{O}_4$  by means of magnetic susceptibility and heat capacity measurements on both polycrystalline and single crystalline samples as well as neutron powder diffraction measurements. We find that this system shows a spin-glass ground state with the transition temperature around  $T \sim 21$  K, in contrast to the static antiferromagnetic order reported in earlier literature. In addition, we reveal a field-induced magnetic ordering, which displays strong magnetic anisotropy character.

**10:12AM K5.00010 Orbital degeneracy near the itinerant electron limit in  $\text{CoV}_2\text{O}_4$** <sup>1</sup>, D. REIG-IPLESSIS, D. CASAVANT, University of Illinois, V. O. GARLEA, A. A. ACZEL, M. FEYGENSON, J. NEUEFEIND, Oak Ridge National Lab, H. D. ZHOU, University of Tennessee, S. E. NAGLER, Oak Ridge National Lab, G. J. MACDOUGALL, University of Illinois — Vanadium spinels,  $\text{AV}_2\text{O}_4$  have both magnetic frustration and orbital degeneracy on the  $V^{3+}$  sublattice, which lead to strong coupling of the orbital, lattice and spin degrees of freedom. Additionally, upon decreasing the V-V distance, the material is predicted to go from a Mott insulator to a metallic phase. Of all the materials in the  $\text{AV}_2\text{O}_4$  series,  $\text{CoV}_2\text{O}_4$  is closest to the predicted transition, and it's debated whether it may be fully described by either localized or itinerant electrons pictures. In all other studied vanadium spinels, there is a cubic to tetragonal transition associated with ordering of the degenerate  $V^{3+}$  orbitals, consistent with a local orbital picture but, this transition is surprisingly absent from  $\text{CoV}_2\text{O}_4$  despite being an insulator with local spins. In this talk we present recent high resolution neutron diffraction and inelastic scattering measurements by our group on powders of  $\text{CoV}_2\text{O}_4$ . Diffraction data show there is small but clear first order structural transition present which correlates with canting of the  $V^{3+}$  spins, while inelastic data are well described by a local spinwave picture. We discuss how these results contribute evidence of a local orbital ordering phase in the region near electron itinerancy.

<sup>1</sup>This work was sponsored by NSF grant DMR-145526

**10:24AM K5.00011 Spin Dynamics and Two-Dimensional Correlations in the FCC Antiferromagnetic  $\text{Sr}_2\text{YRuO}_6$** , STEVEN DISSELER, J. W. LYNN, NIST Center for Neutron Research, Gaithersburg, Maryland 20899, USA, R. F. JARDIM, Instituto de Física, Universidade de São Paulo 05315-970, Brazil, M. S. TORIKACHVILI, Department of Physics, San Diego State University, San Diego, California 92182, USA, E. GR, Institute of Physics "Gleb Wataghin," University of Campinas - UNICAMP, Campinas, São Paulo 13083-859, Brazil — The face-centered cubic lattice of  $\text{Ru}^{5+}$  spins in the double perovskite  $\text{Sr}_2\text{YRuO}_6$  shows a delicate three dimensional antiferromagnetic (AFM) ground state composed of stacked square AFM layers. We present new inelastic neutron scattering data taken on this state revealing a gapped low-energy excitation band that may be modeled by a simple  $J_1 - J_2$  interaction scheme allowing quantitative comparison of similar materials. At higher temperatures, the low-energy excitation spectrum is dominated by a quasi-elastic component associated with size fluctuations of two-dimensional AFM clusters that exhibit asymmetric correlations even at low temperatures. Thus, the FCC lattice in general and the double perovskite structure in particular emerge as hosts of both two-dimensional and three-dimensional dynamics resulting from frustration.

**10:36AM K5.00012 Unanticipated spin gap measured in the frustrated quasi-FCC  $d^3$  double perovskites  $\text{La}_2\text{LiXO}_6$  ( $X = \text{Ru, Os}$ )**, DALINI D MAHARAJ, GABRIELE SALA, CASEY A MARJERRISON, JOHN GREEDAN, BRUCE GAULIN, McMaster University, MATTHEW STONE, Spallation Neutron Source, Oak Ridge National Laboratory — There is much current interest in the influence of strong spin-orbit (SO) interactions on exotic ground state selection in new 4d and 5d magnets, particularly involving  $4d^5$  Ir. Here we consider double perovskites of the form  $\text{A}_2\text{BB}'\text{O}_6$  which are based on heavy 4d or 5d magnetic ions, where the SO interaction is expected to be significant as it increases as  $\sim Z^4$ . The double perovskite structure can accommodate a variety of magnetic ions on the B' site, providing a playground for systematic studies of the exotic ground states stabilized by strong SO coupling. Here, we report inelastic neutron scattering (INS) measurements conducted on the frustrated monoclinic magnets,  $\text{La}_2\text{LiXO}_6$  ( $X = \text{Ru, Os}$ ), wherein the magnetic moments decorate a quasi face-centered-cubic lattice. Our results show the development of a spin gap in the spin excitation spectrum of size  $\Delta_{\text{Os}} = 8$  meV and  $\Delta_{\text{Ru}} = 2.5$  meV concomitant with  $T_N$ , which is unexpected for orbitally quenched  $d^3$  systems. We liken these results to INS results obtained for  $\text{Ba}_2\text{YXO}_6$  and  $\text{La}_2\text{NaXO}_6$ , which were also shown to exhibit spin gaps that correlate with  $T_N$ . We shall discuss trends observed in these three  $d^3$  double perovskite families which correlate strong SO coupling, spin gap and  $T_N$ .

**10:48AM K5.00013 Raman spectroscopy study of spin-orbital liquid candidate  $\text{FeSc}_2\text{S}_4$** <sup>1</sup>, STREIT CUNNINGHAM, K.W. PLUMB, Department of Physics and Astronomy, Johns Hopkins University, Baltimore, Maryland, USA, J.R. MOREY, T.M. MCQUEEN, Department of Chemistry, Johns Hopkins University, Baltimore, Maryland, USA, S. KOOHPAYEH, C.L. BROHOLM, NATALIA DRICHKO, Department of Physics and Astronomy, Johns Hopkins University, Baltimore, Maryland, USA — The A-site cubic spinel  $\text{FeSc}_2\text{S}_4$ , containing  $\text{Fe}^{2+}$  ions in a tetrahedral  $\text{S}_4$  environment, represents a rare candidate of a spin-orbital liquid, where spin and orbital order remain suppressed down to the lowest measurable temperature [1]. We studied phonon spectrum and orbital excitations in  $\text{FeSc}_2\text{S}_4$  by Raman spectroscopy on single crystals. At temperatures below 100K we observe widening of sulfur  $330 \text{ cm}^{-1}$   $T_{2g}$  and  $365 \text{ cm}^{-1}$   $A_{1g}$  phonon modes with an additional weak mode emerging at  $400 \text{ cm}^{-1}$ . These changes can indicate weak lattice distortions associated with the sulfur sites. Below 100K we also observe orbital excitations at frequencies of approximately  $2000 \text{ cm}^{-1}$ . We discuss the result in terms of a competition of spin-orbital liquid and a magnetically ordered state. [1] L. Mittelstadt et al., Phys. Rev. B 91 125112 (2015).

<sup>1</sup>The work at IQM was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Material Sciences and Engineering, under Grant No. DEFG02-08ER46544.

## Wednesday, March 16, 2016 8:00AM - 11:00AM – Session K6 GMAG DMP: Ruthenates 302 - Songxue Chi, Oak Ridge National Laboratory

**8:00AM K6.00001 Tuning quantum properties in bilayer ruthenates**, XIANGLIN KE, Michigan State University — The mutual coupling among spin, charge, lattice and orbital degrees of freedom in transition-metal oxide materials often leads to the competition of various types of energetic states. This makes such materials dramatically susceptible to external parameters, giving rise to novel physical properties and rich phase diagrams. In this talk, I shall use a bilayer ruthenate,  $\text{Ca}_3\text{Ru}_2\text{O}_7$ , as an example to discuss the emergent phenomena achieved by systematically tuning materials magnetic and electronic properties via chemical doping, magnetic field, and pressure. I shall show that this system provides a rare opportunity to investigate the interplay between correlated metal and Mott insulator. This work was done in collaboration with M. Zhu, T. Tao, S. D. Mahanti, Z. Q. Mao, J. Peng, T. Hong, W. Tian, H. Cao, C. R. dela Cruz, D. Singh, and K. Prokes.

**8:36AM K6.00002 Metamagnetism and Nonlinear Susceptibilities in the Bilayer Ruthenate  $\text{Sr}_3\text{Ru}_2\text{O}_7$** <sup>1</sup>, D. PHELAN, Argonne National Labs, B. SHIVARAM, Univ of Virginia, A. VECCHIONE, ROSALBA FITTIPALDI, CNR-SPIN and Dipartimento di Fisica, Salerno, Italy — We report measurements of the third and fifth order nonlinear susceptibilities in the correlated oxide metamagnet,  $\text{Sr}_3\text{Ru}_2\text{O}_7$  for both orientations of the magnetic field, H parallel to the c-axis and in the basal plane. In both geometries we observe peaks in the temperature dependence of the higher order susceptibilities. The position in temperature where the peak in the fifth order susceptibility occurs is at half the temperature where a peak in the third order susceptibility is seen. The latter in turn is at half the temperature where the peak in the linear susceptibility is known to occur. This simple scaling is common to both orientations of the magnetic field. These results will be discussed in the context of similar work with heavy fermion metamagnets<sup>1</sup>.

<sup>1</sup>"Universality in the Magnetic Response of Metamagnetic Metals", B.S. Shivaram, D.G. Hinks, and Pradeep Kumar, Phys. Rev. B89, 241107(R), 2014.

**8:48AM K6.00003 Structure-magnetism correlation induced by Mn substitution in bilayered perovskite  $\text{Sr}_3(\text{Ru}_{1-x}\text{Mn}_x)_2\text{O}_7$** <sup>1</sup>, QIANG ZHANG, Louisiana State Univ - Baton Rouge, FENG YE, SONGXUE CHI, Oak Ridge National Laboratory, DALGIS MESA, Louisiana State Univ - Baton Rouge, WEI TIAN, Oak Ridge National Laboratory, RONGYING JIN, WARD PLUMMER, JIANDI ZHANG, Louisiana State Univ - Baton Rouge — Elastic neutron scattering technique was employed to investigate the effect of Mn substitution on the structure, magnetism and their correlation in  $\text{Sr}_3(\text{Ru}_{1-x}\text{Mn}_x)_2\text{O}_7$  (x=6%, 12% and 16%) crystals. While parent compound  $\text{Sr}_3\text{Ru}_2\text{O}_7$  is paramagnetic, a small amount of Mn substitution induces an E-type antiferromagnetic order. With the increase of Mn substitution from 6 % to 16%, the ordered moment at Ru/Mn site increases significantly with an enhanced  $T_N$  from 20 K for x=6 % to 80 K for x= 16%, and the in-plane magnetic correlation lengths increase to achieve the maximum for x= 16% as indicated by the resolution-limited linewidth of the H-scans through  $\mathbf{Q}_{\text{AFM}}=(0.5, 0, 0)$ . Accompanied by the enhancement of  $T_N$ , the (Ru/Mn) $\text{O}_6$  octahedron rotation is found to be suppressed simultaneously, suggesting a correlation between (Ru/Mn) $\text{O}_6$  octahedron rotation and magnetism due to Mn substitution. Our findings indicate that Mn substitution on Ru in  $\text{Sr}_3\text{Ru}_2\text{O}_7$  has a significant effect on the microscopic structure and magnetism as well as the correlations between them.

<sup>1</sup>This work is supported by the U.S. Department of Energy under EPSCoR Grant No. DE-SC0012432 with additional support from the Louisiana Board of Regents.

**9:00AM K6.00004 Magnetic phase separation in double layer ruthenates  $\text{Ca}_3(\text{Ru}_{1-x}\text{Ti}_x)_2\text{O}_7$** , JIN PENG, Nanjing University, JINYU LIU, JIN HU, ZHIQIANG MAO, Tulane University, XIAOSHAN WU, Nanjing University — Ti doping of a small concentration in the double-layered ruthenate  $\text{Ca}_3(\text{Ru}_{1-x}\text{Ti}_x)_2\text{O}_7$  was previously found to induce an unusual magnetic phase transition from a metallic antiferromagnetic state formed from anti-parallel stacking of ferromagnetic bilayers (AFM-b) to a nearest-neighbor antiferromagnetic state (G-AFM) with Mott insulating properties; the critical Ti concentration for the transition is near  $x = 0.03$ . In this article, we conducted systematic studies on this magnetic transition near the critical composition through detailed magnetization measurements. We found that no intermediate magnetic phases exist between AFM-b and G-AFM states; this is contrasted with manganites where a similar magnetic phase transition takes place through the presence of several intermediate magnetic phases. The AFM-b-to-G-AFM transition in  $\text{Ca}_3(\text{Ru}_{1-x}\text{Ti}_x)_2\text{O}_7$  happens through a phase separation process; the AFM-b and G-AFM phases coexist in the 2-5

**9:12AM K6.00005 Field-controlled spin-density-wave order and quantum criticality in  $\text{Sr}_3\text{Ru}_2\text{O}_7$** , STEPHEN HAYDEN, University of Bristol — The quasi-2D metamagnetic perovskite metal  $\text{Sr}_3\text{Ru}_2\text{O}_7$  has been an enigma for the last decade. The application of a large magnetic field of 8T parallel to the c-axis creates a new phase at low temperatures. This phase shows "electronic nematic" properties in that strong anisotropy its resistivity can be created by tilting the field away from the c-axis. In addition, measurement of transport and thermodynamic properties suggest that the phase is at the centre of a quantum critical region. Here we use neutron scattering to show that the magnetic field actually induces spin-density-wave magnetic order in the proximity of a metamagnetic critical endpoint. In fact,  $\text{Sr}_3\text{Ru}_2\text{O}_7$  can be tuned through two magnetically-ordered SDW states which exist over relatively small ranges in field ( $\mu_0$  0.4 T). Their origin is probably due to the electronic fine structure near the Fermi energy. The magnetic field direction is shown to control the SDW domain populations which naturally explains the strong resistivity anisotropy or "electronic nematic" behaviour observed in this material. We find that  $\text{Sr}_3\text{Ru}_2\text{O}_7$  is also unique in that its quantum critical region is controlled by overdamped incommensurate low-energy spin fluctuations with a diverging relaxation time. The low-energy electronic properties reflect the presence of these fluctuations and, in particular, the field-dependent low-temperature specific heat is proportional to the spin relaxation rate. [Based on C. Lester, S. Ramos, R. S. Perry at el. Natural Materials 14, 373 (2015).]

**9:48AM K6.00006 Magnetic-field-induced first-order phase transitions in  $\text{Ca}_3(\text{Ru}_{1-x}\text{Fe}_x)_2\text{O}_7$  with unusual irreversible behaviors**, MENGZE ZHU, Michigan State Univ, JIN PENG, Nanjing Univ, China, TAO ZOU, Michigan State Univ, TAO HONG, Oak Ridge National Lab, KAREL PROKES, Helmholtz Zentrum Berlin, Germany, S. D. MAHANTI, Michigan State Univ, ZHIQIANG MAO, Tulane University, XIANGLIN KE, Michigan State Univ — Neutron diffraction measurements reveal a magnetic-field-induced incommensurate-commensurate magnetic structure transition in a bilayer ruthenate  $\text{Ca}_3(\text{Ru}_{1-x}\text{Fe}_x)_2\text{O}_7$  ( $x = 0.05$ ). The transition is of first-order in nature, and exhibits intriguing irreversible behaviors at low temperature, i.e. the zero-field incommensurate state before and after field sweeping showing very distinct magnetic ordering wave vectors. The difference in the wavelength of magnetic ordering is strongly temperature-dependent, and disappears gradually as temperature raises. This unusual irreversibility in magnetic ordering vector is rarely observed, and in disagreement with phase coexistence phenomena that is commonly seen in other irreversible first-order phase transitions. Nevertheless, our results demonstrate that thermal fluctuations also play an essential role in this unusual behavior.

**10:00AM K6.00007 Unconventional Magnetic Domains in Triple-layered  $\text{Sr}_4\text{Ru}_3\text{O}_{10}$** <sup>1</sup>, KAI DU, SEONG JOON LIM, JAE WOOK KIM, Rutgers Univ, GANG CAO, University of Kentucky, SANG WOOK CHEONG, Rutgers Univ, RUTGERS CENTER FOR EMERGENT MATERIAL TEAM, CENTER FOR ADVANCED MATERIALS, UNIVERSITY OF KENTUCKY COLLABORATION — A plethora of fascinating phenomena including p-wave superconductivity in  $\text{Sr}_2\text{RuO}_4$  (n=1) and hybrid improper ferroelectricity in  $\text{Ca}_3\text{Ru}_2\text{O}_7$  (n=2) have been observed in Ruddlesden-Popper ruthenates  $(\text{Ca}, \text{Sr})_{n+1}\text{Ru}_n\text{O}_{3n+1}$ . The triple-layered  $\text{Sr}_4\text{Ru}_3\text{O}_{10}$  (n=3) is believed to have an intriguing complex magnetic state, compared with its neighboring bi-layered meta-magnetic  $\text{Sr}_3\text{Ru}_2\text{O}_7$  (n=2) and ferromagnetic  $\text{SrRuO}_3$  (n= $\infty$ ). The phase competition nature associated with this complexity is considered to be responsible for its novel properties such as coupled anisotropic magnetism and transport, low frequency quantum oscillations and sharp magneto-resistivity steps, which are still not well understood yet. To better understand its microscopic mechanism, we studied the magnetic domain structure on  $\text{Sr}_4\text{Ru}_3\text{O}_{10}$  using low-temperature magnetic force microscopy. The observed unique domain structures in  $\text{Sr}_4\text{Ru}_3\text{O}_{10}$  may shed lights on its microscopic phase competition nature and lead to a deeper understanding on its relations with other layered ruthenates.

<sup>1</sup>This work is funded by the Gordon and Betty Moore Foundations EPIQS Initiative through Grant GBMF4413 to the Rutgers Center for Emergent Materials.

**10:12AM K6.00008 Dynamical mean field study of ferromagnetism and correlation strength in cubic barium ruthenate: results and comparison to strontium and calcium ruthenate**, QIANG HAN, Department of Physics, Columbia University, New York, New York 10027, USA, HUNG DANG, Institute for Theoretical Solid State Physics, JARA-FIT and JARA-HPC, RWTH Aachen University, 52056 Aachen, Germany, ANDREW MILLIS, Department of Physics, Columbia University, New York, New York 10027, USA — We present density functional plus dynamical mean field studies of cubic BaRuO<sub>3</sub> using interaction parameters previously found to be appropriate for the related materials CaRuO<sub>3</sub> and SrRuO<sub>3</sub>. The calculated trends in material properties across this family of compounds are in good agreement with experiment and the results provide insights into the origin of magnetism and the role of the van Hove singularity in the physics of Hund's metals.

**10:24AM K6.00009 Ferromagnetic cluster glass state induced by non-magnetic ions in a paramagnetic host**, TAKAFUMI D. YAMAMOTO, Department of Physics, Nagoya University, Nagoya 464-8602, RYUJI OKAZAKI, Department of Physics, Faculty of Science and Technology, Noda 278-8510, HIROKI TANIGUCHI, ICHIRO TERASAKI, Department of Physics, Nagoya University, Nagoya 464-8602 — A paramagnetic metal CaRuO<sub>3</sub> has been known to show unique impurity effects, where a magnetic ordering is induced by a partial substitution of transition metal ions for Ru. Since this phenomenon occurs regardless of the magnetism of the substituted ions, it must reflect a magnetic instability of this ruthenate. Understanding such physical properties is one of intriguing issues in condensed matter physics.

In this talk, we report an unconventional magnetic state induced by substituting non-magnetic Sc<sup>3+</sup> ions. We find that the static magnetic susceptibilities of all Sc-substituted samples show ferromagnetic-like features below 40 K, while the Curie-Weiss temperature dramatically changes with increasing  $x$ . This inconsistency is a sign of *non-uniform magnetic system*. We propose a phenomenological model and show that the static magnetic properties can be described as a volume average of a paramagnetic component originated from Ru<sup>4+</sup> ions and a ferromagnetic one driven by Sc substitution [T. D. Yamamoto *et al.*, JPSJ **84**, 014708 (2015)]. Furthermore our dynamic magnetic measurements reveal a ferromagnetic cluster glass state embedded in the paramagnetic and metallic host of CaRuO<sub>3</sub>.

**10:36AM K6.00010 Suppression of ferromagnetism and observation of quantum well states in epitaxial thin films of the cubic ruthenate BaRuO<sub>3</sub>**, BULAT BURGANOV, Department of Physics, Cornell University, HANJONG PAIK, Department of Materials Science and Engineering, Cornell University, KYLE SHEN, Department of Physics, Cornell University, DARRELL SCHLOM, Department of Materials Science and Engineering, Cornell University — The pseudocubic perovskite ruthenates ARuO<sub>3</sub>, where A is alkaline earth metal, are correlated materials where Hund's coupling drives correlations and leads to a low coherence scale, large renormalization, and formation of local moments. The ferromagnetic BaRuO<sub>3</sub> has an ideal cubic structure and a larger bandwidth, compared to its GdFeO<sub>3</sub>-distorted counterparts, CaRuO<sub>3</sub> and SrRuO<sub>3</sub>. In stark contrast to SrRuO<sub>3</sub>, which is a Fermi liquid below  $T_C$ , BaRuO<sub>3</sub> exhibits critical fluctuations near  $T_C$  that are enhanced under hydrostatic pressure, which suppresses the Fermi liquid coherence scale and  $T_C$  and drives a crossover into non-FL regime. Here we use ARPES to characterize the momentum-resolved electronic structure of strained ultrathin BaRuO<sub>3</sub> films grown in situ by molecular beam epitaxy. The films on STO (001) are metallic down to 2 u.c. thickness and manifest clearly defined subbands of well-defined quasiparticles which arise due to quantum confinement effects. We observe that the bands are moderately renormalized compared to bare GGA bands and discover that the ferromagnetism can be suppressed in the atomically thin limit. We discuss our results on BaRuO<sub>3</sub> in the context of our recent ARPES studies of the other perovskite ruthenates, SrRuO<sub>3</sub> and CaRuO<sub>3</sub>.

**10:48AM K6.00011 Antiferromagnetism in Bulk Rutile RuO<sub>2</sub>**<sup>1</sup>, T. BERLIJN, Oak Ridge National Laboratory, P. C. SNIJDERS, P. R. C. KENT, T. A. MAIER, Oak Ridge National Laboratory, University of Tennessee, H.-D. ZHOU, University of Tennessee, H.-B. CAO, O. DELAIRE, Y. WANG, Oak Ridge National Laboratory, M. KOEHLER, University of Tennessee, H. H. WEITERING, University of Tennessee, Oak Ridge National Laboratory — While bulk rutile RuO<sub>2</sub> has long been considered to be a Pauli paramagnet, we conclude it to host antiferromagnetism based on our combined theoretical and experimental study. This constitutes an important finding given the large amount of applications of RuO<sub>2</sub> in the electrochemical and electronics industry. Furthermore the high onset temperature of the antiferromagnetism around 1000K together with the high electrical conductivity makes RuO<sub>2</sub> unique among the ruthenates and among oxide materials in general.

<sup>1</sup>This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

## Wednesday, March 16, 2016 8:00AM - 11:00AM –

**Session K7 DMP FIAP: Dopants and Defects in Semiconductors: Nitrides** 303 - Christopher Van de Walle, UCSB

**8:00AM K7.00001 Point and Extended Defects in GaN-based Materials**, JAMES SPECK, UCSB Materials Department — In this presentation, the origin and evolution of threading dislocations in GaN heteroepitaxy are reviewed. For heteroepitaxial of GaN on most substrates (e.g., sapphire, MgAl<sub>2</sub>O<sub>4</sub>, SiC, ...) high temperature GaN grows in a Volmer-Weber mode. Threading dislocations result from island coalescence. The evolution of threading dislocations has been extensively modeled. Tensile stress generation via threading dislocation inclination is a major ongoing issue in GaN growth. We review older and more recent work on the impact of threading dislocations in GaN materials properties and device performance. Finally, we review recent work from our group on stress relaxation in nonpolar and semipolar GaN. We demonstrate the first GaN-based laser diodes grown on intentionally stress-relaxed buffer layers and we demonstrate control of relaxation in semipolar laser diodes by selective area growth.

**8:36AM K7.00002 Impact of defects on efficiency of nitride devices**<sup>1</sup>, CHRIS VAN DE WALLE, Univ of California - Santa Barbara — Nitride semiconductors are the key materials for solid-state lighting and also increasingly for power electronics. In both bulk crystals and epitaxial layers, point defects may act as compensating centers, charge traps, or radiative or nonradiative recombination centers. Unintentional impurities often play an equally important role; for instance, carbon that is unavoidably incorporated during metal-organic chemical vapor deposition (MOCVD) acts as a source of yellow luminescence [1]. Theoretical advances now enable us to calculate the energetics as well as electronic and optical properties of point defects with unprecedented accuracy [2]. In AlN, we have identified the defects that lead to characteristic luminescence and absorption lines [3]. Both point defects and impurities can affect the radiative efficiency of light emitters. We have developed a first-principles methodology [4] to determine nonradiative carrier capture coefficients. Accurate calculations of electron-phonon coupling, combined with results for defect formation energies and charge-state transition levels [5], enable the calculation of nonradiative capture rates for electrons and holes and the evaluation of Shockley-Read-Hall coefficients. This approach allows us to identify specific defects that play a key role in limiting the efficiency of nitride semiconductor devices.

1. J. L. Lyons, A. Janotti, and C. G. Van de Walle, Phys. Rev. B **89**, 035204 (2014).
2. C. Freysoldt *et al.*, Rev. Mod. Phys. **86**, 253 (2014).
3. Q. Yan, A. Janotti, M. Scheffler, and C. G. Van de Walle, Appl. Phys. Lett. **105**, 111104 (2014).
4. A. Alkauskas, Q. Yan, and C. G. Van de Walle, Phys. Rev. B **90**, 075202 (2014).
5. J. L. Lyons, A. Alkauskas, A. Janotti, and C. G. Van de Walle, Phys. Stat. Sol. B **252**, 900 (2015).

<sup>1</sup>Work performed in collaboration with A. Alkauskas, C. Dreyer, A. Janotti, J. Lyons, D. Wickramaratne, J. Shen, and Q. Yan, and supported by DOE and NSF.

**9:12AM K7.00003 Saturation Behavior of Eu ion emission in GaN**, NATALIE HERNANDEZ, Lehigh University, BRANDON MITCHELL, University of Mount Union, YASUFUMI FUJIWARA, Osaka University, VOLKMAR DIEROLF, Lehigh University — Europium doped Gallium Nitride (GaN:Eu) has been recognized as a candidate for the red-emitting active layer in nitride-based light emitting diodes. To better comprehend the excitation energy transfer from the excited GaN host to the Eu ion, we performed an extensive analysis of GaN:Eu and GaN co-doped with Eu and other dopants (Silicon and Magnesium). We determined how various growth parameters manipulated site formations and measured the optical accessibility of the Eu ions within the GaN host and the excitation efficiency of the energy transfer between the host material and the Eu ions. Furthermore, we derived a model for the saturation behavior of the emission of Eu ions within GaN. Our results suggest that the saturation behavior is strongly influenced by different crystal growth specifications and co-dopants.

**9:24AM K7.00004 Hydrogen-carbon complexes and the blue luminescence band in GaN**,<sup>1</sup> DENIS DEMCHENKO, Virginia Commonwealth Univ, IBRAHIMA DIALLO, MICHAEL RESHCHIKOV, Virginia Commonwealth University — The blue luminescence band with a maximum at 3.0 eV and the zero-phonon line at 3.33 eV (labeled BL2) is observed in high-resistivity GaN. Under prolonged ultraviolet (UV) light exposure, the BL2 band transforms into the yellow luminescence (YL) band with a maximum at 2.2 eV. Our calculations using hybrid functionals suggest that the BL2 band is related to a hydrogen-carbon defect complex, most likely  $C_N O_N - H_i$ . The complex creates defect transition level close to the valence band, which is responsible for the BL2 band. Under UV illumination the complex dissociates, leaving as byproduct the source of the YL band ( $C_N O_N$  or  $C_N$ ) and interstitial hydrogen.

<sup>1</sup>The work was supported by the National Science Foundation (DMR-1410125) and the Thomas F. and Kate Miller Jeffress Memorial Trust.

**9:36AM K7.00005 Impact of point defects on III-nitride tunnel devices**,<sup>1</sup> DARSHANA WICKRAMARATNE, Materials Department, UC Santa Barbara, JOHN LYONS, Center for Functional Nanomaterials, Brookhaven National Laboratory, CHRIS G. VAN DE WALLE, Materials Department, UC Santa Barbara — Heterostructures using GaN and InGaN are being pursued in designs of tunnel field-effect-transistors (TFETs) to enable low-power switching devices. Point defects and impurities in these heterostructures can adversely affect the performance of these devices through Shockley-Read-Hall (SRH) and Trap-Assisted-Tunneling (TAT) processes. Using first-principles calculations based on a hybrid functional, we calculate the thermodynamic and charge-state switching levels as well as nonradiative recombination rates of point defects and impurities in GaN and InGaN. Gallium vacancies and their complexes, in particular, are found to be potentially detrimental centers. We then investigate how these defects can contribute to SRH and TAT processes in a nitride TFET device.

<sup>1</sup>This work was supported by the Center for Low Energy Systems Technology (LEAST), one of the six SRC STARnet Centers, sponsored by MARCO and DARPA.

**9:48AM K7.00006 Density Functional Theory Calculations of Activation Energies for Carrier Capture by Defects in Semiconductors**, N. A. MODINE, A. F. WRIGHT, S. R. LEE, Sandia National Laboratories — The rate of defect-induced carrier recombination is determined by both defect levels and carrier capture cross-sections. Density functional theory (DFT) has been widely and successfully used to predict defect levels, but only recently has work begun to focus on using DFT to determine carrier capture cross-sections. Lang and Henry developed the theory of carrier-capture by multiphonon emission in the 1970s and showed that carrier-capture cross-sections differ between defects primarily due to differences in their carrier capture activation energies. We present an approach to using DFT to calculate carrier capture activation energies that does not depend on an assumed configuration coordinate and that fully accounts for anharmonic effects, which can substantially modify carrier activation energies. We demonstrate our approach for intrinsic defects in GaAs and GaN and discuss how our results depend on the choice of exchange-correlation functional and the treatment of spin polarization. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

**10:00AM K7.00007 First-principles identification of optically active  $Er^{3+}$  centers in GaN**, KHANG HOANG, North Dakota State University — Rare-earth (RE) doped III-nitrides are of great interest for optoelectronic and spintronic applications. The identification of optically active RE centers in these materials has however been challenging, both in experimental and theoretical/computational studies. In this talk, we present a hybrid density functional study of the interaction between the erbium (Er) dopant and wurtzite GaN, including intrinsic point defects and other impurities that may be present in the host material. Particularly, we investigate the structure, energetics, and transition levels of the Er impurity and its complexes with N and Ga vacancies, substitutional C and O impurities, and H interstitials. In light of our results, we identify possible luminescent  $Er^{3+}$  centers in Er-doped GaN and discuss the role of these centers in the excitation of the Er 4f-electron core.

**10:12AM K7.00008 Native defects in GaN: a hybrid functional study**<sup>1</sup>, IBRAHIMA CASTILLO DIALLO, DENIS DEMCHENKO, None — Intrinsic defects play an important role in the performance of GaN-based devices. We present hybrid density functional calculations of the electronic and possible optical properties of interstitial N ( $N_i - N_i$ ), N antisite ( $N_{Ga}$ ), interstitial Ga ( $Ga_i$ ), Ga antisite ( $Ga_N$ ), Ga vacancy ( $V_{Ga}$ ), N vacancy ( $V_N$ ) and Ga-N divacancies ( $V_{Ga}V_N$ ) in GaN. Our results show that the vacancies display relatively low formation energies in certain samples, whereas antisites and interstitials are energetically less favorable. However, interstitials can be created by electron irradiation. For instance, in 2.5 MeV electron-irradiated GaN samples, a strong correlation between the frequently observed photoluminescence (PL) band centered around 0.85 eV accompanied with a rich phonon sideband of ~0.88 eV and the theoretical optical behavior of interstitial Ga is discussed. N vacancies are found to likely contribute to the experimentally obtained green luminescence band (GL2) peaking at 2.24 eV in high-resistivity undoped and Mg-doped GaN.

<sup>1</sup>National Science Foundation (DMR-1410125) and the Thomas F. and Kate Miller Jeffress Memorial Trust.

**10:24AM K7.00009 Native point defects and doping in  $ZnGeN_2$** <sup>1</sup>, DMITRY SKACHKOV, WALTER LAMBRECHT, Case Western Reserve University — A computational study within the framework of density functional theory is presented for native defects and doping in  $ZnGeN_2$ . We study the three types of vacancies  $V_{Zn}$ ,  $V_{Ge}$ ,  $V_N$ , cation antisite defects  $Zn_{Ge}$ ,  $Ge_{Zn}$ , and potential n-type ( $O_N$ ,  $Ga_{Zn}$ ) and p-type  $Ga_{Ge}$  dopants. The cation antisite defects are found to have significantly lower formation energy than the cation vacancies. The charge neutrality condition pins the Fermi level close to the crossing of the  $Zn_{Ge}^{-1}$  acceptor with the  $Ge_{Zn}^{2+}$  donor, and intrinsic p-type doping would result. The  $V_N$  is found to be a rather deep donor.  $Ge_{Zn}$  is found to behave as a shallow donor. Oxygen impurities are found to strongly prefer the  $O_N$  substitutional site and are found to be shallow donors with a very low energy of formation. Energies of formation of  $Ga_{Zn}$  and  $Ga_{Ge}$  are lower than those of the cation antisites. Thus good solubility is expected and these impurities can hence pin the Fermi level at the crossing of the donor  $Ga_{Zn}^{+1}$  with the acceptor  $Ga_{Ge}^{-1}$ , and efficient p-type doping should result.

<sup>1</sup> Dmitry Skachkov was supported by the U.S. Department of Energy Basic Energy Sciences (DOE-BES) under grant No. ER-46874-SC0008933

**10:36AM K7.00010 Fluorescent Defects in Hexagonal Boron Nitride<sup>1</sup>**, ANNEMARIE L. EXARHOS, KAMERON OSER, DAVID A. HOPPER, RICHARD R. GROTE, LEE C. BASSETT, University of Pennsylvania — Mono- and few-layer hexagonal boron nitride (h-BN) can host defects whose electronic states lie deep within the bandgap, similar to the nitrogen-vacancy color center in bulk diamond. Here, we study defect creation in h-BN through irradiation and thermal annealing. We employ confocal photoluminescence (PL) imaging and spectroscopy under various excitation energies on both supported and suspended h-BN to identify and characterize the emission of isolated defect centers. Polarization- and temperature-dependent measurements of the observed PL are used to map out the electronic structure of the defects, enabling optical control of fluorescent defects in h-BN. This knowledge, coupled with the spatial confinement to 2D and the unique electrical, optical, and mechanical properties of h-BN, will enable the use of these defects for quantum sensing and other applications in quantum information processing.

<sup>1</sup>Work supported by the ARO (W911NF-15-1-0589) and NSF MRSEC (DMR-1120901).

**10:48AM K7.00011 Unique stability of neutral interstitial hydrogen in cubic BN and diamond<sup>1</sup>**, JOHN L. LYONS, Center for Functional Nanomaterials, Brookhaven National Laboratory, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara — In virtually all semiconductors and insulators, hydrogen interstitial impurities act as negative-U centers, implying that hydrogen is never stable in the neutral charge state. Using hybrid density functional calculations, which are crucial for obtaining accurate properties of defects in semiconductors, we find a different behavior for hydrogen interstitials in diamond and cubic BN. In diamond, we find that hydrogen is a very strong positive-U center, and the neutral charge state of the interstitial is stable over a Fermi-level range of more than 2 eV. In cubic BN, a III-V compound semiconductor with properties similar to diamond, we also find positive-U behavior, though over a much smaller Fermi-level range. We will discuss the electronic-structure origins of this negative-U behavior, and compare with the properties of hydrogen in other materials.

<sup>1</sup>Research done in part at the Center for Functional Nanomaterials, which is a U.S. DOE Office of Science Facility, at Brookhaven National Laboratory under Contract No. DE-SC0012704. Work at UCSB was supported by the National Science Foundation.

## Wednesday, March 16, 2016 8:00AM - 11:00AM – Session K8 DCMP: Superconductivity: Cuprates 304 -

**8:00AM K8.00001 FERMIOLOGY OF THE UNDOPED CUPRATE SUPERCONDUCTOR  $\text{Pr}_2\text{CuO}_4$** , ROSS MCDONALD, LANL, NICHOLAS BREZNAY, UC Berkeley, YOSHIHARU KROCKENBERGER, NTT, KIMBERLY MODIC, ZENGWEI ZHU, LANL, IAN HAYES, NITYAN NAIR, TONI HELM, UC Berkeley, HIROSHI IRIE, HIDEKI YAMAMOTO, NTT, JAMES ANALYTIS, UC Berkeley — Unconventional, high temperature superconductivity consistently appears in the vicinity of suppressed phase transitions, leading to the suggestion that quantum criticality is vital to the physics of these systems. A confounding factor in identifying the role of quantum criticality in the electron-doped cuprates is the competing influence of chemical doping and oxygen stoichiometry. Recent advances in molecular beam epitaxy and preparation of cuprate thin films indicate that annealing can be employed to optimize  $T_c$  via the control of apical oxygen occupancy. For  $\text{Pr}_2\text{CuO}_{4\pm\delta}$  the resulting square planar coordinated structure exhibits a 25 K superconducting transition in the absence of Cerium doping. Using these films and ultra high magnetic fields (>90 T) enables measurements of magnetic quantum oscillations – the first observation of their kind for a cuprate thin film. The oscillation frequency is consistent with the reconstructed Fermi surface of the bulk electron-doped cuprate  $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$ . Furthermore, we observe a mass enhancement, suggesting that tuning these materials via oxygen stoichiometry enables exploration of underlying quantum criticality, providing a new axis with which to explore the physics underlying the electron doped side of the cuprate phase diagram.

**8:12AM K8.00002 Single reconstructed Fermi surface pocket in an underdoped single layer cuprate superconductor**, MUN K. CHAN, National High Magnetic Field Laboratory, Los Alamos National Laboratory, R. D. MCDONALD, B. J. RAMSHAW, K. A. MODIC, National High Magnetic Field Laboratory, Los Alamos National Laboratory, N. BARISIC, Technische Universität Wien, M. GREVEN, University of Minnesota, N. HARRISON, National High Magnetic Field Laboratory, Los Alamos National Laboratory — The observation of a small reconstructed Fermi surface with quantum oscillations in bilayer  $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$  opened a path towards identifying broken symmetry states in underdoped cuprates. However, the multi-frequency spectrum of quantum oscillations and complications from bilayer coupling has rendered such an identification inconclusive. Our high resolution quantum oscillation study of the structurally simpler single layer cuprate  $\text{HgBa}_2\text{CuO}_{4+\delta}$  (Hg1201) reveal a single oscillatory component with no signatures of magnetic breakdown tunneling. From this, we conclude that the reconstructed Fermi surface of Hg1201 is comprised of only a single pocket with negligible c-axis warping. Quantitative modeling of these results allow us to determine that biaxial charge-density-wave order is responsible for Fermi surface reconstruction. We find that the characteristic reconstruction gap is a significant fraction of the pseudogap energy. ‘Criss-crossed’ uniaxial charge stripes is ruled out as a viable alternative to biaxial order within a  $\text{CuO}_2$  plane for Hg1201.

**8:24AM K8.00003 Crystal Growth and Electronic Raman Scattering Study of Model High- $T_c$  Cuprate  $\text{HgBa}_2\text{CaCu}_2\text{O}_{6+\delta}$** , LICHEN WANG, YUAN LI, XIANGPENG LUO, JIARUI LI, School of Physics, Peking University, YUAN LI'S GROUP IN ICQM TEAM — In this talk, I will report our recent progress on crystal growth of  $\text{HgBa}_2\text{CaCu}_2\text{O}_{6+x}$  (Hg1212), which possesses a simple tetragonal crystal structure and the highest ambient-pressure  $T_c$  (128 K) among all cuprate superconductors with two  $\text{CuO}_2$  sheets in the primitive cell. Improvement in single-crystal synthesis was made possible by using self-designed high-pressure furnaces and a two-layer encapsulation method, and we demonstrate that the hole concentration can be homogeneously tuned in the underdoped region by post-growth annealing. Our electronic Raman scattering experiments reveal that the maximum of the d-wave superconducting gap increases from single-layer  $\text{HgBa}_2\text{CuO}_{4+x}$  to double-layer Hg1212. In the same spectra, it is found that the characteristic energy of spin excitations, as manifested by the energy of the two-magnon signal, also increases in a nearly proportional fashion. This result is consistent with the idea that magnetic interactions are closely related to the Cooper pairing mechanism.

**8:36AM K8.00004 Effects of pressure and disorder on superconductivity in  $\text{Ti}_2\text{Ba}_2\text{Ca}_{n-1}\text{Cu}_n\text{O}_{2n+4+\delta}$  ( $n=2,3$ )**, JIAN-BO ZHANG, XIAO-JIA CHEN, Center for High Pressure Science and Technology Advanced Research, Shanghai 201203, China, VIKTOR STRUZHUKIN, Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20015, U.S.A., WENGE YANG, HO-KWANG MAO, Center for High Pressure Science and Technology Advanced Research, Shanghai 201203, China, HAI-QING LIN, Beijing Computational Science Research Center, Beijing 100089, China, YONG-CHANG MA, School of Materials Science and Engineering, Tianjin University of Technology, Tianjin 300384, China, NAN-LIN WANG, International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China — The structural, vibrational, and superconducting properties of nearly optimally doped  $\text{Ti}_2\text{Ba}_2\text{Ca}_{n-1}\text{Cu}_n\text{O}_{2n+4+\delta}$  ( $n=2,3$ ) single crystals are studied at high pressures. While the superconducting transition temperature  $T_c$  of the bilayer system exhibits a parabolic behavior with a maximum around an optimal pressure level, its increased path has a kink in the trilayer compound, indicating a joint effect from the inner  $\text{CuO}_2$  plane. The latter is further supported by the appearance of the two additional Raman modes. At higher pressures, we observe the sudden increase of the full width at half maximum of some lattice modes as well as the anomaly of the lattice parameters at certain pressure. These together contribute the enhanced disorder and the  $T_c$  reduction accordingly. We thus are able to distinguish the contribution to  $T_c$  from the intrinsic pressure variables, disorder, and the  $\text{CuO}_2$  plane number and type in this layered family.

**8:48AM K8.00005 Bulk superconductivity at 84 K in the strongly overdoped regime of cuprates**, ANDREA GAUZZI, YANNICK KLEIN, IMPMC-Sorbonne Universities, ELVEZIO MORENZONI, Paul Scherrer Institut, MIKKO NISULA, MAARIT KARP-PINEN, Aalto University, MASSIMO MAREZIO, CRESTA-CNRS, THEODORE H. GEBALLE, Stanford University — By means of magnetic susceptibility, specific heat and muon-spin relaxation ( $\mu$ SR) measurements, we report on bulk superconductivity at 84 K in high-pressure oxidized  $\text{Cu}_{0.75}\text{Mo}_{0.25}\text{Sr}_2\text{YCu}_2\text{O}_{7.54}$ . A record short apical Cu-O distance and a large excess of electronic specific heat at low temperature give evidence of hole overdoping,  $p \approx 0.43$  hole/Cu, well beyond the superconducting dome relating  $T_c$  and  $p$ , considered universally valid for cuprates, where a normal Fermi liquid behavior is expected. On the other hand, the superfluid density measured by means of  $\mu$ SR is similar to that of optimally doped  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ , which indicates that the extra-holes do not contribute to superconductivity, thus leading to a phase separation between superconducting and normal carriers, or that Cooper pairs are strongly localized. In both cases, the unexpected observation of high  $T_c$  in the strongly overdoped regime constitutes a further open issue for the theoretical explanation of superconductivity in cuprates.

**9:00AM K8.00006 Enhanced Surface Superconductivity in Single Crystal  $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$** , IVAR MARTIN, Argonne National Laboratory, XIAN YANG TEE, Nanyang Technological University, Singapore, TOSHIMITSU ITO, TOMOHARU USHIYAMA, YASUhide TOMIOKA, National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan, CHRISTOS PANAGOPOULOS, Nanyang Technological University, Singapore — Surfaces of materials often possess properties which are distinctly different from their bulk. The atomic structure can develop intricate new patterns due to surface reconstruction and the electronic properties can be very distinct, as most dramatically manifested in topological insulators. However, more subtle collective phenomena such as superconductivity are not as strongly affected by the presence of surfaces. Here, we report an unprecedented finding of enhanced superconductivity at the ab-plane surface of high- $T_c$  cuprate  $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ . Spatially-resolved electrical and thermoelectric transport measurements detect a superconducting surface below the transition temperature  $T_{cs}$  which is considerably higher than the bulk  $T_c$ . The effect is pronounced in the region of charge carrier doping ( $x$ ) with strong spin-charge stripe correlations. Notably, for  $x = 0.12$ ,  $T_{cs}$  reaches 36 K, exceeding even the highest reported bulk  $T_c$  in this material for any doping. Possible interpretations for the novel effect are discussed.

**9:12AM K8.00007 Vortex Lattice Formation in High Magnetic Fields in an Underdoped Single Crystal of Hg1201 from  $^{17}\text{O}$  NMR**, JEONGSEOP LEE, YIZHOU XIN, W. P. HALPERIN, Northwestern University, A. P. REYES, P. L. KUHN, National High Magnetic Field Laboratory — The vortex lattice in  $\text{HgBa}_2\text{CuO}_{4+\delta}$  forms at a vortex melting temperature,  $T_v$ , typically  $\sim 40\text{K}$  for underdoped crystals with a hole doping  $\sim 0.11$ . We present our results from  $^{17}\text{O}$  NMR for investigation of the vortex lattice as a function of external magnetic field up to 30 T and temperature as low as 5 K. The vortex contribution to the NMR linewidth can be separated from inhomogeneous broadening by deconvolution of the normal state spectra which was measured separately above,  $T_v$ . The vortex melting temperature was measured for two underdoped samples marked by the onset of extra linewidth broadening due to the inhomogeneous magnetic field distribution from the solid vortex lattice consistent with transverse relaxation measurements. We have found evidence for a change in the vortex lattice symmetry as a function of external fields. This work was supported by the DOE BES under grant No. DE-FG02-05ER46248 and the NHMFL through the NSF and State of Florida. [1] V. F. Mitrovic, *et al.*, Nature, **413**, 501-504 (2001).

**9:24AM K8.00008 Broken bond symmetry assists stripe pinning in superconducting  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$** <sup>1</sup>, JOHN TRANQUADA, Brookhaven Natl Lab, H. JACOBSEN, U. Copenhagen, I.A. ZALIZNYAK, M. HUECKER, G.D. GU, BNL, A.T. SAVICI, B. WINN, ORNL, S. CHANG, NCNR — There has been evidence for quite some time for some degree of charge and spin stripe order in  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  (LSCO). This has been a bit surprising as the crystal structure is supposed to lack the anisotropic Cu-O bonds that lead to robust stripe pinning in  $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ . Using neutron scattering measurements on the HYSPEC instrument at the Spallation Neutron Source, we have discovered evidence for broken bond symmetry and strong associated lattice fluctuations in an LSCO crystal with  $x = 0.07$  [1]. The broken bond symmetry occurs within the orthorhombic phase. We also observe quasielastic incommensurate spin excitations that coexist with the bulk superconductivity, suggesting some degree of pair-density-wave order in the superconducting state. [1] H. Jacobsen *et al.*, Phys. Rev. B (accepted); arXiv:1508.02429.

<sup>1</sup>Work at BNL supported by Office of Basic Energy Sciences, US DOE, under Contract No. DE-SC00112704.

**9:36AM K8.00009 Neutron scattering study of the antiferromagnetic response of  $\text{HgBa}_2\text{CuO}_{4+\delta}$** <sup>1</sup>, YANG TANG, MUN CHAN, CHELSEY DOROW, MIKE VEIT, YANG GE, MARTIN GREVEN, University of Minnesota, LUCILE MANGIN-THRO, YVAN SIDIS, PHILIPPE BOURGES, Laboratoire Louis Brillouin, France, XUDONG ZHAO, Jilin University, China, PAUL STEFFENS, Institut Laue Langevin, France, ANDREW CHRISTIANSON, DOUGLAS ABERNATHY, Oak Ridge National Laboratory, JITAE PARK, Forschungs-Neutronenquelle Heinz Maier-Leibnitz — Antiferromagnetic correlations have been argued to be the cause of the  $d$ -wave superconductivity and of the pseudogap phenomena exhibited by the cuprates. Although neutron scattering experiments of the antiferromagnetic response have been reported for a number of cuprates, results for structurally simple  $\text{HgBa}_2\text{CuO}_{4+\delta}$  (Hg1201) have begun to emerge only recently. Specifically, we have found for moderately-doped Hg1201 ( $T_c \approx 71\text{ K}$ , pseudogap temperature  $T^* \approx 305\text{ K}$ ) that the two most prominent features of the magnetic spectrum reported for other cuprates are absent: the X-shaped 'hourglass' response and the resonance mode in the superconducting state. Instead, the response of Hg1201 is Y-shaped, gapped, and significantly enhanced below  $T^*$  [1]. Here we will discuss our ongoing efforts to understand the doping dependence of the AF response in Hg1201. [1] M. K. Chan *et al.*, arXiv:1402.4517.

<sup>1</sup>Work supported by the DOE Office of Basic Energy Sciences.

**9:48AM K8.00010 Dynamics of quasiparticles and antiferromagnetic correlations in electron-doped cuprate  $\text{La}_{2-x}\text{Ce}_x\text{CuO}_{4\pm\delta}$  (LCCO)**, I. M. VISHIK, F. MAHMOOD, Z. ALPICHSEV, Massachusetts Institute of Technology, J. S. HIGGINS, R. L. GREENE, University of Maryland, N. GEDIK, Massachusetts Institute of Technology — We studied quasiparticle dynamics in thin films of the electron-doped cuprate  $\text{La}_{2-x}\text{Ce}_x\text{CuO}_4$  (LCCO) via optical pump-probe spectroscopy. In underdoped LCCO, the quasiparticle recombination dynamics imply a nodeless superconducting gap, which can be realized with  $d_{x^2-y^2}$  symmetry if a nodal hole-pocket is absent. Meanwhile, optimally doped LCCO shows recombination dynamics consistent with line nodes. Above  $T_c$ , fluence-dependent dynamics indicate a fully-formed gap in the density of states, which is associated with antiferromagnetic correlations, and limits can be placed on the correlation length and time.

**10:00AM K8.00011 A close look at antiferromagnetic phase boundary in multidimensional phase diagram of electron-doped copper oxide**, HESHAN YU, GE HE, Chinese Academy of Sci (CAS), ZIQUAN LIN, Huazhong University of Science & Technology, JIE YUAN, BEIYI ZHU, YI-FENG YANG, TAO XIANG, Chinese Academy of Sci (CAS), FEO.V. KUSMARTSEV, Department of Physics, Loughborough University, LIANG LI, JUNFENG WANG, Huazhong University of Science & Technology, KUI JIN, Chinese Academy of Sci (CAS) — In copper-oxide superconductors, spin fluctuations play a predominant role in electron pairing with electron dopants yet composite orders veil the nature of superconductivity for hole-doped family. However, in electron-doped ones the ending point of AFM is still in controversy for different probes or its sensitivity to oxygen content. Here, by carefully tuning the oxygen content, a systematic study of Hall signal and magnetoresistivity up to 58 Tesla on optimally doped  $\text{La}_{2-x}\text{Ce}_x\text{CuO}_{4\pm\delta}$  ( $x = 0.10$ ) thin films identifies two characteristic temperatures at 62.5 K (error is 7.5 K) and 25 K (error is 5 K). The former is quite robust whereas the latter becomes flexible with increasing magnetic field, thereby linked to two- and three-dimensional AFM, evident from the multidimensional phase diagram as a function of oxygen as well as Ce dopants. Consequently, the observation of extended AFM phase in contrast to  $\mu\text{SR}$  probe corroborates an elevated critical doping in field, providing an unambiguous picture to understand the interactions between AFM and superconductivity.

**10:12AM K8.00012 Superconductivity and planar hole densities in the cuprates from NMR**, JUERGEN HAASE, MICHAEL JURKUTAT, University of Leipzig, DAMIAN RYBICKI, AGH University of Science and Technology — We show how nuclear magnetic resonance (NMR) of  $^{63}\text{Cu}$  and  $^{17}\text{O}$  provides a quantitative measure of the charge distribution in the ubiquitous  $\text{CuO}_2$  plane, the common structural feature of cuprate physics. The various materials are found to differ significantly in the local charge distribution, while the total charge per  $\text{CuO}_2$  matches expectation from stoichiometry. Using the local charges on Cu and O measured by NMR, a new three-dimensional cuprate phase diagram is drawn that consistently encompasses all cuprate materials. These appear ordered according to their maximum  $T_c$ . It is the sharing of the inherent Cu hole with O that sets an upper limit for  $T_c$ , and it correlates with the superfluid density measured by  $\mu\text{SR}$ , over all cuprate families.

**10:24AM K8.00013 Change of carrier density at the pseudogap critical point of a cuprate superconductor**, LOUIS TAILLEFER, SVEN BADOUX, GAEL GRISSONNANCHE, NICOLAS DOIRON-LEYRAUD, University of Sherbrooke, Sherbrooke, Canada, WOJCIECH TABIS, FRANCIS LALIBERTE, BAPTISTE VIGNOLLE, DAVID VIGNOLLES, JEROME BEARD, CYRIL PROUST, LNCMI, Toulouse, France, DOUG BONN, RUIXING LIANG, WALTER HARDY, University of British Columbia, Vancouver, Canada — The pseudogap is a central puzzle of cuprate superconductors. Its connection to the Mott insulator at low doping  $p$  remains ambiguous and its relation to the charge order that reconstructs the Fermi surface at intermediate  $p$  is still unclear. Here we use measurements of the Hall coefficient in magnetic fields up to 88 T to show that Fermi-surface reconstruction by charge order in  $\text{YBa}_2\text{Cu}_3\text{O}_y$  ends sharply at a critical doping  $p = 0.16$ , distinctly lower than the pseudogap critical point at  $p^* = 0.19$ . This shows that pseudogap and charge order are separate phenomena. We then find that the change of carrier density from  $n = 1 + p$  in the conventional metal at high  $p$  to  $n = p$  in the lightly doped regime at low  $p$  starts at  $p^*$ . This shows that pseudogap and antiferromagnetic Mott insulator are linked.

**10:36AM K8.00014 Charge order and the pseudogap in the underdoped cuprates: a quantum oscillation study**, YU-TE HSU, MATE HARTSTEIN, Cavendish Laboratory, University of Cambridge, NEIL HARRISON, MUN CHAN, KIMBERLY MODIC, Los Alamos National Laboratory, JUAN PORRAS, TOSHINAO LOEW, MATHIEU LE TACON, BERNHARD KEIMER, Max Planck Institute for Solid State Research, SUCHITRA SEBASTIAN, Cavendish Laboratory, University of Cambridge — I will present quantum oscillation results on the underdoped copper-oxide superconductors to address the question of the interplay of the charge ordered ground state with the pseudogap. Specifically we experimentally distinguish between the two cases where charge order reconstructs a large paramagnetic Fermi surface predicted by band structure, or where charge order reconstructs a truncated Fermi surface where the density of states is restricted to the nodal region, as observed in the pseudogap state.

**10:48AM K8.00015 Anomalous suppression of energy gap near the antinode in Bi2212**, ALFRED ZONG, Massachusetts Institute of Technology, SUDI CHEN, YU HE, Stanford University, MAKOTO HASHIMOTO, SLAC National Accelerator Laboratory, SHIGEYUKI ISHIDA, YOSHIYUKI YOSHIDA, AIST, Japan, ZHI-XUN SHEN, Stanford University — An energy gap holds special importance in the study of high- $T_c$  superconductors (HTSC) as it is often associated with the order parameter of complex phases in these materials. In hole-doped cuprates around optimal doping, past experiments suggest the presence of two momentum-anisotropic energy gaps originating from  $d$ -wave superconductivity and pseudogap. Here we report an anomalous energy gap suppression near the antinode in overdoped Bi2212 that persists from  $T \ll T_c$  to  $T > T_c$ . Our data imply that the suppression may not originate from pair-breaking scattering, but can be phenomenologically described by higher harmonics of a  $d$ -wave gap. It is important to uncover the origin of this suppression, which is instrumental in understanding the complex landscape of interacting order parameters in cuprate HTSCs.

## Wednesday, March 16, 2016 8:00AM - 11:00AM –

Session K9 DMP: Superlattices & Nanostructures (Wires, Dots, etc): Optical Phenomenona

305 - Andrey Kiselev, HRL Laboratories, LLC

**8:00AM K9.00001 Spin polarization and spatial texture in quantum dots**, GARNETT BRYANT, National Institute of Standards and Technology — Spins in semiconductor quantum dots (QD) are promising qubits. Zeeman-split states form two-level systems with pseudo spin 1/2. Rotations of these qubits typically use magnetic fields B. However, this pseudo spin is not the physical spin of the state. Due to confinement, strain and strong spin-orbit coupling, the physical spin can be strongly mixed and spatially varying in the QD. We use atomistic tight-binding theory for strained InAs/GaAs and strain-free GaAs/AlAs QDs to investigate the influence of strain, QD geometry and magnetic field orientation on spin polarization and spatial texturing. For electrons, with weak spin-orbit coupling, spin is almost fully polarized and nearly aligned with B. For holes, with strong spin-orbit coupling, there can be incomplete spin polarization and spin locked to the QD axis, rather than B, even for B far off the QD axis. Spatial spin texturing occurs on the atomic scale with spin flipping between nearby atoms. In the Voigt configuration, hole spin remains nearly locked locally to the QD axis, but with opposite orientation on opposite sides of the dot, creating a spin-dipole. The influence of this spin polarization and spatial texturing on spin manipulation, exchange interaction and decoherence will be discussed.

**8:12AM K9.00002 Photon Statistics of Quantum Dot Resonance Fluorescence under the Influence of an Above Band-Gap Laser**, DISHENG CHEN, GARY LANDER, KYLE KROWPMAN, West Virginia University, GLENN SOLOMON, Joint Quantum Institute, NIST & University of Maryland, Gaithersburg, MD, EDWARD FLAGG, West Virginia University — We study the statistical behavior of resonance fluorescence from self-assembled InAs quantum dots (QDs) as a function of the density of free charge carriers introduced by an above band-gap laser. Second-order correlation measurements show bunching behavior that changes with above-band laser power and is absent in purely above-band excited emission. Resonant photoluminescence excitation spectra indicate that the QD experiences discrete spectral shifts and continuous drift due to changes in the local charge environment. These spectral changes, combined with tunneling of charges from the environment to the QD, provide an explanation of the bunching observed in the correlations.

**8:24AM K9.00003 Hole spins in quantum dot molecules: novel tuning by GaBiAs barriers**, JACKSON FLOWERS, GARNETT BRYANT, National Institute of Standards and Technology, MATTHEW DOTY, University of Delaware — Hole spins in semiconductor quantum dots (QD) are promising qubits. Tunneling in vertical quantum dot molecules (QDM) provides additional freedom to use fields to manipulate hole g-factors and induce spin mixing. Interdot barriers made from GaBiAs should provide novel opportunities to further engineer these hole spin properties, because heavy- and light-holes in GaBiAs are modified by the Bi concentration without affecting conduction electrons or split off bands. For low Bi concentrations, GaBiAs provides a lower barrier for hole tunneling, allowing hole tunneling more comparable to electron tunneling and enhancing opportunities for g-factor modification. We use atomistic tight-binding theory for InAs QDMs with GaBiAs in the interdot barrier to assess the utility of this barrier material. We model the alloy barrier regions both with the virtual crystal approximation and with random realizations of atomic configurations for the alloy region in the barrier. Results are presented for electron and hole energies in QDMs with GaBiAs barriers as a function of applied electric and magnetic fields. These results allow us to quantify g-factor modification and hole-spin mixing in asymmetric structures to show how different GaBiAs barrier configurations modify hole spin physics in QDMs.

**8:36AM K9.00004 Tunable emission from InAs quantum dots gated with graphene<sup>1</sup>**, LAURA KINNISCHTZE, University of Rochester, Department of Physics & Astronomy, KENNETH GOODFELLOW, University of Rochester, Institute of Optics, CHITRALEEMA CHAKRABORTY, University of Rochester, Materials Science, YIMING LAI, ANTONIO BADOLATO, University of Rochester, Department of Physics & Astronomy, NICK VAMIVAKAS, University of Rochester, Institute of Optics — We demonstrate Stark shifted photo-luminescence from InAs quantum dots (QD) using an n-i-Schottky diode where graphene has been used as the Schottky barrier material. This hybrid photonic device is motivated by the need for tunable single photon sources with high flux and storage capabilities. Photonic crystal nanocavities decorated with a single QD provide a rich environment for coupling spins and photons, in addition to accessing cavity quantum electrodynamic physics. Methods currently used for electrically tuning the QD inside the cavity suffer from a loss of the cavity quality factor, or high leakage currents in the diode which impacts the spin-photon coupling of the device. Our measurements are a first step towards using a graphene flake to electrically tune the emission of a strongly coupled QD-cavity system.

<sup>1</sup>NSF grant no. DMR-1309734

**8:48AM K9.00005 Electronic Structure and Optical Properties of Spectrally Uniform Nanotemplate-Directed InGaAs/GaAs Quantum Dots in Regular Arrays.<sup>1</sup>**, JIEFEI ZHANG, Dept. of Physics and Astronomy, Univ. of Southern California, SIYUAN LU, IBM Thomas J. Watson Research Center, Yorktown Heights, ANUPAM MADHUKAR, Mork Family Dept. of Chemical Engineering and Materials Science — Spectrally uniform single photon emitters in spatially regular arrays are highly sought for their potential use in quantum information processing systems. We have utilized nanotemplate-directed on-site growth of quantum dots (NTQDs) approach[1] that exploits engineered surface stress to provide preferred direction for adatom migration during growth to synthesize regular arrays of single InGaAs/GaAs QDs of controlled flat-top pyramidal shape residing on GaAs(001) nanomesa arrays[2]. The GaAs/In<sub>0.5</sub>Ga<sub>0.5</sub>As/GaAs NTQDs reported here are spectrally uniform within 5nm over 1000um<sup>2</sup>, order of magnitude better than island and colloidal quantum dots. Photoluminescence (PL) and PL excitation studies of individual NTQDs shows that first excited electron state and dense hole states are, respectively, ~40meV and ~10meV higher than ground state. Electrons escape out of QDs through thermally activated tunneling to first excited electron state, which is also manifest in the temperature-dependent behavior of the QD PL decay time. Suitability of such arrays of NTQDs as single photon emitter array will be discussed. [1] A. Konkar, et. al., Jour. Cryst. Growth, 150, 311 (1995) [2] J. Zhang et. al., Jour. Vac. Sc. Tech. B32, 02C106 (2014)

<sup>1</sup>work supported by AFOSR and ARO

**9:00AM K9.00006 Localized magnetoplasmons in quantum dots: Scrutinizing the eligibility of FIR, Raman, and electron energy-loss spectroscopies**, M. KUSHWAHA, Rice University — We report on a one-component, quasi-zero dimensional, quantum plasma exposed to a parabolic potential and an applied magnetic field in the symmetric gauge. If the size of such a system as can be realized in the semiconducting quantum dots is on the order of the de-Broglie wavelength, the electronic and optical properties become highly tunable. Then the quantum size effects challenge the observation of many-particle phenomena such as the magneto-optical absorption, Raman intensity, and electron-energy-loss spectrum. An exact analytical solution of the problem leads us to infer that these many-particle phenomena are, in fact, dictated by the generalized Kohn's theorem in the long-wavelength limit. Maneuvering the confinement and/or the magnetic field furnishes the resonance energy capable of being explored with the FIR, Raman, or electron-energy-loss spectroscopy. This implies that either of these probes should be competent in observing the localized magnetoplasmons in the system. A deeper insight into the physics of quantum dots is paving the way for their implementation in such diverse fields as quantum computing and medical imaging<sup>1</sup>. 1. M.S. Kushwaha, Unpublished.

**9:12AM K9.00007 Influence of Indium Segregation on InGa<sub>N</sub>/Ga<sub>N</sub> QD Band Alignment**, CHRISTIAN GREENHILL, ALEXANDER CHANG, JENNA WALRATH, T. FROST, P.K. BHATTACHARYA, RACHEL GOLDMAN, University of Michigan — InGa<sub>N</sub>/Ga<sub>N</sub> QD systems are promising for optoelectronic devices, such as photovoltaics, light emitters, and lasers due to their high mobility, high absorption coefficient, and direct wide bandgap. However, indium segregation within InGa<sub>N</sub> quantum structures can lead to inefficiencies in device performance and has not been investigated in InGa<sub>N</sub>/Ga<sub>N</sub> QD systems. Using scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS), we have investigated the influence of indium nanostructure on the band structure of single or multi-layered InGa<sub>N</sub>/Ga<sub>N</sub> QDs. We observe a mixture of indium mounds and QDs in the single layered InGa<sub>N</sub>/Ga<sub>N</sub> QD system, where local STS measurements suggest a gradient in indium concentration across the indium mound. Furthermore, STM imaging suggests a higher density of InGa<sub>N</sub>/Ga<sub>N</sub> QDs for multi-layered InGa<sub>N</sub>/Ga<sub>N</sub> QDs compared to that of a single layered InGa<sub>N</sub>/Ga<sub>N</sub> QDs, where STS measurements suggest indium clustering within InGa<sub>N</sub> QDs. We discuss the comparison of the band structure of InGa<sub>N</sub>/Ga<sub>N</sub> mounds vs. QD systems.

**9:24AM K9.00008 Droplet heteroepitaxy of zinc-blende vs. wurtzite Ga<sub>N</sub> quantum dots**, C REESE, S JEON, Department of Materials Science and Engineering - University of Michigan, T HILL, C JONES, Department of Physics - University of Michigan, S SHUSTERMAN, Soreq Nuclear Research Center, Y YACOBY, The Hebrew University of Jerusalem, R CLARKE, H DENG, Department of Physics - University of Michigan, RS GOLDMAN, Department of Materials Science and Engineering - University of Michigan — We have developed a Ga<sub>N</sub> droplet heteroepitaxy process based upon plasma-assisted molecular-beam epitaxy. Using various surface treatments and Ga deposition parameters, we have demonstrated polycrystalline, zinc-blende (ZB), and wurtzite (WZ) Ga<sub>N</sub> quantum dots (QDs) on Si(001), r-Al<sub>2</sub>O<sub>3</sub>, Si(111), and c-GaN substrates. For the polar substrates (i.e. Si(111) and c-GaN), high-resolution transmission electron microscopy and coherent Bragg rod analysis reveals the formation of coherent WZ Ga<sub>N</sub> QDs with nitridation-temperature-dependent sizes and densities. For the non-polar substrates (i.e. Si(001) and r-Al<sub>2</sub>O<sub>3</sub>), QDs with strong near-band photoluminescence emission are observed and ZB Ga<sub>N</sub> QD growth on Si(001) is demonstrated for the first time.

**9:36AM K9.00009 Hydrothermal Synthesis and Photoluminescence of Boron Nitride Quantum Dots**, HONGLING LI, ROLAND YINGJIE TAY, SIU HON TSANG, EDWIN HANG TONG TEO, Nanyang Tech Univ — Boron nitride quantum dots (BNQDs), as a new member of heavy metal-free quantum dots, have attracted great interest owing to its unique structure as well as fascinating physical/chemical properties. However, it is still a challenge to controllably synthesize high quality BNQDs with high quantum yield (QY), uniform size and strong luminescence. Here we present a facile and effective approach to controllably fabricate BNQDs by sputter-solvothermal technique. Encouragingly, the as-prepared BNQDs possess strong blue luminescence with high QY of up to 19.5%, which can be attributed to the synergic effect of size, surface chemistry and edge defects. In addition, the size of the BNQDs could be controlled with a narrow size distribution of 1.32 nm and the smallest average size achieved is 2.62 nm with an average thickness of ~3 atomic layers. Furthermore, the as-prepared BNQDs are non-toxic to cells and show nanosecond-scaled lifetimes and little photobleaching effect. Therefore, it is believed that BNQDs are promising as one of the novel heavy metal-free QDs for multi-purpose applications in a range of fields. Moreover, this synthesis concept is expected to open a new window to controllably prepare other heavy metal-free QDs, as well as to understand their luminescence mechanism.

**9:48AM K9.00010 Insight into Factors Affecting the Presence, Degree, and Temporal Stability of Fluorescence Intensification on ZnO Nanorod Ends**, MANPREET SINGH, Georgetown University, RUIBIN JIANG, The Chinese University of Hong Kong, DANIEL S. CHOI, Georgetown University, JIANFANG WANG, The Chinese University of Hong Kong, JONG-IN HAHM, Georgetown University, GU TEAM, CUHK TEAM — We present a combined experimental and simulation study identifying the key physical and optical parameters affecting the presence and degree of fluorescence intensification measured on zinc oxide nanorod (ZnO NR) ends. We aim to provide an insight into the unique optical phenomenon of fluorescence intensification on NR ends (*FINE*) through experimental and simulation approaches and to elucidate the key factors affecting the occurrence, degree, and temporal stability of *FINE*. Specifically, we examined the effect of the length, width, and growth orientation of single ZnO NRs on the NR-enhanced biomolecular emission profile after decorating the NR surfaces with different amounts and types of fluorophore-coupled protein molecules. We quantitatively and qualitatively profiled the biomolecular fluorescence signal from individual ZnO NRs as a function of both position along the NR long axis and time. Additionally, we employed finite-difference time-domain methods to examine both near- and far-field emission characteristics when considering various scenarios of fluorophore locations, polarizations, spectroscopic characteristics, and NR dimensions. Our efforts may provide a deeper insight into the unique optical phenomenon of *FINE* and further be beneficial to highly miniaturized biodetection favoring the use of single ZnO NRs.

**10:00AM K9.00011 Scattering Intensity and Directionality Probed Along Individual Semiconducting Oxide Nanorods with Precisely Controlled Light Polarization and Nanorod Orientation**, DANIEL S. CHOI, MANPREET SINGH, JONG-IN HAHM, Georgetown University — We elucidate the light-matter interaction properties of individual semiconducting oxide nanorods (NRs) with a monochromatic beam of linearly polarized light that scatters elastically from the NRs by performing forward scattering in a dark-field setting. Specifically, individual NRs of ZnO, SnO<sub>2</sub>, ITO, and ZTO are probed. We precisely control the electric field vector of the incident light and the NR orientation within the plane of light interaction, and spatially resolve the scattering response from different interaction points along the NR long axis. We then discern the effects of light polarization, analyzer angle, and NR orientation on the intensity and directionality of the optical responses both qualitatively and quantitatively along the length of the single NRs. We identify distinctive, forward scattering profiles from individual NRs subject to various incident light polarizations and NR orientations. Fundamental light interaction behavior of the NRs is likely to govern their functional outcomes in photonics, optoelectronics, and sensor devices. Hence, our efforts providing much needed insight into unique optical responses from individual 1D semiconducting oxide nanomaterials can be highly beneficial in developing next-generation optoelectronic systems and optical biodetectors with improved device efficiency and sensitivity.

**10:12AM K9.00012 Exploring the Nature of Exciton Localization in Quasi One-Dimensional GaAs/AlGaAs Quantum Well Tube Nanowires<sup>1</sup>**, HOWARD JACKSON, BEKELE BADADA, TENG SHI, LEIGH SMITH, Department of Physics, University of Cincinnati, CHANGLIN ZHENG, Monash Centre for Electron Microscopy, Monash University, JOANNE ETHERIDGE, Monash Centre for Electron Microscopy and Department of Materials Engineering, Monash University, NIAN JIANG, HOE TAN, CHANNUPATI JAGADISH, Department of Electronic Materials Engineering, Australian National University — We explore the nature of exciton localization in single GaAs/AlGaAs nanowire quantum well tube (QWT) devices using photocurrent (PC) spectroscopy combined with simultaneous photoluminescence (PL) and photoluminescence excitation (PLE) measurements. Excitons confined to GaAs quantum well tubes of 8 and 4 nm widths embedded into an AlGaAs barrier are seen to ionize at high bias. Spectroscopic signatures of the ground and excited states confined to the QWT seen in PL, PLE and PC data are consistent with simple numerical calculations. The demonstration of good electrical contact with the QWTs enables the study of Stark effect shifts in the sharp emission lines of excitons localized to quantum dot-like states within the QWT. Atomic resolution cross-sectional TEM measurements, an analysis of the temperature dependence of PL and time-resolved PL as well as the quantum confined Stark effect of these dots provide insights into the nature of the exciton localization in these nanostructures.

<sup>1</sup>We acknowledge the financial support of NSF DMR 1507844, DMR 151373 and ECCS 1509706 and the Australian Research Council.

**10:24AM K9.00013 Surface sensitivity to dielectric environment of optical and magneto-optical properties in magnetoplasmonic nanodisks**, CÉSAR AURELIO HERREÑO-FIERRO<sup>1</sup>, Universidad Distrital F. J. de C., EDGAR J. PATINO, Universidad de los Andes, GASPAS ARMELLES, ALFONSO CEBOLLADA, Instituto de Microelectrónica de Madrid (CNM-CSIC) — The optical, ellipsometric and magneto-optical surface sensitivity to dielectric environment of magnetoplasmonic nanodisks is experimentally studied. Here the shift of the corresponding spectral structures as a function of the thickness of a coating SiO<sub>2</sub> layer is characterized. Our results reveal that the so called pseudo-Brewster Angle, easily identified in the ellipsometric phase ( $\Delta$ ) spectrum, is up to four times more sensitive than the conventional features used in Surface Plasmon Resonance (SPR) based sensors. These results highlight the need of investigating the factual implementation of this technique to develop improved ellipsometric-phase based transducers for bio-chemical sensing purposes.

<sup>1</sup>Email: caherrenof@udistrital.edu.co

**10:36AM K9.00014 Size and Morphology Dependent Raman Scattering**, XIANGHUA ZENG, CHUAN HU, JIEYA CUI, Yangzhou Univ — Through thermal evaporation, ripple-like CdS nanobelts (NBs) and ZnS:Al nanowires (NWs) were prepared. Room-temperature photoluminescence spectra showed two luminescence peaks at approximately 513 and 725 nm from the ripple-like CdS NBs, the two peaks can be ascribed to the near band gap transition and defect emissions, respectively. Raman spectra showed that the intensities of the longitudinal optical (LO) phonon and its replica peaks from the ripple-like CdS NBs are more than 4 times larger than those from the normal CdS NBs. The Huang–Rhys parameter *S* calculated from the intensity ratio of the 2LO to 1LO phonon increases from 3.21 to 3.56 for normal and ripple-like NBs, which is indicative of a strong exciton-phonon coupling interaction dominated mainly by a Fröhlich interaction through the charge transfer. The results from the ZnS:Al NWs exhibited that the morphology of ZnS:Al NWs greatly influences on the Raman scattering, while the Al-dopant concentration has a smaller effect on the Raman scattering. The Raman scattering intensity of the pine leaf-like morphological ZnS:Al NWs displayed more than eight times larger than the bulk one, which can be explained as a polarization dependent behavior and a multiple scattering.

**10:48AM K9.00015 Multiple-pulse superradiance from an optically induced harmonic confinement in a semiconductor microcavity**<sup>1</sup>, CHIH WEI LAI<sup>2</sup>, WEI XIE<sup>3</sup>, FENG-KUO HSU, Michigan State University, YI-SHAN LEE, SHENG-DI LIN, National Chiao Tung University — We report the observation of macroscopic harmonic states in an optically induced confinement in a highly photoexcited semiconductor microcavity at room temperature. The spatially photomodulated refractive index changes result in the visualization of harmonic states in a micrometer-scale optical potential at quantized energies up to 4 meV even in the weak-coupling plasma limit. We characterize the time evolution of the harmonic states directly from the consequent pulse radiation and identify sequential multiple  $\sim 10$  ps pulse lasing with different emitting angles and frequencies. Such multiple-pulse coherent radiation is attributed to superradiance from correlated electron-hole pairs in a high-density plasma.

<sup>1</sup>This work is supported by NSF grant DMR-09055944.

<sup>2</sup>Current address: US Army Research Laboratory

<sup>3</sup>Current address: East China Normal University

**Wednesday, March 16, 2016 8:00AM - 11:00AM —**

**Session K11 DMP GMAG: Electronic Structure and Magnetism in Fe-based Superconductors**

**II** 307 - Emilia Morosan, Rice University

**8:00AM K11.00001 Orbital-dependent electron correlation effects in iron-based superconductors**, MING YI, Univ of California - Berkeley — The iron chalcogenide superconductors constitute arguably one of the most intriguing families of the iron-based high temperature superconductors given their ability to superconduct at comparable temperatures as the iron pnictides, despite the lack of similarities in their magnetic structures and Fermi surface topologies. In particular, the lack of hole Fermi pockets at the Brillouin zone center posts a challenge to the previous proposal of spin fluctuation mediated pairing via Fermi surface nesting. In this talk, using angle-resolved photoemission spectroscopy measurements, I will present evidence that show that instead of Fermi surface topology, strong electron correlation observed in electron bandwidth is an important ingredient for superconductivity in the iron chalcogenides. Specifically, I will show i) there exists universal strong orbital-selective renormalization effects and proximity to an orbital-selective Mott phase in  $\text{Fe}_{1+y}\text{Te}_{1-x}\text{Se}_x$ ,  $\text{A}_x\text{Fe}_{2-y}\text{Se}_2$ , and monolayer FeSe film on  $\text{SrTiO}_3$  [1,2], and ii) in  $\text{Rb}_x\text{Fe}_2(\text{Se}_{1-x}\text{S}_x)_2$ , where sulfur substitution for selenium continuously suppresses superconductivity down to zero, little change occurs in the Fermi surface topology while a substantial reduction of electron correlation is observed in an expansion of the overall bandwidth, implying that electron correlation is one of the key tuning parameters for superconductivity in these materials. [1] M. Yi et al. Phys. Rev. Lett. 110, 067003 (2013). [2] M. Yi et al. Nat. Comm. 6, 7777 (2015). [3] M. Yi et al. arXiv: 1505.06636.

**8:36AM K11.00002 Bandwidth-controlled metal-superconductor-insulator phase diagram in iron-chalcogenides**, XIAOHAI NIU, SUDI CHEN, JUAN JIANG, ZIRONG YE, TIANLUN YU, DIFEI XU, MIN XU, YU FENG, YAJUN YAN, BINPING XIE, JUN ZHAO, Fudan University, DACHUN GU, LILING SUN, Institute of Physics, Chinese Academy of Sciences, QIANHUI MAO, HANGDONG WANG, MINGHU FANG, Zhejiang University, C. J. ZHANG, High Magnetic Field Laboratory, Chinese Academy of Sciences and University of Science and Technology of China, J. P. HU, Institute of Physics, Chinese Academy of Sciences, ZHE SUN, National Synchrotron Radiation Laboratory, University of Science and Technology of China, DONGLAI FENG, Fudan University — Using angle-resolved photoemission spectroscopy, we studied isovalently doped  $\text{K}_{x-y}\text{Fe}_{2-z}\text{Se}_{2-z}\text{S}_z$ ,  $\text{Rb}_{x-y}\text{Fe}_{2-z}\text{Te}_{2-z}\text{S}_z$  and  $(\text{Ti,K})_{x-y}\text{Fe}_{2-z}\text{Se}_{2-z}\text{S}_z$ , in which the superconducting transition temperature decreases with either positive or negative chemical pressures. The bandwidths of Fe 3d bands in the energy window of [0, -0.5] eV in these materials change systematically with doping: with the decreasing of bandwidth, the ground state evolves from a metal to a superconductor, and eventually to an insulator. This systematic study of electronic structures discovered the correlation-driven insulator state by tuning the bandwidth, which is independent with carrier density. The results also indicate that moderate correlation strength is beneficial to enhance superconductivity.

**8:48AM K11.00003 ARPES investigation of heavily hole-doped Fe-based superconductor  $(\text{Ba,K})\text{Fe}_2\text{As}_2$** , XUN SHI, PIERRE RICHARD, PENG ZHANG, AMBROISE VAN ROEKEGHEM, TIAN QIAN, JIANGPING HU, HONG DING, Chinese Academy of Sci (CAS), DELONG FANG, HAIHU WEN, Nanjing University, NAN XU, MING SHI, Paul Scherrer Institut, TIMUR KIM, MORITZ HOESCH, Diamond Light Source, XIANHUI CHEN, University of Science and Technology of China, PHOTOELECTRON SPECTROSCOPY RESEARCH TEAM, NANJING UNIVERSITY COLLABORATION, PAUL SCHERRER INSTITUT COLLABORATION, DIAMOND LIGHT SOURCE COLLABORATION, UNIVERSITY OF SCIENCE AND TECHNOLOGY OF CHINA COLLABORATION — A Lifshitz transition occurs in the  $(\text{Ba,K})\text{Fe}_2\text{As}_2$  family upon K doping and electron pocket are absent in the heavily doped compounds, including  $\text{KFe}_2\text{As}_2$ . The pairing symmetry is argued to undergoes a phase transition due to the existence of gap node(s) reported in various experiments. In this work we present angle-resolved photoemission spectroscopy and scanning tunneling spectroscopy studies of  $\text{KFe}_2\text{As}_2$ . We observe a van Hove singularity (vHs) in proximity of the Fermi level ( $E_F$ ), which locates in the middle of the principal axes of the first Brillouin zone. The density-of-states at  $E_F$  mainly comes from the vHs whereas it is non-gapped in the superconducting state. Our observation provides natural explanations for many novel behaviors in this material. In particular, it is consistent with our measurements of the gap structure in  $\text{Ba}_{0.1}\text{K}_{0.9}\text{Fe}_2\text{As}_2$ . All these results suggest that Cooper pairing is induced by a strong-coupling mechanism.

**9:00AM K11.00004 Persistence of Dirac Node near Antiferromagnetic-to-Superconducting Phase Boundary in  $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$** , HITOSHI TAKITA, NAOYA KISHIMOTO, YOUSUKE NAKASHIMA, Hiroshima University, AKIHIRO INO, MASASHI ARITA, HIROHUMI NAMATAME, MASAKI TANIGUCHI, Hiroshima Synchrotron Radiation Center, YOSHIHIRO AIURA, IZUMI HASE, HIROSHI EISAKI, KUNIHITO KIHOU, CHUL-HO LEE, AKIRA IYO, National Institute of Advanced Industrial Science and Technology, MASAMICHI NAKAJIMA, Osaka University, SHIN-ICHI UCHIDA, University of Tokyo, HIROSHIMA UNIVERSITY TEAM, HIROSHIMA SYNCHROTRON RADIATION CENTER TEAM, NATIONAL INSTITUTE OF INDUSTRIAL SCIENCE AND TECHNOLOGY TEAM, OSAKA UNIVERSITY TEAM, UNIVERSITY OF TOKYO TEAM — Since the ground state of iron-pnictides changes from an antiferromagnetic (AF) phase to a superconducting (SC) phase, the evolution of electronic structure has attracted much attention. However, systematic investigation has been hindered by the intricate multiple bands arising from the orbital degree of freedom of iron 3d states. Here we performed a polarization-dependent ARPES study of  $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$  across the AF-SC phase boundary. The doping-dependence of ARPES spectra has shown that the Dirac node reported in the AF phase of  $\text{BaFe}_2\text{As}_2$  persists in  $x = 0.04$  near the AF-SC phase boundary, and that it disappears in the SC phase of  $x = 0.05$ . We parametrized the cone-like dispersion in  $x = 0.04$ . The polarization-dependence of our ARPES spectra is consistent with the view that the Dirac node is protected by Berry phase arising from orbital degree of freedom under the inversion symmetry.

**9:12AM K11.00005 orbital selective correlation reduce in collapse tetragonal phase of  $\text{CaFe}_2(\text{As}_{0.935}\text{P}_{0.065})_2$  and electronic structure reconstruction studied by angle resolved photoemission spectroscopy**, LINGKUN ZENG, Chinese Academy of Sci (CAS) — We performed an angle-resolved photoemission spectroscopy (ARPES) study of the  $\text{CaFe}_2(\text{As}_{0.935}\text{P}_{0.065})_2$  in the collapse tetragonal(CT) phase and uncollapse tetragonal(UCT) phase. We find in the CT phase the electronic correlation dramatically reduces respectively to UCT phase. Meanwhile, the reduction of correlation in CT phase show an orbital selective effect: correlation in  $d_{xy}$  reduces the most, and then  $d_{xz/yz}$ , while the one in  $d_{z^2-r^2}$  almost keeps the same. In CT phase, almost all bands sink downwards to higher binding energy, leading to the hole like bands around Brillouin zone(BZ) center sink below  $E_F$  compared with UCT phase. However, the electron pocket around Brillouin Zone(BZ) corner(M) in UCT phase, forms a hole pocket around BZ center(Z point) in CT phase. Moreover, the  $d_{xy}$  exhibits larger movement down to higher binding energy, resulting in farther away from  $d_{yz/xz}$  and closer to  $d_{xy}$ . We propose the electron filling, namely high spin state in UCT phase to low spin state in CT phase(due to competing between crystal structure field and Hund's coupling), other than the Fermi surface nesting might be responsible for the absent of magnetic ordering.

**9:24AM K11.00006 Effect of directional strain on the phase diagram of  $\text{Ca}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$** , A. E. BÖHMER, G. DRACHUK, M. A. TANATAR, S. L. BUD'KO, R. PROZOROV, P. C. CANFIELD, Ames Laboratory and Iowa State University — The iron-based superconductor  $\text{Ca}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$  is exceptionally sensitive to directional stress with *ab*-plane compression stabilizing and *c*-axis compression de-stabilizing the orthorhombic antiferromagnetic phase [1]. Due to differential thermal expansion between a sample and a substrate, an effective in-plane compressive strain can be exerted on it upon cooling. We found that this strain induces a phase transition even in overdoped compositions where the usual magneto-structural transition, observed in underdoped compounds, does not occur in the unstrained state. The induced transition has been characterized by 4-probe resistivity, elastoresistivity (the derivative of resistivity with respect to deformations), polarized light microscopy and Mössbauer spectroscopy. We found a pronounced increase of the resistivity and a divergence of the elastoresistivity coefficients, which is a signature of the tetragonal-to-orthorhombic transition in other iron-based superconductors. The polarized light images directly show the formation of a particularly rich domain pattern below the transition in these samples. This work was supported by the Ames Laboratory, US DOE, under Contract No. DE-AC02-07CH11358. [1] Bud'ko et al., PRB 88,064513 (2013).

**9:36AM K11.00007 Quantum fluctuations in iron-pnictide superconductor  $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$** , LEI SHU, Z. F. DING, J. ZHANG, C. TAN, K. HUANG, Fudan University, Shanghai, China, L. LIU, S. CHEUNG, Y. J. UEMURA, Columbia University, D. E. MACLAUGHLIN, University of Riverside, O. O. BERNAL, California State University, Los Angeles, P.-C. HO, California State University, Fresno, D. HU, Chinese Academy of Sciences, P.C. DAI, Rice University — Muon-spin-relaxation/rotation ( $\mu\text{SR}$ ) experiments were performed on single crystals of iron-pnictide superconductors  $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$  ( $x = 0.28, 0.30$ , and  $0.33$ ). Our preliminary results reveal that the static muon relaxation rate from ZF- $\mu\text{SR}$  measurements is temperature independent through  $T_c$ , suggesting that time reversal symmetry is preserved in the superconducting state. Above  $T_c$ , the field dependence of muon relaxation rate shows NFL behaviors for optimal composition  $x = 0.3$ . A maximum of zero temperature penetration depth at  $x = 0.3$  is also observed.

<sup>1</sup>This work was supported by Chinese NSF, grant 1147060, US NSF, grant DMR-1506677 and DMR-1105380.

**9:48AM K11.00008 Soft-mode transitions of alkaline-earth 122 pnictides<sup>1</sup>**, MICHAEL WIDOM, Carnegie Mellon University, KHANDKER QUADER, Kent State University — A-122 pnictides (A=Ca, Sr, Ba) exhibit three pressure-driven transitions: a first order enthalpic transition at  $P_H$  from the striped AFM orthorhombic (OR) to a tetragonal (T) or a collapsed tetragonal (cT) phase; a transition at  $P_M > P_H$  from the metastable AFM OR to a T or cT phase; a Lifshitz transition at  $P_L$  that causes T to collapse to a cT phase. Transitions at  $P_H$  and  $P_L$  were previously examined through total energy and band structure calculations<sup>23</sup>. Here we address the transition at  $P_M$ , beyond which the metastable AFM OR state ceases to exist. We show this transition occurs through a loss of elastic stability caused by softening of a shear mode associated with stretching along the *c*-axis. Simultaneously, magnetism and orthorhombicity approach limiting values with an approximately square-root singularity<sup>4</sup>. Together these suggest a strong magneto-elastic coupling that may be relevant to a further understanding of the A-122-pnictides under pressure.

<sup>1</sup>This work was supported in part by the DOE under grant DE-SC0014506

<sup>2</sup>M. Widom and K. Quader, Phys. Rev. B 88, 045117 (2013)

<sup>3</sup>K. Quader and M. Widom, Phys. Rev. B 90, 144512 (2014)

<sup>4</sup>M. Widom and K. Quader, arXiv:1508.07932

**10:00AM K11.00009 Correlation driven dimensional reduction in a two orbital Hubbard model**, ANAMITRA MUKHERJEE, University of Tennessee, Knoxville, Tennessee 37996, USA, National Institute of Science Education and Research, India, NIRAVKUMAR D. PATEL, ADRIANNA MOREO, ELBIO DAGOTTO, University of Tennessee, Knoxville, Tennessee 37996, USA — We apply a recently developed many-body technique that allows for the incorporation of thermal effects, to a two orbital Hubbard model of relevance for the pnictides. In this Mean Field-Monte Carlo (MF-MC) approach, we first perform a mean field (MF) decomposition of the Hubbard model and then treat the mean field parameters via the standard finite-temperature classical Monte Carlo (MC). We have earlier established [1] that for the one orbital Hubbard model, this MF-MC approach provides remarkable improvement over simple finite-temperature mean field methods and is in good agreement with Determinantal Quantum Monte Carlo results. In this talk we will discuss our MC-MF results applied to the two orbital Hubbard model with degenerate  $dxz$  and  $dyz$  orbitals for the undoped pnictides [2]. The onsite repulsion strength  $U$  vs. temperature phase diagram is rich and has a narrow window of nematicity above the Neel temperature. Our main result is the discovery of a novel intermediate coupling regime characterized by an unexpected spontaneous dimensional reduction that renders one direction insulating and the other metallic. [1] A. Mukherjee, et. al. Phys. Rev. B 90, 205133 (2014). [2] A. Mukherjee, et. al. arXiv:1510.04902

**10:12AM K11.00010 Testing The Constrained-Path Quantum Monte Carlo Method Using A One Dimensional Three Orbital Hubbard Model.**, GUANGKUN LIU, Univ of Tennessee, Knoxville and Beijing Normal University, NITIN KAUSHAL, Univ of Tennessee, Knoxville, CHRIS BISHOP, SHUHUA LIANG, Univ of Tennessee, Knoxville and ORNL, SHAOZHI LI, STEVE JOHNSTON, Univ of Tennessee, Knoxville, ELBIO DAGOTTO, Univ of Tennessee, Knoxville and ORNL — The “sign problem” usually prevents the large scale quantum Monte Carlo simulations of the multi-orbital Hubbard models. Projecting from a variety of initial states constructed via the Hartree-Fock technique, a constrained-path quantum Monte Carlo [1] (CPQMC) simulation has been carried out for the full one-dimensional three-orbital Hubbard model [2] and also for the same model but neglecting the pair-hopping and spin-flip interactions. The corresponding phase diagrams varying electronic density  $n$  and Hubbard  $U$  are constructed. Extensive comparisons with density matrix renormalization group and determinant quantum Monte Carlo results demonstrate that CPQMC is capable of capturing the physics of the orbital-selective Mott phase [2,3]. Our results also suggest that the spin-flip and pair-hopping interactions only have a limited effect on multi-orbital Hubbard model phase diagrams. [1] Guangkun Liu, Zhongbing Huang, and Yongjun Wang, J. Phys.: Condens. Matter 26, 325601(2014) [2] Julian Rincon, Adriana Moreo, Gonzalo Alvarez, and Elbio Dagotto, Phys. Rev. Lett. 112 106405 (2014) [3] Julian Rincon, Adriana Moreo, Gonzalo Alvarez, and Elbio Dagotto, Phys. Rev. B 90 241105(R)(2014)

**10:24AM K11.00011 Density Matrix Renormalization Group Study of a One Dimensional Three-Orbital Hubbard Model: The role of pair hopping and spin-flip interactions.** , NITIN KAUSHAL, GUANGKUN LIU, CHRIS BISHOP, SHUHUA LIANG, SHAOZHI LI, STEVE JOHNSTON, Department of Physics and Astronomy, The University of Tennessee, Knoxville, ELBIO DAGOTTO, Department of Physics and Astronomy, The University of Tennessee, Knoxville and Oak Ridge National Laboratory — Using the Density Matrix Renormalization Group technique, we extensively study a three-orbital Hubbard model in one dimension without pair hopping and spin-flip Hund interactions. The phase diagram varying the electronic density  $n$  and Hubbard  $U$  is constructed and compared against previous results obtained using the full interaction Hamiltonian [1]. Our results suggest that spin-flip and pair hopping terms are not crucially important to address the orbital-selective Mott phase [1]. This analysis paves the way to study multiorbital Hubbard models using techniques such as the Constrained-Path Quantum Monte Carlo (CPQMC) and Determinant Quantum Monte Carlo (DQMC) methods since they perform better, reducing for instance the severity of the “sign problem”, in the absence of pair hopping and spin flip terms in the interaction.

[1] Julian Rincon et al., *Phys. Rev. Lett.* **112**, 106405 (2014), Julian Rincon et al., *Phys. Rev. B* **90**, 241105 (2014)

replacing MAR16-2015-020199

**10:36AM K11.00012 Doping Evolution of Electronic Properties of FeSe/SrTiO<sub>3</sub> Films** , BING SHEN, YONG HU, DEFA LIU, JIANWEI HU, Department of Physics, Chinese Academy of Sciences, LILI WANG, XUCUN MA, QIKUN XUE, Department of Physics, Tsinghua University, CHUANGTIAN CHEN, ZUYAN XU, Technical Institute of Physics and Chemistry, ZHOU, Institute of Physics, Chinese Academy of Sciences — The latest discovery of high-temperature superconductivity in FeSe has attracted extensive attention. Our previous ARPES studies on the single-layer and double-layer FeSe/SrTiO<sub>3</sub> films from N-phase to S phase by vacuum annealing and get superconductivity in the S phase. Here we report on the doping evolution of electronic properties of double-layer FeSe/SrTiO<sub>3</sub> films doped and it remains in the semiconducting/insulating state. We will present our new ARPES results on the FeSe/SrTiO<sub>3</sub> films with different layers (1UC, 2UC, 3UC) by potassium deposition, to increase the carrier concentration. As the result, we observed the evolution of electronic properties with different layers. This systematic study will provide insight in understanding the evolution of electronic properties from multiple-layer FeSe film and eventually to the bulk FeSe superconductor.

and MAR16-2015-004498

**10:48AM K11.00013 Electronic structure and lattice dynamics at the interface of single layer FeSe and SrTiO<sub>3</sub>**<sup>1</sup> , TOWFIQ AHMED, Los Alamos Natl Laboratory, ALEXANDER BALATSKY, Los Alamos Natl Lab and Nordita, JIAN-XIN ZHU, Los Alamos National Laboratory — Recent discovery of high-temperature superconductivity with the superconducting energy gap opening at temperatures close to or above the liquid nitrogen boiling point in the single-layer FeSe grown on SrTiO<sub>3</sub> has attracted significant interest. It suggests that the interface effects can be utilized to enhance the superconductivity. It has been shown recently that the coupling between the electrons in FeSe and vibrational modes at the interface play an important role. Here we report on a detailed study of electronic structure and lattice dynamics in the single-layer FeSe/SrTiO<sub>3</sub> interface by using the state-of-art electronic structure method within the density functional theory. The nature of the vibrational modes at the interface and their coupling to the electronic degrees of freedom are analyzed. In addition, the effect of hole and electron doping in SrTiO<sub>3</sub> on the electron-mode coupling strength is also considered. [1] Q. Y. Wang et al., *Chin. Phys. Lett.* **29**, 037402 (2012); [2] Jian-Feng Ge et al., *Nature Mater.* **14**, 285 (2014).

<sup>1</sup>This work was carried out under the auspices of the National Nuclear Security Administration of the U.S. DOE at LANL under Contract No. DE-AC52-06NA25396, and was supported by the DOE Office of Basic Energy Sciences.

## Wednesday, March 16, 2016 8:00AM - 11:00AM — Session K12 DCMP: Topological Insulators: Towards Applications 308 -

**8:00AM K12.00001 Plasmon-enhanced electron-phonon coupling in Dirac surface states of the thin-film topological insulator Bi<sub>2</sub>Se<sub>3</sub>** , YURI D. GLINKA, SERCAN BABAKIRAY, DAVID LEDERMAN, West Virginia University — Raman measurements of a Fano-type surface phonon mode associated with Dirac surface states (SS) in Bi<sub>2</sub>Se<sub>3</sub> topological insulator thin films allowed an unambiguous determination of the electron-phonon coupling strength in Dirac SS as a function of film thickness ranging from 2 to 40 nm. A non-monotonic enhancement of the electron-phonon coupling strength with maximum for the 8-10 nm thick films was observed. The non-monotonicity is suggested to originate from plasmon-phonon coupling which enhances electron-phonon coupling when free carrier density in Dirac SS increases with decreasing film thickness and becomes suppressed for thinnest films when anharmonic coupling between in-plane and out-of-plane phonon modes occurs. The observed about four-fold enhancement of electron-phonon coupling in Dirac SS of the 8-10 nm thick Bi<sub>2</sub>Se<sub>3</sub> films with respect to the bulk samples may provide new insights into the origin of superconductivity in this-type materials and their applications.

**8:12AM K12.00002 Inverse spin-galvanic effect in topological-insulator graphene heterostructures.**<sup>1</sup> , MARTIN RODRIGUEZ-VEGA, The College of William and Mary , GEORG SCHWIETE, JAIRO SINOVA, Institut für Physik, Johannes Gutenberg Universität Mainz, ENRICO ROSSI, The College of William and Mary — We study theoretically the inverse spin-galvanic effect in heterostructures formed by a layer of a three dimensional strong topological insulator (TI) and a graphenic layer (single layer graphene, and bilayer graphene). We also consider trilayer structures in which a ferromagnetic thin film is added on top of the graphenic layer. We consider the cases of coherent, and random tunneling between states in the TI and the graphenic layer. We obtain the strength of the inverse spin-galvanic effect, taking into account both intraband and interband contributions, as a function of the system's parameters both for the case in which the disorder is short-range and for the case in which the disorder is long-range as when charge impurities are the dominant source of disorder. We find that for a large range of system's parameters the presence of the graphenic layer enhances the strength of the inverse spin-galvanic effect. Finally, we discuss the relevance of our results for recent experiments.

<sup>1</sup>Work supported by ONR-N00014-13-1-0321 and NSF-DMR-1455233.

**8:24AM K12.00003 Non-local magnetoelectric effects via Coulomb interaction in TI-FMI heterostructures<sup>1</sup>**, STEFAN REX, Department of Physics, Norwegian University of Science and Technology, FLAVIO S. NOGUEIRA, IFW Dresden, and Ruhr-Universität Bochum, ASLE SUDBØ, Department of Physics, Norwegian University of Science and Technology — Magnetic order on the surface of a 3D topological insulator (TI) has been predicted to evoke a topological magnetoelectric effect (TME) by the breaking of time-reversal invariance. In the TME, an electric field leads to a magnetic polarization in the same direction as the field and vice versa. Here, we consider heterostructures of TI and ferromagnetic insulator (FMI) layers. We show that in the presence of long-range Coulomb interactions the magnetization couples non-locally to the fluctuating electric field (non-local TME) by performing a field-theoretic calculation of the vacuum polarization. In addition, we obtain a Landau-Lifshitz equation for the magnetization dynamics, and find that charged magnetic textures lead to a net magnetization even at a large distance. Such textures can be induced by an external electric field with nonzero in-plane divergence. We apply this effect to a FMI-TI-FMI trilayer heterostructure with two parallel interfaces being well-separated by the bulk TI, where we propose to non-locally control the magnetic texture at one interface by proper gating of the other interface. A preprint can be found at arXiv:1510.04285

<sup>1</sup>Supported by the Norwegian Research Council, Grants 205591/V20 and 216700/F20, and the Collaborative Research Center SFB 1143 "Correlated Magnetism: From Frustration to Topology"

**8:36AM K12.00004 Electric field induced quantum anomalous Hall effect in two-dimensional antiferromagnetic triphenyl-lead lattice**, HYUN-JUNG KIM, Korea Inst for Advanced Study, CHAOKAI LI, International Center for Quantum Materials, Peking University, JI FENG, Peking University, ZHENYU ZHANG, University of Science and Technology of China, JUN-HYUNG CHO, Hanyang University — The tuning of topological states is of significant fundamental and practical importance in contemporary condensed matter physics, for which the extension to two-dimensional (2D) organometallic systems is particularly attractive.[1] Using first-principles calculations, we find that a 2D hexagonal triphenyl-lead lattice composed of only main group elements is susceptible to a magnetic instability, characterized by an antiferromagnetic (AFM) insulating state with a renormalized valley gaps with gap difference of 24 meV due to the spin and valley coupling. This AFM state will be subject to a anomalous valley Hall effect under the action of Berry curvature-induced spin and valley currents via, for example, injection of circularly polarized light.[2] Furthermore, such a AFM band insulator can be tuned into a topologically nontrivial quantum anomalous Hall state with a Chern number of one by the application of an out-of-plane electric field. These findings further enrich our understanding of 2D hexagonal organometallic lattices for potential applications in spintronics and valleytronics. [1] M. Z. F. Wang, Z. Liu, and F. Liu, Nat. Comm. 4, 1471 (2013) [2] X. Li, T. Cao, Q. Niu, J. Shi, and J. Feng, Proc. Natl. Acad. Sci. 110, 2738 (2012)

**8:48AM K12.00005 A generalized spin diffusion equation with four electrochemical potentials for channels with spin-orbit coupling<sup>1</sup>**, SHEHRIN SAYED, Electrical and Computer Engineering, Purdue University, West Lafayette, IN 47907, SEOKMIN HONG, Intel Corporation, SUPRIYO DATTA, Electrical and Computer Engineering, Purdue University, West Lafayette, IN 47907 — We will present a general semiclassical theory for an arbitrary channel with spin-orbit coupling (SOC) [1], that uses four electrochemical potential ( $U+$ ,  $D+$ ,  $U-$ , and  $D-$ ) depending on the sign of  $z$ -component of the spin (up ( $U$ ), down ( $D$ )) and the sign of the  $x$ -component of the group velocity ( $+$ ,  $-$ ). This can be considered as an extension of the standard spin diffusion equation [2] that uses two electrochemical potentials for up and down spin states, allowing us to take into account the unique coupling between charge and spin degrees of freedom in channels with SOC. We will describe applications of this model to answer a number of interesting questions in this field such as: (1) whether topological insulators can switch magnets, (2) how the charge to spin conversion is influenced by the channel resistivity, and (3) how device structures can be designed to enhance spin injection. [1] S. Hong, S. Sayed, and S. Datta, "Spin Circuit Model for 2D Channels with Spin-Orbit Coupling". (Under Review). [2] T. Valet, and A. Fert, "Theory of the perpendicular magnetoresistance in magnetic multilayers", Phys. Rev. B, 48, 7099, 1993.

<sup>1</sup>This work was supported by FAME, one of six centers of STARnet, a Semiconductor Research Corporation program sponsored by MARCO and DARPA.

**9:00AM K12.00006 Measurements of current-induced spin polarizations in topological insulators Bi<sub>2</sub>Te<sub>2</sub>Se and Bi<sub>2</sub>Se<sub>3</sub> thin flakes.**, JIFA TIAN, IRENEUSZ MIOTKOWSKI, Department of Physics and Astronomy, Purdue University, SEOKMIN HONG, SUPRIYO DATTA, Birck Nanotechnology Center, Purdue University, YONG CHEN, Department of Physics and Astronomy, Purdue University — Topological insulators (TIs) possess nontrivial spin-momentum-locked topological surface states (TSS). Real TI can also host trivial surface 2DEG with strong Rashba spin-orbit coupling derived from the bulk states. Both TSS and Rashba 2DEG can generate current induced spin polarization, although the dominant helicities of their spin-momentum locking (SML) are expected to be opposite. Here, we report spin potentiometric measurements in exfoliated bulk-insulating Bi<sub>2</sub>Te<sub>2</sub>Se and bulk-metallic Bi<sub>2</sub>Se<sub>3</sub> thin flakes. In both materials, the voltage measured by a FM electrode shows a hysteretic step-like change when the FM magnetization is switched by an in-plane magnetic field. The trend of the voltage change can be reversed by reversing the direction of the dc current, and the amplitude of the spin signal increases linearly with increasing bias current. Such a spin signal is consistent with a current induced spin polarization arising from a helical SML. However, the observed trend of the voltage change is opposite between Bi<sub>2</sub>Te<sub>2</sub>Se and Bi<sub>2</sub>Se<sub>3</sub>, suggesting opposite signs of dominant spin helicity that we attribute to TSS and Rashba 2DEG respectively.

**9:12AM K12.00007 Spintronics device made of topological materials<sup>1</sup>**, JIANGSHENG WU, ZHANGSHENG SHI, MAOJI WANG, South University of Science and Technology of China — Topological Materials is a new state of matter of which the bulk states are gapped insulator or superconductor while the surface states are gapless metallic states. Such surface states are robust against local disorder and impurities due to its nontrivial topology. It induces unusual transport properties and shows nontrivial topological spin texture in real space. We have made use of these two exotic properties to make application in spintronics. For example, we propose to make spin-filter transistor using of 1D or 2D quantum anomalous Hall insulator or 2D topological Weyl semimetal, we also propose a device to measure the spin-polarization of current, a device to generate entangled electron pairs.

<sup>1</sup>Startup funds of SUSTC, Shenzhen Peacock Plan, Shenzhen Free Exploration Plan with grant number JCYJ20150630145302225

**9:24AM K12.00008 Topological Insulator and Thermoelectric Effects**, YONG XU, Department of Physics, Tsinghua University, Beijing 100084, China — The recent discovery of topological insulator (TI) offers new opportunities for the development of thermoelectricity, because many TIs (like Bi<sub>2</sub>Te<sub>3</sub>) are excellent thermoelectric materials. In this talk, I will first introduce our theoretical predictions of anomalous Seebeck effect and strong size effect in TI [PRL 112, 226801 (2014)]. Then I will report our recent proof experiments, which find in TI thin films that (i) the hole-type Seebeck effect and the electron-type Hall effect coexist in the same TI sample for all the measured temperatures (up to 300 K), and (ii) the thermoelectric properties depend sensitively on the film thickness. The unconventional phenomena are revealed to be closely related to the topological nature of the material. These findings may inspire new ideas for designing TI-based high-efficiency thermoelectric devices.

**9:36AM K12.00009 Electric-field control of spin-orbit torque in magnetically doped topological insulators<sup>1</sup>**, YABIN FAN, QIMING SHAO, XUFENG KOU, PRAMEY UPADHYAYA, KANG WANG, University of California, Los Angeles — Recent advances of spin-orbit torques (SOTs) generated by topological insulators (TIs) [1-2] have drawn increasing interest to the spin-momentum locking feature of TIs' surface states, which can potentially provide a very efficient means to generate SOTs for spintronic applications. In this presentation, we will show the magnetization switching through current-induced giant SOT in both TI/Cr-doped TI bilayer [1] and uniformly Cr-doped TI films [3]. In particular, we show that the current-induced SOT has significant contribution from the spin-momentum locked surface states of TIs. We find that the spin torque efficiency is in general three orders of magnitude larger than those reported in heavy metal/ferromagnetic heterostructures. In the second part, we will present the electric-field control of the giant SOT in magnetically doped TIs [3], which suggests promising gate-controlled spin-torque device applications. The giant SOT and efficient current-induced magnetization switching exhibited by the magnetic TIs may lead to innovative spintronic applications such as ultralow power dissipation memory and logic devices. [1] Y. Fan, *et al.*, *Nature Mater.* **13**, 699-704 (2014). [2] A. R. Melnik, *et al.*, *Nature* **511**, 449-451 (2014). [3] Y. Fan, *et al.*, *under preparation*.

<sup>1</sup>We acknowledge the supports from DARPA, FAME, SHINES and ARO programs.

**9:48AM K12.00010 Optical Control of Ferromagnetism in a Magnetically-Doped Topological Insulator<sup>1</sup>**, ANDREW L. YEATS, PETER J. MINTUN, Institute for Molecular Engineering, University of Chicago, Chicago, IL 60637, YU PAN, ANTHONY RICHARDELLA, NITIN SAMARTH, Dept. of Physics, Penn State University, University Park, PA 16802, DAVID D. AWSCHALOM, Institute for Molecular Engineering, University of Chicago, Chicago, IL 60637 — Many proposed experiments involving topological insulators (TIs) require spatial control over time-reversal symmetry and chemical potential. We demonstrate micron-scale optical control of both magnetization and chemical potential in thin films of Cr-doped (Bi,Sb)<sub>2</sub>Te<sub>3</sub>. By optically modulating the coercivity of the films, we write and erase arbitrary spatial configurations of their magnetization, which we then image with Kerr microscopy. Additionally, by optically manipulating a space charge layer in the underlying SrTiO<sub>3</sub> substrates, we can control the local chemical potential of the films. This allows us to write and erase *p-n* junctions in the films, which we image with photocurrent microscopy<sup>2</sup>. Both effects persist for > 16 hours. We will present systematic Kerr microscopy, photocurrent microscopy, and electrical transport studies of these materials and various electronic and magnetic structures patterned on them. We will discuss the prospects for using these optical phenomena to study and control the unique physics of TIs, such as edge-state transport in the quantum anomalous Hall regime.

<sup>1</sup>This work is supported by ONR, AFOSR-MURI, ARO, and NSF.

<sup>2</sup>A. L. Yeats, Y. Pan, A. Richardella, P. J. Mintun, N. Samarth, and D. D. Awschalom, *Science Advances* **1**, e1500640 (2015).

**10:00AM K12.00011 Edge channel transport in a HgTe waveguide modulated by two magnetic barriers<sup>1</sup>**, FENG ZHAI, University of Puerto Rico at Mayaguez, XUANPING JIN, Zhejiang Normal University, JUNQIANG LU, University of Puerto Rico at Mayaguez — we investigate the effects of a magnetic double barrier on the ballistic transport properties of edge-states in a HgTe waveguide with inverted band structures. When its energy is in the bulk gap and close to the bulk conduction band of leads, the electron incident from a quantum spin Hall (QSH) state can be almost totally reflected as the two magnetic barriers are in the antiparallel configuration. For the magnetic double barrier in the parallel configuration, the same electron can transmit nearly perfectly for a proper spin orientation. In the antiparallel configuration, the spin polarization of the output current vanishes. This distinction in the transmission indicates that the proposed edge-state device has two functions: magnetic switching and spin filtering. Our calculations also indicate that nonuniform magnetic fields can break the QSH states more effectively than uniform ones.

<sup>1</sup>This work was supported by the NSFC (grant 11174252) and by the NSF EPSCOR (grant 1010094).

**10:12AM K12.00012 Dynamical electron compressibility in the 3D topological insulator Bi<sub>2</sub>Se<sub>3</sub>**, ANDREAS INHOFER, Laboratoire Pierre Aigrain, ENS Paris, BADIH ASSAF, Département de Physique, ENS Paris, QUENTIN WILMART, Laboratoire Pierre Aigrain, ENS Paris, LOUIS VEYRAT, CHRISTIAN NOWKA, JOSEPH DUFOULEUR, ROMAIN GIRAUD, SILKE HAMPEL, BERND BUECHNER, IFW-Dresden, Institute for Solid State Research, GWENDAL FVE, JEAN-MARC BERROIR, BERNARD PLACAIS, Laboratoire Pierre Aigrain, ENS Paris — Measurements of the quantum capacitance  $c_q$ , related to the electron compressibility  $\chi = c_q/e^2$  is a sensitive tool to probe the density of states. In a topological insulator (TI) the situation is enriched by the coexistence and the interplay of topologically protected surface states and massive bulk carriers. We investigate top-gate metal-oxide-TI capacitors using Bi<sub>2</sub>Se<sub>3</sub> thin crystals at GHz frequencies. These measurements provide insight into the compressibility of such a two electron-fluid system. Furthermore, the dynamical response yields information about electron scattering properties in TIs. More specifically, in our measurements we track simultaneously the conductivity  $\sigma$  and the compressibility as a function of a DC-gate voltage. Using the Einstein relation  $\sigma = c_q D$ , we have access to the gate dependence of the electron diffusion constant  $D(V_g)$ , a signature of the peculiar scattering mechanisms in TIs.

**10:24AM K12.00013 Observation of Majorana fermion states in rf-SQUIDs constructed on Pb-Bi<sub>2</sub>Te<sub>3</sub> surface**, LI LU, YUAN PANG, JIE SHEN, FANMING QU, ZHAOZHENG LYU, JUNHUA WANG, JUNYA FENG, JIE FAN, GUANGTONG LIU, ZHONGQING JI, XIUNIAN JING, CHANGLI YANG, Institute of Physics, Chinese Academy of Sciences, QINGFENG SUN, X. C. XIE, Peking University, LIANG FU, Massachusetts Institute of Technology — Recently, much attention has been paid to search for Majorana fermions in solid-state systems. Among various proposals there is one based on radio-frequency superconducting quantum interference devices (rf-SQUIDs), in which a  $4\pi$ -periodic current-phase relation is expected if Majorana fermion states exist. In this talk we report observations of truncated  $4\pi$ -periodic (i.e.,  $2\pi$ -periodic but fully skewed) oscillatory patterns of contact resistance, on rf-SQUIDs constructed on the surface of three-dimensional topological insulator Bi<sub>2</sub>Te<sub>3</sub>. The results reflect the existence of Majorana fermion states in the devices.

**10:36AM K12.00014 Quantum well states in Rashba semiconductor BiTeI<sup>1</sup>**, YANG HE, ZHIHUI ZHU, Harvard University, MOHAMMAD HAMIDIAN, Harvard University; Cornell University, PENGCHENG CHEN, YAU CHUEN YAM, JENNIFER HOFFMAN, Harvard University; The University of British Columbia — BiTeI displays large Rashba-type spin splitting in both valence and conduction bands. In this work, we use scanning tunneling microscopy to reveal the bipolar nature of BiTeI, confirming the previously observed p-n junction electronic structure. We also discover two-dimensional quantum well states both below and above the semiconducting gap on the Te-terminated surface. This work sheds light on the origin of the giant Rashba splitting in the system.

<sup>1</sup>This effort is funded by the NSF grant DMR-1410480.

**10:48AM K12.00015 Kondo and Majorana doublet interactions in quantum dots**, YOUNGHYUN KIM, UC Santa Barbara, DONG E. LIU, Microsoft Research Station Q, ERIKAS GAIDAMAUSKAS, JENS PAASKE, KARSTEN FLENSBERG, Niels Bohr Institute, University of Copenhagen, ROMAN LUTCHYN, Microsoft Research Station Q — We study the properties of a quantum dot coupled to a normal lead and a time-reversal topological superconductor with Majorana Kramers pair at the end. We explore the phase diagram of the system as a function of Kondo and Majorana-induced coupling strengths using perturbative renormalization group study and slave-boson mean-field theory. We find that, in the presence of coupling between a quantum dot and a Majorana doublet, the system flows to a new fixed point controlled by the Majorana doublet, rather than the Kondo coupling, which is characterized by correlations between a localized spin and the fermion parity of each spin sector of the topological superconductor. We find that this fixed point is stable with respect to Gaussian fluctuations. We also investigate the effect of spin-spin interaction between a quantum dot and Majorana doublet and compare the result with a case where a normal lead is directly coupled to Majorana doublet.

**Wednesday, March 16, 2016 8:00AM - 11:00AM –**  
**Session K13 DAMOP DCOMP: Application of Monte Carlo Techniques to Cold Atom Systems**  
309 - Barry Schneider, NIST/NSF

**8:00AM K13.00001 Coexistence, Interfacial Energy and the Fate of Microemulsions of 2D Dipolar Bosons**, MASSIMO BONINSEGNI, University of Alberta — The superfluid-crystal quantum phase transition of a system of purely repulsive dipolar bosons in two dimensions has been the subject of a lot of theoretical study, mainly because of some intriguing predictions by Spivak and Kivelson (2004) regarding an exotic, intermediate "microemulsion" that should appear at low temperature between the crystal and the superfluid. We investigated this scenario by means of Quantum Monte Carlo simulations at zero temperature, determined freezing and melting densities, and estimated the energy per unit length of a macroscopic interface separating the coexisting crystal and superfluid phases. The results rule out quantitatively the microemulsion scenario for any physical realization of this system, given the exceedingly large predicted size of the bubbles. Reference: S. Moroni and M. Boninsegni, Phys. Rev. Lett. **113**, 240407 (2014)

**8:36AM K13.00002 Quantum spin dynamics and entanglement in systems with long-range interactions<sup>1</sup>**, ANA M REY, JILA, NIST and University of Colorado at Boulder — One of the fundamental goals of modern quantum sciences is to learn how to control and manipulate non-equilibrium many-body systems and use them to make powerful and improved quantum devices, materials and technologies. However, out-of-equilibrium systems are complex, typically strongly correlated and entangled, and thus to model them we are in an urgent need of new methodologies. In this talk I will discuss new theoretical methods that we have developed to investigate emergent non-equilibrium phenomena in driven-dissipative spin systems interacting via long-range interactions. I will show we can capture the dynamics of correlations and entanglement in close systems and the interplay between dissipation and entanglement in open quantum systems including spin-boson models. As a specific application I will discuss the use of our methods to model the spin dynamics exhibited by arrays of trapped ions with controllable long-range interactions. I will show that our predictions are consistent with recent experimental measurements. I will also discuss new protocols to diagnostic and characterize entanglement based on well-established NMR protocols

<sup>1</sup>This work is supported by NSF, ARO, AFOSR-MURI, and NIST

**9:12AM K13.00003 Universal scaling of density and momentum distributions in Lieb-Liniger gases<sup>1</sup>**, MARCOS RIGOL, The Pennsylvania State University — We present numerically exact results for the scaling of density and momentum distribution functions of harmonically trapped one-dimensional bosons with repulsive contact interactions. We consider systems in the continuum [1], and in the presence of a lattice [2,3], both in the ground state [1,2] and at finite temperature [1,3]. We use path integral quantum Monte Carlo with worm updates in calculations at finite interaction strengths, and the Bose-Fermi mapping in the Tonks-Girardeau limit. We first discuss the homogeneous case and, within the local density approximation, use it to motivate the scaling in the presence of a harmonic trap. For the momentum distribution function, we pay special attention to the high momentum tails and their  $k^{-4}$  asymptotic behavior. When available, we compare our results to experimental measurements of the momentum distribution function of ultracold bosonic gases in two-dimensional optical lattices.

References:

- [1] W. Xu and M. Rigol. Universal scaling of density and momentum distributions in Lieb-Liniger gases. arXiv:1508.07011.
- [2] M. Rigol and A. Muramatsu. Universal properties of hard-core bosons confined on one-dimensional lattices. Phys. Rev. A **70**, 031603(R) (2004).
- [3] M. Rigol. Finite-temperature properties of hard-core bosons confined on one-dimensional optical lattices. Phys. Rev. A **72**, 063607 (2005).

<sup>1</sup>We acknowledge support from the National Science Foundation Grant No. PHY13-18303 and the Office of Naval Research

**9:48AM K13.00004 Cooling Atomic Gases With Disorder<sup>1</sup>**, RICHARD SCALETTAR, University of California, Davis — Cold atomic gases have proven capable of emulating a number of fundamental condensed matter phenomena including Bose-Einstein condensation, the Mott transition, Fulde-Ferrell-Larkin-Ovchinnikov pairing and the quantum Hall effect. Cooling to a low enough temperature to explore magnetism and exotic superconductivity in lattices of fermionic atoms remains a challenge. We propose a method to produce a low temperature gas by preparing it in a disordered potential and following a constant entropy trajectory to deliver the gas into a non-disordered state which exhibits these incompletely understood phases. We show, using quantum Monte Carlo simulations, that we can approach the Neel temperature of the three-dimensional Hubbard model for experimentally achievable parameters. Recent experimental estimates suggest the randomness required lies in a regime where atom transport and equilibration are still robust. Thereza Paiva, Ehsan Khatami, Shuxiang Yang, Valery Rousseau, Mark Jarrell, Juana Moreno, Randall G. Hulet, and Richard T. Scalettar, arXiv:1508.02613

<sup>1</sup>This work was supported by the NNSA SSAA program.

**10:24AM K13.00005 Diagrammatic Monte Carlo study of mass-imbalanced Fermi-polaron system**, LOUE POLLET, Department of Physics, LMU Munich — After a brief introduction and review of diagrammatic Monte Carlo, I present our results for the three-dimensional Fermi-polaron system with mass-imbalance, where an impurity interacts resonantly with a noninteracting Fermi sea whose atoms have a different mass. This method allows to go beyond frequently used variational techniques by stochastically summing all relevant impurity Feynman diagrams up to a maximum expansion order limited by the sign problem. The polaron energy and quasiparticle residue can be accurately determined over a broad range of impurity masses. Furthermore, the spectral function of an imbalanced polaron demonstrates the stability of the quasiparticle and allows to locate in addition also the repulsive polaron as an excited state. The quantitative exactness of two-particle-hole wave-functions is investigated, resulting in a relative lowering of polaronic energies in the mass-imbalance phase diagram. The contact coefficient for the mass-balanced polaron system is found in good agreement with variational methods. Mass-imbalanced systems can be studied experimentally by ultracold atom mixtures like  $^6\text{Li}$ - $^{40}\text{K}$ . I will discuss some open questions and links with recent experiments.

**Wednesday, March 16, 2016 8:00AM - 11:00AM –**

**Session K14 GSNP GSOF: Extreme Mechanics: Topology in Mechanics** 310 - Pedro Reis, Massachusetts Institute of Technology

**8:00AM K14.00001 Topological mechanics of gyroscopic meta-materials**, WILLIAM IRVINE, University of Chicago — Topological mechanical meta-materials are artificial structures whose unusual properties are protected very much like their electronic and optical counterparts. I will present an experimental and theoretical study<sup>1</sup> of a new kind of active meta-material comprised of coupled gyroscopes on a lattice that breaks time-reversal symmetry. The vibrational spectrum displays a sonic gap populated by topologically protected edge modes which propagate in only one direction and are unaffected by disorder. We observe these edge modes in experiment and verify their robustness to disorder and the insertion of obstacles. Controlled distortions of the underlying lattice can induce a topological phase transition that switches the edge mode chirality. This effect allows the direction of the edge current to be determined on demand.

<sup>1</sup>Topological mechanics of gyroscopic meta-materials, Lisa M. Nash, Dustin Kleckner, Alismari Read, Vincenzo Vitelli, Ari M. Turner and William T.M. Irvine, PNAS (In press).

**8:36AM K14.00002 Kirigami!**, RANDALL KAMIEN, Univ of Pennsylvania — We explore and develop a simple set of rules that apply to cutting, pasting, and folding honeycomb lattices. We consider origami-like structures that are extrinsically flat away from zero dimensional sources of Gaussian curvature and one-dimensional sources of mean curvature, and our cutting and pasting rules maintain the intrinsic bond lengths on both the lattice and its dual lattice. We find that a small set of rules is allowed providing a framework for exploring and building kirigami - folding, cutting, and pasting the edges of paper.

**9:12AM K14.00003 Mechanisms and nonlinear waves from topological modes**, BRYAN CHEN, UMass Amherst — Topological protection can arise in mechanical structures such as linkages, frames, or rigid origami. The key ingredients are a balance of degrees of freedom and constraints away from the boundaries. In this setting certain zero energy modes of the system can be made robust against a broad class of perturbations and noise. However, since there are no restoring forces to these modes to linear order, they result in flexes and mechanisms which must be treated as nonlinear waves. I will discuss several simple and concrete examples which illustrate these ideas.

**9:48AM K14.00004 Topological Toughening of graphene and other 2D materials**, HUAJIAN GAO, Brown University — It has been claimed that graphene, with the elastic modulus of 1TPa and theoretical strength as high as 130 GPa, is the strongest material. However, from an engineering point of view, it is the fracture toughness that determines the actual strength of materials, as crack-like flaws (i.e., cracks, holes, notches, corners, etc.) are inevitable in the design, fabrication, and operation of practical devices and systems. Recently, it has been demonstrated that graphene has very low fracture toughness, in fact close to that of ideally brittle solids. These findings have raised sharp questions and are calling for efforts to explore effective methods to toughen graphene. Recently, we have been exploring the potential use of topological effects to enhance the fracture toughness of graphene. For example, it has been shown that a sinusoidal graphene containing periodically distributed disclination quadrupoles can achieve a mode I fracture toughness nearly twice that of pristine graphene. Here we report working progresses on further studies of topological toughening of graphene and other 2D materials. A phase field crystal method is adopted to generate the atomic coordinates of material with specific topological patterns. We then perform molecular dynamics simulations of fracture in the designed samples, and observe a variety of toughening mechanisms, including crack tip blunting, crack trapping, ligament bridging, crack deflection and daughter crack initiation and coalescence.

**10:24AM K14.00005 Control of defect localization in crystalline wrinkling by curvature and topology**<sup>1</sup>, FRANCISCO LOPEZ JIMENEZ, MIT — We investigate the influence of curvature and topology on crystalline wrinkling patterns in generic elastic bilayers. Our numerical analysis predicts that the total number of defects created by adiabatic compression exhibits universal quadratic scaling for spherical, ellipsoidal and toroidal surfaces over a wide range of system sizes. However, both the localization of individual defects and the orientation of defect chains depend strongly on the local Gaussian curvature and its gradients across a surface. Our results imply that curvature and topology can be utilized to pattern defects in elastic materials, thus promising improved control over hierarchical bending, buckling or folding processes. Generally, this study suggests that bilayer systems provide an inexpensive yet valuable experimental test-bed for exploring the effects of geometrically induced forces on assemblies of topological charges.

<sup>1</sup>Joint work with Norbert Stoop, Romain Lagrange, Jorn Dunkel and Pedro M. Reis

**Wednesday, March 16, 2016 8:00AM - 11:00AM –**

**Session K15 DCMP DMP: Transport in Graphene and 1D Structures** 314 - Kurt Gaskill, Naval Research Laboratory

**8:00AM K15.00001 Unconventional 1/f noise in Graphene on SrTiO<sub>3</sub> substrate**, ANINDITA SAHOO, Department of Physics, Indian Institute of Science, Bangalore-560012, India, ROALD RUITER, TAMALIKA BANERJEE, Zernike Institute for Advanced Materials, University of Groningen, Groningen, The Netherlands, ARINDAM GHOSH, Department of Physics, Indian Institute of Science, Bangalore-560012, India — Electrical transport in graphene has been of great interest in both fundamental and applied research. The impact of the substrate is critical to the operation of graphene field effect transistors (FET), which can modify several transport parameters as well as low frequency 1/f noise. Replacing the usual SiO<sub>2</sub>/Si<sup>++</sup> substrate with SrTiO<sub>3</sub> [STO] having high dielectric constant, has opened up new possibilities, leading to large doping, higher mobility, and also hysteretic transfer characteristics for memory applications. We have studied 1/f noise in dual-gated single layer graphene (SLG) FET sandwiched between STO (substrate) and mechanically exfoliated hexagonal boron-nitride (dielectric for the top gate). The area normalized noise amplitude of SLG on STO followed an unexpected 'W'-shape dependence of gate-bias with the central peak at Dirac point in conflict with the usual 'V', 'M' or 'Λ'-type dependence of SLG noise on SiO<sub>2</sub>. We discuss possible microscopic mechanisms for such behavior, considering the role of puckering of oxygen atoms introducing inward dipole moments that can form a new source of electrostatically tunable scattering mechanism at the graphene-STO interface.

**8:12AM K15.00002 1/f Noise in Gated Epitaxial Graphene Nanoribbons**, OWEN VAIL, JEREMY YANG, ANNA MIETTINEN, JOHN HANKINSON, School of Physics, Georgia Institute of Technology, CLAIRE BERGER, School of Physics, Georgia Institute of Technology, CNRS-Institut Neel, WALTER DE HEER, ZHIGANG JIANG, School of Physics, Georgia Institute of Technology — Epitaxial Graphene Nanoribbons (EGNR) grown on sidewall SiC have gained interest as a high-quality interconnect enabling room temperature ballistic transport over micron lengths. To be useful as an interconnect a proper characterization of the noise level in the EGNR needs to be determined. Toward this end, we fabricated EGNR devices with an Aluminum-Oxide top gate and use field effect to tune the fermi energy in the graphene channel. Our studies of the electronic noise and its dependence on the charge density in the ribbon reveal information about the subband structure of the density of states in addition to the ribbon's spectral density at low frequencies. Comparisons to the widely reported 1/f noise in silicon and other forms of graphene provide strong references for analyzing our results.

**8:24AM K15.00003 Theoretical study of the crossover into hydrodynamic regime in graphene<sup>1</sup>**, DEREK HO, INDRA YUDHISTIRA, National University of Singapore, BEN YU-KUANG HU, University of Akron, SHAFFIQUE ADAM, National University of Singapore and Yale-NUS College — Experiments on graphene have recently succeeded in entering the hydrodynamic regime, as demonstrated by successful observations of strong violation of Wiedemann-Franz law [1], the Gurzhi effect and electronic Poiseuille flow [2]. It is known that electronic systems enter the hydrodynamic regime when electron-electron scattering dominates over electron-impurity and electron-phonon scattering. However, a quantitative study of this transition from the Fermi liquid to hydrodynamic regime is still lacking. In view of this, we quantitatively analyze the electron-electron, electron-impurity and electron-phonon scattering rates as a function of temperature, charge doping and disorder (charge puddle) strength. This yields a quantitative understanding of the onset of hydrodynamic electronic behavior in graphene samples. [1] J. Crossno et al., arXiv: 1509.04713v1 (2015). [2] D. A. Bandurin et al., arXiv: 1509.04165 (2015).

<sup>1</sup>This work is supported by the National Research Foundation of Singapore under its Fellowship program (NRF-NRFF2012-01) and by the Singapore Ministry of Education and Yale-NUS College through Grant No. R-607-265-01312.

**8:36AM K15.00004 Observation of insulating behavior and strong localization in suspended monolayer graphene<sup>1</sup>**, CENK YANIK, YASER VAHEB, ABDULKADIR CANATAR, VAHID SAZGARI, ISMET I. KAYA, Sabanci University, QUANTUM TRANSPORT AND NANOELECTRONICS LABORATORY TEAM — Dirac point of graphene is known to be inaccessible due to the electron hole puddles which screen the neutrality point and makes the minimum conductance limited to the order of  $e^2/h$ . However, in extremely clean suspended graphene samples, there is a possibility to observe a diverging resistance approaching the charge neutrality point via yet to be understood localization or Boltzmann transport mechanism. We observe a resistance in excess of  $10^6 \Omega$  near the charge neutrality point in a very high quality suspended monolayer graphene in the absence of magnetic field. The sample exhibits negative magnetoresistance indicating a strong localization effect at low charge carrier densities. The possible origins of these observations will be discussed in the context of the transport mechanisms mentioned above.

<sup>1</sup>This work is supported by TUBITAK under grant number 112T990

**8:48AM K15.00005 ABSTRACT WITHDRAWN —**

**9:00AM K15.00006 Approaching Collimation with a Graphene-based Quantum Point Contact**, GRACE PAN, Department of Physics, Yale University, MENYOUNG LEE, Department of Physics, Stanford University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Japan, DAVID GOLDBABER-GORDON, Department of Physics, Stanford University — Quantum point contacts (QPCs) are narrow constrictions on the order of the Fermi wavelength that bridge together two electrically conducting regions. QPCs display sensitive conductance quantization and are a classic playing field to illustrate clean, ballistic transport in low-dimensional materials. However, graphene-based QPCs are challenging to fabricate, in part due to two reasons: edge disorder that suppresses conductance quantization and imperfect gate depletion leading to charge puddles. Using graphene-boron nitride heterostructures, we demonstrate improvements over a simple etch and Au-gating method by introducing a protective alumina dielectric layer. We use this method to create two QPCs in series and explore potential electron-beam collimation at low magnetic field, in the spirit of Molenkamp (1990).

**9:12AM K15.00007 Realizing 1-D conducting channel between oppositely gated regions in bilayer graphene.**, JANGHEE LEE, Pohang University of Science and Technology, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, HU-JONG LEE, Pohang University of Science and Technology — The band gap of bilayer graphene (BLG) can be tuned by applying an external electric field perpendicular to the plane of a BLG sheet. If direction of the electric fields in two adjacent regions in BLG are opposite, one-dimensional (1-D) conducting channel emerges at the boundary between two regions with chiral nature. In this presentation, we introduce a method for fabricating two pairs of split-gates attached to BLG, which is sandwiched between two atomically clean hexagonal boron nitride (h-BN) single crystals and thus allows ballistic transport of carriers at least within the device size. Current-voltage characteristics show a large transport gap, which is comparable to the results obtained from optical measurements and numerical calculations. Opening the band gap in two adjacent regions of the BLG flake by oppositely gated electric fields, we observed metallic behavior in transport characteristics along the boundary between the two regions although the resistance of two gapped regions are a few hundreds of  $k\Omega$ . These results indicate that a 1-D conducting channel formed between the two regions where the induced band gaps were inverted to each other. The formation of this 1-D conducting channel mimics the topological edge conducting channels emerging at the boundary of a two-dimensional topological insulator and may be utilized for applying BLG to valleytronics

**9:24AM K15.00008 Orientation-independent conductance step of graphene nanoribbons**, JI-HAE CHOI, SANG-HOON LEE, MINSOO KIM, Pohang Univ of Sci & Tech, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, HU-JONG LEE, SEUNG-HOON JHI, Pohang Univ of Sci & Tech, CNPL TEAM, QTS TEAM, ULTRA-HIGH PRESSURE PROCESSES GROUP TEAM — Low-energy electronic structure of graphene is characterized by the states from two inequivalent valleys at K and K' points that have opposite chirality. In graphene nanoribbons (GNRs), the K and K' valleys, when projected into one-dimensional (1D) Brillouin zone, can be mixed due to the edge termination. The degree of mixing determines the electronic property of GNRs. However, non-valley mixing properties have been hardly observed so far. In this work, we made effective 1D transport channels by gate-defined carrier guiding. They exhibit a quantum conductance step of  $4e^2/h$ , which is the characteristic of non-mixed valleys. To verify these experimental results, we performed both first-principles and tight-binding calculations of GNRs with arbitrary axial orientations. Calculated band structures and quantum conductance of GNRs show zero-energy flat bands and a conductance step of  $4e^2/h$  except armchair-edge GNRs. We find that this is a consequence of generic zigzag-type boundary conditions of GNRs with arbitrary axial orientations except armchair-edge cases

**9:36AM K15.00009 Theoretical Study of All-Electrical Quantum Wire Valley Filters in Bilayer Graphene<sup>1</sup>**, YU-SHU WU, National Tsing-Hua University, Taiwan, NING-YUAN LUE, YEN-CHUN CHEN, NTHU, Taiwan, JIA-HUEI JIANG, NTHU, Taiwan, MEI-YIN CHOU, AS, Taiwan — Graphene electrons carry valley pseudospin, due to the double valley degeneracy in graphene band structure.[1] In gapped graphene, the pseudospin is coupled to an in-plane electric field, through the mechanism of valley-orbit interaction (VOI).[2] Based on the VOI, a family of electrically-controlled valleytronic devices have been proposed. Here, we report the theoretical study of a recently proposed valley filter consisting of a Q1D channel in bilayer graphene defined and controlled by electrical gates. We discuss two types of calculations – those of energy subband structure in the channel and electron transmission through a valley valve consisting of two proposed filters. For the former, we have developed a tight binding formulation in the continuum limit. For the latter, we employ the recursive Green's function method. Results from the calculations will be presented. References [1] Rycerz et al., Nat. Phys. 3, 172 (2007); Xiao et al., Phys. Rev. Lett. 99, 236809 (2007). [2] Wu et al., Phys. Rev. B 84, 195463 (2011); ibid B 86, 045456 (2012); ibid B 86, 165411 (2012); ibid B 88, 125422 (2013).

<sup>1</sup>Financial support by MoST, Taiwan, ROC is acknowledged.

**9:48AM K15.00010 Transport measurements in quasi-one dimensional graphene wires**, VARUN HARBOLA, MENYOUNG LEE, Physics department, Stanford University, DAVID GOLDBABER-GORDON, Physics department, Stanford Univ, TAKASHI TANIGUCHI, KENJI WATANABE, National institute of material science, Japan — ABSTRACT: Recent developments have enabled fabrication of high mobility graphene structures. The elastic mean free path in the 2D bulk of the graphene can be greater than ten microns, whereas the graphene can be patterned to widths of 1 micron or below. Thus, we can make structures for which bulk elastic scattering can be neglected. We experimentally study the role of other length scales, such as electron-electron scattering length, cyclotron length, and the width of the graphene ribbon, on transport properties.

**10:00AM K15.00011 Near-field study of domain walls in bilayer graphene**, LILI JIANG, ZHIWEN SHI, FENG WANG, Univ of California - Berkeley — Domain wall in bilayer graphene is emerging as a fascinating one-dimensional system due to the presence of structural soliton and electrically valley Hall boundary states. They are expected to process unusual electronic and optical properties because of the modification of atomic structures. We systematically study the bilayer graphene domain walls with different configurations including lines, circles and networks using scanning near-field optical microscopy (SNOM). The SNOM technique provides a convenient way to investigate domain walls in ambient condition. Our results suggest that bilayer graphene domain wall is an interesting and rich system for fundamental research about light-matter interactions.

**10:12AM K15.00012 Optical signatures of a hypercritical 1D potential in a 2D Dirac metal**, BOR-YUAN JIANG, GUANGXIN NI, Univ of California - San Diego, CHENG PAN, Univ of California - Riverside, ZHE FEI, Univ of California - San Diego, BIN CHENG, CHUN NING LAU, MARC BOCKRATH, Univ of California - Riverside, DIMITRI BASOV, MICHAEL FOGLER, Univ of California - San Diego — Generation of quasi-bound states in graphene near strong charged perturbations is a solid-state analog of atomic collapse of superheavy elements or particle production by hypothetical cosmic strings. We show, for the case of a linelike perturbation, that as the perturbation grows in strength, quasi-bound states are generated sequentially. Each of these critical events is signaled by a sharp change in the local optical conductivity. Tunable linelike perturbations can be realized in experiment using nanowire or nanotube electrostatic gates. We report measurements of local conductivity for such systems obtained through near-field optical microscopy.

**10:24AM K15.00013 Electronic transport across linear defects in graphene**, ANA L C PEREIRA, CARLOS J PAEZ, State University of Campinas, JOO NUNO B RODRIGUES, National University of Singapore, NUNO M R PERES, Universidade do Minho - Portugal — Graphene is being proposed for a variety of new electronic devices. However, the required high-quality electrical properties are affected by the formation of polycrystalline structures, which are practically unavoidable by the growth methods known so far. As such, the scattering problem of an electron off a grain boundary becomes relevant. We investigate the low-energy electronic transport across grain boundaries in graphene ribbons and in ?nite ?akes. Using the recursive Greens-function method, we compute the electronic transmittance across different types of grain boundaries in graphene ribbons and ?akes. We use the charge and current density spatial distributions to enhance our understanding of their electronic transport properties, and ?nd that electronic transport depends both on the grain boundaries microscopic details and on their orientation. We consider extended linear defects of type 585 and 5757, and also a spatial region where the grain boundary is composed by the superposition of two monolayer domains. In addition, we employ the transfer-matrix formalism to analytically study the electronic transport across a class of zigzag grain boundaries with periodicity 3. We ?nd that these grain boundaries give rise to intervalley scattering.

**10:36AM K15.00014 Theoretical investigation of graphene on STO(111) surface**, DONGHAN SHIN, ALEXANDER A. DEMKOV, Univ of Texas, Austin — Graphene, a two-dimensional electronic system which consists of a single layer of graphite, is considered a possible candidate for nano-electronic applications as it has a very high electron mobility. One of the problems in realizing this in practice is the difficulty of doping. Using density functional theory we explore the possibility of field-doping graphene by placing a graphene sheet on a (111)-oriented SrTiO3 (STO) surface that is highly polar. We investigate the electronic structure of the system. Our results suggest that two conduction channels can form near the Fermi level. One is mainly composed of  $\pi$ -like carbon based orbitals, while the other is localized at the oxide surface.

**10:48AM K15.00015 Critical Delocalization of Chiral Zero Energy Modes in Graphene<sup>1</sup>**, AIRES FERREIRA, Department of Physics, University of York, York YO10 5DD, United Kingdom, EDUARDO MUCCIOLO, Department of Physics, University of Central Florida, Orlando, Florida 32816, USA — Graphene subjected to chiral-symmetric disorder is believed to host zero energy modes (ZEMs) resilient to localization, as suggested by the renormalization group analysis of the underlying nonlinear sigma model. We report accurate quantum transport calculations in honeycomb lattices with in excess of  $10^9$  sites and fine meV resolutions. The Kubo dc conductivity of ZEMs induced by vacancy defects (chiral BDI class) is found to match  $4e^2/(\pi h)$  within 1% accuracy, over a parametrically wide window of energy level broadenings and vacancy concentrations. Our results disclose an unprecedentedly robust metallic regime in graphene, providing strong evidence that the early field-theoretical picture for the BDI class is valid well beyond its controlled weak-coupling regime.

<sup>1</sup>A.F. acknowledges the financial support of the Royal Society, UK.

**Wednesday, March 16, 2016 8:00AM - 11:00AM –**

**Session K16 DMP: 2D Devices: Black Phosphorous** 315 - Marija Drndic, University of Pennsylvania

**8:00AM K16.00001 Black phosphorus for future devices**, VINCENT MEUNIER, Rensselaer Polytechnic Institute — Black phosphorus (or phosphorene at the monolayer limit) has attracted significant attention as an emerging 2D material due to its unique properties compared with well-explored graphene and transition metal dichalcogenides such as MoS<sub>2</sub> and WSe<sub>2</sub>. In bulk form, this mono-elemental layered structure is a highly anisotropic semiconductor with a bandgap of 0.3 eV which presents marked distinctions in optical and electronic properties depending on crystalline directions. In addition, black phosphorus possesses a high carrier mobility, making it promising for applications in high frequency electronics. A large number of characterization studies have been performed to understand the intrinsic properties of BP. Here I will present a number of investigations where first-principles modelling was combined with scanning tunneling microscopy (STM) [1], Raman spectroscopy [2], and transmission electron microscopy (TEM) [3] to assist in the design of phosphorene-based devices.<sup>1</sup> I will provide an overview of these studies and position them in the context of the very active research devoted to this material. In particular, I will show how low-frequency Raman spectra provide a unique handle on the physics of multilayered systems and how BP's structural anisotropy weaves its way to its unusual polarization dependent Raman signature. Finally, I will show recent progress where nanopores, nanobridges, and nanogaps have been sculpted directly from a few-layer BP sample using a TEM, and indicate the potential use of these results on the creation of phosphorene-based nanoelectronics. I will conclude this talk with a critical look at the issues of phosphorene stability under ambient conditions. References: [1] Nano Lett. 14, 6400-6406 (2014); [2] ACS Nano, 2015, 9 (6), pp 6333-6342 (2015); [3] unpublished

<sup>1</sup>Collaborators on this research include: Liangbo Liang, Bobby G. Sumpter, Alex Puzetzy, Minghu Pan, (Oak Ridge National Laboratory), Marija Drndic (University of Pennsylvania), Mildred Dresselhaus, Xi-Ling, Shengxi Huang (Massachusetts Institute of Technology)

**8:36AM K16.00002 Strain Engineering of Phosphorene via Bending**, DEEPTI VERMA, Department of Chemical Engineering and Materials Science, University of Minnesota, TRAIAN DUMITRICA, Department of Mechanical Engineering, University of Minnesota — Phosphorene (PE) - the newly discovered 2D derivative of Phosphorus - has an inherent band gap and a high current on/off ratio. Manipulating strain in PE films - strain engineering (SE) - will offer the opportunity to further tailor its electronic properties. Using objective boundary conditions (OBC) coupled with density functional tight binding model (DFTB), we calculate bending rigidity of PE and its 2D allotropes by modeling bent PE as large diameter nanotubes (PNTs). OBCs not only allow for drastic reductions in the number of atoms in simulations but also enable simulations of chiral PNTs, which is impossible with periodic boundary conditions. At the same time, the method describes how bending influences the electronic structure. We establish a robust platform for achieving SE for anisotropic 2D films. Using results from our calculations and orthotropic thin shell model we develop equivalent continuum structure (ECS) for PE and its allotropes upon bending. The developed ECS can be used for performing finite element simulations of PE films on substrates.

**8:48AM K16.00003 Quantum Hall Effect in Black Phosphorus/hBN Heterostructures**, FANGYUAN YANG, LIKAI LI, Fudan University, Collaborative Innovation Center of Advanced Microstructures, Nanjing, GUO JUN YE, University of Science and Technology of China, Collaborative Innovation Center of Advanced Microstructures, Nanjing, ZUOCHENG ZHANG, Tsinghua University, ZENGWEI ZHU, Wuhan National High Magnetic Field Center and School of Physics, Huazhong University of Science and Technology, WEN KAI LOU, Chinese Academy of Sciences, University of Science and Technology of China, LIANG LI, Wuhan National High Magnetic Field Center and School of Physics, Huazhong University of Science and Technology, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, KAI CHANG, Chinese Academy of Sciences, University of Science and Technology of China, YAYU WANG, Tsinghua University, XIAN HUI CHEN, University of Science and Technology of China, Collaborative Innovation Center of Advanced Microstructures, Nanjing, YUANBO ZHANG, Fudan University, Collaborative Innovation Center of Advanced Microstructures, Nanjing — Black phosphorus field effect transistors have emerged as a new two-dimensional electron system (2DES) with high mobility. We achieved high mobilities by placing black phosphorus thin flakes on atomically flat hBN substrates. The mobility is further improved by placing a graphite back gate very close to the 2DES, which screens charged impurities. In this talk, we will present our observation of the integer quantum Hall effect in high mobility black phosphorus 2DEG. Temperature and angular dependent measurements reveal a wealth of information on the charge carriers in this new 2DES.

**9:00AM K16.00004 Fabrication of suspended few-layer black phosphorus nanopores and nanoribbons via electron beam nanosculpting**, PAUL MASIH DAS, Department of Physics and Astronomy, University of Pennsylvania, GOPINATH DANDA, Department of Electrical and Systems Engineering, University of Pennsylvania, WILLIAM PARKIN, Department of Physics and Astronomy, University of Pennsylvania, ANDREW CUPO, NEERAV KHARCHE, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, XI LING, SHENGXI HUANG, MILDRED DRESSSELHAUS, Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, VINCENT MEUNIER, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, MARIJA DRNDIC, Department of Physics and Astronomy, University of Pennsylvania — We present nanopores, nanoribbons, and nanogaps in suspended few-layer black phosphorus (BP) flakes that have been realized using in situ transmission electron microscope nanosculpting. Few-layer BP flakes were first produced through a liquid exfoliation procedure and suspended on holey SiN<sub>x</sub> membranes. We investigate the structural characteristics of few-layer BP and further show the time-dependent properties of various nanostructures under exposure to an electron beam. It is shown that high-resolution structural modification of nanopores and nanoribbons can be achieved with nanometer-scale precision on timescales of a few minutes. We also used density functional theory to provide a model for the observed anisotropy in edge formation by computing energy barriers for various edge geometries.

**9:12AM K16.00005 Highly Anisotropic intrinsic electronic transport properties of monolayer and bilayer phosphorene from first principles<sup>1</sup>**, ZHENGHE JIN, JEFFREY MULLEN, KI WOOK KIM, North Carolina State University — We present an analysis of the electron(hole)-phonon scattering in monolayer and bilayer phosphorene using first principles. Density Functional Theory (DFT) and Density Functional Perturbation Theory (DFPT) are used to calculate the scattering matrix elements and full band Monte Carlo carrier transport simulation is employed to obtain the intrinsic electron/hole mobility. Room temperature mobility and saturation velocity in monolayer and bilayer phosphorene are extracted and significant layer number dependence in the mobility is revealed which results from the carrier-phonon interaction matrix elements. The transport properties are also varied with the crystal orientation with anisotropy mobility mostly attributed to the anisotropic band structure and effective masses. Our calculation reveals monolayer phosphorene has anisotropic hole transport property with the room temperature mobility in the armchair direction (458 cm<sup>2</sup>/Vs) about five times larger than in the zigzag direction (90 cm<sup>2</sup>/Vs). For bilayer phosphorene, the mobility on both directions increases to 1610 cm<sup>2</sup>/Vs and 760 cm<sup>2</sup>/Vs along armchair and zigzag direction respectively. The increased mobility in bilayer is consistent with the experiments which revealed low field mobility of over one thousand in multiple layer phosphorene structure, which provides optimal material for channel in field-effect transistor and a good opportunity for high-performance p-type device.<sup>1</sup> This work was supported, in part, by SRC/NRI SWAN.

**9:24AM K16.00006 Realize Dirac cones in compressed black phosphorus**, LI YANG, RUIXIANG FEI, VY TRAN, Department of Physics, Washington University — Using the k-p theory and first-principles simulations, we predict that applying a moderate uniaxial or hydrostatic pressure (>0.6GPa) on bulk or multilayer black phosphorus (BP) can diminish its bandgap and produce one-dimensional and even two-dimensional (2D) Dirac cones. Similar to topological insulators, these 2D Dirac cones result from two competing mechanisms: the unique linear band dispersion tends to open a gap via a "pseudo-spin-orbit" coupling, while the band symmetries preserve the material's gapless spectrum. In particular, these Dirac cones in BP are bulk states that do not require time-reversal symmetry, thus they can keep the high carrier mobility even in the presence of surface or magnetic perturbations. Finally, our predictions have been confirmed by recent experiments.

**9:36AM K16.00007 Extraordinary Bending Effects in MoS<sub>2</sub>, Phosphorene, and Graphene Nanoribbons<sup>1</sup>**, LIPING YU, ADRIENN RUZSINSZKY, JOHN PERDEW, Temple University — The two-dimensional (2D) materials show great potential for flexible electronics and energy applications. They have remarkable mechanical, electronic, thermal and optical properties, which are often coupled to each other. In this talk, we shall present our first principles study on the bending effects in the electronic structure of MoS<sub>2</sub>, phosphorene, and graphene nanoribbons. We predict that mechanical bending, as a unique attribute of thin 2D materials, can be used to control conductivity and Fermi-level shift. We find that bending can control the charge localization of top valence bands in both MoS<sub>2</sub> and phosphorene nanoribbons. The donor-like in-gap edge-states of armchair MoS<sub>2</sub> ribbon and their associated Fermi-level pinning can be removed by bending. A bending-controllable new in-gap state and accompanying direct-indirect gap transition are predicted in armchair phosphorene nanoribbon. We demonstrate that such emergent bending effects are realizable in experiment and can be attributed to the highly non-uniform and enormously large local in-plane strains induced by bending. The bending stiffness as well as the effective thickness of 2D materials are also derived from first principles.

<sup>1</sup>The work was supported as part of the Center for the Computational Design of Functional Layered Materials, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science

**9:48AM K16.00008 Synthesis of black phosphorus films and particles by ultra-fast laser ablation<sup>1</sup>**, GANG QIU, QIONG NIAN, YEXIN DENG, BIWEI DENG, SHENGYU JIN, ADAM CHARNAS, GARY CHENG, PEIDE YE, Purdue University — Few-layer black phosphorus (BP) has become one of top interests among various 2D materials because of its outstanding electrical and optical properties. However, availability of large size BP thin films stands as a major roadblock against further research and its applications. Here we report a method of synthesis BP films and particles by employing ultra-fast laser ablation. We demonstrated that arbitrary BP film patterns can be defined by laser direct writing. BP particles were also achieved as byproduct through manipulating laser power and frequency. Physical mechanism of laser ablation process was investigated, which also provides an optimizing strategy of improving BP thin film quality.

<sup>1</sup>The work was supported in part by NSF ECCS-1449270, NSF/AFOSR EFRI 2DARE Program, and ARO W911NF-15-1-0574

**10:00AM K16.00009 Quasiparticle Band Gap and Band Gap Reduction of Multi-Layer Black Phosphorus in an External Electric Field**, VY TRAN, LI YANG, Washington University in St Louis — Few-layer black phosphorus has emerged as a promising 2D semiconductor due to its highly tunable, direct band gap. In this talk, we examine the tunability of the band gap with respect to the number of layers and the under an external electric field. Using the results of DFT as well as many-body GW calculations, we explore the mechanism for the band gap reduction when increasing the number of layers in black phosphorus. We propose a simple model that describes this behavior, allowing us to calculate the band gap of multi-layer black phosphorus under an external electric field. The results are checked against *ab-initio* calculations, which shows excellent agreement. This allows us to overcome the limitations of DFT and predict the band gap for much larger layer numbers and electric field strength.

**10:12AM K16.00010 An Accurate and Compact Tight-binding Model for Phosphorene**, CARLOS PAEZ, ANA PEREIRA, University of Campinas, EDUARDO MUCCILO, University of Central Florida — In recent years, a variety of tight-binding models have been proposed for phosphorene. Although capturing key features such as the main band gap and the effective masses near the gamma point, they are not sufficiently accurate for the determination of electronic transport properties, particularly when probing states near the vicinity of extreme points of the valence and conduction bands. We propose a new tight-binding model parameterization based on the hybridization of s and p orbitals. For that purpose, we use the Slater-Koster method to construct a four-band model. We optimized the tight-binding parameters to fit the main features of *ab-initio* electronic band structure calculations and to reproduce the correct orbital composition at high-symmetry and low-symmetry points. Using this new tight-binding model, we compute some electronic transport properties of phosphorene ribbons in the presence of disorder.

**10:24AM K16.00011 Weak Localization in few layer Black Phosphorus**, NATHANIEL GILLGREN, YANMENG SHI, TIMOTHY ESPIRITU, University of California Riverside, KENJI WATANABE, TAKAHASHI TANIGUCHI, National Institute for Materials Science, CHUN NING (JEANIE) LAU, University of California Riverside — Few-layer black phosphorus has recently attracted interest from the scientific community due to its high mobility, tunable band gap, and large anisotropy. Recent experiments have demonstrated that black phosphorus provides a promising candidate to explore the physics of 2D semiconductors. In this study we explore the magnetotransport of few-layer black phosphorus-boron nitride heterostructure devices at low magnetic fields. Weak localization is observed at low temperatures. We extract the dephasing length and measure its dependence on temperature, carrier density and electric field.

**10:36AM K16.00012 Chemically Controlling Black Phosphorus Exfoliation to Achieve Variable-Sized Phosphorene<sup>1</sup>**, AMY NG, THOMAS SUTTO, US Naval Research Laboratory, YEXIN DENG, Purdue University, RHONDA STROUD, TODD BRINTLINGER, US Naval Research Laboratory, PEIDE YE, Purdue University, NABIL BASSIM, US Naval Research Laboratory — Phosphorene is the 2-dimensional form of phosphorus and a close relative of graphene. It has a nonzero fundamental band gap that gives rise to semiconductor properties, which makes it highly desirable for numerous applications in optoelectronics and as a replacement channel for conventional semiconductor devices. However, difficulties in isolating large area single-, few-, or multi-layer sheets are an impediment to realizing the aforementioned applications. We are investigating multiple chemical routes for optimal production of phosphorene sheets. Utilizing various solvent systems, ranging from a simple ethanol to dimethylformamide to more viscous ionic liquids, we have obtained flakes of differing thicknesses and sizes. We characterized the structure and composition of the resulting phosphorene sheets with aberration-corrected scanning transmission electron microscopy in addition to optical/macroscopic studies. Flake size, quality, and quantity obtained as a function of the solvent system, where factors such as viscosity, surface tension, chemical behavior, and degree of agitation, will be presented.

<sup>1</sup>This work was supported by the Office of Naval Research.

**10:48AM K16.00013 Negative differential resistance observed from vertical  $p^{+}-n^{+}$  junction device with two-dimensional black phosphorous<sup>1</sup>**, DAEYEONG LEE, YOUNG DAE JANG, JAEHWAN KWEON, JUNGJIN RYU, EUYHEON HWANG, WON JONG YOO<sup>2</sup>, Sungkyunkwan Univ. (SKKU), SAMSUNG-SKKU GRAPHENE/2D CENTER (SSGC) COLLABORATION — A vertical  $p^{+}-n^{+}$  homojunction was fabricated by using black phosphorus (BP) as a van der Waals two-dimensional (2D) material. The top and bottom layers of the materials were doped by chemical dopants of gold chloride ( $AuCl_3$ ) for p-type doping and benzyl viologen (BV) for n-type doping. The negative differential resistance (NDR) effect was clearly observed from the output curves of the fabricated BP vertical devices. The thickness range of the 2D material showing NDR and the peak to valley current ratio of NDR are found to be strongly dependent on doping condition, gate voltage, and BP's degradation level. Furthermore, the carrier transport of the  $p^{+}-n^{+}$  junction was simulated by using density functional theory (DFT) and non-equilibrium Green's function (NEGF). Both the experimental and simulation results confirmed that the NDR is attributed to the band-to-band tunneling (BTBT) across the 2D BP  $p^{+}-n^{+}$  junction, and further quantitative details on the carrier transport in the vertical  $p^{+}-n^{+}$  junction devices were explored, according to the analyses of the measured transfer curves and the DFT simulation results.

<sup>1</sup>This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MEST) (2013R1A2A2A01015516).

<sup>2</sup>corresponding author. Email address: yoojw@skku.edu

**Wednesday, March 16, 2016 8:00AM - 11:00AM –**

**Session K17 DCMP DMP: Many-body Interactions in Graphene** 316 - Vikram Deshpande, University of Utah

**8:00AM K17.00001 Gate-tunable electron focusing across graphene p-n junction**, SHAOWEN CHEN, Columbia University, ZHENG HAN, Institute of Metal Research, Chinese Academy of Sciences, LEI WANG, Cornell University, CORY DEAN, JAMES HONE, Columbia University — Electrons moving across a ballistic semiconductor junction experience a change in trajectory described by an electronic version of Snell's law. In the case of a barrier separating regions of  $n$  and  $p$  type carriers, negative refraction is expected, which theoretically leads to a Veselago type of electron focusing. Being a ballistic bipolar 2D system, hexagonal Boron Nitride-encapsulated graphene is expected to be a model system to realize this effect, however, robust demonstration of veselago lensing has remained limited. We describe novel methods to fabricate high quality graphene p-n junctions with atomically sharp boundaries. Using a magnetic focusing measurement scheme, we demonstrate unambiguous signatures of negative refraction in these devices. Our observations are in good agreement with simulations and shed light on future application for electronic optics in ballistic graphene.

**8:12AM K17.00002 Dynamical polarizability of the 2D pseudospin-1 dice lattice**, JOHN MALCOLM, ELISABETH NICOL, Guelph-Waterloo Physics Institute, University of Guelph — The two-dimensional dice lattice is composed of three triangular sublattices whose low-energy excitation spectrum consists of Dirac-Weyl fermions with pseudospin-1. The energy dispersion has two Dirac cones, like the pseudospin-1/2 two-triangular-sublattice graphene, with an additional third band exactly at zero energy. We present theoretical results for the electronic dynamical polarization function in the material. This is a fundamental entity in many-body physics, renormalizing the Coulomb interaction through the dielectric function. From the polarization function we also obtain the Lindhard function, the plasmon branch, and can discuss other screening effects. These are contrasted with those of graphene.

**8:24AM K17.00003 Dynamical Energy Gap Engineering in Graphene via Oscillating Out-of-Plane Deformations<sup>1</sup>**, NANCY SANDLER, DAWEI ZHAI, Department of Physics and Astronomy, Ohio University — The close relation between electronic properties and mechanical deformations in graphene has been the topic of active research in recent years. Interestingly, the effect of deformations on electronic properties can be understood in terms of pseudo-magnetic fields, whose spatial distribution and intensity are controllable via the deformation geometry. Previous results showed that electromagnetic fields (light) have the potential to induce dynamical gaps in graphene's energy bands, transforming graphene from a semimetal to a semiconductor [1, 2]. However, laser frequencies required to achieve these regimes are in the THz regime, which imposes challenges for practical purposes. In this talk we report a novel method to create dynamical gaps using oscillating mechanical deformations, i.e., via time-dependent pseudo-magnetic fields. Using the Floquet formalism we show the existence of a dynamical gap in the band structure at energies set by the frequency of the oscillation, and with a magnitude tuned by the geometry of the deformation. This dynamical-mechanical manipulation strategy appears as a promising venue to engineer electronic properties of suspended graphene devices. [1] Syzranov et al. Phys. Rev. B 78, 045407 (2008). [2] Oka et al. Phys. Rev. B 79, 081406(R) (2009).

<sup>1</sup>Work supported by NSF-DMR 1508325.

**8:36AM K17.00004 Hyperfine interaction in hydrogenated graphene**, NOEL GARCIA, International Iberian Laboratory (INL), MANUEL MELLE, Centro Algoritmi, Universidade do Minho, JOAQUIN FERNANDEZ-ROSSIER, International Iberian Laboratory (INL) — We study the hyperfine interaction of Hydrogen chemisorbed in graphene nanostructures with a gap in their spectrum, such as islands and ribbons. Chemisorption of Hydrogen on graphene results in a bound in-gap state that hosts a single electron localized around the adatom. Using both density functional theory and a four-orbital tight-binding model we study the hyperfine interaction between the hydrogen nuclear spin and the conduction electrons in graphene. We find that the strength of the hyperfine interaction decreases for larger nanostructures for which the energy gap is smaller. We then compare the results of the hyperfine interaction for large nanostructures with those of graphene 2D crystal with a periodic arrangement of chemisorbed Hydrogen atoms, obtaining very similar results. The magnitude of the hyperfine interaction is about 150 MHz, in line with that of Si:P. We acknowledge financial support by Marie-Curie-ITN 607904-SPINOGRAPH.

**8:48AM K17.00005 Two-particle vortices in graphene<sup>1</sup>**, MIKHAIL PORTNOI, University of Exeter, CHARLES DOWNING, University of Strasbourg — We show that a pair of two-dimensional massless Dirac-Weyl fermions can form a bound state independently on the sign of the inter-particle interaction potential, as long as this potential decays at large distances faster than Kepler's inverse distance law. The coupling occurs only at the Dirac point, when the charge carriers lose their chirality. These bipartite states must have a non-zero internal angular momentum, meaning that they only exist as stationary vortices. This leads to the emergence of a new type of energetically-favorable quasiparticles: double-charged zero-energy vortices. Their bosonic nature allows condensation and gives rise to Majorana physics without invoking a superconductor. The presence of dark-matter-like silent immobile vortices explains a range of poorly understood experiments in gated graphene structures at low doping.

<sup>1</sup>This work was supported by EU H2020 RISE project CoExAN, EU FP7 ITN NOTEDEV and FP7 IRSES project InterNoM.

**9:00AM K17.00006 Local density of states in bilayer graphene with 1D potential well**, AKIHIRO OKAMOTO, TAKEHITO YOKOYAMA, SHUICHI MURAKAMI, Department of Physics, Tokyo Institute of Technology — Monolayer graphene shows anomalous behaviors at the scattering by a 1D potential well due to the massless Dirac fermions, and it is called Klein paradox. In contrast, bilayer graphene shows different behaviors at the scattering by the potential well, and is attributed to the massive chiral fermions with a parabolic dispersion. We then expect that bound states at the 1D potential well for the two cases are different, due to the different effective models and the K and K' points. In the present work, we calculate bound states induced by a 1D potential well, and compare them with the properties of 1D edge states. In particular, in the bilayer graphene, there are two types of bound states, both of which have a parabolic dispersion near K and K' points, and we describe how the dispersion changes by the change of the potential strength. We then calculate the local density of states at various positions, contributed by the scattering states and the bound states by the 1D potential well, and discuss how they depend on the potential strength.

**9:12AM K17.00007 Non-perturbative renormalization group calculation of the quasi-particle velocity and the dielectric function of graphene.**, ANAND SHARMA, CARSTEN BAUER, ANDREAS RUECKRIEGEL, PETER KOPIETZ, Univ Frankfurt — We use a nonperturbative functional renormalization group approach to calculate the renormalized quasiparticle velocity  $v(k)$  and the static dielectric function  $\epsilon(k)$  of suspended graphene as function of an external momentum  $k$ . We fit our numerical result for  $v(k)$  to  $v(k)/v_F = A + B \ln(\Lambda_0/k)$ , where  $v_F$  is the bare Fermi velocity,  $\Lambda_0$  is an ultraviolet cutoff, and  $A = 1.37$ ,  $B = 0.51$  for the physically relevant value ( $e^2/v_F = 2.2$ ) of the coupling constant. In stark contrast to calculations based on the static random-phase approximation, we find that  $\epsilon(k)$  approaches unity for  $k \rightarrow 0$ . Our result for  $v(k)$  agrees very well with a recent measurement by Elias *et al.* [Nat. Phys. **7**, 701 (2011)]. With in the same approximation, we also explore an alternative scheme in order to understand the true nature of the low energy (momentum) behavior in graphene.

**9:24AM K17.00008 Majorana Zero Modes in Graphene**, PABLO SAN-JOSE, CSIC - Madrid, JOSE L. LADO, International Iberian Nanotechnology Laboratory (INL), RAMN AGUADO, CSIC - Madrid, FRANCISCO GUINEA, Instituto Madrileo de Estudios Avanzados en Nanociencia (IMDEA-Nanociencia), JOAQUIN FERNANDEZ-ROSSIER, Departamento de Fisica Aplicada, Universidad de Alicante — A clear demonstration of topological superconductivity (TS) and Majorana zero modes remains one of the major pending goal in the field of topological materials. One common strategy to generate TS is through the coupling of an s-wave superconductor to a helical half-metallic system. Numerous proposals for the latter have been put forward in the literature, most of them based on semiconductors or topological insulators with strong spin-orbit coupling. Here we demonstrate an alternative approach for the creation of TS in graphene/superconductor junctions without the need of spin-orbit coupling. Our prediction stems from the helicity of graphene's zero Landau level edge states in the presence of interactions, and on the possibility, experimentally demonstrated, to tune their magnetic properties with in-plane magnetic fields. We show how canted antiferromagnetic ordering in the graphene bulk close to neutrality induces TS along the junction, and gives rise to isolated, topologically protected Majorana bound states at either end. We also discuss possible strategies to detect their presence. Remarkable progress has recently been reported in the fabrication of the proposed type of junctions, which offers a promising outlook for Majorana physics in graphene systems.

**9:36AM K17.00009 Electron interactions in graphene through an effective Coulomb potential<sup>1</sup>**, JOAO N. B. RODRIGUES, Centre for Advanced 2D Materials and Department of Physics, National University of Singapore, SHAFFIQUE ADAM, Centre for Advanced 2D Materials and Department of Physics, National University of Singapore and Yale-NUS College — A recent numerical work [H.-K. Tang *et al.*, PRL **115**, 186602 (2015)] considering graphene's  $\pi$ -electrons interacting through an effective Coulomb potential that is finite at short-distances, stressed the importance of the  $sp^2$ -electrons in determining the semimetal to Mott insulator phase transition in graphene. Some years ago, I. F. Herbut [PRL **97**, 146401 (2006)] studied such a transition by mapping graphene's  $\pi$ -electrons into a Gross-Neveu model. From a different perspective, D. T. Son [PRB **75**, 235423 (2007)] put the emphasis on the long-range interactions by modelling graphene as Dirac fermions interacting through a bare Coulomb potential. Here we build on these works and explore the phase diagram of Dirac fermions interacting through an effective Coulomb-like potential screened at short-distances. The interaction potential used allows for analytic results that controllably switch between the two perspectives above.

<sup>1</sup>This work was supported by the Singapore National Research Foundation (NRF-NRFF2012-01 and CA2DM medium-sized centre program) and by the Singapore Ministry of Education and Yale-NUS College (R-607-265-01312).

**9:48AM K17.00010 Quasiparticle weight and renormalized Fermi velocity of graphene with long-range Coulomb interactions<sup>1</sup>**, HO-KIN TANG, JIA NING LEAW, J. N. B. RODRIGUES, Department of Physics, National University of Singapore, P. SENGUPTA, School of Physical and Mathematical Sciences, Nanyang Technological University, F. F. ASSAAD, Institut für Theoretische Physik und Astrophysik, Universität Würzburg, S. ADAM, Department of Physics, National University of Singapore — In this work, we study the effects of realistic Coulomb interactions in graphene using a projective quantum Monte Carlo simulation of electrons at half-filling on a honeycomb lattice. We compute the quasiparticle residue, the renormalized Fermi velocity and the antiferromagnetic order parameter as a function of both the long-range and short-range components of the Coulomb potential. We find that the Mott insulator transition is determined mostly by the short-range interaction and is consistent with the Gross-Neveu-Yukawa critical theory. Far from the critical point and in the semi-metallic regime, we find that the Fermi-velocity and quasiparticle residue are influenced by the long-range tail of the Coulomb potential, and for very small interaction strength are consistent with predictions of first order perturbation theory. For experimentally relevant and stronger values of the long-range interaction, our numerical data contradicts prediction from both perturbation theory and the renormalization group approaches.

<sup>1</sup>This work was supported by Singapore National Research Foundation (NRF-NRFF2012-01 and CA2DM mid-size Centre), Singapore Ministry of Education (Yale-NUS College R-607-265-01312 and MOE2014-T2-2-112), and DFG Grant No. AS120/9-1.

**10:00AM K17.00011 Snake states and their symmetries in graphene**, RAKESH TIWARI, University of Basel, YANG LIU, MATEJ BRADA, Loughborough University, C. BRUDER, University of Basel, F. V. KUSMARTSEV, Loughborough University, E. J. MELE, University of Pennsylvania — Snake states are open trajectories for charged particles moving in two dimensions under the influence of a spatially varying perpendicular magnetic field. They can also occur in a constant perpendicular magnetic field when the particle density is made nonuniform as realized at a pn junction in a semiconductor, or in graphene. We examine the correspondence of such trajectories in monolayer graphene in the quantum limit for two families of domain walls: (a) a uniform doped carrier density in an antisymmetric perpendicular magnetic field and (b) antisymmetric carrier density distribution in a uniform perpendicular magnetic field. Although, these families support different internal symmetries, the pattern of the boundary and interface currents is the same in both cases. We demonstrate that these two physically different situations are gauge equivalent when rewritten in a Nambu doubled formulation of the two limiting problems. Using gauge transformations in particle-hole space to connect these two problems, we map the protected interfacial modes to the Bogoliubov quasiparticles of an interfacial one-dimensional p-wave paired state.

**10:12AM K17.00012 A complete set of data to characterize loop braiding statistics in (3+1)-D topological phases**, DOMINIC ELSE, Department of Physics, University of California, Santa Barbara, CHETAN NAYAK, Microsoft Research, Station Q, University of California, Santa Barbara — In (2+1)-D, topological phases of matter can be classified by the braiding statistics of their particle-like excitations. Similarly, in (3+1)-D one expects topological phases to be characterized by the braiding statistics of their excitations, which may be particle-like or loop-like. A “braiding” of loop-like excitations is any continuous deformation of some collection of (possibly linked) loops which eventually returns the loops to their original locations. Here, we identify a finite set of basic data which determines the amplitude for *any* loop braiding in an abelian (3+1)-D topological phase. This includes the “three-loop braiding” recently considered by several authors, but also all other possible braidings. Our basic data are the natural generalization of the  $F$  and  $R$  symbols of (2+1)-D topological phases to (3+1)-D. From a mathematical point of view, we expect them to correspond to a “ribbon 2-category”.

**10:24AM K17.00013 A Bosonic Analogue of a Topological Dirac Semi-Metal<sup>1</sup>**, MATTHEW LAPA, University of Illinois at Urbana-Champaign, GIL YOUNG CHO, Korea Advanced Institute of Science and Technology, TAYLOR HUGHES, University of Illinois at Urbana-Champaign — We construct a bosonic analogue of a two-dimensional topological Dirac Semi-Metal (DSM). The low-energy description of the most basic 2D DSM model consists of two Dirac cones at positions  $\pm \mathbf{k}_0$  in momentum space. The local stability of the Dirac cones is guaranteed by a composite symmetry  $Z_2^{T\mathcal{I}}$ , where  $T$  is time-reversal and  $\mathcal{I}$  is inversion. This model also exhibits interesting time-reversal and inversion symmetry breaking electromagnetic responses. In this work we construct a bosonic analogue of a DSM by replacing each Dirac cone with a copy of the  $O(4)$  Nonlinear Sigma Model (NLSM) with topological theta term and theta angle  $\theta = \pm\pi$ . One copy of this NLSM also describes the gapless surface termination of the 3D Bosonic Topological Insulator (BTI). We compute the time-reversal and inversion symmetry breaking electromagnetic responses for our model and show that they are twice the value one gets in the DSM case. We also investigate the local stability of the individual  $O(4)$  NLSM's in the BSM model. Along the way we clarify many aspects of the surface theory of the BTI including the electromagnetic response, the charges of vortex excitations, and the stability to symmetry-allowed perturbations.

<sup>1</sup>NSF CAREER DMR-1351895

**10:36AM K17.00014 Hydrodynamic & Transport Properties of Dirac Materials in the Quantum Limit**, MATTHEW GOCHAN, KEVIN BEDELL, Boston College — Dirac materials are a versatile class of materials in which an abundance of unique physical phenomena can be observed. Such materials are found in all dimensions, with the shared property that their low-energy fermionic excitations behave as massless Dirac fermions and are therefore governed by the Dirac equation. The most popular Dirac material, its two dimensional version in graphene, is the focus of this work. We seek a deeper understanding of the interactions in the quantum limit within graphene. Specifically, we derive hydrodynamic and transport properties, such as the conductivity, viscosity, and spin diffusion, in the low temperature regime where electron-electron scattering is dominant. To conclude, we look at the so-called universal lower bound conjectured by the anti-de Sitter/conformal field theory (AdS/CFT) correspondence for the ratio of shear viscosity to entropy density ratio. The lower bound, given by  $\eta/s \geq \hbar/(4\pi k_B)$ , is supposedly obeyed by all quantum fluids. This leads us to ask whether or not graphene can be considered a quantum fluid and perhaps a “nearly perfect fluid” (NPF); if this is the case, is it possible to find a violation of this bound at low temperatures.

**10:48AM K17.00015 Matrix Product State approach to quantum Hall quasielectrons**, HANS HANSSON, EDDY ARDONNE, JONAS KJLL, Stockholm University — Matrix product state (MPS) techniques have been successfully used to study quasiholes in different quantum Hall states. In particular it has provided a numerically very efficient way to calculate statistical braiding phases. So far it has been hard to generalize these methods to also describe quasielectrons. Using recently developed techniques for constructing explicit wave functions for the abelian quantum Hall hierarchy, we suggest a new way to construct MPS wave functions for states containing quasielectrons, and also for Abelian hierarchy states.

## Wednesday, March 16, 2016 8:00AM - 11:00AM –

Session K18 GMAG DMP FIAP: Spin-Hall III 317 - Benjamin Jungfleisch, Argonne National Laboratory

**8:00AM K18.00001 Anomalous Hall effect in antiferromagnetic GdPtBi**, TAKEHITO SUZUKI, ARAVIND DEVARAKONDA, YU-TING LIU, JOSEPH CHECKELSKY, Massachusetts Inst of Tech-MIT — The Berry phase of the electronic wave function is responsible for a transverse velocity of conducting carriers which results in anomalous Hall conductivity. This effect has been extensively investigated in ferromagnetic systems, but less is known in antiferromagnets. We have synthesized single crystals of GdPtBi, a metallic system which exhibits antiferromagnetic ordering below the transition temperature  $T_N = 9$  K. We have investigated the electrical transport and magnetic properties of these crystals and found a distinct anomalous Hall effect response. We will discuss these observations in the context of the known mechanisms for anomalous velocity in ferromagnets and recent models unique to antiferromagnetic systems.

**8:12AM K18.00002 Spin transport in antiferromagnetic insulator detected by spin pumping**, WEI CAO, YI LI, WILLIAM BAILEY, Columbia Univ — Spin transport in antiferromagnetic insulators has drawn attention recently. Prior work has been done on the spin diffusion length of different antiferromagnetic materials via inverse spin hall effect. In this work, we measure the spin pumping of Py/Cu/CoO to characterize the absorption of spin current in the CoO layer. The series of Py/Cu/CoO (t) with changing the thickness of CoO layer indicates that there is a Gilbert damping enhancement of 0.001 in saturation at about 2 nm at room temperature. The spin mixing conductance obtained from this experimental series and from Py (t)/Cu/CoO series is  $2.4 \text{ nm}^{-2}$  and  $3.2 \text{ nm}^{-2}$ , respectively. We also measured the spin pumping of the Py/Cu/CoO sample at low temperatures. The Gilbert damping exhibits a positive peak at about 280 K, which is close to the  $Nel$  temperature of CoO. Our work shows a finite spin mixing conductance in Py/Cu/CoO and the spin diffusion length of CoO is quite small at room temperature. We also find that its Gilbert damping reaches its maximum value at  $Nel$  temperature.

**8:24AM K18.00003 Spin current control of damping in YIG/Pt nanowires**, CHRISTOPHER SAFRANSKI, IGOR BARSUKOV, HAN KYU LEE, University of California Irvine, TOBIAS SCHNEIDER, Helmholtz-Zentrum Dresden Rossendorf, ALEJANDRO JARA, ANDREW SMITH, University of California Irvine, HOUCHEH CHANG, 3 Colorado State University, YAROSLAV TSEKOVNYAK, University of California Los Angeles, MINGZHONG WU, 3 Colorado State University, ILYA KRIVOROTOV, University of California Irvine — Understanding of spin transport at ferromagnet/normal metal interfaces is of great importance for spintronics applications. We report the effect of pure spin currents in YIG(30 nm)/Pt(6 nm) nanowires. The samples show magneto-resistance from two distinct mechanisms: (i) spin Hall magnetoresistance (SMR) and (ii) inverse spin Hall effect (ISHE) along with spin Seebeck current (SSC) induced by Ohmic heating of the Pt layer. Using the SMR and ISHE effects, we measure the spin wave eigenmodes by spin-torque ferromagnetic resonance (ST-FMR). Direct current applied to the Pt layer results in injection of spin Hall current into YIG that acts as damping or anti-damping spin torque depending on the polarity. In addition, Ohmic heating gives rise to a SSC acting as anti-damping regardless of current polarity. ST-FMR reveals current-induced variation of the spin wave mode linewidth that is asymmetric in the bias current and decreases to zero for anti-damping spin Hall current. Near this current, we observe complex interaction among the spin wave eigenmodes that we assess using micromagnetic simulations. Our results advance understanding of magnetization dynamics driven by pure spin currents.

**8:36AM K18.00004 Spin Circuit Representation of Spin Pumping in Topological Insulators<sup>1</sup>**, KUNTAL ROY, Purdue University — Earlier we developed spin circuit representation of spin pumping and combined it with the spin circuit representation for the inverse spin Hall effect to show that it reproduces the established results in literature [1]. Here we construct the spin circuit representation of spin pumping in topological insulators. The discovery of spin-polarized surface states in three-dimensional (3D) topological insulators (TIs) with strong spin-orbit coupling is promising for the development of spintronics. There is considerable bulk conduction too in 3D TIs (e.g., Bi<sub>2</sub>Se<sub>3</sub>) apart from possessing the surface states. We utilize the spin circuit model for spin orbit torques in topological insulator surface states [2] to develop the equivalent circuit model of spin pumping in topological insulators. Such equivalent circuit model developed here can be utilized to analyze available experimental results and evaluate more complex structures. [1] K. Roy et al., Spin Circuit Representation for Spin Pumping Phenomena, in APS March Meeting, Session Y28.12 (2015). [2] S. Hong, Spin Circuit Model for Spin-Orbit Torque in 2D Channels, in APS March Meeting, Session G52.1 (2015).

<sup>1</sup>This work was supported by FAME, one of six centers of STARnet, a Semiconductor Research Corporation program sponsored by MARCO and DARPA

**8:48AM K18.00005 Spin pumping from a ferromagnet into a hopping insulator: Role of resonant absorption of magnons<sup>1</sup>**, MIKHAIL RAIKH, YUE ZHANG, DMYTRO PESIN, Univ of Utah — Motivated by recent experiments [1,2,3] on spin pumping from a ferromagnet into organic materials in which the charge transport is due to hopping, we study theoretically the generation and propagation of spin current in a hopping insulator. Unlike metals, the spin polarization at the boundary with ferromagnet is created as a result of magnon absorption within pairs of localized states and it spreads following the current-carrying resistor network (although the charge current is absent). We consider a classic resonant mechanism of the ac absorption in insulators and adapt it to the absorption of magnons. A strong enhancement of pumping efficiency is predicted when the Zeeman splitting of the localized states in external magnetic field is equal to the frequency of ferromagnetic resonance. Under this condition the absorption of a magnon takes place within *individual* sites.

[1] K. Ando *et al.*, Nat. Mater. **12**, 622 (2013).

[2] S. Watanabe *et al.*, Nat. Phys. **10**, 308 (2014).

[3] Z. Qiu *et al.*, AIP Advances **5**, 057167 (2015).

<sup>1</sup>This work was supported by the NSF MRSEC program at the University of Utah under Grant No. DMR 1121252 (Z.Y. and M.E.R.) and by the NSF Grant No. DMR 1409089 (D.A.P.).

**9:00AM K18.00006 Detection of topological surface states by spin pumping at room temperature**, Y. T. FANCHIANG, C. K. CHENG, M. HONG, Graduate Institute of Applied Physics and Department of Physics, National Taiwan University, Taipei 10617, Taiwan, H. Y. LIN, K. H. CHEN, S. R. YANG, C. N. WU, J. KWO, Department of Physics, National Tsing Hua University, Hsinchu 30013, Taiwan, S. F. LEE, Institute of Physics, Academia Sinica, Taipei 11529, Taiwan — Spin pumping on heterostructures made of ferrimagnetic YIG film and topological insulator Bi<sub>2</sub>Se<sub>3</sub> films has been performed at room temperature. In the presence of topological interface states, spin pumping induced non-equilibrium spin density caused significant resonance field shifts ( $H_{\text{res}}$  shifts) of YIG/Bi<sub>2</sub>Se<sub>3</sub> with respect to bare YIG. The uncommon  $H_{\text{res}}$  shifts correspond to clearly resolved changes of gyromagnetic ratio of YIG. As the Bi<sub>2</sub>Se<sub>3</sub> thickness varied from 4 nm to 20 nm, increasing  $H_{\text{res}}$  shifts were observed, while the enhancement of damping constant saturated at the spin diffusion length of Bi<sub>2</sub>Se<sub>3</sub>, suggesting the two parameters were of different origins. Bi<sub>2</sub>Se<sub>3</sub> thickness dependence of spin pumping revealed that Rashba-split 2DEG has comparable effects on the magnetization dynamics. From the change of gyromagnetic ratio, we calculated the imaginary part of spin mixing conductance to be one order of magnitude larger than the real part. Our results showed that with clean and well-defined interface, spin pumping may serve as an effective way to detect spin-polarized surface states.

**9:12AM K18.00007 Current-induced spin and orbital magnetizations in tellurium**, TAIKI YODA, MOTOAKI HIRAYAMA, TAKEHITO YOKOYAMA, Department of Physics, Tokyo Institute of Technology, SHOJI ISHIBASHI, TAKASHI MIYAKE, Nanosystem Research Institute, AIST, SHUICHI MURAKAMI, Department of Physics, Tokyo Institute of Technology, TIES, Tokyo Institute of Technology — Tellurium has a characteristic helical lattice structure, and lacks inversion and mirror symmetries. Such chiral crystals lead to various novel phenomena. For example, we have shown that spin and orbital magnetizations are induced by an electric current in chiral crystals[1]. In our presentation, we calculate the current-induced spin and orbital magnetization in tellurium by using first-principles calculations. The calculations show that both spin and orbital magnetizations are induced parallel to the electric current. In tellurium we found that the orbital magnetization is larger than the spin magnetization by two orders of magnitude. The spin magnetization is induced by the current via the spin-orbit coupling. Therefore, the induced spin magnetization is limited by the size of the spin-orbit coupling. On the other hand, the orbital magnetization is determined by crystal structure without spin-orbit coupling. By using a chiral crystal, a magnetization can be induced by an electric current without ferromagnets and the spin-orbit coupling. [1]Yoda, T. et al. Sci. Rep. **5**, 12024

**9:24AM K18.00008 Enhanced spin Hall ratios by Al and Hf impurities in Pt thin films<sup>1</sup>**, MINH-HAI NGUYEN, MENGNAO ZHAO, DANIEL C. RALPH, ROBERT A. BUHRMAN, Cornell Univ — The spin Hall effect (SHE) in Pt has been reported to be strong and hence promising for spintronic applications. In the intrinsic SHE mechanism, which has been shown to be dominant in Pt, the spin Hall conductivity  $\sigma_{SH}$  is constant, dependent only on the band structure of the spin Hall material. The spin Hall ratio  $\theta_{SH} = \sigma_{SH} / \rho$ , on the other hand, should be proportional to the electrical resistivity  $\rho$  of the spin Hall layer. This suggests the possibility of enhancing the spin Hall ratio by introducing additional diffusive scattering to increase the electrical resistivity of the spin Hall layer. Our previous work has shown that this could be done by increasing the surface scattering by growing thinner Pt films in contact with higher resistivity materials such as Ta. In this talk, we discuss another approach: to introduce impurities of metals with negligible spin orbit torque into the Pt film. Our PtAl and PtHf alloy samples exhibit strong enhancement of the spin Hall torque efficiency with impurity concentration due to increased electrical resistivity.

<sup>1</sup>Supported in part by Samsung Electronics

**9:36AM K18.00009 Large Spin Hall Angle in Vanadium Film**, TAO WANG, Department of Physics and Astronomy, University of Delaware, Newark, DE 19716 USA, XIN FAN, Department of Physics and Astronomy, University of Denver, Denver, CO 80208 USA, WENRUI WANG, Department of Physics, University of Illinois, Urbana, IL 61801 USA, YUNSONG XIE, MUHAMMAD A. WARS, JUN WU, YUNPENG CHEN, Department of Physics and Astronomy, University of Delaware, Newark, DE 19716 USA, VIRGINIA O. LORENZ, Department of Physics, University of Illinois, Urbana, IL 61801 USA, JOHN Q. XIAO, Department of Physics and Astronomy, University of Delaware, Newark, DE 19716 USA — We report the large spin Hall angle observed in Vanadium film with small grain size and distorted lattice parameter. The spin Hall angle is quantified by measuring current-induced spin-orbit torque in V/CoFeB bilayer using optical spin torque magnetometer based on polar magneto-optical Kerr effect (MOKE). The spin Hall angle as large as  $\theta_{SH} = -0.071$  has been observed in V/CoFeB bilayer Structural analysis, using X-ray diffraction (XRD), transmission electron microscopy (TEM) and selected area electron diffraction (SAED), confirms films grown at room temperature have very small grain size and enlarged lattice parameter. The Vanadium films with distorted crystal structure also have high resistivity ( $>200 \mu\Omega\bullet\text{cm}$ ) and long spin diffusion length ( $\sim 16.3 \text{ nm}$ ) measured via spin pumping experiment. This finding of spin Hall effect enhancement in more disordered structure will provide insights for understanding and exploiting materials with strong spin orbit interaction, especially in light 3d transition metals which promise long spin diffusion length.

**9:48AM K18.00010 Spin-orbit torques and charge pumping in crystalline magnets**, CHIARA CICCARELLI, Univ of Cambridge — In magnetic crystals with an inversion asymmetric unit cell a non-zero global spin-polarization is generated by an electrical current, which acts with a torque on the magnetisation exciting magnetic dynamics [1]. This relativistic non-equilibrium spin phenomenon also has a reciprocal effect in which the excitation of magnons results in the pumping of a charge current [2]. The possibility to manipulate/read magnetism with electrical currents is highly relevant for magnetic memories and other spintronic devices. I will start by reviewing our recent research on spin-orbit torques (SOTs) in crystalline magnets, in particular our very recent measurements of the crystalline SOT at room temperature in half-Heusler NiMnSb thin films. With this experiment we are able to fully characterise magnitude and symmetry of the SOTs [3, 4]. I will then talk about the first demonstration of magnonic charge pumping in crystal magnet GaMnAs [2]. In this effect, which is the reciprocal effect of SOTs, the precessing ferromagnet pumps a charge current. Differently from spin pumping, which is commonly used to electrically detect magnetization dynamics, in charge pumping magnons are converted within the ferromagnet into high-frequency currents via the relativistic spin-orbit interaction, without the need of a secondary spin-charge conversion element, such as heavy metals with large spin Hall angle. References 1. Chernyshov et al., Nature Physics 5, 656 (2009). 2. Ciccarelli et al., Nature nanotechnology 10, 50 (2014). 3. Fang et al., Nature Nanotechnology 6, 413 (2011). 4. Kurebayashi et al., Nature Nanotechnology 9, 211 (2014).

**10:24AM K18.00011 Experiment study on special anisotropy of spin mixing conductance**, XIAOLONG FAN, HENGAN ZHOU, Lanzhou University, LI MA, SHIMING ZHOU, Tongji University, DESHENG XUE, Lanzhou University — Spin pumping, a promising technique for generating pure spin current via ferromagnetic resonance (FMR), can pump nonequilibrium magnetization through the interface between normal metal (NM) and ferromagnetic metal or ferromagnetic insulator. The efficiency of spin current injection is determined by spin mixing conductance (SMC). In this work, we systematically investigate the values of the SMC in NM(Pt, Pd, W, Mo)/YIG systems. By using cavity FMR, we found that the SMC has in-plane isotropy but out-of-plane anisotropy. The values of SMC show maximum when magnetization is along film normal. We also used electrical detection of inverse spin Hall voltage to double check the anisotropy of SMC. We attribute such anisotropy to the interfacial spin orbit coupling.

**10:36AM K18.00012 Moderate Positive Spin Hall Angle in Uranium<sup>1</sup>**, MARTA ANGUERA, SIMRAN SINGH, ENRIQUE DEL BARCO, University of Central Florida, ROSS SPRINGELL, University of Bristol, CASEY W. MILLER, Rochester Institute of Technology — We will present results on FMR and voltage measurements of magnetic damping and the inverse spin Hall effect, respectively, in Ni<sub>80</sub>Fe<sub>20</sub>/Uranium bilayers. A pure spin current is injected into an Uranium film from the ferromagnetic resonance dynamics of the magnetization of an adjacent Ni<sub>80</sub>Fe<sub>20</sub> (permalloy) film. The spin current generated is then converted into an electric field by the inverse spin Hall effect. Our results suggest a spin mixing conductance of order  $2 \times 10^{19} \text{ m}^{-2}$  and a positive spin Hall angle of 0.004, which are both unexpected based on trends in d-electron systems. These results support the idea that materials with unfilled f-electron orbitals may require additional exploration for spin physics.

<sup>1</sup>Work at UCF was supported by NSF-ECCS grant 1402990. Work at RIT was supported by NSF-ECCS Grant 1515677.

**10:48AM K18.00013 Thickness dependence of inverse spin Hall effect in Au and W studied using YIG-based spin pumping**, KENG-YUAN MENG, JACK BRANGHAM, JAMES GALLAGHER, SISHENG YU, SHANE WHITE, WILLIAM RUANE, ROHAN ADUR, CHRIS HAMMEL, FENGYUAN YANG, The Ohio State University — Yttrium iron garnet (YIG) is an excellent material for generating pure spin currents due to its narrow ferromagnetic resonance (FMR) linewidth and low damping. High quality YIG thin films are deposited by off-axis magnetron sputtering, followed by in-situ deposition of Au and W layers of varying thicknesses. Using the inverse spin-Hall effect (ISHE) in the Au and W layers, we study FMR-driven spin pumping from YIG thin films (16nm) into each metal at thicknesses of 2-50nm. Gilbert damping of these bilayers are obtained with variable frequency FMR measurements. Spin transport parameters, including the spin diffusion length in metal, spin mixing conductance at the interfaces and spin hall angles, are also determined.

## Wednesday, March 16, 2016 8:00AM - 11:00AM —

Session K19 GMAG DMP FIAP: III-V Magnetic Semiconductors 318 - Paul Crowell, University of Minnesota

**8:00AM K19.00001 An X-ray standing wave study of the diluted magnetic semiconductor Ga(Mn)As**, SLAVOMIR NEMSAK, Forschungszentrum Juelich, CHENG-TAI KUO, UC Davis, CHRISTOPH SCHLUETER, Diamond Light Source, MATHIAS GEHLMANN, Forschungszentrum Juelich, SHIH-CHIEH LIN, UC Davis, SVEN DOERING, MARKUS ESCHBACH, EWA MLYNCZAK, LUKASZ PLUCINSKI, Forschungszentrum Juelich, STEPHAN BOREK, JAN MINAR, University Muenchen, HIDEO OHNO, Tohoku University, TIEN-LIN LEE, Diamond Light Source, CLAUS M. SCHNEIDER, Forschungszentrum Juelich, CHARLES S. FADLEY, UC Davis — We have combined the recently developed techniques of soft x-ray standing-wave angle-resolved photoemission (SW-ARPES) [Gray et al., EPL 104, 17004 (2013)] and hard x-ray ARPES (HARPES) [Gray et al., Nature Mat. 11, 957 (2012)] so as to be able to use single-crystal Bragg reflection to create the SW [Thiess et al., Sol. St. Comm. 150, 553 (2010)], thus permitting the first measurements of momentum- and element- resolved bulk electronic structure. The strengths of the SW-HARPES method are demonstrated using the dilute magnetic semiconductor Ga<sub>(1-x)</sub>Mn<sub>x</sub>As. A strong SW is generated by Bragg reflection of ca. 3 keV x-rays from the (111) planes of both undoped GaAs and Mn-doped thin films with x=0.05. Due to the uneven occupancy of (111) planes by either Ga(Mn) or As atoms, the element-specific band structure can be obtained with a help of the SW modulation in core levels. Apart from the site specific decomposition of the electronic structure, the SW measurements also confirmed a substitutional presence of Mn atoms at the Ga sites. This technique should be applicable to a broad range of complex materials.

**8:12AM K19.00002 Magnetism and Mn Clustering in (In, Mn)Sb Magnetic Semiconductors.<sup>1</sup>**, BRUCE WESSELS, JINDONG LIU, MICAH HANSON, JOHN PETERS, Northwestern University — Magnetic semiconductors doped with transition metal elements such as (In,Mn)Sb and (Ga,Mn)Sb are considered ideal systems for spintronic devices such as magnetic junction transistors. The magnetic behavior of these semiconductors is largely influenced by magnetic atom distribution, electronic structure, and chemical state. The Mn distribution and phase composition in (In, Mn)Sb films grown by metal-organic vapor phase epitaxy (MOVPE) were determined using X-ray photoelectron spectroscopy (XPS). From XPS the spin-orbit splitting energy of the Mn 2p core-level was found to increase with increasing Mn concentration. The measured magnetic moment per Mn atom decreases with increasing Mn concentration, which is attributed to atomic-scale clusters that are ferromagnetic or ferrimagnetic. The magnetic properties in conjunction with XPS analysis indicate that atomic-scale Mn clusters could be responsible for the high-temperature magnetism of greater than 400 K in (In,Mn)Sb. These results demonstrate the potential of modifying the magnetic properties of (In,Mn)Sb films by controlling Mn concentration or phase composition.

<sup>1</sup>This work was supported by the NSF under grant DMR-1305666.

**8:24AM K19.00003 Electronic structure near the Fermi level in the ferromagnetic semiconductor GaMnAs studied by ultrafast time-resolved light-induced reflectivity measurements<sup>1</sup>**, TOMOAKI ISHII, TADASHI KAWAZOE, Univ of Tokyo, YUSUKE HASHIMOTO, Radboud Univ Nijmegen, HIROSHI TERADA, IRIYA MUNETA, MOTOICHI OHTSU, MASAOKI TANAKA, SHINOBU OHYA, Univ of Tokyo — The determination of the Fermi level ( $E_F$ ) position is important to understand the origin of the ferromagnetism in ferromagnetic semiconductor GaMnAs. The recent transient reflectivity (TR) spectroscopy measurement, which is potentially sensitive to the absorption edges, indicated that the  $E_F$  exists in the valence band [1]. However, the pump fluence in this study is rather high, and the accumulation of photo-carriers can shift the absorption edges. Thus, the definition of both the band gap and  $E_F$  is obscure. Here, we have performed TR spectroscopy measurements on GaMnAs films with the pump fluence carefully controlled to suppress the accumulation of photo-carriers. The energy resolution of the TR spectrum was improved to 0.5 meV. The data shows light-induced change in the reflectivity spectra which is attributed to the band-gap renormalization and band filling. We have reproduced the observed TR spectra using the Kramers-Kronig relation and found the Mn-induced electronic states near the  $E_F$  in the band gap. [1] T. de Boer et al., Phys. Rev. B 85, 033202 (2012).

<sup>1</sup>This work was partially supported by Grants-in-Aids for Scientific Research including Specially Promoted Research and Project for Developing Innovation Systems of MEXT.

**8:36AM K19.00004 High Field Magnetic Circular Dichroism in Ferromagnetic InMnSb and InMnAs<sup>1</sup>**, M. A. MEEKER, B. A. MAGILL, G. A. KHODAPARAST, Virginia Tech, D. SAHA, C. J. STANTON, University of Florida, S. MCGILL, NHMFL, Florida, B. W. WESSELS, Northwestern Univ. — An understanding of the fundamental interactions in narrow gap ferromagnetic semiconductors such as InMnAs and InMnSb has been developed primarily from static magnetization and electrical transport measurements. In this study, to provide a better understanding of the coupling of the Mn impurities to the conduction and valence bands through the sp-d exchange interactions, we have performed magnetic circular dichroism measurements (MCD) on MOVPE grown InMnAs and InMnSb. In our samples, the Mn content varies from 2% to 10.7% and all the samples have Curie temperatures above 300 K. The samples were photo-excited using a Quartz Tungsten Halogen lamp with energies ranging between 0.92-1.45 eV, and in magnetic fields up to 31 T. The temperatures ranged from 15-190 K. Comparison of the observed MCD with theoretical calculations provides a direct method to probe the band structure including the temperature dependence of the spin-orbit split-off bandgap and g-factors, as well as a means to estimate the sp-d coupling constants.

<sup>1</sup>Supported by the AFOSR through grant FA9550-14-1-0376, NSF-Career Award DMR-0846834, NSF-DMR-60035274, NSF-DMR-1305666, NSF MRI program (DMR-1229217).

**8:48AM K19.00005 Spin-dependent transport properties of a GaMnAs-based vertical spin metal-oxide-semiconductor field-effect transistor structure<sup>1</sup>**, TOSHIKI KANAKI, HIROKATSU ASAHARA, SHINOBU OHYA, MASAOKI TANAKA, The University of Tokyo — Spin metal-oxide semiconductor field-effect transistors (spin MOSFETs) [1] are one of the most promising devices for the post-scaling era. In previous studies on spin MOSFETs[2,3], the drain-source current was controlled by the gate-source voltage and magnetization configuration of the source and drain; however, the magnetoresistance (MR) ratios (0.1% [2] and 0.005% [3]) were too small to be put into practical applications, and thus spin MOSFET with a high MR ratio is strongly required. Here, we study a GaMnAs-based vertical spin-MOSFET structure. We successfully modulate the drain-source current  $I_{DS}$  by  $\sim 0.5$  (–0.5) % with a gate-source voltage of  $-10.8$  (+10.8) V and also modulate  $I_{DS}$  by up to 60 % with changing the magnetization configuration of the GaMnAs source/drain at 3.5 K. The MR ratio is more than two orders of magnitude higher than that obtained in the previous studies on spin MOSFETs[2,3][4] [1] S. Sugahara and M. Tanaka, APL 84, 2307 (2004). [2] R. Nakane et al., JJAP 49, 113001 (2010). [3] T. Sasaki et al., Phys. Rev. Appl. 2, 034005 (2014). [4] T. Kanaki et al., submitted; arXiv:1510.07497.

<sup>1</sup>This work is supported by Grants-in-Aid for Scientific Research including the Specially Promoted Research and the Project for Developing Innovation Systems of MEXT.

**9:00AM K19.00006 Ferromagnetism in Silicon Single Crystals with Positively Charged Vacancy Clusters<sup>1</sup>**, YU LIU, Helmholtz Zentrum Dresden-Rossendorf, XINGHONG ZHANG, QUAN YUAN, JIECAI HAN, Harbin Institute of Technology, SHENGQIANG ZHOU, Helmholtz Zentrum Dresden-Rossendorf, BO SONG, Harbin Institute of Technology — Defect-induced ferromagnetism provides an alternative for organic and semiconductor spintronics. Here, we investigated the magnetism in Silicon after neutron irradiation and try to correlate the observed magnetism to particular defects in Si. Commercially available p-type Si single crystal wafer is cut into pieces for performing neutron irradiations. The magnetic impurities are ruled out as they can not be detected by secondary ion mass spectroscopy. With positron annihilation lifetime spectroscopy, the positron trapping center corresponding to lifetime 375 ps is assigned to a kind of stable vacancy clusters of hexagonal rings (V6) and its concentration is enhanced by increasing neutron doses. After irradiation, the samples still show strong diamagnetism. The weak ferromagnetic signal in Si after irradiation enhances and then weakens with increasing irradiation doses. The saturation magnetization at room temperature is almost the same as that at 5 K. The X-ray magnetic circular dichroism further provides the direct evidence that Silicon is the origin of this ferromagnetism. Using first-principles calculations, it is found that positively charged V6 brings the spin polarization and the defects have coupling with each other.

<sup>1</sup>The work is financially supported by the Helmholtz Postdoc Programme (Initiative and Networking Fund, PD-146).

### 9:12AM K19.00007 Microscopic understanding of spin current probed by shot noise<sup>1</sup>, TOMONORI

ARAKAWA, Department of Physics, Graduate School of Science, Osaka University, 560-0043, Toyonaka, Osaka — The spin currents is one of key issue in the spintronics field and the generation and detection of those have been intensively studied by using various materials. The analysis of experiments, however, relies on phenomenological parameters such as spin relaxation length and spin flip time. The microscopic nature of the spin current such as energy distribution and energy relaxation mechanism, has not yet well understood. To establish a better microscopic understanding of spin currents, I focused on the shot noise measurement which is well established technique in the field of mesoscopic physics [Y. M. Blanter and M. Büttiker, Phys. Rep. 336, 1 (2000)]. Although there are many theoretically works about shot noise in the presence of spin currents, for example detection of spin accumulation [J. Meair, P. Stano, and P. Jacquod, Phys. Rev. B 84 (2011).], estimation of spin flip currents, and so on, these predictions have never been experimentally confirmed. In this context, we reported the first experimental detection of shot noise in the presence of the spin accumulation in a (Ga,Mn)As/tunnel barrier/n-GaAs based lateral spin valve device [T. Arakawa et al., Phys. Rev. Lett. 114, 016601 (2015)].

Together with this result, we found however that the effective temperature of the spin current drastically increases due to the spin injection process. This heating of electron system could be a big problem to realize future spin current devices by using quantum coherence, because the effective temperature rise directly related to the destruction of the coherence of the spin current. Therefore, then we focused on the mechanism of this heating and the energy relaxation in a diffusive channel. By measuring current noise and the DC offset voltage in the usual non-local spin valve signal as a function of the spin diffusion channel length, we clarified that the electron-electron interaction length, which is the characteristic length for the relaxation of the electron system, is much longer than the spin relaxation length. In other words, the spin currents in such a semiconducting material can be strongly out of equilibrium. In this invited talk, I will present a series of experimental work on the spin current in a (Ga,Mn)As/tunnel barrier/n-GaAs based lateral spin valve device, mainly probed by the current noise measurement. Finally I hope I will mention about our future plan to cool down the effective temperature of the spin current by using superconductivity.

<sup>1</sup>This work was partially supported by JSPS KAKENHI Grant Numbers 26220711, 25887037, 25103003, and 15K17680.

### 9:48AM K19.00008 Physical Properties of Fe-doped Ba(Mn<sub>1-x</sub>Fe<sub>x</sub>)<sub>2</sub>Sb<sub>2</sub> Single Crystals, ZHENYU

DIAO, JIANNENG LI, AHMAD US SALEHEEN, TAPAS SAMANTA, W.ADAM PHELAN, SHANE STADLER, RONGYING JIN, Department of Physics and Astronomy, Louisiana State University — BaMn<sub>2</sub>Sb<sub>2</sub> forms the ThCr<sub>2</sub>Si<sub>2</sub>-type crystal structure and has the magnetic semiconducting ground state. In attempt to alter its ground-state properties, Mn is partially substituted by Fe resulting in Ba(Mn<sub>1-x</sub>Fe<sub>x</sub>)<sub>2</sub>Sb<sub>2</sub>. While the doped system remains the same structure for  $x \leq 0.5$ , its electrical and thermal conductivity decreases with increasing  $x$ , suggesting that doping-induced disorder plays an important role. Magnetically, we find that, with increasing  $x$ , the magnetic transition temperature  $T_M$  decreases (from 700 K for  $x = 0$  to 500 K for  $x = 0.5$ ) but magnetic susceptibility increases above and below  $T_M$ . These and low-temperature magnetization anisotropy suggest the canted-antiferromagnetic configuration with net magnetic moment in BaMn<sub>2</sub>Sb<sub>2</sub>. The antiferromagnetic interaction is gradually suppressed upon Fe doping, leading to the enhanced ferromagnetic component in Ba(Mn<sub>1-x</sub>Fe<sub>x</sub>)<sub>2</sub>Sb<sub>2</sub>.

### 10:00AM K19.00009 Magnetic Coupling in FeBi<sub>2</sub>Se<sub>4</sub> and FeSb<sub>2</sub>Se<sub>4</sub> from first principles, LOGAN

WILLIAMS, EMMANOUIL KIOUPAKIS, JUAN LOPEZ, PIERRE FERDINAND P. POUDEU, University of Michigan — Spintronic devices offer benefits in power efficiency and size reduction over current electronics, but require the development of semiconductor materials with favorable magnetic properties. Specifically, a high ferromagnetic-to-paramagnetic Curie transition temperature is required for spintronics operation at room temperature. FeBi<sub>2</sub>Se<sub>4</sub> and FeSb<sub>2</sub>Se<sub>4</sub> are two n and p-type magnetic semiconductors, respectively, with Curie transition temperatures of 450K. We employ first-principles calculations based on density functional theory to examine the magnetic coupling mechanisms in these materials. Our results indicate that antisite defects of Fe upon the Bi/Sb sites are crucial to the ferromagnetic coupling of the Fe magnetic moments in the crystals. This research was supported by the National Science Foundation CAREER award through Grant No. DMR-1254314. Computational Resources were provided by the DOE NERSC facility.

### 10:12AM K19.00010 Strain fields and electronic structure of CrN<sup>1</sup>, TOMAS ROJAS, SERGIO E. ULLOA,

Ohio University — Chromium nitride (CrN) has a promising future for its resistance to corrosion and hardness, and very interesting magnetic and electronic properties. CrN presents a phase transition in which the crystal structure, magnetic ordering and electronic properties change at a (Nel) temperature  $\sim 280$  K. Thin films from different labs exhibit different conductance behavior at low temperature. We study the unusual electronic and magnetic properties of thin layers. For that purpose we develop a tight binding Hamiltonian based on the Slater-Koster approach, and estimate the interaction between the Cr-3d and N-2p orbitals, by analyzing the band structure and comparing it with ab initio calculations performed using the LSDA+U method [1]. These calculations show the system to behave as a semiconductor below the Nel temperature. Based on our model we calculate the effective masses and analyze the effect of strain fields in the electronic structure in order to understand the electronic behavior near the phase transition. [1] A. Herwadkar and W. Lambrecht, Phys. Rev. B 79(3), 035125 (2009).

<sup>1</sup>Supported by NSF DMR-1508325

### 10:24AM K19.00011 Observation of the room-temperature local ferromagnetism and its nanoscale growth in the ferromagnetic semiconductor GeFe<sup>1</sup>, Y. K. WAKABAYASHI, S. SAKAMOTO, The Univ.

of Tokyo, Y. TAKEDA, JAEA, K. ISHIGAMI, Y. TAKAHASHI, Y. SAITOH, The Univ. of Tokyo, H. YAMAGAMI, JAEA, A. FUJIMORI, M. TANAKA, S. OHYA, The Univ. of Tokyo — Group-IV-based ferromagnetic semiconductor GeFe is expected to be efficient spin injectors and detectors in group-IV-based semiconductor devices, because it can be epitaxially grown on Si and Ge substrates [1,2] and the  $T_C$  can be increased up to 210 K by annealing [3]; however, detailed microscopic understanding of the ferromagnetism is lacking. In this study, we have investigated the local magnetic properties of the GeFe films, using soft X-ray magnetic circular dichroism. We found that nanoscale local ferromagnetic regions formed in the high-Fe-content regions exist even at room temperature, well above the Curie temperature of 20 - 100 K. We also observed the intriguing nanoscale growth process of the local ferromagnetic regions in which they expand as temperature decreases, followed by a transition of the entire film into a ferromagnetic state at the Curie temperature [4]. References [1] Y. Ban, Y. Wakabayashi et al., AIP Adv. 4, 097108 (2014). [2] Y. K. Wakabayashi et al., Phys. Rev. B, 90, 205209 (2014). [3] Y. K. Wakabayashi et al., J. Appl. Phys. 116, 173906 (2014). [4] Y. K. Wakabayashi et al., arXiv:1502.00118 (2015).

<sup>1</sup>This work was partly supported by Giant-in-Aids for Scientific Research including Specially Promoted Research, Project for Developing Innovation Systems of MEXT, and FIRST program of JSPS.

**10:36AM K19.00012 Magnon-drag and thermomagnetic transport properties of Ca doped YIG<sup>1</sup>**, YUANHUA ZHENG, BIN HE, The Ohio State University - Columbus, XI CHEN, JIANSHI ZHOU, University of Texas at Austin, LI SHI, ROBERTO MYERS, JOSEPH HEREMANS, The Ohio State University - Columbus — Yttrium-iron garnet (YIG) is an insulating ferromagnet commonly used to study various spin transport phenomena: in conjunction with a Pt film, it generates the well-known spin-Seebeck effect [1]. Because of the close relationship between the spin-Seebeck effect and the magnon-drag charge Seebeck effect [2], we investigate the thermoelectric transport properties of an electrically conducting bulk YIG crystal doped p-type with Ca. A large and sharp change in the thermopower of Ca:YIG near the Curie temperature has been observed, which is potentially explained by the magnon-drag model. We present the temperature dependence of electrical conductivity, magneto-thermopower, and Hall coefficient of Ca:YIG. Photo-excitation of the carriers from the valence band into the Ca level results in photoconductivity and photo-Seebeck effects as well. [1] Jin et al., *Phys. Rev. B* 92, 054436 (2015) [2] Lucassen et al., *Appl. Phys. Lett.* 99 262506 (2011)

<sup>1</sup> Acknowledgement: ARO MURI W911NF-14-1-0016

**10:48AM K19.00013 Infrared Kerr measurements on ferromagnetic silicon and silicon carbide**, JUNGRYEOL SEO, ALOK MUKHERJEE, MUMTAZ MURAT ARIK, JOHN CERNE, Department of Physics, University at Buffalo, Buffalo, NY, USA, YU LIU, SHENGQIANG ZHOU, ROMAN BTTGER, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstrae 400, 01328 Dresden, Germany, BO SONG, Harbin Institute of Technology, Nangang, Harbin, Heilongjiang, China, GANG WANG, Institute of physics, Chinese Academy of Sciences, Haidian, Beijing, China — We measure the infrared (100-1000 meV) Kerr angle in ferromagnetic silicon and silicon carbide. The samples were either neutron irradiated or aluminum doped to induce ferromagnetic behavior. The samples are studied in the 10-300K temperature range at magnetic fields up to 7T. We also explore the dependence of the magneto-optical signal on samples with different irradiation exposure levels. This study provides new information on the optical, magnetic, and electronic properties of these materials. Work supported by NSF-DMR1410599 and the Helmholtz Postdoctoral Program PD-146.

**Wednesday, March 16, 2016 8:00AM - 11:00AM –**  
**Session K20 DCOMP: Quantum Many-Body Systems and Methods I** 319 - Nicola Lanata, Rutgers University

**8:00AM K20.00001 Continuous-time auxiliary field quantum Monte Carlo study of charge ordering in two-dimensional extended Hubbard model.**, HANNA TERLETSKA, University of Michigan, TIANRAN CHEN, West Chester University of Pennsylvania, EMANUEL GULL, University of Michigan — The competition between local and non-local long-range Coulomb repulsions in strongly interacting electron systems leads to emergence of complex charge ordering phases. To perform the quantum many-body simulations of such effects, we extend the existing continuous-time auxiliary field quantum Monte Carlo method to incorporate the non-local density-density interactions. We apply the developed method to the two-dimensional extended Hubbard model (with all range of non-local interactions) at and away from the half-filling. We explore the properties of the model in different parameter regimes of short and long range interactions, temperature and fillings.

**8:12AM K20.00002 Diagrammatic Monte Carlo for Dual Fermions**, SERGEI ISKAKOV, EMANUEL GULL, Univ of Michigan - Ann Arbor — The dual fermion series is a diagrammatic extension of the dynamical mean field theory that includes non-local dynamic correlations. Evaluating this series analytically has proven to be challenging. In this talk we show results for a diagrammatic Monte Carlo method that stochastically samples two-particle vertex diagrams of the dual fermion perturbation series. We present an introduction to the method and show applications to correlated systems.

**8:24AM K20.00003 The numerical renormalization group and multi-orbital impurity models**, ANDREAS WEICHELBAUM, K. M. STADLER, J. VON DELFT, Ludwig Maximilians University, Munich, Germany, Z. P. YIN, G. KOTLIAR, Rutgers University, Piscataway, New Jersey, ANDREW MITCHELL, Utrecht University, The Netherlands — The numerical renormalization group (NRG) is a highly versatile and accurate method for the simulation of (effective) fermionic impurity models. Despite that the cost of NRG is exponential in the number of orbitals, by now, symmetric three-band calculations have become available on a routine level. [1] Here we present a recent detailed study on the spin-orbital separation in a three-band Hund metal with relevance for iron-pnictides via the dynamical mean field theory (DMFT). [2] In cases, finally, where the orbital symmetry is broken, we demonstrate that interleaved NRG [3] still offers an accurate alternative approach within the NRG with dramatically improved numerical efficiency at comparable accuracy relative to conventional NRG.

[1] Weichselbaum, *Annals of Physics* **327**, 2972 (2012)

Stadler et al, *PRL* **115**, 136401 (2015)

Mitchell et al, *PRB* **89**, 121105(R) (2014)

**8:36AM K20.00004 DFT+DMFT calculation of band gaps for the transition metal monoxides NiO, CoO, FeO and MnO.**<sup>1</sup>, LONG ZHANG, Department of Physics, University of Florida, Gainesville, Florida, USA, PETER STAAR, Institute for Theoretical Physics, ETH Zurich, Switzerland, ANTON KOZHEVNIKOV, Swiss National Supercomputing Centre, ETH Zurich, Switzerland, THOMAS SCHULTHEISS, Institute for Theoretical Physics, ETH Zurich, Switzerland, HAI-PING CHENG, Department of Physics, University of Florida, Gainesville, Florida, USA — We report calculated spectral functions of the four late transition metal monoxides MnO, FeO, CoO and NiO in the paramagnetic phase. We used density functional theory (DFT) in combination with dynamic mean field theory (DMFT), which gives much better description of band gaps. Both projected Wannier orbitals and the on-site screened Coulomb interactions are obtained from DFT ground states to ensure consistency. Because of the p-d hybridization in these materials, we calculated Coulomb interactions for the dp model as well as the d-dp model using the cRPA method. With the standard fully localized limit double counting correction, we found that the d-dp model gives results in better agreement with experiments. This work was supported by the US Department of Energy (DOE), Office of Basic Energy Sciences (BES), under Contract No. DE-FG02-02ER45995.

<sup>1</sup>supported by the US Department of Energy (DOE), Office of Basic Energy Sciences (BES), under Contract No. DE-FG02-02ER45995

**8:48AM K20.00005 Probing many body effects using Fourier Transform Scanning Tunneling Spectroscopy: Can spin-orbit splitting in dispersion be observed in q-space?** , GELAREH FARAH, Univ of British Columbia, UBC LABORATORY FOR ATOMIC IMAGING RESEARCH (LAIR)) TEAM — Well studied surface systems such as Ag and Cu provide a safe platform to test novel spectroscopy methods that can have extended applications in near future. Our current focus is given to Fourier Transform Scanning Tunneling Spectroscopy (FT-STs) that allows us to study scattering effects (quasiparticle interactions - namely QPI) of CO and Co on Cu(111) surface. Magnetic Co adatoms are expected to generate a spin-orbit split in dispersion in QPI(q) space, the existence of which is confirmed by the k-space angle-resolved photo-emission spectroscopy (ARPES) of Cu(111) surface in the recent years. Hence the previously observed electron-phonon kink and spin-orbit splitting of the dispersion, as well as the scattering properties of CO molecules and Co adatoms, should also be observable in QPI space via FT-STs of Cu(111), and compatible with previous studies on similar systems. We are using a low temperature (4.2 K) commercial Scanning Tunneling Microscope (CREATEC STM) that operates using Nanonis electronic controllers and software which allows us to perform FT-STs as well as topological imaging.

**9:00AM K20.00006 Deconfined criticality in "easy-plane"  $SU(N)$  anti-ferromagnets<sup>1</sup>** , JONATHAN D'EMIDIO, GANPATHY MURTHY, RIBHU KAUL, University of Kentucky — Motivated by evidence for deconfined criticality in  $SU(N)$  anti-ferromagnets, we investigate the phase diagram of these models in the case where the  $SU(N)$  symmetry is reduced to rotations about the diagonal generators ("easy-plane" symmetry). We carry out extensive numerical simulations using quantum Monte Carlo, revealing a first-order magnetic to valence bond solid phase transition that becomes a continuous deconfined transition at large  $N$ . We support our numerical data by performing epsilon expansions of the easy-plane deformed  $CP^{N-1}$  field theory near both the upper and lower critical dimensions. This renormalization group analysis shows that the symmetric deconfined fixed point is unstable in the presence of easy-plane anisotropy, resulting in a runaway flow for intermediate values of  $N$  and a flow towards a stable easy-plane deconfined fixed point at large  $N$ , which is consistent with the critical behavior of our lattice models.

<sup>1</sup>This research was partially financially supported by NSF DMR-1056536.

**9:12AM K20.00007 Magnetic transitions and quantum criticality in the three-dimensional Hubbard model<sup>1</sup>** , THOMAS SCHÄFER, Institute of Solid State Physics, Vienna University of Technology, Vienna, Austria, ANDREY KATANIN, Institute of Metal Physics, Ural Federal University, Ekaterinburg, Russia, KARSTEN HELD, ALESSANDRO TOSCHI, Institute of Solid State Physics, Vienna University of Technology, Vienna, Austria — We analyze the (quantum) critical properties of the simplest model for electronic correlations, the Hubbard model, in three spatial dimensions by means of the dynamical mean field theory (DMFT, including all local correlations) and the dynamical vertex approximation (D $\Gamma$ A, including non-local correlations on all length scales). Both in the half-filled/unfrustrated [1] and in the hole-doped system [2] the transition temperature is significantly lowered by including non-local fluctuations.

In the latter case, however, the magnetic order becomes incommensurate, eventually leading to a complete suppression of the order and giving rise to a magnetic quantum critical point (QCP) at zero temperature [2]. We analyze the (quantum) critical properties of this QCP (e.g. critical exponents) and relate our findings to the standard theory of quantum criticality in metals, the Hertz-Millis-Moriya theory.

[1] G. Rohringer, A. Toschi, A. A. Katanin, and K. Held, Phys. Rev. Lett. **107**, 256402 (2011).

[2] T. Schäfer, A. A. Katanin, K. Held, and A. Toschi, in preparation.

<sup>1</sup>Solids4Fun, Austrian Science Fund (FWF, project ID 1243)

**9:24AM K20.00008 A Multiorbital DMFT Analysis of Electron-Hole Asymmetry in the Dynamic Hubbard Model** , CHRISTOPHER POLACHIC, Williams Baptist College, FRANK MARSIGLIO, University of Alberta — The dynamic Hubbard model (DHM) improves on the description of strongly correlated electron systems provided by the conventional single-band Hubbard model through additional electronic degrees of freedom, namely a second, higher energy orbital and associated hybridization parameters for interorbital transitions. The additional orbital in the DHM provides a more realistic modeling of electronic orbital "relaxation" in real lattices. One result of orbital relaxation is a clear electron-hole asymmetry, absent in the single-band case. We have employed the computational technique of dynamical mean field theory, generalized to the two-orbital case, to study this asymmetry with respect to varying system parameters, including both intersite and intrasite orbital hybridization as well as the role played by Mott physics. Our results stand in good agreement with previous exact diagonalization studies of the DHM.

**9:36AM K20.00009 Interlaced coarse-graining for the dynamical cluster approximation<sup>1</sup>** , URS HAEHNER, ETH Zurich, PETER STAAR, IBM Research - Zurich, MI JIANG, ETH Zurich, THOMAS MAIER, Oak Ridge National Laboratory, THOMAS SCHULTHEISS, ETH Zurich — The negative sign problem remains a challenging limiting factor in quantum Monte Carlo simulations of strongly correlated fermionic many-body systems. The dynamical cluster approximation (DCA) makes this problem less severe by coarse-graining the momentum space to map the bulk lattice to a cluster embedded in a dynamical mean-field host. Here, we introduce a new form of an interlaced coarse-graining and compare it with the traditional coarse-graining. We show that it leads to more controlled results with weaker cluster shape and smoother cluster size dependence, which with increasing cluster size converge to the results obtained using the standard coarse-graining. In addition, the new coarse-graining reduces the severity of the fermionic sign problem. Therefore, it enables calculations on much larger clusters and can allow the evaluation of the exact infinite cluster size result via finite size scaling. To demonstrate this, we study the hole-doped two-dimensional Hubbard model and show that the interlaced coarse-graining in combination with the DCA<sup>+</sup> algorithm permits the determination of the superconducting  $T_c$  on cluster sizes, for which the results can be fitted with the Kosterlitz-Thouless scaling law.

<sup>1</sup>This research used resources of the Oak Ridge Leadership Computing Facility (OLCF) awarded by the INCITE program, and of the Swiss National Supercomputing Center. OLCF is a DOE Office of Science User Facility supported under Contract DE-AC05-00OR22725.

**9:48AM K20.00010 Diagrammatic Monte Carlo sampling of the dual-fermion expansion for the Hubbard model** , JAN GUKELBERGER, University of Sherbrooke, EVGENY KOZIK, King's College London, HARTMUT HAFERMANN, Huawei Technologies Co. Ltd. — The dual-fermion approach provides a formally exact prescription for calculating the properties of a correlated electron system in terms of a diagrammatic expansion around dynamical mean-field theory (DMFT). The approach can address the full range of interactions, is exact in both the weak- and strong-coupling limits, and naturally incorporates long-range correlations beyond the reach of current cluster extensions to DMFT. Practical implementations have so far been limited to leading-order or ladder-type approximations to the expansion. In this work we compute the dual-fermion expansion for the Hubbard model to higher orders by means of a diagrammatic Monte Carlo algorithm which stochastically samples all diagram topologies. This approach allows a systematic check for the convergence of the series and hence provides a route towards a fully controlled treatment of correlated electrons.

**10:00AM K20.00011 Hubbard operator density functional theory for Fermionic lattice models**, ZHENGQIAN CHENG, CHRIS MARIANETTI, Columbia Univ — We formulate an effective action as a functional of Hubbard operator densities whose stationary point delivers all local static information of the interacting lattice model. Using the variational principle, we get a self-consistent equation for Hubbard operator densities. The computational cost of our approach is set by diagonalizing the local Fock space. We apply our method to the one and two band Hubbard model (including crystal field and on-site exchange) in infinite dimensions where the exact solution is known. Excellent agreement is obtained for the one-band model. In the two-band model, good agreement is obtained in the metallic region of the phase diagram in addition to the metal-insulator transition. While our approach does not address frequency dependent observables, it has a negligible computational cost as compared to dynamical mean field theory and could be highly applicable in the context total energies of strongly correlated materials and molecules.

**10:12AM K20.00012 Towards an ab-initio treatment of nonlocal electronic correlations with dynamical vertex approximation<sup>1</sup>**, ANNA GALLER, PATRIK GUNACKER, JAN TOMCZAK, PATRIK THUNSTRÖM, KARSTEN HELD, Vienna University of Technology — Recently, approaches such as the dynamical vertex approximation (DΓA) [1] or the dual-fermion method [2] have been developed. These diagrammatic approaches are going beyond dynamical mean field theory (DMFT) by including nonlocal electronic correlations on all length scales as well as the local DMFT correlations. Here we present our efforts to extend the DΓA methodology to ab-initio materials calculations (ab-initio DΓA) [3]. Our approach is a unifying framework which includes both GW and DMFT-type of diagrams, but also important nonlocal correlations beyond, e.g. nonlocal spin fluctuations. In our multi-band implementation we are using a worm sampling technique [4] within continuous-time quantum Monte Carlo in the hybridization expansion to obtain the DMFT vertex, from which we construct the reducible vertex function using the two particle-hole ladders. As a first application we show results for transition metal oxides. [1] A. Toschi, A. A. Katanin, and K. Held, Physical Review B 75, 045118 (2007). [2] A. N. Rubtsov, M. I. Katsnelson, A. I. Lichtenstein, Physical Review B 77, 033101 (2008). [3] A. Toschi et al., Annalen der Physik 523, 698 (2011) [4] P. Gunacker et al., Physical Review B 92, 155102 (2015)

<sup>1</sup>Support by the ERC project AbinitioDGA (306447) is acknowledged.

**10:24AM K20.00013 Extremely Correlated Fermi Liquid theory: Imposing the hole density sum-rule<sup>1</sup>**, B. SRIRAM SHASTRY, Univ of California-Santa Cruz — The analytical theory of extremely strongly correlated Fermi liquids (ECFL) for the large U models, when applied to Cuprate superconductors in the nodal direction, provides ARPES spectral line shapes that are very close to experiments. Approximate lowest order calculations within this formalism also closely reproduce the spectral line shapes for the single impurity Anderson model found using the Numerical Renormalization Group. Similarly excellent comparison is possible with the Dynamical Mean Field Theory self energy for the Hubbard model in high dimensions. However these calculations yields too large an energy scale for frequency dependence, in the proximity of integer (or Mott) filling. We show that the theory permits the imposition of sum rules for hole density, rather than the electron density used earlier, on the Greens functions of the theory. The numerical results of these variants are presented, and compared to the earlier calculations. The new results go a long way towards resolving the energy scale problem, while retaining the excellence of line shapes.

<sup>1</sup>The work at UCSC was supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES) under Award FG02-06ER46319.

**10:36AM K20.00014 Space-time separation of electronic correlations**, JAN M. TOMCZAK, THOMAS SCHÄFER, BENJAMIN KLEBEL, ALESSANDRO TOSCHI, Vienna University of Technology — While second-order phase transitions always cause strong nonlocal fluctuations, their effect on spectral properties crucially depends on the dimensionality. First, we show that for the important case of three dimensions the electron self-energy is well separable into a local dynamical part and static nonlocal contributions[1]. In particular, using the dynamical vertex approximation for the doped 3D Hubbard model, we demonstrate that the quasiparticle weight remains essentially momentum independent, despite overall large nonlocal corrections to the self-energy when approaching the spin-ordered state. This generalizes earlier empirical findings of this property in the iron pnictides[2] and transition metal oxides[3] based on Hedin's *GW* approximation. With this insight, we here propose a "space-time-separated" scheme for many-body perturbation theory that is up to ten times more efficient than current implementations. Finally, we discuss limits of the space-time separation of correlation effects by studying the crossover from three to two dimensions.

[1] T. Schäfer, A. Toschi, JMT. PRB 91, 121107(R) (2015)

[2] JMT, M. van Schilfgaarde, G. Kotliar. PRL 109, 237010 (2012)

[3] JMT, M. Casula, T. Miyake, S. Biermann PRB 90, 165138 (2014)

**10:48AM K20.00015 Computation of ab initio energy savings due to magnetic interactions<sup>1</sup>**, ALEXANDER MUNOZ, LUCAS WAGNER, Univ of Illinois - Urbana — The double-exchange mechanism [1] is the traditional explanation for antiferromagnetic coupling between magnetic ions. In this theory, the energy savings within the context of a hopping model is derived from kinetic energy terms. However, the connection to ab initio energy savings to our knowledge has not been studied using an explicitly correlated theory that can obtain quantitative accuracy. Our study focuses on determining, from ab initio calculations, whether the origin of interactions in magnetic systems is explainable through conventional arguments. To this end, we investigate the contributions (kinetic, ionic, electron-electron) to the total energy of the (Mn-O-Mn)<sup>+2</sup> system using quantum Monte Carlo techniques. We will report on progress in elucidating the connection between the ab initio energy savings and the effective model energy savings that result in an antiferromagnetic interaction in this system. [1] Zener. Phys. Rev. , 403 (1951)

<sup>1</sup>L.K. Wagner was supported by NSF DMR 1206242.

## Wednesday, March 16, 2016 8:00AM - 10:36AM —

Session K21 DCMP GPC: Geophysics and Planetary Science 320 - Arianna Gleason, Los Alamos National Laboratory

**8:00AM K21.00001 Ab initio Raman spectroscopy of water under extreme conditions**, VIKTOR ROZSA, DING PAN, QUAN WAN, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago — Water exhibits one of the most complex phase diagrams of any binary compound. Despite extensive studies, the melting lines of high-pressure ice phases remain very controversial, with reports differing by hundreds of Kelvin. The boundary between ice VII and liquid phase is particularly disputed, with recent work exploring plasticity and amorphization mediating the transition. Raman measurements are often used to fingerprint melting, yet their interpretation is difficult without atomistic modeling. Here, we report a study of high P/T water where we computed Raman spectra using a method [1] combining ab initio molecular dynamics and density functional perturbation theory, as implemented in the Qbox code [2]. Spectra were computed for the liquid at 10 and 20 GPa, both at 1000 K, and for solid ice VII (20 GPa, 500 K). Decomposing the spectra into inter and intra molecular contributions provided insight into the dynamics of the hydrogen-bonded network at extreme conditions. The relevance of our simulation results for models of water in Earth, Uranus, and Neptune will be discussed, and an interpretation of existing experiments at high pressure will be presented. [1] Wan, Q., Spanu, L., Galli, G., Gygi, F., J. Chem. Theory Comput. 9, 4124. (2013) [2] <http://qboxcode.org>

**8:12AM K21.00002 Conductivity and Correlations in Fe at Earth Core Conditions**, R.E. COHEN, Carnegie Inst for Science and LMU, PENG ZHANG, Department of Physics, Xi'an Jiaotong University, KRISTJAN HAULE, Dept. Physics, Rutgers University — We have computed electrical conductivity in iron at Earth core conditions self-consistently within many-body theory using DFT/DMFT. We find that electron correlations are important even in the generation of Earth's magnetic field. Earth's magnetic field was believed to arise from thermal convection of molten iron alloy in Earth's outer core, but density functional theory (DFT) calculations suggested that the conductivity of iron is too high to support thermal convection, so that new geodynamo models were being developed. The DFT computations for resistivity were based on the scattering of electrons off of atomic vibrations, or electron-phonon (e-p) scattering. We applied self-consistent density functional theory plus dynamical mean-field theory (DFT+DMFT) to iron and found that at high temperatures electron-electron (e-e) scattering is comparable to the e-p scattering, bringing theory into agreement with experiments and solving the transport problem in Earth's core, consistent with the conventional thermal geodynamo [Peng, Cohen, and Haule, Nature 517, 605, 2015]. How electron correlations change with pressure, and how this affects material properties, will be discussed. This work is supported by the US National Science Foundation and the ERC Advanced grant ToMCA<sup>2</sup>.

**8:24AM K21.00003 A Green Function Approach to the Effects of Core-state Overlap on Interatomic Interactions at Extreme Densities**, YANG WANG, Pittsburgh Supercomputing Center, Carnegie Mellon University, G MALCOLM STOCKS, Materials Science and Technology Division, Oak Ridge National Laboratory — Under extreme conditions of temperature and pressure, interatomic separations in condensed matter can approach a small fraction of those under normal laboratory conditions. For example, during high-energy ( $\sim 100$  keV) radiation damage cascades, interatomic separations can be as small as  $0.5\text{\AA}$ . Under such conditions, core states between neighboring atoms could overlap and must be included as band states. Here we use Greens function method in the framework of multiple scattering theory, also known as Korringa-Kohn-Rostoker (KKR) electronic structure methods, to seamlessly integrate these core overlap effects within an all-electron *ab initio* approach. To accomplish these we use multiple integration contours in the complex plane that incorporate states normally treated as bound atomic levels. We show results for Ni and NiFe alloys in extreme densities ( $a/a_0 \sim 0.3$ ) to illustrate the convergence of the method with respect to which core states are banded as well as the angular momentum cut-off required to establish absolute convergence of the total energies. Results are compared with those of plane-wave methods for different choices of the underlying pseudo potential to establish the range of validity of the various approaches.

**8:36AM K21.00004 Dissolved carbon in extreme conditions characterized by first principles simulations<sup>1</sup>**, DING PAN, GIULIA GALLI, Institute for Molecular Engineering, the University of Chicago — One key component to understanding carbon transport in the Earth interior is the determination of the molecular species formed when carbon bearing materials are dissolved in water at extreme conditions. We used first principles molecular dynamics to investigate oxidized carbon in water at high pressure (P) and high temperature (T), up to the conditions of the Earth's upper mantle. Contrary to popular geochemistry models assuming that  $\text{CO}_2$  is the major carbon species present in water, we found that most of the dissolved carbon at 10 GPa and 1000 K is in the form of solvated  $\text{CO}_3^{2-}$  and  $\text{HCO}_3^-$  anions. We also found that ion pairing between alkali metal cations and  $\text{CO}_3^{2-}$  or  $\text{HCO}_3^-$  anions is greatly affected by P-T conditions, decreasing with pressure along an isotherm. Our study shows that it is crucial to take into account the specific molecular structure of water under extreme conditions and the changes in hydrogen bonding occurring at high P and T, in order to predict chemical reactions in dissolved carbon. Our findings also shed light on possible reduction mechanisms of  $\text{CO}_2$  when it is geologically stored, depending on the availability of water.

<sup>1</sup>The work is supported by the Sloan Foundation through the Deep Carbon Observatory

**8:48AM K21.00005 ABSTRACT WITHDRAWN —**

**9:00AM K21.00006 Novel stable compounds in the Mg-Si-O system under exoplanet pressures and their implications in planetary science**, HAIYANG NIU, State Univ of NY- Stony Brook, ARTEM OGANOV, Skolkovo Institute of Science and Technology, XINGQIU CHEN, DIANZHONG LI, Institute of Metal Research — The Mg-Si-O system is the major Earth and rocky planet-forming system. Here, through quantum variable-composition evolutionary structure explorations, we have discovered several unexpected stable binary and ternary compounds in the Mg-Si-O system. Besides the well-known  $\text{SiO}_2$  phases, we have found two extraordinary silicon oxides,  $\text{SiO}_3$  and  $\text{SiO}$ , which become stable at pressures above 0.51 TPa and 1.89 TPa, respectively. In the Mg-O system, we have found one new compound,  $\text{MgO}_3$ , which becomes stable at 0.89 TPa. We find that not only the  $(\text{MgO})_x(\text{SiO}_2)_y$  compounds, but also two  $(\text{MgO}_3)_x(\text{SiO}_3)_y$  compounds,  $\text{MgSi}_3\text{O}_{12}$  and  $\text{MgSiO}_6$ , have stability fields above 2.41 TPa and 2.95 TPa, respectively. The highly oxidized  $\text{MgSi}_3\text{O}_{12}$  can form in deep mantles of mega-Earths with masses above  $20 M_\oplus$  ( $M_\oplus$ :Earth's mass). Furthermore, the dissociation pathways of pPv- $\text{MgSiO}_3$  are also clarified, and found to be different at low and high temperatures. The low-temperature pathway is  $\text{MgSiO}_3 \Rightarrow \text{Mg}_2\text{SiO}_4 + \text{MgSi}_2\text{O}_5 \Rightarrow \text{SiO}_2 + \text{Mg}_2\text{SiO}_4 \Rightarrow \text{MgO} + \text{SiO}_2$ , while the high-temperature pathway is  $\text{MgSiO}_3 \Rightarrow \text{Mg}_2\text{SiO}_4 + \text{MgSi}_2\text{O}_5 \Rightarrow \text{MgO} + \text{MgSi}_2\text{O}_5 \Rightarrow \text{MgO} + \text{SiO}_2$ . Present results are relevant for models of the internal structure of giant exoplanets, and for understanding the high-pressure behavior of materials.

**9:12AM K21.00007 Spin crossover in solid and liquid (Mg,Fe)O at extreme conditions<sup>1</sup>**, LARS STIXRUDE, Department of Earth Sciences, University College London, EERO HOLMSTROM, Department of Applied Physics, COMP Centre of Excellence, Aalto University, Finland — Ferroperricite,  $(\text{Mg,Fe})\text{O}$ , is a major constituent of the Earth's lower mantle (24-136 GPa). Understanding the properties of this component is important not only in the solid state, but also in the molten state, as the planet almost certainly hosted an extensive magma ocean initially. With increasing pressure, the Fe ions in the material begin to collapse from a magnetic to a nonmagnetic spin state. This crossover affects thermodynamic, transport, and electrical properties. Using first-principles molecular dynamics simulations, thermodynamic integration, and adiabatic switching, we present a phase diagram of the spin crossover. In both solid and liquid, we find a broad pressure range of coexisting magnetic and non-magnetic ions due to the favorable enthalpy of mixing of the two. In the solid increasing temperature favors the high spin state, while in the liquid the opposite occurs, due to the higher electronic entropy of the low spin state. Because the physics of the crossover differ in solid and liquid, melting produces a large change in spin state that may affect the buoyancy of crystals freezing from the magma ocean in the earliest Earth.

<sup>1</sup>This research was supported by the European Research Council under Advanced Grant No. 291432 MoltenEarth (FP7/2007-2013)

**9:24AM K21.00008 Amorphization and nanocrystallization of silicon under laser shock compression: bridging experiment with atomic simulation.**<sup>1</sup>, SHITENG ZHAO, BIMAL KAD, ERIC HAHN, Univ of California - San Diego, BRUCE REMINGTON, CHRISTOPHER WEHRENBURG, Lawrence Livermore National Laboratory, EDUARDO BRINGA, Universidad Nacional de Cuyo, CHANNING HUNTINGTON, HYE-SOOK PARK, Lawrence Livermore National Laboratory, KARREN MORE, Oak Ridge National Laboratory, MARC MEYERS, Univ of California - San Diego — Terawatt, nanosecond-duration, laser-driven, shock compression and recovery experiments on [001] silicon unveiled remarkable structural changes above a pressure threshold. Two distinct amorphous regions were identified: (a) a bulk amorphous layer close to the surface and (b) amorphous bands initially aligned with {111} slip planes. Further increase of the laser energy leads to the re-crystallization of amorphous silicon into nanocrystals with high concentration of nano-twins. Shock-induced defects play a very important role in the onset of amorphization. Calculations of the free energy changes with pressure and shear, using the Patel-Cohen methodology, are in agreement with the experimental results. Molecular dynamics simulation corroborates the amorphization, showing that it is initiated by the nucleation and propagation of partial dislocations. The nucleation of amorphization is analyzed by classical nucleation theory.

<sup>1</sup>This research is funded by a UC Research Laboratories Grant (09-LR-06-118456-MEYM) and a National Laser Users Facility (NLUF) Grant (PE-FG52-09NA-29043)

**9:36AM K21.00009 First-principles study of the amorphization of stishovite by isotropic volume expansion**, MASAOKI MISAWA, FUYUKI SHIMOJO, Kumamoto University, RAJIV K. KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, University of Southern California — Simple synthesis of ceramics with high hardness and high toughness from Earth-abundant materials is one of the most important issues in materials science. Nishiyama et al. synthesized nano-crystalline stishovite with extremely high toughness and high hardness via compression and decompression of silica, and proposed fracture-induced amorphization mechanisms for the toughening [1]. Furthermore, it was shown that the toughening mechanisms are effective even in nanoscale order [2]. Our first-principles molecular dynamics simulations have shown rapid amorphization of stishovite within picoseconds under increasing volume, thus substantiating the proposed amorphization mechanisms. Furthermore, we have calculated the critical stress, energy difference, and energy barrier for the crystalline-to-amorphous structural transition. [1] N. Nishiyama et al., Scientific Reports 4, 6558 (2014). [2] K. Yoshida et al., Scientific Reports 5, 10993 (2015).

**9:48AM K21.00010 Phase diagram of the itinerant helical magnet MnSi at high pressures and strong magnetic fields**, SERGEI STISHOV, Russian Acad of Sci-Troitsk — We performed a series of resistivity, heat capacity and ultrasound speed measurements of a MnSi single crystal at high pressures and strong magnetic fields [1-3]. Two notable features of the phase transition in MnSi that disappear on pressure increase are a sharp peak marking the first order phase transition and a shallow maximum, situated slightly above the critical temperature and pointing to the domain of prominent helical fluctuations. The longitudinal and transverse ultrasound speeds and attenuation were measured in a MnSi single crystal in the temperature range of 2-40 K and magnetic fields to 7 Tesla. The magnetic phase transition in MnSi in zero magnetic field is signified by a quasi-discontinuity in the  $c_{11}$  elastic constant, which almost vanishes at the skyrmion - paramagnetic transition at high magnetic fields. The powerful fluctuations at the minima of  $c_{11}$  make the mentioned crossing point of the minima and the phase transition lines similar to a critical end point, where a second order phase transition meets a first order one.

1. Alla E. Petrova and Sergei M. Stishov, Phys. Rev. B 86, 174407 (2012)
2. V. A. Sidorov, et al., Phys. Rev. B 89, 100403(R) (2014)
3. A. E. Petrova and S. M. Stishov, Phys. Rev. B 91, 214402 (2015)

**10:00AM K21.00011 A DFT+DMFT study of magnetic properties of FeO at high pressure.**, PENG ZHANG<sup>1</sup>, Department of Physics, Xi'an Jiaotong university & Geophysical Laboratory, RONALD COHEN<sup>2</sup>, Extreme Materials Initiative, Geophysical Laboratory, Carnegie Institution for Science, Washington, D.C. USA, K. HAULE, Department of Physics and Astronomy, Rutgers University, NJ, USA — FeO is an insulator with anti-ferromagnetic (AFM) spin ordering at ambient pressure. When external pressure is increased, the Néel temperature first increases at the pressure below 40 GPa. Experiments show the AFM ordering collapses at high pressures. Using the density functional theory plus dynamical mean-field theory (DFT+DMFT), we examined the nature of magnetic collapse of FeO and derived its magnetic phase diagram up to 180 GPa. We found coexistence of high spin-low spin transition and paramagnetic-AFM transition, both driven by increased pressure. The high spin-low spin transition is result of partition and pairing of 3d electrons in iron. The local moment of iron atom after high spin-low spin transition is small but finite up to 180 GPa.

<sup>1</sup>Carnegie Institution for Science, Washington, D.C. USA

<sup>2</sup>Department for Geo- und Umweltwissenschaften, Ludwig-Maximilians-Universität, Munich, Germany

**10:12AM K21.00012 Effects of composition and iron spin state on the structural transition of (Mg,Fe)CO<sub>3</sub> in the Earth's lower mantle**, HAN HSU, SHENG-CHIEH HUANG, National Central University, CHENG-RONG HSING, CHING-MING WEI, Academia Sinica — Iron-bearing magnesium carbonates (Mg,Fe)CO<sub>3</sub> are believed the major carbon carriers in the Earth's deep lower mantle; knowledge of their physical properties is thus essential to understand the Earth's deep carbon cycle. It is known that (Mg,Fe)CO<sub>3</sub> ferromagnesite is stable up to 80-100 GPa. At 45-50 GPa, ferromagnesite undergoes a high-spin to low-spin crossover, accompanied by a volume reduction and elastic anomalies. Above 100 GPa, ferromagnesite goes through a complicated structural transition, which is still a subject under debate. So far, several distinct high-pressure (Mg,Fe)CO<sub>3</sub> structures have been inferred from experiments, including  $P2_1/c$  [1] and  $Pmm2$  phases [2]. In theory,  $C2/m$  [3] and  $P-1$  phases [4] have been suggested, but the  $Pmm2$  phase is not found. One possible reason for this discrepancy is that the above-mentioned calculations are based on pure MgCO<sub>3</sub>, while experiments were performed using (Mg,Fe)CO<sub>3</sub> with high iron concentration (>50%). Here, we use density functional theory + self-consistent Hubbard  $U$  (DFT+ $U_{sc}$ ) calculations to study this structural transition. The effects of composition and iron spin state on these (Mg,Fe)CO<sub>3</sub> phases are also discussed. [1] E. Boulard et al., Proc. Natl. Acad. Sci. USA **108**, 5184 (2011). [2] J. Liu et al., Sci. Rep. **5**, 7640 (2015). [3] A. R. Oganov et al., Earth Planet. Sci. Lett. **273**, 38 (2008). [4] C. J. Pickard and R. J. Needs, Phys. Rev. B **91**, 104101 (2015).

**10:24AM K21.00013 Gravitational Collapse and Shocks in Two-Phase Celestial Bodies**, MICHAEL GRINFELD, The U.S. Army Research Laboratory, PAVEL GRINFELD, Drexel University, Department of Mathematics — The phenomenon of gravitational collapse (GC) is well-known in theoretical astro- and planetary physics. It occurs when the incompressibility of substances is unable to withstand the pressure due to gravitational forces in celestial bodies of sufficiently large mass. The GC never occurs in incompressible models – homogeneous or layered. This situation changes dramatically when different incompressible layers appear to be different phases of the same chemical substance and the mass exchange between the phases can occur due to phase transformation. The possibility of destabilization in such system becomes realistic, as it was first discovered in the Ramsey static analysis [1,2]. We will present our generalization of the Ramsey's results using dynamic approach. [1] W.H. Ramsey, "On the instability of small planetary cores", Mon. Not. R. Astron. Soc. **110** (4), 325-338 (1950). [2] H. Jeffreys, "The Earth: Its Origin, History, and Physical Constitution". Cambridge University Press (1976).

**Wednesday, March 16, 2016 8:00AM - 10:48AM –**

**Session K22 DCOMP: Predicting and Classifying Materials via High-Throughput Databases and Machine Learning II** 321 - Dimitrios Papaconstantopoulos, George Mason University

**8:00AM K22.00001 An Automated Application Framework to Model Disordered Materials Based on a High Throughput First Principles Approach**, COREY OSES, Duke Univ, KESONG YANG, UC San Diego, STEFANO CURTAROLO, Duke Univ, DUKE UNIV COLLABORATION, UC SAN DIEGO COLLABORATION — Predicting material properties of disordered systems remains a long-standing and formidable challenge in rational materials design. To address this issue, we introduce an automated software framework capable of modeling partial occupation within disordered materials using a high-throughput (HT) first principles approach. At the heart of the approach is the construction of supercells containing a virtually equivalent stoichiometry to the disordered material. All unique supercell permutations are enumerated and material properties of each are determined via HT electronic structure calculations. In accordance with a canonical ensemble of supercell states, the framework evaluates ensemble average properties of the system as a function of temperature. As proof of concept, we examine the framework's final calculated properties of a zinc chalcogenide ( $\text{ZnS}_{1-x}\text{Se}_x$ ), a wide-gap oxide semiconductor ( $\text{Mg}_x\text{Zn}_{1-x}\text{O}$ ), and an iron alloy ( $\text{Fe}_{1-x}\text{Cu}_x$ ) at various stoichiometries.

**8:12AM K22.00002 An Extensive Database of Electronic Structure Calculations between Transition Metals<sup>1</sup>**, SHEREEF SAYED, DIMITRIOS PAPACONSTANTOPOULOS, George Mason Univ — Density Functional Theory and its derived application methods, such as the Augmented Plane Wave (APW) method, have shown great success in predicting the fundamental properties of materials. In this work, we apply the APW method to explore the properties of diatomic pairs of transition metals in the CsCl structure, for all possible combinations. A total of 435 compounds have been studied. The predicted Density of States, and Band Structures are presented, along with predicted electron-phonon coupling and Stoner Criterion, in order to identify potential new superconducting or ferromagnetic materials. This work is performed to demonstrate the concept of high-throughput calculations at the crossing-point of Big Data and materials science.

<sup>1</sup>US Dept of Energy

**8:24AM K22.00003 High throughput ab-initio modeling of proton transport in solid electrolytes**, JANAKIRAMAN BALACHANDRAN, LIANSHAN LIN, PANCHAPAKESAN GANESH, Oak Ridge National Laboratory — Solid oxide materials that can selectively transport protons have great potential for fuel cell applications. However several fundamental questions remain unanswered such as (a) How do the dopants organize at various dopant concentrations, (b) How spatial organization of dopants influence proton migration energy, (c) How disorder and strain in a material influence its ionic transport. In this work we have developed an integrated high throughput framework to calculate proton transport properties by integrating open source packages (such as pymatgen, fireworks) The high throughput framework scales well on supercomputing clusters. We have used this framework to analyze over 100 perovskites compounds with over 12 different dopant atoms. These computational models enable us to obtain insights how the proton transport properties depend on host and dopant atoms. Further, we also perform ab-initio modeling to understand how dopants spatially organize at different dopant concentrations, and how this spatial organization affects proton conductivity. This analysis enabled us to obtain fundamental insights on why proton conductivity decreases in Y doped BaZrO<sub>3</sub> at high dopant concentrations.

**8:36AM K22.00004 From organized high throughput data to phenomenological theory: The example of dielectric breakdown**, CHIHO KIM, University of Connecticut, GHANSHYAM PILANIA, Los Alamos National Laboratory, RAMPI RAMPRASAD, University of Connecticut — Understanding the behavior (and failure) of dielectric insulators experiencing extreme electric fields is critical to the operation of present and emerging electrical and electronic devices. Despite its importance, the development of a predictive theory of dielectric breakdown has remained a challenge, owing to the complex multiscale nature of this process. Here, we focus on the *intrinsic* dielectric breakdown field of insulators—the theoretical limit of breakdown determined purely by the chemistry of the material, *i.e.*, the elements the material is composed of, the atomic-level structure, and the bonding. Starting from a benchmark dataset (generated from laborious first principles computations) of the intrinsic dielectric breakdown field of a variety of model insulators, simple predictive phenomenological models of dielectric breakdown are distilled using advanced statistical or machine learning schemes, revealing key correlations and analytical relationships between the breakdown field and easily accessible material properties. The models are shown to be general, and can hence guide the screening and systematic identification of high electric field tolerant materials.

**8:48AM K22.00005 The Robustness of Cluster Expansion: Assessing the Role of Relaxation<sup>1</sup>**, ANDREW H. NGUYEN, CONRAD W. ROSENBROCK, GUS L. W. HART, Brigham Young Univ - Provo — Cluster expansion (CE) has been used widely in combination with first-principles calculations to predict stable structures of metal alloys. CE treats alloys as a purely configuration problem, *i.e.*, a problem in the distribution of the alloying elements on a fixed lattice. CE models are usually built from data taken from “relaxed” first-principles calculations where the individual atoms assume positions that minimize the total energy. A perennial question in the cluster expansion community is how the accuracy of the CE is affected by relaxations—technically, the formalism of CE breaks down when the underlying lattice is not preserved—but practitioners often argue that there is a one-to-one correspondence between relaxed and unrelaxed structures so that the formalism holds. We quantify the effect of relaxation on the robustness of cluster expansions by comparing CE fits for relaxed and unrelaxed data sets. Our results give a heuristic for when CE models can be trusted.

<sup>1</sup>ONR (MURI N00014-13-1-0635)

**9:00AM K22.00006 The New NRL Crystallographic Database<sup>1</sup>**, MICHAEL MEHL, Naval Research Laboratory, Washington DC 20375, STEFANO CURTAROLO, DAVID HICKS, CORMAC TOHER, Duke University, Durham, NC, OHAD LEVY, Duke University, Durham, NC and NRCN, Israel, GUS HART, Brigham Young University, Provo, Utah — For many years the Naval Research Laboratory maintained an online graphical database of crystal structures for a wide variety of materials. This database has now been redesigned, updated and integrated with the AFLOW framework for high throughput computational materials discovery (<http://materials.duke.edu/afLOW.html>). For each structure we provide an image showing the atomic positions; the primitive vectors of the lattice and the basis vectors of every atom in the unit cell; the space group and Wyckoff positions; Pearson symbols; common names; and Strukturbericht designations, where available. References for each structure are provided, as well as a Crystallographic Information File (CIF). The database currently includes almost 300 entries and will be continuously updated and expanded. It enables easy search of the various structures based on their underlying symmetries, either by Bravais lattice, Pearson symbol, Strukturbericht designation or commonly used prototypes. The talk will describe the features of the database, and highlight its utility for high throughput computational materials design.

<sup>1</sup>Work at NRL is funded by a contract with the Duke University Department of Mechanical Engineering.

**9:12AM K22.00007 First-principles determination of low-energy structures in epitaxially-strained perovskite SrMnO<sub>3</sub>** , JIALAN ZHANG, KARIN RABE, Rutgers, The State University of New Jersey — Using a physically-motivated form for the energy as a function of magnetic ordering and lattice distortions around the high symmetry reference structure, we present a systematic method for determining the ground state and low-energy structures of transition-metal ABO<sub>3</sub> compounds from first principles. The structural information obtained through this method forms the foundation for the first-principles structural determination of the structure of perovskite oxide superlattices. The method is demonstrated for SrMnO<sub>3</sub>, which has a nontrivial phase sequence with varying epitaxial strain that has been of recent interest both in first-principles and experimental investigations.

**9:24AM K22.00008 Finding new ternary transition metal selenides and sulphides<sup>1</sup>** , AWADHESH NARAYAN, ANKITA BHUTANI, JAMES N. ECKSTEIN, DANIEL P. SHOEMAKER, LUCAS K. WAGNER, Univ of Illinois - Urbana — The transition metal oxides exhibit many interesting physical properties, and have been explored in detail over time. Recently, the transition metal chalcogenides including selenium and sulfur have been of interest because of their correlated electron properties, as seen in the iron based superconductors and the layered transition metal dichalcogenides. However, the chalcogenides are much less explored than the oxides, and there is an open question of whether there may be new materials heretofore undiscovered. We perform a systematic combined theoretical and experimental search over ternary phase diagrams that are empty in the Inorganic Crystal Structure Database containing cations, transition metals, and one of selenium or sulfur. In these 27 ternary systems, we use a probabilistic model to reduce the likelihood of false negative predictions, which results in a list of 24 candidate materials. We then conduct a variety of synthesis experiments to check the candidate materials for stability. While the prediction method did obtain compositions that are stable, none of the candidate materials formed in our experiments. We come to the conclusion that these phase diagrams are either truly empty or have unusual structures or synthesis requirements.

<sup>1</sup>This work was supported by the Center for Emergent Superconductivity, Department of Energy Frontier Research Center under Grant No. DEAC0298CH1088

**9:36AM K22.00009 High-Throughput Identification of Unique Structure Prototypes in the Inorganic Crystal Structure Database** , DAVID HICKS, CORMAC TOHER, OHAD LEVY, STEFANO CURTAROLO, Duke Univ — High-throughput computational assessment of materials properties is currently a major component of the effort to develop new useful materials by uncovering trends and correlations between structures, compositions, and functionalities. Efficient implementation of this approach thus requires a systematic identification of distinct material structure prototypes. We have developed a robust algorithm that calculates the level of similarity between crystal structures independent of the unit cell representation, using the comparison method proposed by Burzlaff [1]. This algorithm has been implemented in the high-throughput framework, Automatic Flow (AFLOW) [2], and applied to the Inorganic Crystal Structure Database (ICSD) [3] entries in the AFLOWLIB.org [4] online repository. We have determined the uniqueness statistics for the ICSD and have created a comprehensive set of the unique structural prototypes represented in it. [1] H. Burzlaff and Y. Malinovsky Acta Cryst. A53, 217-224 (1997). [2] S. Curtarolo et al. Comp. Mater. Sci. 58, 218-226 (2012). [3] FIZ Karlsruhe and NIST, Inorganic Crystal Structure Database, <http://icsd.fiz-t.karlsruhe.de/icsd/> [4] S. Curtarolo et al. Comp. Mater. Sci. 58, 227-235 (2012).

**9:48AM K22.00010 Prediction of the first stable compound with flat hexagonal tin layers<sup>1</sup>** , JUNPING SHAO, CLEMENT BEAUFILS, ALEKSEY KOLMOGOROV, Binghamton University, SUNY — An analysis of stability trends in a large family of metal stannides has directed our attention towards a previously unknown compound featuring a backbone of flat hexagonal tin layers. Ab initio calculations show that this compound is at least metastable under ambient conditions and is furthermore stabilized under pressure. Compounds with such layered frameworks may possess exotic electronic properties and also serve as precursors for the synthesis of 2D derivatives.

<sup>1</sup>Supported by NSF Grant DMR-1410514

**10:00AM K22.00011 Can k-point integration for metals be dramatically improved?** , GUS HART, JEREMY JORGENSEN, Brigham Young University, PRIYA GOPAL, Central Michigan University, MARCO BUONGIORNO-NARDELLI, University of North Texas — Our group has spent hundreds of millions of cpu hours calculating the energies of different materials and their competing structures. The energy of the occupied electron states is a small part of the total energy of a given material, but electron energy accounts for almost all of the numerical error in these calculations (at least in metals). Current methods of integrating electron band energies are simple (usually rectangle rule + smearing) but converge very slowly, requiring many, many k-points, even for simple metals. But integration approaches with better convergence rates, such Gauss quadrature, are hard to utilize. Because of the multivalued nature of electron bands (leading to crossings, kissings, etc.) standard interpolation methods are ineffective. We will discuss a number of improvements we have made and discuss a possible solution to the interpolation problem.

**10:12AM K22.00012 The Quantum Monte Carlo Database: towards high-accuracy and high-throughput calculation of material properties** , JOSHUA SCHILLER, University of Illinois at Urbana-Champaign, RAYMOND PLANTE, National Institute of Standards and Technology, LUCAS WAGNER, ELIF ERTEKIN, University of Illinois at Urbana-Champaign — Quantum Monte Carlo (QMC) techniques comprise a class of promising methods that offer a path towards higher accuracy for materials property prediction. However, their application in bulk materials has historically been limited to one-at-a-time evaluation of a given material. While these results often provide benchmark-level accuracy for quantities of interest, they do not allow for high-throughput analysis of the data since each calculation is done slightly differently. We present a combined data format and automatic generation platform based on the QWalk code for QMC data: QMCDB. This platform collects QMC results and provenance information automatically and stores the information in a database. We will report on the construction of this database and what lessons can be learned about using QMC for high-throughput applications.

**10:24AM K22.00013 Predictive modeling of surface morphology of multicomponent catalysts for their optimum performance** , ALTAF KARIM, SYED ISLAMUDDIN SHAH, COMSATS Institute of Information Technology, Islamabad, Pakistan — Multi-component microstructures of artificially engineered catalysts are promising for the best ever performance in alternative fuel production. We have designed and implemented a set of intelligent algorithms capable of predicting the surface morphology of multicomponent catalysts for their optimum performance. For example we come up with three kinds of different catalysts. Based on a database obtained from the density functional theory based kinetic Monte Carlo simulations, the first kind of single component catalytic surface promotes and helps dissociative adsorption of chemical species, but it hinders the diffusion of intermediate species. On the other hand, the second kind of single component catalytic surface promotes the diffusion of intermediate species, but suppresses the reactions and desorption processes. However the third kind of single component catalytic surfaces can significantly enhance reactions among intermediate species. Therefore no single component material surface would be a suitable candidate for becoming a good catalyst. However a combination of all above mentioned kind of materials may exhibit the maximum ever performance. Our algorithm models the surface morphology of these multicomponent catalysts by varying the surface area of each component and also by changing the shape of each component in such a way that the catalyst gives the highest rate of chemical formation. Our results confirm the best ever performance of our artificially engineered catalysts.

**10:36AM K22.00014 Doping Li and K into  $\text{Na}_2\text{ZrO}_3$  Sorbent to Improve Its  $\text{CO}_2$  Capture Capability**, YUHUA DUAN, DOE-National Energy Technology Laboratory — Carbon dioxide is one of the major combustion products which once released into the air can contribute to global climate change. Solid sorbents have been reported in several previous studies to be promising candidates for  $\text{CO}_2$  sorbent applications due to their high  $\text{CO}_2$  absorption capacities at moderate working temperatures. However, at a given  $\text{CO}_2$  pressure, the turnover temperature ( $T_t$ ) of an individual solid capture  $\text{CO}_2$  reaction is fixed and may be outside the operating temperature range ( $\Delta T_o$ ) for a particular capture technology. In order to shift such  $T_t$  for a solid into the range of  $\Delta T_o$ , its corresponding thermodynamic property must be changed by changing its structure by reacting (mixing) with other materials or doping with other elements. As an example, by combining thermodynamic database searching with *ab initio* thermodynamics calculations, in this work, we explored the Li- and K-doping effects on the  $T_t$  shifts of  $\text{Na}_2\text{ZrO}_3$  at different doping levels. The obtained results showed that compared to pure  $\text{Na}_2\text{ZrO}_3$ , the Li- and K-doped mixtures  $\text{Na}_{2-\alpha}\text{M}_\alpha\text{ZrO}_3$  ( $\text{M}=\text{Li, K}$ ) have lower  $T_t$  and higher  $\text{CO}_2$  capture capacities.

## **Wednesday, March 16, 2016 8:00AM - 11:00AM –**

**Session K23 DMP DCOMP: Focus Topic: Computational Materials Discovery and Design - Structure Prediction and Phase Diagrams** 322 - Stephan Lany, National Renewable Energy Laboratory

**8:00AM K23.00001 Entropy descriptors and Entropy Stabilized Oxides**, STEFANO CURTAROLO, Duke University — In this presentation we will discuss the development of entropy descriptors for the AFLOWLIB.org *ab-initio* repository and the path leading to the synthesis of the novel entropy stabilized oxides. [Nat. Comm. 6:8485 (2015)]. Research sponsored by DOD-ONR N000141310635 and N000141512863.

**8:36AM K23.00002 Computational Discovery of New Heusler Compounds: Structures, Stabilities, and Applications**, JIANGANG HE, VINAY HEGDE, CHRIS WOLVERTON, Department of Materials Science and Engineering, Northwestern University — Since their discovery by Fritz Heusler in 1903, Heusler compounds,  $\text{X}_2\text{YZ}$ , have been attracting a lot of research attention and have been intensely studied for their potential usage in spintronics, shape-memory devices, superconductors, thermoelectrics, topological insulators, and other applications. However, although more than 1000 Heusler compounds have been reported experimentally or computationally, a lot of potential Heusler compounds have not been explored yet due to complexities involved in dealing with such a huge phase space. As searching for new compounds experimentally is an expensive and a lengthy process, in this talk, we will demonstrate how to use a multi-step high-throughput computational screening method to predict several hundreds new stable and metastable Heusler compounds from 186588 compositions. As an example application, we will illustrate how to find age hardening precipitates using our screening strategy

**8:48AM K23.00003 Discovering complete pressure-temperature phase diagrams with Hamiltonian Monte Carlo nested sampling**, ROBERT BALDOCK, University of Cambridge, NOAM BERNSTEIN, Naval Research Laboratory, LIVIA BARTÓK-PARTÁY, GÁBOR CSÁNYI, University of Cambridge — Nested sampling is a Monte Carlo algorithm that can be used to efficiently calculate the complete configurational density of states in a material that undergoes multiple first-order phase transitions. From the density of states one can calculate the partition function as an explicit function of temperature and perform statistical mechanics from first principles. Indeed, we have shown how nested sampling can be used to automatically discover complete pressure-temperature phase diagrams with no prior knowledge of the locations of phase transitions or the structures of phases. In this talk I will present a new version of the nested sampling algorithm, based on a modified Hamiltonian ("Hybrid") Monte Carlo scheme. This new scheme reduces the scaling of a general nested sampling calculation. In particular the new algorithm expedites the sampling of atomic configuration spaces in condensed phases, and permits one to perform nested sampling calculations at a fraction of the cost required by ordinary nested sampling with standard Monte Carlo.

**9:00AM K23.00004 Equilibrium phase diagrams of alloys using nested sampling**, NOAM BERNSTEIN, Naval Research Laboratory, ROBERT J N BALDOCK, LIVIA BARTÓK-PARTÁY, GÁBOR CSÁNYI, Cambridge University — Temperature-pressure-composition phase diagrams describe the structures of materials in thermal equilibrium, and are an essential tool in understanding material properties. Predicting phase diagrams is challenging, even given a description of the interatomic interactions, because of the need to sample a very large configuration space. Nested sampling (NS) has been shown to be an efficient tool for calculating the partition function, and therefore all thermodynamic properties and ensemble averages, by systematically sampling the configuration space of isolated and periodic systems. Its effectiveness comes from sampling starting from high energy, where barriers are relatively low and equilibration is relatively fast, and iteratively eliminating a fixed *fraction* of the remaining configuration space. We present an application of NS at constant pressure to the phase diagram of a model binary alloy, CuAu, using an embedded atom method potential. We identify phase transitions indicated by peaks in the calculated specific heat, and the dominant phase at each temperature from ensemble-averaged structural ordering, as represented by quantities such as the radial distribution function. These results demonstrate the power of NS as a method for calculating complete phase diagrams.

**9:12AM K23.00005 Taking Materials Design Into The Space Of Polymorphs: Structure Predictions And Realizability<sup>1</sup>**, VLADAN STEVANOVIC, Colorado School of Mines — The phenomenon of polymorphism exemplifies the significance of structural degrees of freedom in determining physical properties of solids. Classic case is elemental carbon with markedly different mechanical, optical and electronic properties between its graphite and diamond forms. To harness the richness of this phenomenon and extend rational materials design into the space of polymorphs, there is a need for developing approaches that are capable of exploring systematically and efficiently the potential energy surface, and (desirably) assist in experimental realization of different structures. While the former presents a common place in the field of structure predictions, less attention is given to the latter. Namely, available experimental data indicate that the energy above the ground state alone is insufficient to quantify the realizability of different structures. For example, MgO crystallizes exclusively as the rocksalt despite the predicted existence of a number of low-energy structures. Similarly, ZnO is realized in the wurtzite, zincblende and a relatively high-energy rocksalt structure, again, apparently disregarding a number of theoretically predicted low-energy structures. In this talk I will present recent attempts to tackle these issues focused on partially ionic systems. The structure prediction part is carried out by performing local DFT relaxations on a large set of random superlattices (RSLs) with atoms distributed randomly over different planes in a way that favors cation-anion coordination. Second, application of the RSL sampling to a range of binary ionic systems such as MgO, ZnO, SnO<sub>2</sub> and other, reveals that the frequency of occurrence of a given structure offers an estimate of the volume of configuration space occupied by the corresponding local minimum, which is shown to be connected to the realizability of different structures.

<sup>1</sup>This work is part of the Center for Next Generation of Materials by Design, a US DOE funded Energy Frontier Research Center.

**9:48AM K23.00006 Prediction of boron carbon nitrogen phase diagram**, SANXI YAO, Carnegie Mellon Univ, HANTAO ZHANG, Univ of Science and Technology of China, MICHAEL WIDOM, Carnegie Mellon Univ — We studied the phase diagram of boron, carbon and nitrogen, including the boron-carbon and boron-nitrogen binaries and the boron-carbon-nitrogen ternary. Based on the idea of electron counting and using a technique of mixing similar primitive cells, we constructed many "electron precise" structures. First principles calculation is performed on these structures, with either zero or high pressures. For the BN binary, our calculation confirms that a rhombohedral phase can be stabilized at high pressure, consistent with some experimental results. For the BCN ternary, a new ground state structure is discovered and an Ising-like phase transition is suggested. Moreover, we modeled BCN ternary phase diagram and show continuous solubility from boron carbide to the boron subnitride phase.

**10:00AM K23.00007 Design and discovery of heterostructural alloys**, AARON HOLDER, SEBASTIAN SIOL, PAUL NDIONE, HAOWEI PENG, ANDRIY ZAKUTAYEV, STEPHAN LANY, NREL, BETHANY MATTHEWS, JANET TATE, Oregon State Univ., BRIAN GORMAN, Colorado School of Mines, ROY GORDON, Harvard, LAURA SCHELHAS, MIKE TONEY, SLAC — The tailoring of materials properties by alloying is routinely utilized to design materials for targeted technological applications. Despite the great successes of alloying in isostructural systems, heterostructural alloying remains a fundamentally unexplored area. In heterostructural alloys, the crossover between different crystal structures enables a new parameter for control over structure and properties by variation of the composition. Here, we present a complementary theoretical and experimental investigation of novel semiconducting metal chalcogenide alloys to develop design principles and approaches for utilizing heterostructural alloying as a materials design strategy. We use *ab initio* methods to predict the structural and electronic properties of novel alloys with commensurate and incommensurate lattice symmetries. Non-equilibrium deposition methods are employed to overcome thermodynamic solubility limits and produce metastable thin-film samples across the entire alloy composition range. The prediction, theory-guided combinatorial synthesis, and characterization of heterostructural alloys demonstrate the design and discovery of functional metastable materials. Our approach establishes a new route for the control of structure-property and composition-structure relationships by accessing non-equilibrium phase space to develop new materials with uniquely tailored properties.

**10:12AM K23.00008 Informatics-aided computational design of functional layered oxides**, PRASANNA V BALACHANDRAN, Los Alamos National Laboratory, Los Alamos, NM, JOSHUA YOUNG, Department of Materials Science and Engineering, Drexel University, Philadelphia, PA, TURAB LOOKMAN, Los Alamos National Laboratory, Los Alamos, NM, JAMES RONDINELLI, Department of Materials Science and Engineering, Northwestern University, Evanston, IL — We discuss a data-driven *ab initio* protocol with predictive capability to design and accelerate the discovery of noncentrosymmetric (NCS) inorganic oxides. Our approach synergistically integrates applied group theory, materials informatics and density functional theory (DFT) to uncover geometry-chemistry-symmetry guidelines for computational design of new NCS materials, specifically oxygen octahedra containing basic building units. Using this approach, we identify new and previously unknown compositions with potential for realizing NCS structures in the bulk  $n=1$  Ruddlesden-Popper (RP) oxides. We then validate our predictions using DFT calculations. Our approach enables rational design and engineering of both crystal structures and functionalities.

**10:24AM K23.00009 Computational Discovery of Materials Using the Firefly Algorithm<sup>1</sup>**, GUILLERMO AVENDAO-FRANCO, ALDO ROMERO, West Virginia University — Our current ability to model physical phenomena accurately, the increase computational power and better algorithms are the driving forces behind the computational discovery and design of novel materials, allowing for virtual characterization before their realization in the laboratory. We present the implementation of a novel firefly algorithm, a population-based algorithm for global optimization for searching the structure/composition space. This novel computation-intensive approach naturally take advantage of concurrency, targeted exploration and still keeping enough diversity. We apply the new method in both periodic and non-periodic structures and we present the implementation challenges and solutions to improve efficiency. The implementation makes use of computational materials databases and network analysis to optimize the search and get insights about the geometric structure of local minima on the energy landscape. The method has been implemented in our software PyChemia, an open-source package for materials discovery.

<sup>1</sup>We acknowledge the support of DMREF-NSF 1434897 and the Donors of the American Chemical Society Petroleum Research Fund for partial support of this research under contract 54075-ND10

**10:36AM K23.00010 Superconductivity in metastable phases of phosphorus-hydride compounds under high pressure<sup>1</sup>**, JOSE FLORES LIVAS, University of Basel, MAXIMILIAN AMSLER, Northwestern University, ANTONIO SANNA, Max-Planck Institut für Mikrostrukturphysik, CHRISTOPH HEIL, LILIA BOERI, Graz University of Technology, GIANNI PROFETA, Dipartimento di Fisica Università degli Studi di L'Aquila, CHRIS WOLVERTON, Northwestern University, STEFAN GOEDECKER, University of Basel, E. K. U. GROSS, Max-Planck Institut für Mikrostrukturphysik — Recently, compressed phosphine was reported to metallize at pressures above 45 GPa, reaching a superconducting transition temperature ( $T_c$ ) of 100 K at 200 GPa. However, neither the exact composition nor the crystal structure of the superconducting phase have been conclusively determined. In this work the phase diagram of  $\text{PH}_n$  ( $n = 1, 2, 3, 4, 5, 6$ ) was extensively explored by means of *ab initio* crystal structure prediction methods. The results do not support the existence of thermodynamically stable  $\text{PH}_n$  compounds, which exhibit a tendency for elemental decomposition at high pressure even when vibrational contributions to the free energies are taken into account. Although the lowest energy phases of  $\text{PH}_{1,2,3}$  display  $T_c$ 's comparable to experiments, it remains questionable if the measured values of  $T_c$  can be fully attributed to a phase-pure compound of  $\text{PH}_n$ .

<sup>1</sup>This work was done within the NCCR MARVEL project

**10:48AM K23.00011 Hybrid MC/MD Method For High Entropy Alloy<sup>1</sup>**, BOJUN FENG, MICHAEL WIDOM, Carnegie Mellon University — High entropy alloys (HEA) are materials that contain multiple components of elements consisting of a single solid solution phase which could make the entropy of mixing very high. From recent investigations, HEAs possess promising properties such as strength at high temperature, tensile strength, thermal stability and corrosion resistance. In this talk, a hybrid Molecular Dynamics (MD)/Monte Carlo (MC) simulation method is introduced to the computational analysis of HEA, treating atomic displacement by MD as well as swapping atomic species by MC. This method efficiently models the phase separation and short range order by swapping between different types of atoms, while structural deviation from the perfect lattice sites of atoms is equilibrated quickly by MD. We apply this method to HfNbTaZr HEA modeled using an embedded-atom potential. The result gives a strong phase separation of Hf-Zr and Nb-Ta pairs shown by the pair correlation function. Diffuse scattering patterns are predicted and compared to experiments.

<sup>1</sup>DOE Grant No. DE-SC0014506

**Wednesday, March 16, 2016 8:00AM - 11:00AM –**  
**Session K24 DMP: Many-Body Perturbation Theory for Electronic Excitations: Theoretical Spectroscopy** 323 - Claudia Draxl, Humboldt University

**8:00AM K24.00001 DFT+ $U(\omega)$ : Frequency-dependent Hubbard  $U$  correction**, DAVID D. O'REGAN, Trinity College Dublin, NICOLA MARZARI, Ecole Polytechnique Fédérale de Lausanne (EPFL) — In contemporary first-principles atomistic simulation based on DFT, the augmentation of approximate exchange-correlation functionals with spatially or energetically localized corrections, such as DFT+ $U$ , is a successful approach for improving its applicability to strongly interacting systems. Electronic screening is a dynamical process, and since the Hubbard  $U$  parameter, in particular, is a measure of the screened Coulomb interaction, its frequency-dependent generalisation for the dynamical regime is possible. We introduce a conceptually pragmatic and computationally straightforward method, named DFT+ $U(\omega)$ , for calculating and incorporating strong dynamical screening effects in spectroscopic calculations based on Kohn-Sham DFT. Our method is designed to be a minimal dynamical extension of DFT+ $U$ , one in which computing approximate dynamical Hubbard  $U$  functions only requires functionality that is widely available. We demonstrate our effective plasmon fitting and self-energy approximation scheme for DFT+ $U(\omega)$ , which enables the resulting low-energy dynamical model to be solved at the  $G_0W_0$  level, and beyond, efficiently and effectively.

**8:12AM K24.00002 RIXS of Ammonium Nitrate using OCEAN**, JOHN VINSON, TERRENCE JACH, NIST, Gaithersburg, MD, MATTHIAS MUELLER, RAINER UNTERUMSBERGER, BURKHARD BECKHOFF, PTB, Berlin, Germany — The OCEAN code allows for calculations of near-edge x-ray spectroscopies using a *GW*/Bethe-Salpeter equation (BSE) approach. Here we present an extension of the code for calculating resonant inelastic x-ray scattering (RIXS). Recent work has shown that peak-specific broadening of nitrogen  $K\alpha$  emission in nitrates is due to a valence-band lifetime that is an order of magnitude shorter than that of the nitrogen 1s hole, an inversion of the usual assumption that valence holes have longer lifetimes than core-level holes. Using the BSE, including *GW* corrections to the DFT energies, as implemented in OCEAN we are able to compare calculations of RIXS with measured spectra of the same. By utilizing an approach free from fitting parameters we are able to identify the origins of various broadening effects observed in experiment.

**8:24AM K24.00003 Signatures of correlation in transition metal oxides**, MATTEO GATTI, LSI, Ecole Polytechnique, France, MATTEO GUZZO, Humboldt-Universität zu Berlin, Germany, LUCIA REINING, LSI, Ecole Polytechnique, France — Photoemission satellites are a genuine fingerprint of electronic correlation that cannot be interpreted within the quasiparticle band-structure picture. Here we show that they can be understood in terms of the coupling between different elementary excitations, as in the case of plasmon sidebands. Using examples from different correlated materials, we discuss how this coupling can be explained by advanced calculations based on first-principles many-body perturbation theory that combine *GW*-like approximations for the self-energy with the cumulant expansion of the Green's function [1-3]. This approach is not limited to low-energy satellites, but allows for a consistent explanation of signatures of correlation over a wide range of binding energies. [1] M. Guzzo *et al.*, Phys. Rev. Lett. **107**, 166401 (2011). [2] M. Gatti and M. Guzzo, Phys Rev B **87**, 155147 (2013). [3] M. Gatti *et al.*, Phys. Rev. Lett. **114**, 116402 (2015).

**8:36AM K24.00004 High-resolution Valence and Core Excitation Spectra via First-Principles Calculations and Experiment**<sup>1</sup>, ERIC SHIRLEY, NIST, F. FOSSARD, ONERA-CNRS, LEM, K. GILMORE, ESRF, G. HUG, ONERA-CNRS, LEM, J.J. KAS, J.J. REHR, F. VILA, U. Wash., Seattle — We calculate the optical and C K-edge near edge spectra of crystalline and molecular  $C_{60}$  measured with high-resolution electron energy-loss spectroscopy. The calculations are carried out using at least three different methods: Bethe-Salpeter calculations using the NIST Bethe-Salpeter Equation solver (NBSE) in the valence and OCEAN (Obtaining Core Excitation with Ab initio methods and NBSE) suite [Gilmore *et al.*, Comp. Phys. Comm., (2015)]; excited-core-hole calculations using XCH [D. Prendergast and G. Galli, Phys. Rev. Lett. **96**, 215502 (2006)]; and constrained occupancy using StoBe (Stockholm-Berlin core-excitation code) [StoBe-deMon version 3.0, K. Hermann *et al.* (2009)]. They include self-energy effects, lifetime-damping, and Debye-Waller effects. A comparison of spectral features to those observed illustrates the sensitivity of certain features to computation details (e.g., self-energy corrections and core-hole screening). This may point to limitations of various approximations, e.g. in conventional BSE paradigm and/or the incomplete treatment of vibrational effects.

<sup>1</sup>Supported in part by DOE BES Grant DE-FG03-97ER45623 (JJR, JJK, FV)

**8:48AM K24.00005 Obtaining X-ray absorption near-edge structure for transition metal oxides via the Bethe-Salpeter equation**, YUFENG LIANG, Lawrence Berkeley National Lab, The Molecular Foundry, JOHN VINSON, National Institute of Standards and Technology, SRI PEMMARAJU, Lawrence Berkeley National Lab, The Molecular Foundry, ERIC SHIRLEY, National Institute of Standards and Technology, DAVID PRENDERGAST, Lawrence Berkeley National Lab, The Molecular Foundry — Transition metal oxides are an important class of materials featured with strongly correlated effects. Most interesting and yet to-be-unveiled physics is associated with the metal 3d orbitals, which can be probed by X-ray absorption near-edge spectroscopy. A thorough interpretation of the x-ray spectroscopy is often accompanied with first-principles simulations of structures, electronic properties and the corresponding x-ray spectra. However, the simulation for TMOs is particularly challenging with the localized 3d orbitals. Most previous studies relied on the ground-state calculations without the core-hole as a compromise. Other treated the excited atom as a charged impurity but the calculated spectra turn out to be even more deviated from experiments [1]. Here, we present the first study for the O K-edge for several typical TMOs via solving the Bethe-Salpeter equation (BSE). We have found that electron-core-hole interactions can alter the absorption spectra significantly. Our study helps to disentangle core-hole effects from the intrinsic electron correlations and hence facilitates the development of more advanced many-electron theories. [1] Isao Tanaka, Teruyasu Mizoguchi, and Tomoyuki Yamamoto J. Am. Ceram. Soc., **88** [8] 20130209 (2005)

**9:00AM K24.00006 First-Principles Study of Frequency-Dependent Resonant Raman Scattering**, YANNICK GILLET, Université catholique de Louvain, STEFAN KONTUR, Humboldt-Universität zu Berlin, MATTEO GIANTOMASSI, Université catholique de Louvain, CLAUDIA DRAXL, Humboldt-Universität zu Berlin, XAVIER GONZE, Université catholique de Louvain — A resonance phenomenon appears in the Raman response when the exciting light has frequency close to electronic transitions. Unlike for molecules and for graphene, the theoretical prediction of such frequency-dependent Raman response of crystalline systems has remained a challenge. Indeed, many Raman intensity first-principle calculations are nowadays done at vanishing light frequency, using static Density-Functional Perturbation Theory, thus neglecting the frequency dependence and excitonic effects. Recently, we proposed a finite-difference method for the computation of the first-order frequency-dependent Raman intensity [1], with excitonic effects described by the Bethe-Salpeter equation. We found these to be crucial for the accurate description of the experimental enhancement for laser photon energies around the gap. In this work, we generalize this approach to the more complex second-order Raman intensity, with phonon losses coming from the entire Brillouin zone. Interestingly, even without excitonic effects, one is able to capture the main relative changes in the frequency-dependent Raman spectrum at fixed laser frequencies. The excitonic effects are discussed. [1] Y. Gillet, M. Giantomassi, X. Gonze, Phys. Rev. B **88**, 094305 (2013).

**9:12AM K24.00007 Cumulant approach for electronic excitations in x-ray and electron spectra**<sup>1</sup>, J. J. REHR, Univ of Washington — A quantitative treatment of electronic excitations and other many-body effects in x-ray and electron spectra has long been challenging. Physically, electronic correlations and atomic vibrations lead to inelastic losses and damping effects that are ignored in ground state methods or approximations such as TDDFT. Quasi-particle (QP) approaches such as the *GW* approximation yield significant improvements, as demonstrated in real-space Greens function [1] and *GW*/Bethe-Salpeter equation [2] calculations, but still ignore multi-electron excitations. Recently such excitations have been treated with considerable success using cumulant expansion techniques and the quasi-boson approximation [3,4]. In this beyond QP approach, excitations such as plasmons and electron-hole excitations appear as satellites in the spectral function. The method naturally accounts for multiple-satellites and can be extended to include extrinsic losses and interference effects. Extensions for effects of vibrations and strong correlations including charge-transfer satellites may also be possible [5]. These advances are illustrated with a number of applications.

[1] John J. Rehr *et al.*, Comptes Rendus Physique **10**, 548 (2009).

[2] K. Gilmore *et al.*, Comput. Phys. Comm. **197**, 109 (2015).

[3] L. Hedin, J. Phys.: Condens. Matter **11**, R489 (1999).

[4] Jianqiang Sky Zhou *et al.*, J. Chem. Phys. **143**, 194109 (2015).

[5] J. J. Kas, *et al.*, Phys. Rev. B **91**, 121112(R) (2015).

<sup>1</sup>Supported by DOE Grant DE-FG02-97ER45623

**9:48AM K24.00008 Real-time cumulant approach for inelastic losses in x-ray spectra<sup>1</sup>**, J. J. KAS, J. J. REHR, U of Washington, J. B. CURTIS, U of Rochester — Intrinsic inelastic losses in core level x-ray absorption (XAS), emission (XES), and x-ray photo-emission spectra (XPS), arise from excitations of the system due to the sudden creation or annihilation of a deep core hole. Additional extrinsic losses arise during the propagation of the photoelectron, and interference processes are also important. These excitations are reflected in the satellite peaks observed in XPS. Formally the distribution of these excitations are described in terms of the core-hole spectral function, which can be calculated in terms of the core-hole Green's function represented in exponential form. Here we discuss an approach for calculating the exponent, or cumulant in terms of local density fluctuations via real-space, real-time time-dependent density functional theory.<sup>2</sup> The role of extrinsic and interference terms is also discussed. Our method is illustrated in calculations of XAS and XPS for number of systems, including weakly correlated as well as *d*- and *f*-electron materials.

<sup>1</sup>Supported by DOE BES Grant DE-FG03-97ER45623

<sup>2</sup>J. J. Kas, F. D. Vila, J. J. Rehr, and S. A. Chambers, Phys. Rev. B **91**, 121112 (2015).

**10:00AM K24.00009 Approaching the quantum limit for plasmonics: linear atomic chains**, EMILY TOWNSEND, GARNETT BRYANT, National Institute of Standards and Technology — Linear atomic chains, such as atom chains on surfaces, linear arrays of dopants in semiconductors, or linear molecules, provide ideal testbeds for studying quantum plasmonics in nanosystems. We study the many-body excitations of finite (10-25) linear atomic chains. We use both time-dependent density functional theory (TDDFT) and exact diagonalization to analyze the excitations. TDDFT reveals optically driven excitations that can be single-particle-like, plasmon-like or mixed states. Such states can have very different dependencies on the electron-electron interaction strength, which can be used to help identify the states. TDDFT can identify plasmonic resonances, but it does not reveal how to quantize them. Exact diagonalization is used to get the full quantum description. However, exact diagonalization results can be very different from TDDFT results. Highly correlated, multi-excitonic states, also strongly dependent on the electron-electron interaction strength, appear in the exact response but not in TDDFT excitation spectra. These excitonic many-body states make it hard to identify plasmonic excitations. Exact results are also strongly dependent on the strength of the exchange interaction. We present these results to show how quantum plasmons appear in linear atomic chains.

**10:12AM K24.00010 On the Role of Fe<sub>2</sub>O<sub>3</sub> Surface States for Water Splitting**, MAYTAL CASPARY TOROKER, Department of Materials Science and Engineering, Technion - Israel Institute of Technology — Understanding the chemical nature and role of electrode surface states is crucial for improved electrochemical cell operation. For iron (III) oxide ( $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>), which is one of the most widely studied anode electrodes used for water splitting, surface states were related to the appearance of a dominant absorption peak during water splitting. The chemical origin of this signature is still unclear and this open question has provoked tremendous debate. In order to pin down the origin and role of surface states, we perform first principle calculations with density functional theory +U on several possible adsorbates at the  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>(0001) surface. We show that the origin of the surface absorption peak could be a Fe-O•type bond that functions as an essential intermediate of water oxidation

**10:24AM K24.00011 Many body calculations of the optoelectronic properties of *h*-AlN: from 3D to 2D<sup>1</sup>**, DENIZ KECIK, National Nanotechnology Research Center, Bilkent University, Ankara 06800, Turkey, CIHAN BACAKSIZ, Department of Physics, Izmir Institute of Technology, 35430 Izmir, Turkey, ENGIN DURGUN, Institute of Materials Science and Nanotechnology, Bilkent University, Ankara 06800, Turkey, TUGRUL SENER, Department of Physics, Izmir Institute of Technology, 35430 Izmir, Turkey — Outstanding electronic and optical properties of graphene, *h*-BN, MoS<sub>2</sub> etc. motivate the further discovery of novel 2D materials such as AlN, a III-V compound, with remarkable features for potential optoelectronic applications, due to its wide indirect band gap. The layer and strain dependent optoelectronic properties of the recently synthesized monolayer hexagonal AlN (*h*-AlN) were investigated using density functional and many body perturbation theories, where RPA and BSE were employed on top of the QP<sub>GW</sub> method. The optical spectra of 1-4 layered *h*-AlN revealed prominent absorption beyond the visible light regime; absorbance within the UV range increasing with the number of layers. In addition, the applied tensile strain (1 – 7%) was observed to gradually redshift the absorption spectra. While the many body corrections induced significant blueshift to the optical spectra, evidence of bound excitons were also found for the layered structures. Hence, the optoelectronic properties of layered *h*-AlN can be tuned by modifying their structure and applying strain, moreover are greatly altered when electron-hole interactions are considered.

<sup>1</sup>This work was supported by the Scientific and Technological Research Council of Turkey (TUBITAK, project no. 113T050).

**10:36AM K24.00012 Putting DFT to the Test: A First-Principles Study of Electronic, Magnetic, and Optical Properties of Co<sub>3</sub>O<sub>4</sub>**, VIJAY SINGH, MONICA KOSA, KOUSHIK MAJHI, DAN THOMAS MAJOR, Department of Chemistry, Bar-Ilan University, Ramat-Gan, Israel, PROF. ARIE ZABAN COLLABORATION — First-principles density functional theory (DFT) and a many-body Green's function method have been employed to elucidate the electronic, magnetic, and photonic properties of a spinel compound, Co<sub>3</sub>O<sub>4</sub>. Co<sub>3</sub>O<sub>4</sub> is believed to be a strongly correlated material, where the on-site Coulomb interaction (*U*) on Co *d* orbitals is presumably important, although this view has recently been contested. The suggested optical band gap for this material ranges from 0.8 to 2.0 eV, depending on the type of experiments and theoretical treatment. Thus, the correlated nature of the Co *d* orbitals in Co<sub>3</sub>O<sub>4</sub> and the extent of the band gap are still under debate, raising questions regarding the ability of DFT to correctly treat the electronic structure in this material. To resolve the above controversies, we have employed a range of theoretical methods, including pure DFT, DFT+U, and a range-separated exchange–correlation functional (HSE06) as well as many-body Green's function theory (i.e., the GW method). We compare the electronic structure and band gap of Co<sub>3</sub>O<sub>4</sub> with available photoemission spectroscopy and optical band gap data and confirm a direct band gap of ca. 0.8 eV. Furthermore, we have also studied the optical properties of Co<sub>3</sub>O<sub>4</sub> by calculating the imaginary part of the dielectric function (Im( $\epsilon$ )), facilitating direct comparison with the measured optical absorption spectra.

**10:48AM K24.00013 Objective performance of the GW approximation and the Bethe-Salpeter Equation for molecules**, FABIEN BRUNEVAL, CEA, SRMP (France) & Dept. of Physics, UC Berkeley & Lawrence Berkeley National Lab (USA), SAMIA M. HAMED, TONATIUH RANGEL-GORDILLO, JEFFREY B. NEATON, Dept. of Physics, UC Berkeley & Lawrence Berkeley National Lab (USA) — We have evaluated the quality of the quasiparticle energies obtained within the *GW* approximation and of the optical excitations with the solution of the Bethe-Salpeter equation (BSE) for molecules. The calculations have been performed with a recently developed code based on Gaussian [1,2] that allowed us to use the exact same techniques as the one employed in traditional quantum chemistry. We demonstrate [3] the extreme sensitivity of the *GW* and BSE results upon the Kohn-Sham starting point. Most of the starting point dependence in BSE is to be ascribed to the underlying *GW* band structure. We highlight the problem of the triplet excitations that are equally underestimated in time-dependent density-functional theory and in BSE. [1] F. Bruneval, J. Chem. Phys. **136**, 194107 (2012). [2] F. Bruneval and M.A.L. Marques, J. Chem. Theory Comput. **9**, 324 (2013). [3] F. Bruneval, S. M. Hamed and J. B. Neaton, J. Chem. Phys. **142**, 244101 (2015).

**Wednesday, March 16, 2016 8:00AM - 11:00AM –**

**Session K25 DCMP: Superconductivity: Theory I** 324 - Harald Jeschke, Goethe-Universitt Frankfurt

**8:00AM K25.00001 Revised phase diagram and anomalous thermal evolution of the antinodal gap and Raman response in high-temperature superconductors**, YUAN ZHOU, Nanjing University and Brookhaven Natl Lab, ZUODONG YU, Nanjing University, WEIGUO YIN, Brookhaven Natl Lab, HAIQING LIN, Beijing Computational Science Research Center, CHANGDE GONG, Nanjing University — The interplay of competing orders is essential to high-temperature superconductivity, which emerges upon suppression of an antiferromagnetic order typically via charge doping. However, where the zero-temperature quantum critical point (QCP) takes place — in terms of the doping level — is still elusive for it is hidden by the superconducting dome. The QCP has long been believed to follow the continuous extrapolation of the characteristic temperature ( $T^*$ ) for a normal-state order, but recently  $T^*$  within the superconducting dome was found to exhibit unexpected back-bending in the cuprate  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$  and the iron-pnictide  $\text{BaFe}_{1-x}\text{Co}_x\text{As}$ . Here we show that the original and the revised phase diagrams can be understood in terms of weak and moderate competitions, respectively, between superconductivity and a pseudogap state such as d-density-wave, based on Ginzburg-Landau theory and the microscopic extended t-J model. We further illustrate that the anomalous thermal dependences of the measured antinodal gap and Raman response in cuprates can be well understood by a two-step evolution, dominated by superconductivity and pseudogap, respectively.

**8:12AM K25.00002 The Andreev reflection in a superconductor-normal metal junction of a doped correlated quantum spin Hall insulator<sup>1</sup>**, YUNG-YEH CHANG, Department of Electrophysics, National Chiao-Tung University, HsinChu, Taiwan, 300, CHUNG-YU MOU, Department of Physics, National Tsing-Hua University, HsinChu, Taiwan 300, CHUNG-HOU CHUNG, Dept. of Electrophysics, Natl. Chiao-Tung Univ., HsinChu, Taiwan, 300; Physics Division, Natl. Center for Theoretical Sciences, HsinChu, Taiwan, 300 — Andreev conductance across a normal metal-superconductor (N-S) junction of doped correlated quantum spin Hall insulator on honeycomb lattice is theoretically studied via Blonder-Tinkham-Klapwijk (BTK) formalism. The normal side is modeled by the doped Kane-Mele (KM) model. The superconducting side is a doped correlated KM t-J model, which has been shown to feature d+id'-wave spin singlet pairing. With increasing intrinsic spin-orbit coupling, the doped KM t-J system undergoes a topological phase transition from the chiral d-wave superconductivity to the  $Z_2$  spin-Chern superconducting phase with helical Majorana fermions at edges. We apply a local strain on the N-S interface to generate an effective Dirac-delta barrier and study the transport near the chiral-helical phase transition in the weak tunneling limit. We explore the Andreev conductance at the K and K Dirac points, respectively and find the distinctive behaviors across the transition. Relevance of our results for the adatom-doped graphene is discussed. Reference: S.J. Sun, C.H. Chung, Y.Y. Chang, W.F. Tsai, and F.C. Zhang, arxiv:1506.02584."

<sup>1</sup>Y.Y. C. acknowledges the support from the MOST grant No.104-2112-M-009 -004 -MY3 and the NCTS of Taiwan, R.O.C.

**8:24AM K25.00003 Macroscopic character of composite high temperature superconducting wires**, STEVEN KIVELSON, Stanford Univ, BORIS SPIVAK, University of Washington — The "d-wave" symmetry of the superconducting order in the cuprate high temperature superconductors is a well established fact, and one which identifies them as "unconventional." However, in macroscopic contexts — including many potential applications (*i.e.* superconducting "wires") — the material is a composite of randomly oriented superconducting grains in a metallic matrix, in which Josephson coupling between grains mediates the onset of long-range phase coherence. Here, we analyze the physics at length scales large compared to the size of such grains, and in particular the macroscopic character of the long-range order that emerges. While XY-superconducting glass order and macroscopic d-wave superconductivity may be possible, we show that under many circumstances — especially when the d-wave superconducting grains are embedded in a metallic matrix — the most likely order has global s-wave symmetry.

**8:36AM K25.00004 Random field disorder and charge order driven quantum oscillations in cuprates**, ANTONIO RUSSO, SUDIP CHAKRAVARTY, UCLA — In the pseudogap regime of the cuprates, charge order breaks a  $Z_2$  symmetry. Therefore, the interaction of charge order and quenched disorder due to potential scattering, can, in principle, be treated as a random field Ising model. A numerical analysis of the ground state of such a random field Ising model reveals local, glassy dynamics in both  $2D$  and  $3D$ . The glassy dynamics are treated as a heat bath which couple to the itinerant electrons, leading to an unusual electronic non-Fermi liquid. If the dynamics are strong enough, the electron spectral function has no quasiparticle peak and the effective mass diverges at the Fermi surface, precluding quantum oscillations. In contrast to charge density,  $d$ -density wave order (reflecting staggered circulating currents) does not directly couple to potential disorder, allowing it to support quantum oscillations. At fourth order in Landau theory, there is a term consisting of the square of the  $d$ -density wave order parameter, and the square of the charge order. This coupling could induce parasitic charge order, which may be weak enough for the Fermi liquid behavior to remain uncorrupted. Here, we argue that this distinction must be made clear, as one interprets quantum oscillations in cuprates.

**8:48AM K25.00005 Onsager rule, quantum oscillation frequencies, and the density of states in the mixed-vortex state of cuprates**, ZHIQIANG WANG, SUDIP CHAKRAVARTY, UCLA — Onsager rule that determines the frequencies of quantum oscillations in high magnetic fields serves as an anchor point. In its absence it would be very difficult to interpret the experimental results, because for each instance the problem would have to be considered anew. In the mixed-vortex state of the underdoped cuprates where, major consequential discoveries have recently taken place, its validity has been recently questioned. Here we show that this rule remains intact to an excellent approximation. The models we consider are fairly general, consisting of a variety of density wave states combined with  $d$ -wave superconductivity. Another exceptionally interesting result from our model calculations is that the oscillations ride on top of a field independent density of states,  $\rho(B)$ , for higher fields. This feature appears to be consistent with the recent specific heat measurements.

**9:00AM K25.00006 Collective modes in non-uniform superconductors**, ANTON VORONTSOV, ANDREW HAMMER, Montana State University — We study dynamics of a superconducting condensate in the presence of a domain wall defect in the order parameter. We find that broken translation and reflection symmetries result in new collective excitations, bound to the domain wall region. Two additional amplitude/Higgs modes lie below the bulk pairbreaking edge  $2\Delta$ ; one of them is a Goldstone mode with vanishing excitation energy. Spectrum of bound collective modes is related to the topological structure and stability of the domain wall. The 'unbound' bulk collective modes and transverse gauge field mostly propagate across the domain wall, but the longitudinal component of the gauge field is completely reflected. Softening of the amplitude mode suggests reduced damping and possible route to its detection in geometrically confined superfluids or in superconductor-ferromagnetic heterostructures.

**9:12AM K25.00007 Quasiclassical approach to magnetic susceptibility<sup>1</sup>**, CAROLINE RICHARD, ANTON VORONTSOV, Montana State University — Quasiclassical theory is a powerful technique that allows calculation of physical observables using just the low-energy states of the system. It is especially useful in studying properties of the non-uniform superfluid phases. We extend this approach to calculate response functions that involve high-energy correlations. Using example of Pauli magnetic susceptibility we employ Andreev approximation to express the spin-spin correlation function near a pairbreaking surface, in terms of low-energy, high-energy and mixed state contributions. This provides a convenient way to calculate response of a non-uniform superconductor at finite  $q$ -vectors.

<sup>1</sup>Supported by RCSA through Cottrell Scholar Award

**9:24AM K25.00008 Boosted one dimensional superconductors on a lattice**, SAYONEE RAY, SUBROTO MUKERJEE, VIJAY B. SHENOY, Indian Institute of Science — We study the effect of a boost (that engenders a current-carrying state) on one dimensional systems of lattice fermions with short-ranged attractive interactions. In the absence of a boost such systems possess algebraic superconducting order. Naively, one might expect a boost to weaken and ultimately destroy superconductivity, as in higher dimensions. However, we show that for one dimensional systems its effect is to *strengthen* the algebraic superconducting order by making correlation functions fall off more slowly with distance. We explain the physical underpinnings of these findings.

**9:36AM K25.00009 Negative isotope effect in Hubbard-Holstein model.**, DA WANG, Nanjing University — In phonon mediated conventional s-wave superconductors, higher-frequency phonon (or smaller atomic mass) leads to a higher superconducting transition temperature, known as the isotope effect. However, in correlated systems, various competing electronic order (such as spin-density-wave, charge-density-wave, and unconventional superconductivity) arises and the effect of electron-phonon coupling on these orders is a long-standing problem. Using the functional renormalization group, here we investigated the interplay between the electron correlation and electron-phonon coupling in the Hubbard-Holstein model on a square lattice. At half-filling, we found spin-density-wave and charge-density-wave phases and the transition between them, while no superconducting phase arises. Upon finite doping, d-wave/s-wave superconductivity emerges in proximity to the spin-density-wave/charge-density-wave phase. Surprisingly, lower-frequency Holstein phonons are either less destructive or even beneficial to the various phases, resulting in a negative isotope effect. For the superconducting phases, such an effect is apparently beyond the Bardeen-Cooper-Schrieffer theory.

**9:48AM K25.00010 The superconducting state of Holstein model using dynamical mean field theory**, CHUNGWEI LIN, BINGNAN WANG, KOON TEO, Mitsubishi Elec Res Lab — To enhance the superconducting temperature within the conventional superconductors, we solve the Holstein model, where conduction electrons are coupled to some boson field, using dynamical mean field theory (DMFT) with the configuration interaction impurity solver. Thanks to the non-perturbative nature of DMFT, we determine the zero-temperature order parameter for a wide range of boson energies to find the optimal range for superconductivity. This is beyond the Migdal-Eliashberg theory where the boson energy is assumed to be small compared to the Fermi energy. The effect of Hubbard on-site repulsion will be also discussed.

**10:00AM K25.00011 Unconventional superconductivity and interaction induced Fermi surface reconstruction in the two-dimensional Edwards model**, DAI-NING CHO, STEFFEN SYKORA, IFW Dresden — We study the possibility of unconventional superconducting pairing in the framework of a novel two-dimensional quantum transport model, where the charge carriers are strongly affected by the correlations and fluctuations of a background medium, described by bosonic degrees of freedom. Using the projective renormalization method (PRM) we find in the half-filled band case an interplay between stable superconducting solutions and a charge-density wave order parameter which determines the ground state in the limit of large bosonic energies. The superconducting pairing mainly appears on a new hole-like Fermi surface, which is formed nearby the center of the Brillouin zone due to strong renormalization of the original fermionic band. In the superconducting state, the Fermi surface splits into two disconnected parts, which are characterized by different sign of the superconducting order parameter.

**10:12AM K25.00012 A comprehensive model for high- $T_c$  based on pair-pair interactions.**, WILLIAM SACKS, ALAIN MAUGER, IMPMC, Sorbonne Universities, France, YVES NOAT, INSP, Sorbonne Universities, France — The superconducting (SC) state of cuprates is characterized by a dome-shaped  $T_c$  versus carrier density and an unconventional *pseudogap* (PG) state above  $T_c$  - basic properties remain highly debated. We have recently proposed a mechanism [1] based on the mutual interaction between incoherent Cooper pairs existing above  $T_c$ . At the critical temperature, this interaction induces a Bose-like condensation leading to the coherent SC state.

Absent in the conventional BCS case, the mutual pair-pair interaction is proportional to the condensate density  $n_{oc}(T)$  but is also related to the quasiparticle excitations. It gives an excellent fit to the DOS as measured by electron tunneling for a wide range of samples and carrier concentration. We conclude that long-range order is achieved by a direct quasiparticle - Cooper-pair coupling.

We then focus on the *temperature dependence* of the thermodynamic functions (condensation energy, entropy, etc.) and of the quasiparticle DOS. We show that these quantities depend on the unique combination of pair (boson) and quasiparticle (fermion) excitations, allowing a qualitative understanding of the phase diagram.

W. Sacks, A. Mauger, Y. Noat, Superconduct. Sci.Technol. **28** 105014, 2015

**10:24AM K25.00013 Two types of superconducting domes in unconventional superconductors**, TANMOY DAS, Indian Institute of Science, Bangalore, CHRISTOS PANAGOPOULOS, Nanyang Technological University, Singapore — In this talk, we present a comprehensive analysis of the SC properties and phase diagrams across several families of unconventional superconductors within the copper-oxides, heavy-fermions, organics, and the recently discovered iron-pnictides, iron-chalcogenides, and oxybismuthides. We find that there are two types of SC domes present in all families of SC materials, arising sometimes as completely isolated, or merged into one, or in some materials only any one of them appears. One of the SC dome appearing at or near a possible QCP usually possesses a lower transition temperature ( $T_c$ ). The other SC dome appearing at a different value of the tuning parameter around a non-Fermi liquid (NFL) state often has higher  $T_c$ . Both SC domes are not necessarily linked to each other, and so does the QCP and NFL state. In materials, where both domes are present, they can be isolated by multiple tuning (such as such as disorder, or pressure, or magnetic field in addition to doping, and vice versa), giving a unique opportunity to decouple the relationship between QCP, NFL, and their role on superconductivity. The systematic study the NFL state might be a generic route to higher- $T_c$  superconductivity.

**10:36AM K25.00014 Theory of pump-probe photoemission from a d-wave superconductor**, BENJAMIN NOSARZEWSKI, BRIAN MORITZ, SLAC National Accelerator Laboratory and Stanford University, ALEXANDER F. KEMPER, North Carolina State University, JAMES K. FREERICKS, Georgetown University, THOMAS P. DEVEREAUX, SLAC National Accelerator Laboratory and Stanford University — Motivated by recent tr-ARPES experiments on high-temperature superconductors, we use the nonequilibrium Keldysh formalism to study the time-resolved photoemission spectra of a model electron-boson coupled system out of equilibrium. We introduce a momentum dependence to the electron-boson coupling to produce a superconducting state with d-wave symmetry. We investigate the nature of quasiparticle relaxation and recombination as well as the signatures of amplitude mode oscillations of the superconducting order parameter. We interpret our results in terms of existing experiments in the cuprates.

**10:48AM K25.00015 First principles calculations of  $\text{La}_2\text{CuO}_4$** , ANDREI PLAMADA, Institute for Theoretical Physics, ETH Zurich, ANTON KOZHEVNIKOV, Swiss National Supercomputer Centre, ETH Zurich, URS HAEHNER, MI JIANG, Institute for Theoretical Physics, ETH Zurich, PETER STAAR, IBM Research - Zurich, THOMAS MAIER, Computer Science and Mathematics Division and Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, THOMAS SCHULTHEISS, Institute for Theoretical Physics, ETH Zurich — We use the DFT+DCA method for a high-end study of the electronic structure properties of  $\text{La}_2\text{CuO}_4$ . The parameters of a tight-binding model are created using the first-principles electronic structure calculations. The all-electron full-potential linearised augmented plane-wave method is used to solve the non-interacting band problem. Then the set of physically relevant Wannier functions is chosen as a basis for the underlying Hubbard model. The Wannier functions and the corresponding non-interacting Hamiltonian  $H_{nm}^0(\mathbf{k})$  are created using the well-established downfolding approach. The screened Coulomb interaction parameters  $U_{nm}$  of the model are computed using the constrained random-phase approximation technique. The double counting term is assumed to be a constant multiplied by the identity operator in the correlated subspace and it is determined based on first-principles considerations. The resulting *ab-initio* parameterisation of the Hubbard model is solved within dynamical cluster approximation (DCA).

**Wednesday, March 16, 2016 8:00AM - 11:00AM –**

**Session K26 DCMP: Insulator: Growth, Structure, Properties, and Defects** 325 - Bharat Jalan,  
University of Minnesota

**8:00AM K26.00001 Nanocrystal Ghosting: Extensive radiation damage in MgO induced by low-energy electrons**, WILLIAM SAWYER, ZACHERY FRANKENFIELD, Deptment of Physics, West Chester University, KENNETH KANE, Deptment of Physics, Virginia Commonwealth University — Radiation damage in magnesium oxide has been an ongoing source of investigation. Early work was motivated by its simple cubic structure and its excellent electrical insulating properties over a wide range of temperatures and mechanical conditions. The goal was to determine its suitability as an electrical insulator in radiation intense environments including nuclear reactors and proposed nuclear fusion devices. During this period experimental results for irradiation of MgO using electrons with energies less than 500 keV produced very limited damage. These results, supported by theoretical arguments, lead to the conclusion that MgO was relatively impervious to damage from electrons with energies below this threshold. More recently its excellent insulating properties and relative mechanical stability combined with an increased interest in nanomaterials applications have created renewed interest in MgO. In this paper direct evidence is presented for extensive radiation damage in MgO nanocrystals from intense irradiation by electrons ( $2 \times 10^4$  electrons/nm<sup>2</sup> sec) with beam energies between 120 keV and 60 keV.

**8:12AM K26.00002 Point defects in yttria-stabilized zirconia**, C. STEPHEN HELLBERG, NOAM BERNSTEIN, STEVEN C. ERWIN, Naval Research Lab — The densification that occurs during sintering of certain ceramics has been observed to occur more rapidly and at lower temperatures when a weak external electric field is applied.<sup>1</sup> We compute the formation energies of point defects in yttria-stabilized zirconia using first principles density functional theory. We examine interstitials, vacancies, and vacancy complexes including Schottky defects in a Y<sub>2</sub>Zr<sub>14</sub>O<sub>31</sub> computational cell, which corresponds to approximately 7 mol% yttria stabilized zirconia. We relate our results to recent experimental work on electric-field-assisted sintering in yttria-stabilized zirconia, showing how the expansion of lattice constants observed in diffraction measurements results from increasing defect densities. 1. Raj, R., Cologna, M., and Francis, J. S. C. Influence of Externally Imposed and Internally Generated Electric Fields on Grain Growth, Diffusional Creep, Sintering and Related Phenomena in Ceramics. *Journal of the American Ceramic Society* 94, 1941 (2011).

**8:24AM K26.00003 Investigation of Defect Structure to Determine the Primary Photorefractive Centers Responsible for Enhanced Beam Coupling in KNbO<sub>3</sub>:Fe**, DEAN EVANS, Air Force Rsch Lab - WPAFB, SERGEY BASUN<sup>1</sup>, Azimuth Corp., AIR FORCE RSCH LAB - WPAFB TEAM, AIR FORCE RSCH LAB - WPAFB TEAM — A series of experiments are used to determine the location of the energy levels of various Fe centers and associated defect centers in KNbO<sub>3</sub>:Fe, as well as conclude which centers are the primary photorefractive centers. In particular, the methods include electron paramagnetic resonance, optical absorption spectroscopy, electric conductivity, and beam coupling. A correlated study using data acquired with these techniques has been performed on as-grown (unreduced) and reduced KNbO<sub>3</sub>:Fe crystals, which identified which Fe centers were reduced and which ones were not. Conditions for an increased electron source population (improved beam coupling performance) was determined and compared to beam coupling results for pure electron, pure hole, and electron-hole competition processes.

<sup>1</sup> Air Force Rsch Lab - WPAFB

**8:36AM K26.00004 Raman and Fluorescence Study of Erbium-Doped Laser-Induced Crystals-in-Glass**, BRIAN KNORR, Fairleigh Dickinson Univ, KEITH VEENHUIZEN, ADAM STONE, Lehigh University, HIMANSHU JAIN, Fairleigh Dickinson Univ, VOLKMAR DIEROLF, Lehigh University — Laser induced crystallization of glasses is a spatially selective process which has the potential to produce photonic integrated circuits in a glass matrix. Low temperature Combined Excitation Emission Spectroscopy in Er:LaBGeO<sub>5</sub> show that erbium incorporates at predominantly one majority site in both glass-ceramics and laser-induced crystals-in-glass, but that other minority sites also exist. The energy levels of the majority site were quantified. The fluorescence characteristics of the erbium ions in any site in the laser-induced crystals were found to be only weakly influenced by the irradiation conditions during growth. On the other hand, a hidden parameter, potentially boron deficiency-related defects, resulted in a significant change in the incorporation behavior of the erbium ions. Simultaneous scanning confocal Raman and fluorescence spectroscopy showed that the energies of the Raman modes are shifted, and the erbium fluorescence intensity varies, in a non-uniform manner, despite the host glass being homogeneously doped, across the cross-sections of laser-induced crystals in glass. These fluctuations within the Raman and fluorescence are spatially correlated, implying that different erbium sites form preferentially at different locations in the crystal cross-section.

**8:48AM K26.00005 Excitons and band edge alignment in CdSe/CdS core-shell nanocrystals: ab initio**, DANYLO ZHEREBETSKYY, LIN-WANG WANG, Materials Sciences Division, Lawrence Berkeley National Laboratory, COMPUTATIONAL MATERIALS SCIENCE AND NANOSCIENCE TEAM — Quantum confinement is a foundational nanoscience concept that allows tuning electronic properties of quantum dots. Core-shell quantum dots are promising nanoparticles and found applications as light-emitting optoelectronic devices and biomarkers [1] due to their robustness and tunability of both core and shell. The fluorescent quantum yield of these quantum dots can achieve 100% [2] even at room temperature [3]. However, to understand many phenomena of carrier dynamics, photoluminescence efficient and Auger effects, fine electronic structures of the exciton are needed. Here, using large scale electronic structure calculations based on charge patching method, we have investigated the exciton binding energy, band alignment between core and shell, charge separation between electron and hole. We will discuss how these can be tuned by changing the core/shell dimensions. 1. Shirasaki Y., Supran G., Bawendi M., Bulović V. *Nature Photonics* 7, 13 (2013). 2. Javaux C. et al, *Nature Nanotech.* 8, 206 (2013) 3. Achieved in Alivisatos lab (2014).

**9:00AM K26.00006 Photocreation and hyperbolic decay of Sb<sup>2+</sup> in Sn<sub>2</sub>P<sub>2</sub>S<sub>6</sub>:Sb.**, SERGEY BASUN, Air Force Res. Lab. WrightPatterson Air Force Base, LARRY HALLIBURTON, Dept of Physics, West Virginia University, SERGEY ODOULOV, ALEXANDR SHUMELYUK, Institute of Physics, 03 650 Kyiv, Ukraine, ALEXANDER GRABAR, Institute of Solid State Physics and Chemistry, DEAN EVANS, Air Force Res. Lab. WrightPatterson Air Force Base — In Sn<sub>2</sub>P<sub>2</sub>S<sub>6</sub>:Sb, photorecharging of Sb<sup>3+</sup> ions to Sb<sup>2+</sup> causes a new interesting phenomenon – photo-sensitizing of photorefraction.[1,2] The decay of the optically produced Sb<sup>2+</sup> ions was directly measured through EPR and was found to have a hyperbolic character:  $\sim 1/(t/\tau+1)$  with an activation energy of 0.42 eV. This decay character and a very similar activation energy were also found in photorefraction and optically induced absorption experiments. The observed hyperbolic decay was explained through the set of rate equations that takes into account the EPR result: only Sb<sup>3+</sup> ions are present in Sn<sub>2</sub>P<sub>2</sub>S<sub>6</sub>:Sb in thermal equilibrium. The long-wavelength onset of the EPR-measured Sb<sup>2+</sup> “photocreation” spectrum together with the activation energy of the Sb<sup>2+</sup> decay allowed to firmly locate the position of the Sb<sup>2+/3+</sup> electron level in the bandgap of Sn<sub>2</sub>P<sub>2</sub>S<sub>6</sub>: 0.42 eV below the conduction band bottom. [1] D. R. Evans, A. Shumelyuk, G. Cook, S. Odoulov. *Opt. Lett.* 36, 454 (2011). [2] Y. Skrypka, A. Shumelyuk, S. Odoulov, S. Basun, D. Evans, *Opt. Comm.* 356, 208 (2015).

**9:12AM K26.00007 Surface Analysis of  $sp^2$  Carbon in Ag and Al Covetic Alloys\***, H M IFTEKHAR JAİM, Materials Science and Engineering Department, University of Maryland, College Park, MD 20742, USA, DANIEL P. COLE, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD 21005, LOURDES G. SALAMANCA-RIBA, Materials Science and Engineering Department, University of Maryland, College Park, MD 20742, USA — Ag, Al-6061 and Al-7075 were doped with carbon by an electrocharging assisted process where high electric current is applied to the molten metal containing particles of activated carbon. This process gives rise to epitaxial growth of graphene nanoribbons (GNR) and carbon nanostructures within the metal matrix. Alloys produced with such technique are named Covetics. Al-6061 and Al-7075 covetics have shown superior mechanical, electrical and anti-corrosion properties. The nanostructured carbon incorporation has been confirmed by XPS, Raman, and TEM studies. Here, we present detailed surface characterization of the carbon nanostructures in these new alloys. Raman and EELS mapping of carbon nanostructure were carried out to identify the nature of bonding, strain and defect characteristics. Mostly, crystalline GNR or graphene sheets were found to create networks with  $sp^2$  character, under compressive strain with high concentration of defects. AFM and KPFM showed contrast in phases and potentials for ribbon like features. Incorporation of  $sp^2$  carbon in metals is an initial step for the integration of carbon nanostructures for future applications requiring high strength and conductivity.

**9:24AM K26.00008 Direct visualization of atomically precise nitrogen-doped graphene nanoribbons.**, HONG-LIANG LU, University of Chinese Academy of Sciences and Institute of Physics, Chinese Academy of Sciences, Beijing 100049, China, YI ZHANG, YANFANG ZHANG, GENG LI, JIANCHEN LU, Institute of Physics and University of Chinese Academy of Sciences, Chinese Academy of Sciences, Beijing 100190, China, XIAO LIN, University of Chinese Academy of Sciences and Institute of Physics, Chinese Academy of Sciences, Beijing 100049, China, SHIXUAN DU, Institute of Physics and University of Chinese Academy of Sciences, Chinese Academy of Sciences, Beijing 100190, China, REINHARD BERGER, XINLIANG FENG, KLAUS MULLEN, Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany, HONG-JUN GAO, Institute of Physics and University of Chinese Academy of Sciences, Chinese Academy of Sciences, Beijing 100190, China — We have fabricated atomically precise nitrogen-doped chevron-type graphene nanoribbons by using the on-surface synthesis technique combined with the nitrogen substitution of the precursors. Scanning tunneling microscopy and spectroscopy indicate that the well-defined nanoribbons tend to align with the neighbors side-by-side with a band gap of 1.02 eV, which is in good agreement with the density functional theory calculation result. The influence of the high precursor coverage on the quality of the nanoribbons is also studied. We find that graphene nanoribbons with sufficient aspect ratios can only be fabricated at sub-monolayer precursor coverage. This work provides a way to construct atomically precise nitrogen-doped graphene nanoribbons.

**9:36AM K26.00009 First-principle study on substrate-induced structures of bismuth adsorption on graphene.**, SHIH-YANG LIN, Department of Physics, National Cheng Kung University, SHEN-LIN CHANG, Department of Electrophysics, National Chiao Tung University, HSIN-HSIEN CHEN, SHU-HSUAN SU, JUNG-CHUN HUANG, MING-FA LIN, Department of Physics, National Cheng Kung University — The geometric and electronic properties of Bi-adsorbed monolayer graphene, enriched by the strong effect of substrate, are investigated by the first-principles calculations. The six-layered substrate, corrugated buffer layer, and slightly deformed monolayer graphene are all simulated. Adatom arrangements are optimized through detailed analyses on adsorption energies and ground-state energies of various adsorption sites, revealing a hexagonal array of Bi atoms dominated by the interactions between buffer layer and monolayer graphene. The increasing temperature can overcome a ~50 meV energy barrier and induce triangular and rectangular nanoclusters. The most stable and the metastable structures agree with the scanning tunneling microscopy measurements. The density of states exhibits a finite value at the Fermi level, a dip at low energy, and a shoulder at ~-0.8 eV, as observed in the experimental measurements of tunneling conductance.

**9:48AM K26.00010 Atomic-scale investigation of grain boundary motion in graphene**, DONGWOOK KIM, Seoul National University, YOUNGKUK KIM, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, JISOON IHM, EUIJOON YOON, GUN-DO LEE, Seoul National University — Grain boundaries (GBs) in graphene can migrate when irradiated by electron beams from a transmission electron microscope (TEM). Here, we present an ab initio study on the atomic scale mechanism for the GB motion with misorientation angle of 30 in graphene. From total energy calculations and energy barrier calculations, we find that a Stone–Wales(SW)-type transformation can occur more easily near GBs than in pristine graphene due to a reduced energy barrier. There are other cases of migration which can be understood by other type of transformation, named evaporation of a carbon dimer. We also find that a mismatch in the crystalline orientation at GBs can drive the evaporation of a carbon dimer easily by greatly reducing the corresponding overall energy barrier. After evaporation of the carbon dimer, the GBs can be stabilized through a series of SW-type transformations that result in GB motion. The GB motion induced by evaporation of the dimer is in excellent agreement with recent TEM experiments.

**10:00AM K26.00011 Rippllocations: A Novel Defect in Layered Materials**, JACOB GRUBER, ANDREW LANG, JUSTIN GRIGGS, GARRITT TUCKER, MICHEL BARSOUM, Drexel Univ — Recently, a new defect, the rippllocation, the mechanical buckling of a single atomic layer, was proposed to explain the behavior of two dimensional materials. Leveraging atomistic simulations, this concept is extended to bulk layered materials. Unlike dislocations, rippllocations do not possess a Burgers vector and do not have polarity. In graphite, rippllocations are attracted both to vacancies, where they can annihilate, and other rippllocations, forming larger complexes and eventually kink boundaries. While some rippllocation behavior can be described by dislocation complexes, the failure of these models to explain core interactions suggests that rippllocations are a fundamentally new class of defect. Furthermore, TEM examination of nanoindented  $Ti_3SiC_2$ , where dislocation theory does not provide a complete description of behavior, reveals the presence of defects with no Burgers vector and with rotation and strain fields similar to those predicted in simulation, suggesting the presences of buckled basal planes. Rippllocations have profound implications for the deformation of plastically anisotropic solids, including graphite, layered silicates and the MAX phases.

**10:12AM K26.00012 Spin chains and electron transfer at stepped silicon surfaces**, STEVEN ERWIN, Naval Research Laboratory, JULIAN AULBACH, RALPH CLAESSEN, JOERG SCHAEFER, Universitaet Wuerzburg — Stepped silicon surfaces oriented between Si(111) and Si(001) show unusual behavior when submonolayer amounts of gold are adsorbed: they self-assemble to form arrays of steps with virtually perfect structural order. Known examples include Si(553), Si(557), and Si(775). For the first two of these there is, in addition, strong theoretical and experimental evidence that the silicon step edges are spin polarized, raising the possibility of a magnetically ordered ground state at a silicon surface. The situation is different, however, for Si(775): theory and experiment both show that spin polarization does not occur. Here we use density-functional theory and scanning tunneling microscopy to develop a physically transparent picture explaining the formation of these 'spin chains' on the family of Si(hhk)-Au surfaces. Specifically, we explain why spin chains form on particular silicon (hhk) orientations but not on others. Finally, we use this understanding to propose strategies for using surface chemistry to control the formation or suppression of spin chains on Si(hhk)-Au surfaces.

**10:24AM K26.00013 Film Growth on Nanoporous Substrate<sup>1</sup>**, XUE ZHANG, JAMES JOY, CHENWEI ZHAO<sup>2</sup>, Brown University, Department of Physics, J.M. XU, Brown University, School of Engineering, JAMES VALLES, Brown University, Department of Physics — Self-ordered nanoporous anodic aluminum oxide (AAO) provides an easy way to fabricate nano structured material, such as nano wires and nano particles. We employ AAO as substrates and focus on the thermally evaporated film growth on the surface of the substrate. With various materials deposited onto the substrate, we find the films show different structures, e.g. ordered array of nano particles for Lead and nanohoneycomb structure for Silver. We relate the differing behaviors to the difference of surface energy and diffusion constant. To verify this, the effect of substrate temperature on the film growth has been explored and the structure of the film has been successfully changed through the process.

<sup>1</sup>We are grateful for the support of NSF Grants No. DMR-1307290.

<sup>2</sup>Currently at Northwestern Polytechnical University, Xi'an, China.

**10:36AM K26.00014 Thermal Expansion of  $\text{ScF}_3$ .** , R. BHANDIA, Occidental College, A. GROCKOWIAK, T. SIEGRIST, T. BESARA, S.W. TOZER, National High Magnetic Field Laboratory, G.M. SCHMIEDESHOFF, Occidental College —  $\text{ScF}_3$  is an insulator, has a cubic crystal structure, and exhibits negative thermal expansion over a very wide temperature range. We will present and discuss thermal expansion measurements made with capacitive and fiber-Bragg-grating dilatometers. Work at Occidental College is supported by the National Science Foundation under DMR-1408598. A portion of this work was funded by the US Department of Energy NNSA SSAA DE-NA0001979, and performed at the National High Magnetic Field Laboratory, which is supported by National Science Foundation Cooperative Agreement No. DMR-1157490 and the State of Florida.

**10:48AM K26.00015 Electronic and optical properties of co-doped  $\text{BaTiO}_3$  with fluorine and nitrogen: A first-principles study.** , JAWAD ALSAEI<sup>1</sup>, Universit of Bahrain, PUAL TANGNEY, ARASH MOSTOFI, Imperial College London — Ferroelectric oxides such as  $\text{BaTiO}_3$  (BTO) are very good candidates for tunable dielectric devices. Tailoring the electronic and optical properties of these materials is usually achieved through means of strain engineering and compositional variations. In this work, we use first-principles calculations to study the effect of the co-substitution of F and N in BTO on its electronic and optical properties. Our simulations suggest that the optical properties are very sensitive to the atomic configuration of the dopant atoms. Our simulations show that the most energetically favorable configuration is that in which the F and N atoms form linear parallel chains of F-Ti-N motif that tend to cluster with each other. This configuration induces a large birefringence that can be further enhanced by means of biaxial strain. Our results shed more light on this particular type of anionic doping that has been rarely studied in the literature [?].

## References

[1] Kumar, N., Pan, J., Aysha, N., Waghmare, U. V., Sundaresan, A., and Rao, C. (2013) Journal of Physics: Condensed Matter 25(34), 345901.

<sup>1</sup>This work has been done while J. Alsaedi was at Imperial College London.

**Wednesday, March 16, 2016 8:00AM - 11:00AM –**  
**Session K27 DMP: Carbon Nanotubes: Electronic, Transport & Sensing** 326 - Yan Li, Peiking University

**8:00AM K27.00001 Carbon nanotube based field-effect transistors: merits and fundamental limits** , LIAN-MAO PENG, Peking University — The development of even more powerful computer systems are made possible by scaling of CMOS transistors, and this simple process has afforded continuous improvement in both the device switch time and integration density. However, CMOS scaling has become very difficult at the 22-nm node and unlikely to be rewarding beyond the 14-nm node. Among other new approaches, carbon nanotube devices are emerging as the most promising technique with unique properties that are ideal for nanoelectronics. In particular, perfect n-type and p-type contacts are now available for controlled injection of electrons into the conduction band and holes into the valence band of the CNT, paving the way for a doping free fabrication of CNT based ballistic CMOS, high performance optoelectronic devices, and integrated circuits [1-3]. These results will be compared with data projected for Si CMOS toward the end of the roadmap at 2026, as well as with those thermodynamic and quantum limits. References: [1] L.-M. Peng, Z.Y. Zhang and S. Wang, Materials Today 17 (2014) 433 [2] L. Ding et al., Nature Communication Published 14 Feb 2012, DOI: 10.1038/ncomms1682; Tian Pei et al., Nano Letters 14 (2014) 3102 [3] S. Wang et al., Nano Letters 11 (2011) 23; L.J. Yang et al., Nature Photonics 5 (2011) 672; H. Xu et al., Nano Letters 14 (2014) 5382

**8:36AM K27.00002 Integration of High-Purity Carbon Nanotube Solution into Electronic Devices** , GEORGE TULEVSKI, IBM TJ Watson Research Center, IBM TJ WATSON RESEARCH CENTER TEAM — Due to their exceptional electronic properties, carbon nanotubes (CNT) are leading candidates to be employed as channel materials in future nanoelectronic devices. A key bottleneck to realizing device integration is the sorting of carbon nanotubes, namely the isolation of high-purity, semiconducting CNT solutions. This talk will describe our efforts in using polymer-based sorting methods to isolate high-density and high-purity semiconducting CNT solutions. We explore the dependence of starting material and polymer to CNT ratio on the effectiveness of the separation. We confirm optically and electrically that the semiconducting purity is >99.99% through several thousand individual device measurements. In addition to single-CNT devices, thin-film transistors were also fabricated and tested. Due to the high purity of the solutions, device switching ( $\sim 10^5 I_{\text{ON}}/I_{\text{OFF}}$ ) was observed at channel lengths below the percolation threshold (<500 nm). Operating below the percolation threshold allows for devices with much higher current densities and effective mobilities as transport is now the result of direct transport as opposed to hopping between CNTs.

**8:48AM K27.00003 One-dimensional quantum transport in hybrid metal-semiconductor nanotube systems.**<sup>1</sup> , MAXIM GELIN, Munich Technical University, IGOR BONDAREV, North Carolina Central University — We study the inter-play between the intrinsic 1D conductance of metallic atomic wires (AWs) and plasmon mediated near-field effects for semiconducting single wall carbon nanotubes (CNTs) that encapsulate AWs of finite length. We use the matrix Green's functions formalism to develop an electron transfer theory for such a hybrid quasi-1D metal-semiconductor nanotube system. The theory predicts Fano resonances in electron transmission through the system. That is the AW-CNT near-field interaction blocks some of the pristine AW transmission band channels to open up new coherent channels in the CNT forbidden gap outside the pristine AW transmission band. This makes the entire hybrid system transparent in the energy domain where neither of the individual pristine constituents, neither AW nor CNT, are transparent. The effect can be used to control electron charge transfer in semiconducting CNT based devices for nanoscale energy conversion, separation and storage [1-3]. — [1]S.Nanot, et al., Sci. Rep. 3, 1335 (2013); [2]M.Barkelid and V.Zwiller, Nature Photo 8, 47 (2014); [3]A.Sharma, et al., Nature Nano DOI:10.1038/nnano.2015.220.

<sup>1</sup>NSF-ECCS-1306871 (M.G.), DOE-DE-SC0007117 (I.B.)

**9:00AM K27.00004 Making End-Bonded Contacts to Carbon Nanotubes** , JIANSHI TANG, QING CAO, GEORGE TULEVSKI, SHU-JEN HAN, IBM Thomas J. Watson Research Center, Yorktown Heights, NY 10598, USA — As a promising candidate for post-Si era, the implementation of carbon nanotube (CNT)-based CMOS technology requires both high-quality channel and electrical contacts that can be scaled down to sub-10 nm. In the efforts of making scalable contacts to CNT, we have recently demonstrated low-resistance end-bonded carbide contacts, formed by the reaction of Mo with CNT through high-temperature annealing (>800 °C) [1]. Such end-bonded contact scheme leads to a size-independent contact resistance of about 30 kilo-ohms, which overcomes the scaling limit of conventional side contacts. In this talk, we will present another strategy to make end-bonded contacts to CNTs through thermal annealing at much lower temperatures (400-600 °C). The contact metals are carefully chosen to have a high carbon solubility, so that the carbon atoms could dissolve into the contacts to inherently form end-bonded contacts. Experimental results, including Raman, SEM, and electrical measurements, with different annealing temperatures will be presented. The length-dependent contact resistance for this new end-bonded contact will be evaluated and compared with that of conventional side contact and also end-bonded carbide contact. [1] Q. Cao, et al., Science, 350, 68-72 (2015).

**9:12AM K27.00005 Carbon nanotube transistor based high-frequency electronics<sup>1</sup>** , MICHAEL SCHROTER, Technical University Dresden — At the nanoscale carbon nanotubes (CNTs) have higher carrier mobility and carrier velocity than most incumbent semiconductors. Thus CNT based field-effect transistors (FETs) are being considered as strong candidates for replacing existing MOSFETs in digital applications. In addition, the predicted high intrinsic transit frequency and the more recent finding of ways to achieve highly linear transfer characteristics have inspired investigations on analog high-frequency (HF) applications. High linearity is extremely valuable for an energy efficient usage of the frequency spectrum, particularly in mobile communications. Compared to digital applications, the much more relaxed constraints for CNT placement and lithography combined with already achieved operating frequencies of at least 10 GHz for fabricated devices make an early entry in the low GHz HF market more feasible than in large-scale digital circuits. Such a market entry would be extremely beneficial for funding the development of production CNTFET based process technology. This talk will provide an overview on the present status and feasibility of HF CNTFET technology will be given from an engineering point of view, including device modeling, experimental results, and existing roadblocks.

<sup>1</sup>Carbon nanotube transistor based high-frequency electronics

**9:48AM K27.00006 Transport properties of C60/nanotube heterostructures** , WU SHI, Lawrence Berkeley National Laboratory; Univ of California, Berkeley, THANG PHAM, HAMID BARZEGAR, Univ of California, Berkeley, ALEX ZETTTL, Lawrence Berkeley National Laboratory; Univ of California, Berkeley — Crystal structures determine the electronic properties. The fullerene C60 is insulating but can become superconducting with Tc above 30 K by inserting atoms or apply a pressure. In addition, Tc changes with the distance between fullerene molecules. Because of relatively weak intermolecular interactions, C60 molecules can even pack into nanowire structures with low dimensional constraints imposed by carbon nanotubes (CNTs) or boron nitride nanotubes (BNNTs). In this study, we will report the characterization of C60/nanotube heterostructures and their transport properties. By filling into nanotubes, C60 molecules form one-dimensional quasi-crystal structures, which are absent in bulk or film forms. The C60-C60 intermolecular distance changes with the tube diameters, which could potentially yield rich transport properties.

**10:00AM K27.00007 Environmental effects on the electrical properties of narrow-gap carbon nanotubes** , LEE ASPITARTE, DAN MCCULLEY, ETHAN MINOT, Oregon State University — Observations of single-walled carbon nanotubes (CNTs) with band gaps of 50 - 100 meV and diameters of approximately 2 nm pose an intriguing puzzle. The orthodox theory of CNTs predicts that such CNTs should have band gaps between 0 and 25 meV, yet these “narrow-gap” CNTs are routinely observed (band gaps in the range 50 – 100 meV). A possible explanation is that strong Coulomb interactions cause a Mott gap in nominally metallic CNTs (Deshpande et al., Science, 2009). To test this hypothesis, we have fabricated field-effect transistor devices from suspended narrow-gap CNTs. We have tested these devices in a variety of dielectric environments, including air, vacuum, TiO<sub>2</sub> coatings, and molecular liquids such as oil, anisole, toluene, isopropanol, and water. In many cases we can relate changes in electrical properties to changes in electrostatic disorder, gate capacitance, mobility and band alignment. We will discuss the possibility of an interaction-driven effect that is changed by the dielectric environment.

**10:12AM K27.00008 Absorption of CO<sub>2</sub> on Carbon-based Sensors: First-Principle Analysis.** , NACIR TIT, Physics Department, UAE University, P.O.Box 15551, Al-Ain, UAE, MOHAMMED ELEZZI, HASAN ABDULLAH, HOCINE BAHLOULI, Physics Department, KFUPM, P.O.Box 1690, Dhahran 31261, Saudi Arabia, ZAIN YAMANI, Center for Research Excellence in Nanotechnology, KFUPM, P.O.Box 5040, Dhahran 31261, Saudi Arabia — We present first-principle investigation of the adsorption properties of CO and CO<sub>2</sub> molecules on both graphene and carbon nano-tubes (CNTs) in presence of metal catalysis, mainly iron (Fe). The relaxations were carried out using the self-consistent-charge density-functional tight-binding (SCC-DFTB) code in neglect of heat effects. The results show the following: (1) Defected graphene is found to have high sensitivity and high selectivity towards chemisorption of CO molecules and weak physisorption with CO<sub>2</sub> molecules. (2) In case of CNTs, the iron “Fe” catalyst plays an essential role in capturing CO<sub>2</sub> molecules. The Fe ad-atoms on the surface of CNT introduce huge density of states at Fermi level, but the capture of CO<sub>2</sub> molecules would reduce that density and consequently reduce conductivity and increase sensitivity. Concerning the selectivity, we have studied the sensitivity versus various gas molecules (such as: O<sub>2</sub>, N<sub>2</sub>, H<sub>2</sub>, H<sub>2</sub>O, and CO). Furthermore, to assess the effect of catalysis on sensitivity, we have studied the sensitivity of other metal catalysts (such as: Ni, Co, Ti, and Sc). We found that CNT-Fe is highly sensitive and selective towards detection of CO and CO<sub>2</sub> molecules. CNT being conductive or semiconducting does not matter much on the adsorption properties.

**10:24AM K27.00009 Detection of the Odor Signature of Ovarian Cancer using DNA-Decorated Carbon Nanotube Field Effect Transistor Arrays** , CHRISTOPHER KEHAYIAS, NICHOLAS KYBERT, JEREMY YODH, A. T. CHARLIE JOHNSON, Univ of Pennsylvania — Carbon nanotubes are low-dimensional materials that exhibit remarkable chemical and bio-sensing properties and have excellent compatibility with electronic systems. Here, we present a study that uses an electronic olfaction system based on a large array of DNA-carbon nanotube field effect transistors vapor sensors to analyze the VOCs of blood plasma samples collected from patients with malignant ovarian cancer, patients with benign ovarian lesions, and age-matched healthy subjects. Initial investigations involved coating each CNT sensor with single-stranded DNA of a particular base sequence. 10 distinct DNA oligomers were used to functionalize the carbon nanotube field effect transistors, providing a 10-dimensional sensor array output response. Upon performing a statistical analysis of the 10-dimensional sensor array responses, we showed that blood samples from patients with malignant cancer can be reliably differentiated from those of healthy control subjects with a p-value of  $3 \times 10^{-5}$ . The results provide preliminary evidence that the blood of ovarian cancer patients contains a discernable volatile chemical signature that can be detected using DNA-CNT nanoelectronic vapor sensors, a first step towards a minimally invasive electronic diagnostic technology for ovarian cancer.

**10:36AM K27.00010 Monitoring DNA polymerase with nanotube-based nanocircuits** , YAN LI, MIROSLAV HODAK, WENCHANG LU, JERRY BERNHOLC, North Carolina State University, PHILIP COLLINS, University of California Irvine — DNA polymerases play an important role in the process of life by accurately and efficiently replicating our genetic information. They use a single-stranded DNA as a template and incorporate nucleotides to create the full, double-stranded DNA. Recent experiments have successfully monitored this process by attaching a Klenow fragment of polymerase I to a carbon nanotube and measuring the current along the tube [1]. Follow-up experiments have shown promise for distinguishing between DNA base pairs when nucleotide analogs are used [2], thus opening a new avenue for DNA sequencing. In this talk, we present results from computational studies on DNA polymerase I nanocircuits. The enzyme was first equilibrated in molecular dynamics and then density functional theory and Keldysh non-equilibrium Green's function methods were used to calculate the ballistic transmission coefficients and currents for different enzymatic states. Our results show significant change in current when the enzyme alternates between open (idle) and closed (synthesizing) states. We can also differentiate between some template bases when modified nucleotides and gate scanning are used. [1] T. J. Olsen et. al., JACS 135, 7855 (2013) [2] K. M. Pugliese et. al., JACS 137, 9587 (2015)

**10:48AM K27.00011 A photonic microscope for observing real-time vibrations of carbon nanotubes**, ARTHUR W. BARNARD, MIAN ZHANG, School of Applied and Engineering Physics, Cornell University, GUSTAVO WIEDERHECKER, Instituto de Física Gleb Wataghin, Universidade Estadual de Campinas, MICHAL LIPSON, School of Electrical and Computer Engineering, Cornell University, PAUL L. MCEUEN, Department of Physics, Cornell University; Kavli Institute at Cornell for Nanoscale Science — Vibrational modes in suspended carbon nanotubes (CNTs) are incredibly responsive to small forces, which makes them a prime candidate as nano-mechanical sensors. However, transducing this mechanical motion into detectable signals is a considerable challenge. Electrical detection, which has been the prevailing method thus far, suffers a significant impedance mismatch to macroscopic electronics and is thus susceptible to noise. We demonstrate an alternative: optical readout of CNT vibrations in real-time. By combining a unique CNT microtweezer platform with a high-finesse optical microdisk resonator, we dramatically enhance the naturally small optical cross-section of CNTs and thereby achieve unprecedented detection sensitivity. With this novel photonic microscope, we directly measure the thermal Brownian motion of CNTs and observe marked spectral diffusion at room temperature, shedding light on CNTs unique thermal physics. By further enhancing the optical coupling, we demonstrate optical amplification of CNT vibrations and directly observe period-doubling in the amplified state.

**Wednesday, March 16, 2016 8:00AM - 11:00AM –**  
**Session K28 DMP: Quantum Anomalous Hall Effect II** 327 - Anthony Richardella, Pennsylvania State University

**8:00AM K28.00001 Searching for better magnetic topological insulator materials for the quantum anomalous Hall effect<sup>1</sup>**, KE HE, Department of Physics, Tsinghua University — The recent experimental observation of the quantum anomalous Hall (QAH) effect in thin films of magnetic topological insulators (TIs) paves the ways for practical applications of dissipationless quantum Hall edge states and for realizations of the novel quantum phenomena such as chiral topological superconductivity and axion magnetoelectric effect. Further studies in these directions require magnetic TI materials that are able to show the QAH effect at higher temperature and with conduction channels of lower dissipation. We have performed systematic study on the QAH effect in magnetically doped TI films with different thicknesses, magnetic dopants and compositions. The results clarify the relations between the QAH effect and energy band structure, electronic localization and ferromagnetism, which not only give a comprehensive understanding on the nature of the QAH effect but also provide insights into designing and fabrication of superior QAH materials.

<sup>1</sup>This work was supported by the National Natural Science Foundation of China, the Ministry of Science and Technology of China, and Collaborative Innovation Center of Quantum Matter of China

**8:36AM K28.00002 Precise Quantization of Anomalous Hall Effect**, ANDREW BESTWICK<sup>1</sup>, Stanford University — In the quantum anomalous Hall effect, electron transport in a magnetically-doped topological insulator takes place through chiral, dissipationless edge channels. In this talk, we discuss the behavior of a nearly ideal implementations of the effect in which the Hall resistance is within a part per 10,000 of its quantized value and the longitudinal resistivity can reach below  $1 \Omega$  per square. Nearly all Cr-doped topological insulator samples demonstrate extreme temperature dependence that is well-modeled by a small effective gap, allowing control over quantization with an unexpected magnetocaloric effect. We also discuss measurements of new device geometries and non-local resistances that identify the sources of dissipation that limit the effect.

<sup>1</sup>(Now at Rigetti Computing)

**9:12AM K28.00003 Distinct Effect of Cr Bulk and Surface Doping on the Local Environment and Electronic Structure of Bi<sub>2</sub>Se<sub>3</sub><sup>1</sup>**, TURGUT YILMAZ, Univ of Connecticut - Storrs, IVO PLETIKOSIC, Princeton University, TONICA VALLA, Brookhaven National Laboratory, BORIS SINKOVIC, Univ of Connecticut - Storrs — We report on studies of Cr doping of Bi<sub>2</sub>Se<sub>3</sub> by comparing surface doped with bulk doped Bi<sub>2</sub>Se<sub>3</sub> films and their electronic and local structures studied by in-situ ARPES and core-level photoemission spectroscopies, respectively. In the case of surface doping we see the evidence for Cr substituting the Bi by observation of the extra feature in the Bi 5d photoemission spectra that increases with doping. On the other hand the Cr 3p spectra show two distinct chemical states indicating that there are two different Cr locations with different local electronic configuration. However, unlike theoretical expectations, the electronic structure measured at 15 K shows that surface states preserve gapless feature with well defined Dirac cone and presence of quantum well states, induced by doping. In contrast, the bulk Cr doped Bi<sub>2</sub>Se<sub>3</sub> films show gapped surface states with gap energy as large as 100 meV even at room temperature, which is far above the reported ferromagnetic transition temperature.

<sup>1</sup>YT and BS acknowledge support from University of Connecticut REP program

**9:24AM K28.00004 Tuning the electronic structure in nearly gapless HgCdTe with temperature: infrared magneto-spectroscopy study**, SEONGPHILL MOON, Natl High Magnetic Field Lab, Florida State University, M. MARCINKIEWICZ, C. CONSEJO, S. RUFFENACH, W. KNAP, F. TEPPE, Laboratoire Charles Coulomb, University of Montpellier, France, J. LUDWIG, Natl High Magnetic Field Lab, Florida State University, K. THIRUNAVUKKARASU, D. SMIRNOV, National High Magnetic Field Laboratory, S. KRISH-TOPIENKO, V. I. GAVRILENKO, Institute for Physics of Macrostructures, Nizhni Novgorod, Russia, S. A. DVORETSKII, N. N. MIKHAILOV, Rzhanelov Institute of Semiconductor Physics, Novosibirsk, Russia — Replace this text with your abstract body. Recently, a temperature-induced transition from a conventional two-dimensional semiconductor to a topological insulator has been demonstrated through magneto transport studies on HgTe/CdHgTe quantum wells [Wiedmann, S. et al. Phys. Rev. B 91, 205311 (2015)]. Here we report on a temperature-driven semiconductor-to-semimetal transition in 3-dimensional CdxHg1-xTe (x=0.15) revealed by infrared magneto-spectroscopy. We show that changing the temperature from 4K to 120K enables continuous tuning of the band structure from inverted to normal alignment through a critical gapless state realized at ~80K, where the inter-Landau level transitions exhibit a characteristic  $\sqrt{B}$  dependence intersecting at zero energy. Using an effective Dirac model, we determine the effective mass and the Fermi velocity for the studied temperature range.

**9:36AM K28.00005 Distorted weak anti-localization effects in Bi<sub>2</sub>Se<sub>3</sub>/La<sub>0.70</sub>Sr<sub>0.30</sub>MnO<sub>3</sub> (TI/FM) heterostructures grown by pulsed laser deposition**, FRANK HUNTE, RAJ KUMAR, YI-FANG LEE, SANDHYARANI PUNUGUPATI, JUSTIN SCHWARTZ, JAY NARAYAN, Materials Science and Engineering, North Carolina State University, Raleigh, NC - 27695 — Topological insulator/ferromagnet (TI/FM) heterostructures with broken time reversal symmetry by interface-induced magnetism are the potential platforms for the observation of novel quantum transport phenomena, magnetic monopoles and exotic quantum magneto-electric effects. TI/FM heterostructures with low Curie temperature ferromagnets i. e. GdN, EuS have been fabricated and studied. One of the challenges encountered with these heterostructures is their low Curie temperatures which limits their potential for applications in spintronic devices at room temperature. To address this issue, we have grown Bi<sub>2</sub>Se<sub>3</sub>/La<sub>0.70</sub>Sr<sub>0.30</sub>MnO<sub>3</sub> (TI/FM) heterostructures by the method of pulsed laser deposition. La<sub>0.70</sub>Sr<sub>0.30</sub>MnO<sub>3</sub> (LSMO) is a strong ferromagnetic material with T<sub>c</sub> ~350 K and Bi<sub>2</sub>Se<sub>3</sub> is the most studied topological insulator. XRD and phi scan results show that epitaxial thin films of Bi<sub>2</sub>Se<sub>3</sub> are grown on the LSMO template. Strong in-plane magnetization is confirmed by magnetometry measurements of the Bi<sub>2</sub>Se<sub>3</sub>/LSMO heterostructure. Magneto-transport measurements show a distorted weak anti-localization effect with hysteretic behavior due to interface induced ferromagnetism in the Bi<sub>2</sub>Se<sub>3</sub> TI films. This work was supported, in part, by National Science Foundation ECCS-1306400.

**9:48AM K28.00006 Growth and Characterization of Mn Doped InAs/GaSb Quantum Wells: Toward a 2D Quantum Anomalous Hall Insulator**, DI XIAO, SUSAN KEMPINGER, NITIN SAMARTH, Department of Physics, The Pennsylvania State University — The new discovery of a class of quantum spin Hall insulators (QSHIs), namely the type-II broken gap InAs/GaSb quantum wells (QWs), has drawn much attention in the condensed matter community. Counter-propagating helical states protected by time reversal symmetry exist at the edge, giving a quantized Hall conductance of  $2e^2/h$ , while the bulk remains insulating in this 2D topological insulator (TI). Compared to other TI systems, InAs/GaSb QW has a great advantage that the band structure, with a small hybridization gap, can be continuously tuned through electric fields, allowing the topological phase transition between trivial and topological phases. A recent theoretical proposal [PRL, 113.14(2014)] indicates that it is possible to keep only one chiral edge state without external magnetic field, i.e. the quantum anomalous Hall (QAH) state, by introducing long-range ferromagnetic order into this QW system. (In,Mn)As and (Ga,Mn)Sb have been well studied as diluted magnetic semiconductors, making Mn-doping a reasonable choice. Here, we present preliminary results on the MBE growth and characterization of electrically-gated Mn doped InAs /GaSb QWs. We will present a discussion of magnetization and magneto-transport measurements. Funded by ONR.

**10:00AM K28.00007 Interface driven states in ferromagnetic topological insulator heterostructures.**<sup>1</sup>, VALERIA LAUTER, Oak Ridge National Lab, FERHAT KATMIS, JAGADEESH MOODERA, Department of Physics, Massachusetts Institute of Technology, Cambridge, MA-02139, USA — The broken time reversal symmetry (TRS) states can be introduced into a topological insulator (TI) material by ferromagnetic ordering at the interface. Recently [1] we demonstrated a fundamental step towards realization of high temperature magnetization in Bi<sub>2</sub>Se<sub>3</sub>-EuS TI-FMI heterostructures through observation of magnetic proximity-induced symmetry breaking on the Bi<sub>2</sub>Se<sub>3</sub> surface via the exchange interaction by depositing EuS film on the top of the Bi<sub>2</sub>Se<sub>3</sub> surface. Here we show that we can independently break the TRS on both surfaces of a TI, which brings the long-range induced magnetism on either or both surfaces of a TI in a controlled way. We provide a depth-sensitive data on details of magnetic proximity effect in hidden interfaces by Polarized Neutron Reflectometry. The proximity coupling strength and penetration depth of magnetism into TI are extracted as functions of temperature, magnetic field and magnetic history. The large neutron absorption of Eu atoms serves as the element sensitivity and enables us to identify such magnetism in TI as proximity magnetism. This provides a next step to realization of complex heterostructures of TI and FMI leading to wide applications in TI-based next generation spintronic devices. [1] F. Katmis, V. Lauter et al, submitted.

<sup>1</sup>Supported by U.S. DOE, Office of Science, BES, MIT MRSEC award DMR-0819762, NSF Grant DMR-1207469, ONR Grant N00014-13-1-0301, NSF grant DMR-1231319.

**10:12AM K28.00008 Step-wise switching of anomalous Hall effect in a topological insulator**<sup>1</sup>, LUKAS ZHAO, ZHIYI CHEN, INNA KORZHOVSKA, SHIHUA ZHAO, LIA KRUSIN-ELBAUM, CCNY - CUNY, MARCIN KONCZYKOWSKI, Ecole Polytechnique — Surfaces of three-dimensional (3D) topological insulators (TIs) have emerged as one of the most remarkable states of condensed quantum matter where exotic charge and spin phases of Dirac particles could arise. The main challenge to finding these phases comes from a non-vanishing conductivity of the bulk. Recently we have demonstrated that we can access 2D surface transport and reach the charge neutrality point (CNP) by compensating intrinsically *p*-type TIs using high energy electron beams, and increase bulk resistivity by orders of magnitude. Here we report a discovery of anomalous Hall signal (AHE) at the CNP in Bi<sub>2</sub>Te<sub>3</sub> of unprecedented appearance; it shows regions of plateaus on sweeping the temperature, where Hall resistivity is flat in temperature, and has sharp (nearly discontinuous) 'steps' in-between the plateaus. The height of the steps increases on cooling, consistently following the ratio of 1:3 with each step. We will show by electrostatically tuning gated structures how this macroscopic switching of spins evolves in the vicinity of CNP and discuss the phenomenon of step-wise AHE in the context of charge inhomogeneities (puddles) and correlations between the localized bulk spins and Dirac spins.

<sup>1</sup>Supported by NSF-DMR-1420634, NSF-DMR-1312483-MWN, and DOD-W911NF-13-1-0159

**10:24AM K28.00009 Prediction of Quantum Anomalous Hall Insulator in Functionalized GaBi Honeycomb**, CHRISTIAN CRISOSTOMO, SUNG-PING CHEN, ZHI-QUAN HUANG, CHIA-HSIU HSU, FENG-CHUAN CHUANG, Natl. Sun Yat-sen U., HSIN LIN, Natl. U. of Singapore, ARUN BANSIL, Northeastern U. — Using first-principles electronic calculations, we predict functionalized GaBi honeycomb under tensile strain to harbor quantum anomalous hall (QAH) insulating phase. A single band inversion at  $\Gamma$  point was found in spin-polarized band structure of half-fluorinated planar strained GaBi. In order to confirm the topological properties, we evaluated the Chern number (C) and found that  $C = 1$ , indicating the presence of QAH phase. Additionally, the same value was also obtained by using hydrogen atoms, instead of fluorine atoms, as the adsorbate in both planar and buckled GaBi. Moreover, the electronic spectrum of a half-fluorinated GaBi nanoribbon with armchair or zigzag edges possess only one edge band crossing the Fermi level within the band gap. Finally, a suitable substrate which could induce the similar effect of half-hydrogenation or half-fluorination on the GaBi honeycomb could be used for spintronic devices.

**10:36AM K28.00010 Metal-to-insulator switching in quantum anomalous Hall states**, LEI PAN, XUFENG KOU, Univ of California - Los Angeles, JING WANG, Stanford university, YABIN FAN, Univ of California - Los Angeles, EUN SANG CHOI, National High Magnetic Field Laboratory, Florida State University, QIMING SHAO, Univ of California - Los Angeles, SHOU CHENG ZHANG, Stanford university, KANG LUNG WANG, Univ of California - Los Angeles — Quantum anomalous Hall effect (QAHE) was recently achieved in magnetic topological insulator films as a form of dissipationless transport without external magnetic field. However, the universal phase diagram of QAHE and its relation with quantum Hall effect (QHE) remain to be investigated. Here, we report the experimental observation of the giant longitudinal resistance peak and zero Hall conductance plateau at the coercive field in the six quintuple-layer (Cr<sub>0.12</sub>Bi<sub>0.26</sub>Sb<sub>0.62</sub>)<sub>2</sub>Te<sub>3</sub> film, and demonstrate the metal-to-insulator switching between two opposite QAHE plateau states up to 0.3 K. The universal QAHE phase diagram is further confirmed through the angle-dependent measurements. Our results address that the quantum phase transitions in both QAHE and QHE regimes are in the same universality class, yet the microscopic details are different.

**10:48AM K28.00011 Investigating dissipation in the quantum anomalous Hall effect**<sup>1</sup>, ELI FOX, ANDREW BESTWICK, DAVID GOLDBABER-GORDON, Stanford University, YANG FENG, YUNBO OU, KE HE, YAYU WANG, QI-KUN XUE, Tsinghua University, XUFENG KOU, LEI PAN, KANG WANG, University of California, Los Angeles — In the quantum anomalous Hall effect, a magnetic exchange gap in a 3D topological insulator gives rise to dissipationless chiral edge states. Though the effect has recently been realized in a family of ferromagnetically-doped (Bi,Sb)<sub>2</sub>Te<sub>3</sub> topological insulator thin films, experiments to date have found non-vanishing longitudinal resistance, contrary to initial theoretical expectations. Proposed sources of this dissipation include extra gapless or activated quasi-helical edge states, thermally activated 2D conduction, and variable-range hopping. Here, we discuss transport measurements of Corbino disk and non-local geometries to identify the mechanism of non-ideal behavior.

<sup>1</sup>This work supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award No. 19-7503.

**Wednesday, March 16, 2016 8:00AM - 11:00AM —**  
**Session K29 DCMP DMP: Topological Insulators: Theory I** 328 - Siddharth Parameswaran, University of California, Irvine

**8:00AM K29.00001 Tunneling Seebeck and Anomalous Nernst effects in three-dimensional topological insulators<sup>1</sup>**, CHENGHAO SHEN, BENEDIKT SCHARF, ALEX MATOS-ABIAGUE, IGOR ZUTIC, State University of New York at Buffalo — We theoretically investigate the longitudinal (Seebeck) and transverse (Nernst) thermopowers generated by thermally-induced tunneling across a magnetic barrier on the surface of a three-dimensional insulator. As a manifestation of Klein tunneling, the tunneling Seebeck coefficient exhibits oscillatory behavior with respect to the barrier thickness. Moreover, in spite of the absence of a source of spin polarization (only the barrier is magnetic), the tunneling anomalous Nernst coefficient is not only finite but can even be much larger than its Seebeck counterpart.

<sup>1</sup>This work was supported by DFG Grant No. SCHA 1899/1-1 (B.S.), U.S. ONR Grant No. N000141310754 (B.S., A.M.-A.), U.S. DOE, Office of Science BES, under Award DE-SC0004890 (I.Z.)

**8:12AM K29.00002 Amperean pairing mediated by magnetic fluctuations at the surface of a topological insulator**, MEHDI KARGARIAN, DMITRY K. EFIMKIN, VICTOR GALITSKI, Department of Physics, University of Maryland, College Park, Maryland 20742 — We study the interface between a three-dimensional topological insulator and a ferromagnetic thin film. Due to the Dirac nature of surface states, in-plane magnetization couples to them as a gauge field, leading to emergent electric and magnetic fields. We argue that magnetic fluctuations mediate strongly anisotropic interaction and can be the origin of an unconventional superconductivity with Amperean pairings.

**8:24AM K29.00003 Edge state contributions to the Loschmidt echo in topological insulators and superconductors**, NICHOLAS SEDLMAYR, Institute of Mathematical and Theoretical Physics, Michigan State University, ELIO KÖNIG, ALEX LEVCHENKO, Department of Physics, University of Wisconsin-Madison — Non-analytic behavior in the time evolution of a quantum system at critical times can be seen in the Loschmidt echo, the overlap between a time evolved state and an initial state. This is referred to as a dynamical phase transition, an analogue of the non-analytic behavior in the free energy across temperature driven phase transitions. In particular it has been demonstrated that in topological systems a quench across the topological phase transition and dynamical phase transitions are intimately related. Here we look at the contribution to the Loschmidt echo of the topologically protected edge states of 1D topological insulators and superconductors. These edge state have already been shown to have interesting contributions to the fidelity and entanglement entropy, which can also be useful for characterizing the topological phases and phase transitions.

**8:36AM K29.00004 Magnetic ordering and quantum anomalous Hall phase of Cr-doped topological insulators: First principles studies<sup>1</sup>**, JEONGWOO KIM, Department of Physics and Astronomy, University of California, Irvine, SEUNG-HOON JHI, Department of Physics, Pohang University of Science and Technology, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine — Realization of transverse electric currents without external magnetic fields, so called the quantum anomalous Hall effect (QAHE), is achieved in Cr-doped topological insulating (Bi,Sb)2Te3 compounds. However, detailed mechanism of QAHE and magnetic ordering in topological insulators (TIs) is still unclear with several models in controversy. We study the origin of QAHE in magnetic impurity-doped TIs using first-principles calculations. We investigate a possibility of the quantum anomalous Hall phase in conventional three-dimensional topological insulators, such as Bi2Se3, Bi2Te3, and Sb2Te3. We find that Sb2Te3 is the most suitable compound for realizing QAHE, because it maintains insulating phase and relatively strong ferromagnetic ordering in a wide range of Cr doping while Bi2Se3 and Bi2Te3 become metallic even by a small amount of Cr doping. Contrary to previous predictions, the kinetic exchange is responsible for the magnetic phase of Cr-doped TIs and it induces spin-polarized valence and conduction bands in Sb2Te3. We also discuss the role of Bi doping in topological surfaces states of Cr-doped Sb2Te3, which leads to QAHE in (Bi,Sb)2Te3.

<sup>1</sup>Work was supported as part of the SHINES, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award No. SC0012670.

**8:48AM K29.00005 Filling-Enforced Quantum Band Insulators in Spin-Orbit Coupled Crystals**, HOI CHUN PO, University of California, Berkeley, HARUKI WATANABE, Massachusetts Institute of Technology, MICHAEL P. ZALETEL, Station Q, Microsoft Research, Santa Barbara, ASHVIN VISHWANATH, University of California, Berkeley; Materials Science Division, Lawrence Berkeley National Laboratories, Berkeley — While band insulators are usually described in wavevector space in terms of fully filled bands, they are sometimes also described in terms of a complementary Wannier picture in which electrons occupy localized, atom-like orbitals. Under what conditions does the latter picture break down? The presence of irremovable quantum entanglement between different sites can obstruct a localized orbital description, which occurs in systems like Chern and topological insulators. We collectively refer to such states as Quantum Band Insulators (QBIs). Here we report the theoretical discovery of a filling-enforced QBI - that is, a free electron insulator in which the band filling is smaller than the minimum number dictated by the atomic picture. Consequently such insulators have no representation in terms of filling localized orbitals and must be QBIs. This is shown to occur in models of certain cubic crystals with non-symorphic space groups. Like topological insulators, filling-enforced QBIs require spin-orbit coupling. However, in contrast, they do not typically exhibit protected surface states. Instead their nontrivial nature is revealed by studying the quantum entanglement of their ground state wavefunction.

**9:00AM K29.00006 Casimir Torque between Topological Insulators: a Physical Implication of the Surface State Hexagonal Warping Effect**, LIANG CHEN, North China Electric Power University, KAI CHANG, Institute of Semiconductors, Chinese Academy of Sciences — We use a variation of the Lifshitz formula to calculate the anisotropic Casimir energy density between two topological insulators in the vacuum. We find that the hexagonal warping effect can induce a Casimir torque between the two topological insulators,  $T_c \propto \sin(6\theta)$  with twisted angle  $\theta$ . The maximal Casimir torque at  $\theta = \pi/12$  is estimated to be  $\sim 10^{-19} N \cdot m/rad$  for Bi<sub>2</sub>Te<sub>3</sub> on the [111] surface when the distance between the two topological insulators is about 20 nm and the surface areas are taken to be  $\sim 1 cm^2$ .

**9:12AM K29.00007 Emergent Topological States at Domain Walls in Bismuth<sup>1</sup>**, JINWOONG KIM, NICHOLAS KIOUSSIS, Department of Physics and Astronomy, California State University, Northridge — The discovery of topological insulators has brought new perceptions in materials science which allows the understanding of material properties as an inevitable result of symmetry and its breaking. Polyacetylene is one example of topological insulators classified by structural symmetry that exhibits zero modes at a domain wall separating two opposite dimerized phases. The sign reversal of the topological mass across a domain wall is not restricted to 1D systems and is ubiquitous in a wide range of 3D materials. Employing both ab initio and model Hamiltonian calculations we have studied the topological properties of structural domain walls in bismuth, which is the 3D analogue of the domain walls in 1D polyacetylene. The model Hamiltonian can be represented to lowest order by two Pauli matrices yielding a mass gap that closes upon dimerization sign reversal. The calculations demonstrate that zero mode states emerge at the domain wall which exhibit quasi-one dimensional linear dispersions. Our results imply that conducting channels may emerge at structural domain walls such as grain boundaries as a consequence of topological protection, whose properties are determined by global rather than local symmetry.

<sup>1</sup>This work is supported by NSF-PREM under Grant No DMR-1205734.

**9:24AM K29.00008 Single-ion magnetic anisotropy of transition metal impurities in  $\text{Bi}_2\text{Se}_3$  bulk and thin film topological insulators**, FHOKRUL ISLAM, ANNA PERTSOVA, Dept. of physics, Linnaeus University, REZA MAHANI, KTH Royal Institute of Technology, CARLO CANALI, Dept. of physics, Linnaeus University — The breaking of time reversal symmetry in a topological insulator (TI) by magnetic doping is one of the most studied phenomena among the properties of Dirac materials. The robustness of the topological surface states (TSS) against magnetic impurities is of critical importance for spin-dependent transport in these systems. The interaction between TSS and magnetic impurities can open a gap, provided that the magnetic order is oriented normal to the surface of the TI. Such gap opening is crucial for realizing TI-based spintronic devices and for the observation of different fundamental phenomena, such as the anomalous quantum Hall effect. Using density functional theory as implemented in the WIEN2k ab-initio package, we have investigated the effect of the magnetization orientation on the gap opening at the Dirac point, for substitutional Mn and Fe impurities on the  $\text{Bi}_2\text{Se}_3$  surface, and have calculated the associated single-ion anisotropy (SIA). We also have studied bulk SIA in order to compare the role played by TSS on the surface SIA.

**9:36AM K29.00009 Strong Correlation effects to Topological Quantum Phase Transitions in Three-Dimensions**, ADRIANO AMARICCI, CNR-IOM, MASSIMO CAPONE, International School for Advanced Studies, JAN BUDICH, University of Innsbruck, Austria, GIORGIO SANGIOVANNI, BJOERN TRAUZETTEL, University of Wuerzburg, Germany — Topological Insulating phases of three dimensions are classified in terms of four  $Z_2$  global invariants. In the non-interacting case the Topological Quantum Phase Transition (TQPT), *i.e.* the sudden change of such invariants, occurs through the continuous closure of the energy gap as long as the symmetries protecting the Topological phase are preserved. However, the recent progress in engineering or predict Topological Insulating states in heavy-elements compounds, pushed the attention to the effects of large electronic interaction. Here we show that strongly correlated 3-dimensional Topological Insulators are characterized by a substantially different physics with respect to their non-interacting counterpart. Our study shows that the TQPT to the Strong Topological Insulator is dominated by the presence of a Quantum Critical Point, the end of a first-order topological transition. In addition we show that the conventional paradigm of a continuous TQPT breaks down for strong enough correlation, through to a discontinuous transition without closure of the spectral gap.

**9:48AM K29.00010 Field theory representation of mixed gauge-gravity symmetry-protected topological invariants, group cohomology and beyond**, JUVEN WANG, Institute for Advanced Study, Princeton, ZHENG-CHENG GU, Perimeter Institute for Theoretical Physics, XIAO-GANG WEN, MIT — The challenge of identifying symmetry-protected topological states (SPTs) is due to their lack of symmetry-breaking order parameters and intrinsic topological orders. For this reason, it is impossible to formulate SPTs under Ginzburg-Landau theory or probe SPTs via fractionalized bulk excitations and topology-dependent ground state degeneracy. However, the partition functions from path integrals with various symmetry twists are universal SPT invariants, fully characterizing SPTs. In this work, we use gauge fields to represent those symmetry twists in closed spacetimes of any dimensionality and arbitrary topology. This allows us to express the SPT invariants in terms of continuum field theory. We show that SPT invariants of pure gauge actions describe the SPTs predicted by group cohomology, while the mixed gauge-gravity actions describe the beyond-group-cohomology SPTs, recently observed by Kapustin. We find new examples of mixed gauge-gravity actions for  $U(1)$  SPTs in 3+1D and 4+1D via the Stiefel-Whitney class and the gravitational Chern-Simons term. [Work based on Phys. Rev. Lett. 114, 031601 (2015) arXiv:1405.7689]

**10:00AM K29.00011 Spin texture of topological surface states of side-surfaces in  $\text{Bi}_2\text{Se}_3$  from first principles<sup>1</sup>**, JOHN VILLANOVA, KYUNGWHA PARK, Virginia Tech - Blacksburg — Topological insulators have recently drawn a lot of attention because of topologically protected surface states with Dirac dispersion and spin-momentum locking induced by time-reversal symmetry and strong spin-orbit coupling, respectively. Recent experiments report interesting transport properties of  $\text{Bi}_2\text{Se}_3$  nanowires and nanoribbons with growth directions normal to the (111) surface. However, most of the studies of  $\text{Bi}_2\text{Se}_3$  are focused on the (111) surface. Additionally, surfaces other than the (111) surface would facilitate hole doping with adatoms since both Bi and Se atoms are present at these other surfaces. We investigate the spin texture and electronic structure of topologically protected surface states of two representative side-surfaces of  $\text{Bi}_2\text{Se}_3$  by using density-functional theory (DFT). In particular, we consider two surfaces normal to the (111) surface, such as  $(1\bar{1}0)$  and  $(11\bar{2})$ , where the former has twofold symmetry and the latter has mirror symmetry. We present our calculated spin textures of the surface states of these side surfaces that qualitatively differ from typical Rashba-like features and from the prediction based on the bulk model Hamiltonian by keeping up to quadratic terms in momentum.

<sup>1</sup>Funding from NSF DMR-1206354 and Computer resources from SDSC Trestles under DMR060009N and VT ARC. Grateful to B. Partoens and C. De Beule for discussion at the early stage of this work.

**10:12AM K29.00012 Domain wall of a ferromagnet on a three-dimensional topological insulator**, RYOHEI WAKATSUKI, MOTOHIKO EZAWA, University of Tokyo, NAOTO NAGAOSA, University of Tokyo, RIKEN Center for Emergent Matter Science (CEMS) — Topological insulators (TIs) show rich phenomena and functions which can never be realized in ordinary insulators. Most of them come from peculiar surface or edge states. Especially, the quantized anomalous Hall effect without an external magnetic field is realized in a two-dimensional ferromagnet on a three-dimensional TI, which supports the dissipationless edge current. Here we demonstrate theoretically that the domain wall of this ferromagnet, which carries edge currents, is charged and can be controlled by an external electric field. The chirality and relative stability of the Neel wall and the Bloch wall depend on the position of the Fermi energy as well as the form of the coupling between the magnetic moment and the orbital of the host TI. These findings will pave a path to utilize the magnets on TI for spintronics applications. R. Wakatsuki, M. Ezawa, and N. Nagaosa, Scientific Reports **5**, 13638 (2015).

**10:24AM K29.00013 Topological phases protected by point group symmetry<sup>1</sup>**, SHENG-JIE HUANG, HAO SONG, MICHAEL HERMELE, University of Colorado Boulder — There has been remarkable progress in the theoretical understanding of symmetry protected topological (SPT) phases. However, most theories focus on internal, or on-site, symmetries, even though spatial symmetries are important in solids. In this talk, we classify bosonic SPT phases protected by crystalline point group symmetry, which we dub point group SPT (pgSPT) phases. Our approach is based on a procedure to reduce a d-dimensional pgSPT phase to lower-dimensional SPT phases protected by internal symmetry. For three-dimensional pgSPT phases, this approach allows us to gain insight into non-trivial properties at symmetry preserving surfaces. In particular, we obtain toy models for the surfaces of certain pgSPT phases at which there is a symmetry preserving  $Z_2$  topological order with anomalous symmetry fractionalization. We also discuss connections between bosonic pgSPT phases and electronic topological crystalline insulators.

<sup>1</sup>This research is supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES) under Award DE-SC0014415

**10:36AM K29.00014 Visualizing competing trends at topological surfaces<sup>1</sup>**, PAOLO SESSI, Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany, RUDRO BISWAS, Department of Physics and Astronomy, Purdue University, 525 Northwestern Avenue West Lafayette, Indiana, USA, THOMAS BATHON, Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany, ALEXANDER BALATSKY, Institute for Materials Science, Los Alamos New Mexico 87545, USA, MATTHIAS BODE, Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — Topological insulators interacting with magnetic impurities are usually described within the framework of gapping the Dirac quasiparticles energy spectrum by time reversal symmetry breaking. However, the overwhelming majority of studies demonstrate the presence of finite density of states near the Dirac node even once the system becomes magnetic. The contradictory observations call for a better understanding of the nature of the mobility and transport in magnetically doped topological insulators. Here, by combining different experimental techniques with theoretical calculations, we map the response of topological states to magnetic impurities at the atomic scale and reveal that, contrary to what generally believed, gapless density of states and magnetic order can coexist.

<sup>1</sup>This work was supported by DFG-SPP1666, US DOE BES E304, ERC DM 321031 and KAW.

**10:48AM K29.00015 Landau Theory of Helical Fermi Liquids**, REX LUNDGREN, University of Texas at Austin, JOSEPH MACIEJKO, University of Alberta — We construct a phenomenological Landau theory for the two-dimensional helical Fermi liquid found on the surface of a three-dimensional time-reversal invariant topological insulator. In the presence of rotation symmetry, interactions between quasiparticles are described by ten independent Landau parameters per angular momentum channel, by contrast with the two (symmetric and antisymmetric) Landau parameters for a conventional spin-degenerate Fermi liquid. We project quasiparticle states onto the Fermi surface and obtain an effectively spinless, projected Landau theory with a single projected Landau parameter per angular momentum channel that captures the spin-momentum locking or nontrivial Berry phase of the Fermi surface. As a result of this nontrivial Berry phase, projection to the Fermi surface can increase or lower the angular momentum of the quasiparticle interactions. We derive equilibrium properties, criteria for Fermi surface instabilities, and collective mode dispersions in terms of the projected Landau parameters. We briefly discuss experimental means of measuring projected Landau parameters.

## Wednesday, March 16, 2016 8:00AM - 11:00AM — Session K30 DMP: Complexity in Ferroic Systems 329 - Manuel Bibes, CNRS Thales

**8:00AM K30.00001 Artificial chemical and magnetic structure at the domain walls of an epitaxial oxide.**, BEATRIZ NOHEDA, Zernike Institute for Advanced Materials, Univ of Groningen — Progress in nanotechnology requires new paradigms for materials synthesis that allow controlling their functionality down to the smallest scales. Here we report a novel two-dimensional ferromagnetic phase that is synthesized at the domain walls (DWs) of the antiferromagnetic insulator TbMnO<sub>3</sub> when grown in thin layers under epitaxial strain. This Mn oxide phase presents an atomic arrangement that does not exist in bulk and cannot be synthesized by standard chemical routes. The number of 2D ferromagnetic sheets can be controlled by tuning the thickness of the thin films, giving rise to volume fractions that go up to 25% of the total film volume. Such novel phases are driven by a unique environment induced by the symmetry breaking and large stresses present at domain walls, which function as nanoreactors. This new class of nanoscale materials may find innovative applications in nanoelectronics and spintronics. The work is published as S. Farokhipoor, C. Magén, S. Venkatesan, J. Íñiguez, C. J. M. Daumont, D. Rubi, E. Snoeck, M. Mostovoy, C. de Graaf, A. Müller, M. Döblinger, C. Scheu, B. Noheda, Nature 515, 379 (2014)

**8:36AM K30.00002 Microscopic order parameters coupling at domain walls and its effect on macroscopic properties.**, SAEEDH FAROKHIPOOR, Department of Materials Science, University of Cambridge, UK, UMUT ADEM, Department of Materials Science, Izmir Institute of Technology, Turkey, ULI ZEITLER, Radboud University, Nijmegen, NL, AGUNG NUGROHO, Faculty of Mathematics and Natural Sciences, Bandung, Indonesia, JOHAN BUURMA, GRAEME BLAKE, BEATRIZ NOHEDA, THOMAS PALSTRA, Zernike Institute for Advanced Materials, University of Groningen, NL — Domain and domain wall (DW) engineering provides an alternative model to tune the physical properties of materials, typically done via conventional materials chemistry. The interplay of coexisting non-ferroelectric structural order parameters, ferroelectric and magnetic order parameters at the DWs in hexagonal manganites provides a new pathway to determine macroscopic properties by tuning the DW characteristics [1]. Here, we report different types of domain structures and DW types associated with the crystal growth conditions in hexagonal manganites. We show that differences in the DW polar state manifest themselves as variations in the conductivity measured macroscopically. Piezo force microscopy and X-ray diffraction enables us to determine the plane of the DWs and hence, their strain state. The latter findings corroborate with the topographical study. Finally, these results show that DWs under strain lower the critical field of the magnetic phase transition compared to samples with strain-free DWs. This work represents the first example of non-local physical properties being determined by the presence of topographically protected DWs. [1] S. Artyukhin et al., Nat Mater 13 (2014)

**8:48AM K30.00003 Visualization of weak ferromagnetic domains in multiferroic hexagonal ferrite thin film<sup>1</sup>**, WEIDA WU, WENBO WANG, Department of Physics and Astronomy, Rutgers University, Piscataway, NJ, 08854 USA, JARRETT A. MOYER, PETER SCHIFFER, Department of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA, JULIA A. MUNDY, DAVID A. MULLER, School of Applied and Engineering Physics, Cornell University, Ithaca, New York 14853, USA, DARRELL G. SCHLOM, Department of Materials Science and Engineering, Cornell University, Ithaca, New York 14853, USA — Hexagonal *h*-LuFeO<sub>3</sub> thin film has been reported to be a room-temperature multiferroic [1]. Extensive studies on high quality MBE thin films revealed a magnetoelectric phase with weak ferromagnetism emerges below  $T_N \sim 147$  K [2]. However, the direct observation of weak ferromagnetic domain structures is still lacking. Here we report cryogenic magnetic force microscopy (MFM) results on 200 nm thick *h*-LuFeO<sub>3</sub> film grown by molecular-beam epitaxy (MBE) on (111)-oriented yttria-stabilized cubic zirconia (YSZ) substrates. Labyrinth-like weak ferromagnetic domain structures were observed with a domain size  $\sim 1 \mu\text{m}$  and domain wall width  $\sim 0.4 \mu\text{m}$ . Field-dependent MFM data indicates the coercive field is  $\sim 2.66$  T at 50 K and  $\sim 3.15$  T at 6 K. [1] W. Wang et al., Phys. Rev. Lett. 110, 237601(2013). [2] J. A. Moyer et al., APL MATER. 2, 012106 (2014).

<sup>1</sup>This work is supported by DOE BES under award DE-SC0008147.

## 9:00AM K30.00004 ABSTRACT WITHDRAWN —

**9:12AM K30.00005 Frequency Dependent Microwave Impedance Microscopy of Ferroelectric Domain Walls**, SCOTT JOHNSTON, ZHI-XUN SHEN, Stanford University — ABO<sub>3</sub> ferroelectrics are known to exhibit domain wall conductivity which is of great fundamental and technological interest. Microwave Impedance Microscopy is a near field measurement technique which allows local, non-contact measurement of AC conductivity and permittivity. In this work, Microwave Impedance Microscopy over a wide frequency range is used to probe the electrical properties of domain walls in ABO<sub>3</sub> ferroelectrics. An unexpected, strong frequency dependence in the microwave dissipation near domain walls is observed.

**9:24AM K30.00006 Spin-phonon interaction of mixed-phase BiFeO<sub>3</sub> films studied by Raman spectroscopy**, YI-CHUN CHEN, YEN-CHIN HUANG, Department of Physics, National Cheng Kung University, WEN-I LIANG, YING-HAO CHU, Department of Material Science and Engineering, National Chiao Tung University — Multiferroic BiFeO<sub>3</sub> (BFO) has ferroelectricity and antiferromagnetism at room temperature, and so was motivated for novel magnetoelectric applications. When a BFO film is epitaxially grown on the LaAlO<sub>3</sub> (LAO) substrate, the strong compressive strain will transform BFO to a mixed-phase state, including rhombohedrally (R-) and tetragonally (T-) distorted monoclinics. The stripe-shape R-BFO is embedded in T-BFO matrix, forming periodic domains which possess enhanced piezoelectric response and spontaneous magnetization. Moreover, the magnetic R-BFO phases can be switched by external electric fields. Here, in order to study the mechanism of strain induced magnetic properties, we report a detailed Raman study of the mixed-phase BFO. The phonons of each phase are distinguished by an in-situ testing system combining an atomic force microscope (AFM) and a Raman spectroscopy. When external magnetic fields are applied, a low-frequency phonon mode of T-BFO phase changes due to the magnetostrictive effect. Variations of mixed-phase phonons versus temperature are also studied, which show that phonon shifts of high-frequency modes are contributed from phonon-phonon anharmonic interaction; by contrast, the shifts of low-frequency modes are due to spin-phonon interactions.

**9:36AM K30.00007 Inducing phase transitions of T-like BiFeO<sub>3</sub> films by low-energy He implantation**, ANDREAS HERKLOTZ, Oak Ridge National Lab, CHRISTIANNE BEEKMAN, Florida State University, STEFANIA FLORINA RUS, National Institute for Research and Development in Electrochemistry and Condensed Matter Romania, ILIA IVANOV, NINA BALKE, THOMAS ZAC WARD, Oak Ridge National Lab — Ferroelectric phase transitions of BiFeO<sub>3</sub> are found to be controllable through the application of single axis, out-of-plane strain. Low-energy He implantation has been deployed to induce out-of-plane strain in T-like BFO films, while the compressive in-plane strain due to the coherent growth on LaAlO<sub>3</sub> substrates remains fixed. Our data shows that He implantation triggers a  $M_C - M_A - T$  phase sequence of the T polymorph that is identical to structural changes that are induced with increasing temperature. Mixed phases nanodomains phases are gradually suppressed and disappear above a certain He doping level. Our data shows that the ferroelectric and optical properties of BiFeO<sub>3</sub> films critically depend on the He doping level. Thus, the results demonstrates that He implantation can be used as an intriguing approach to study lines in the rich phase space of BFO films that cant be accessed by simple heteroepitaxy. This effort was wholly supported by the US Department of Energy (DOE), Office of Basic Energy Sciences (BES), Materials Sciences and Engineering Division, with user projects supported at ORNLs Center for Nanophase Materials Research (CNMS) which is also sponsored by DOE-BES.

**9:48AM K30.00008 ABSTRACT WITHDRAWN —**

**10:00AM K30.00009 Effect of manganese substitution in barium titanate ( $Mn - BaTiO_3$ )<sup>1</sup>**, RAJASEKARAKUMAR VADAPPOO, MUHTAR AHART, Extreme Materials Initiative, Geophysical Laboratory, Carnegie Institution for Science, Washington, DC 20015 USA, R. E. COHEN, Carnegie Institution for Science, Washington, DC USA, Department für Geo- und Umweltwissenschaften, Ludwig-Maximilians-Universitaet, Munich, Germany — Barium titanate single crystals exhibit a very large recoverable nonlinear strain with aging, which is an order higher than the highly strained PZN-PT single crystals.[1] Transition metal dopants improve the electromechanical properties of these classic ferroelectrics and third generation relaxor ferroelectrics.[2] To understand the source of these effects, we systematically investigate the effect of Mn substitution in  $BaTiO_3$  using theory [3] and experiments. Mn substituted  $BaTiO_3$  ceramics were synthesized by solid state reaction. Mn substitution of up to 4 atomic % showed tetragonal phase and further substitution leads to evolution of hexagonal phase. Raman spectra show increasing Mn substitution reduce the intensity of A<sub>1</sub>(TO) and B<sub>1</sub>, E(TO+LO) modes, broaden the E(TO), A<sub>1</sub>(TO) modes and a new peak evolution at  $629\text{ cm}^{-1}$ . Enhanced strain double hysteresis was observed with increase in Mn substitution on electric field. Influence of Mn substitution on dielectric properties will be presented. The enhanced strain properties with aging observed on Mn substituted PIN-PMN-PT crystals is also discussed. References: [1] X. Ren, Nature Mater. 3, 91 (2004). [2] Zhang et al., IEEE Trans. Ultrason.,60, 1572 (2013). [3] J. F. Nossa et al., Phys. Rev. B 91, 214105 (2015).

<sup>1</sup>This work is supported by ONR

**10:12AM K30.00010 Enhanced ferroelectric polarization and potential morphotropic phase boundary in PZT-based alloys**, DAVID PARKER, MICHAEL MCGUIRE, Oak Ridge National Laboratory, DAVID SINGH, Dept. of Physics and Astronomy, University of Missouri, Columbia MO — We present a combined theoretical and experimental study of alloys of the high performance piezoelectric PZT (PbZr<sub>0.5</sub>Ti<sub>0.5</sub>O<sub>3</sub>) with BZnT (BiZn<sub>0.5</sub>Ti<sub>0.5</sub>O<sub>3</sub>) and BZnZr (BiZn<sub>0.5</sub>Zr<sub>0.5</sub>O<sub>3</sub>), focussing on lattice instabilities, atomic displacements and ferroelectric polarization. From theory we find that the 75 - 25 PZT - BZnT alloy has substantially larger cation displacements, and hence ferroelectric polarization than the PZT base material, on the tetragonal side of the phase diagram. We also find a possible morphotropic phase boundary in this system by comparing displacement patterns and optimized c/a ratios. Experiments indicate the feasibility of sample synthesis within this alloy system.

**10:24AM K30.00011 Diffuse Scattering from Relaxor PMN-xPT**, MATTHEW KROGSTAD, Northern Illinois Univ, STEPHAN ROSENKRANZ, RAYMOND OSBORN, JUSTIN WOZNIAC, Argonne Nat'l Lab, FENG YE, Oak Ridge Nat'l Lab., JACOB RUFF, Cornell Univ, PETER GEHRING, NIST, ZUO-GUANG YE, Simon Fraser Univ, DANIEL PHELAN, Argonne Nat'l Lab — Relaxor ferroelectrics possess intriguing electromechanical and dielectric properties, the microscopic physics of which is widely regarded to be related to local, correlated atomic displacements from long-range symmetry. However, despite numerous studies over the last few decades, the details of how short range correlations and disorder drive the relaxor behavior remain unresolved. Single crystal diffuse scattering provides a powerful probe of such deviations from an average structure correlated over varying length scales, and over the last few years, techniques and instruments for measuring diffuse scattering with both x-rays and neutrons have seen a dramatic improvement, allowing for large volumes of reciprocal space to be measured in little time. We present our recent complementary neutron and x-ray measurements on solid solutions of PMN-xPT which revealed new structure to the diffuse scattering of relaxors close to the morphotropic phase boundary.

**10:36AM K30.00012 Structural and Dynamical Properties of Barium Stannate**, D. PHELAN, Argonne National Laboratory, M. J. KROGSTAD, Northern Illinois University / Argonne National Laboratory, A. LOPEZ-BEZANILLA, Argonne National Laboratory, D. PARSHALL, NIST Center for Neutron Research, Y. GIM, S. L. COOPER, University of Illinois, H. ZHENG, Argonne National Laboratory — Barium stannate based perovskites have recently drawn attention due to their potential as transparent conducting oxides and reports of high carrier mobility in La-doped single crystals. Published DFT calculations and experimental results have suggested phonon instabilities at high symmetry zone boundary positions and local octahedral rotations, respectively, for BaSnO<sub>3</sub>. Here, we discuss recent structural measurements of BaSnO<sub>3</sub>, in which we have searched for such distortions by employing a combination of single crystal neutron diffraction and total scattering analysis of powder neutron diffraction. Moreover, we discuss lattice dynamical measurements, comparing phonon dispersion measurements to DFT calculations.

**10:48AM K30.00013 Real-space observation of metal-insulator transition at complex oxide heterointerface with cross-sectional STM**, YA-PING CHIU<sup>1</sup>, National Taiwan Normal University, Taiwan, JHENG-CYUAN LIN, Academia Sinica, Taiwan, TRA-VU THANH, National Chiao Tung University, Taiwan, TAI-TE LIN, PO-CHENG HUANG, National Sun Yat-sen University, Taiwan, BO-CHAO HUANG, Academia Sinica, Taiwan, JIUNN-YUAN LIN, YING-HAO CHU<sup>2</sup>, National Chiao Tung University, Taiwan — We report the direct observation of tunable electronic property through visible light at  $LaAlO_3/SrTiO_3$  (LAO/STO) complex oxide heterointerface using cross-sectional scanning tunneling microscopy and spectroscopy (XSTM/S). Many researches have shown that for the interface to be conducting, the thickness of LAO should be equal to or greater than the critical value 4 unit cells (u.c.). With LAO surface modification by Au clusters, interfacial two-dimensional electron gas presents a giant optical switching effect under visible light illumination. In this study, through the interaction between photons and electrons system, a direct observation of the evolution of electronic structures from insulating to conducting has been revealed in the LAO (3u.c.)/STO model using the technique of cross-sectional scanning tunneling microscopy and spectroscopy. Results clearly reveal the changes in the built-in electric field in LAO and the band bending in the STO adjacent to the interface after light illumination.

<sup>1</sup>National Sun Yat-sen University, Taiwan; Academia Sinica, Taiwan

<sup>2</sup>Academia Sinica, Taiwan

**Wednesday, March 16, 2016 8:00AM - 11:00AM –**

**Session K31 DCP: Advances in Density Functional Theory V** 331 - Michele Pavanello, Rutgers University

**8:00AM K31.00001 Ultrafast Laser-Induced Demagnetization: Identifying the Mechanism with Real-Time TDDFT**, E.K.U. GROSS, Max Planck Institute of Microstructure Physics, Halle, Germany — In the past 2 decades several experiments have demonstrated the laser-induced demagnetization of ferromagnetic solids in less than 100 femto-seconds. This is orders of magnitude faster than the present-day magnetic-field-based technology. To shed light on the underlying microscopic mechanism, we have performed an ab-initio study of Fe, Co, Ni and Cr in short laser pulses, using real-time non-collinear time-dependent spin density functional theory (TDDFT). We show [1] that the demagnetization proceeds in two distinct steps: First, a fraction of the electrons is excited without much change in the total spin polarization. In a second step, the spin magnetic moment of the remaining localized d-electrons decreases through spin-flip transitions induced by spin-orbit coupling. For pulse lengths of a few femto-seconds, the whole process of demagnetization happens in less than 50 femto-seconds. For antiferromagnetic Heusler compounds, such as  $Mn_3Ga$  and  $Ni_2MnGa$ , an even faster process is found where magnetic moment is transferred from one sublattice to the other. Employing a combination [2] of TDDFT with Optimal Control Theory, we furthermore demonstrate how the demagnetization process can be controlled with suitably shaped laser pulses. Finally, we assess the influence of the approximation used for the exchange-correlation (xc) functional by comparing non-collinear LSDA results with a novel xc functional [3] that exerts a local exchange-correlation torque.

1. K. Krieger, J.K. Dewhurst, P. Elliott, S. Sharma, E.K.U. Gross, JCTC **11**, 4870 (2015).

2. A. Castro, J. Werschnik, E.K.U. Gross, Phys. Rev. Lett. **109**, 153603 (2012).

3. F.G. Eich, E.K.U. Gross, Phys. Rev. Lett. **111**, 156401 (2013).

**8:36AM K31.00002 Real-time dynamics of Hubbard-type model systems via a combination of the Kadanoff-Baym formalism with adiabatic TDDFT**, HOPJAN MIROSLAV, Lund University, DANIEL KARLSSON, University of Jyväskylä, SIMON YDMAN, CLAUDIO VERDOZZI, CARL-OLOF ALMBLADH, Lund University — We propose a description of nonequilibrium systems via a simple protocol that combines DFT-exchange-correlation potentials with self-energies of many-body perturbation theory. The approach, aimed to avoid double counting of interactions, is tested against exact results in Hubbard-type systems, with respect to interaction strength, perturbation speed/inhomogeneity, and system dimensionality/size. In many regimes, we observe good agreement with the exact results, and an improvement over the pure adiabatic local TDDFT or the pure Second-Born NEGF approximations. We also address the reasons behind the residual discrepancies, and briefly discuss possible directions for future work.

**8:48AM K31.00003 Electronic stopping in liquid water from first principles: An application of large-scale real-time TDDFT simulations**, KYLE REEVES, YI YAO, YOSUKE KANAI, University of North Carolina at Chapel Hill — Electronic stopping describes the transfer of energy from a highly-energetic charged particle to electrons in a material. This process induces massive electronic excitations via interaction between the material and the highly localized electric field from the charged particle. Understanding this phenomenon in condensed matter systems under proton irradiation has implications in various modern technologies. First-principles simulations, based on our recently-developed large-scale real-time time-dependent density functional theory approach, provide a detailed description of how electrons are excited via a non-equilibrium energy transfer from protons on the attosecond time scale. We apply this computational approach to the important case of liquid water under proton irradiation. Our work reveals several key features of the excitation dynamics at the mesoscopic and molecular levels which support a clearer understanding of the water radiolysis mechanism under proton irradiation. Importantly, we will demonstrate a first-principles determination of the energy transfer rate, (i.e. electronic stopping power) in liquid water, and a comparison to existing empirical models will be presented. We will conclude by discussing how the exchange-correlation approximation influences the calculation of the electronic stopping power.

**9:00AM K31.00004 Electrical conductivity of metals from real-time time-dependent density functional theory**, XAVIER ANDRADE, ALFREDO CORREA, Lawrence Livermore National Laboratory — In this presentation, I will discuss how to apply real-time electron dynamics to study electronic currents in crystalline systems and, in particular, how to use this method to predict electrical conductivities in different regimes. This approach presents many interesting theoretical challenges associated to the representation of bulk systems as infinitely periodic. For example, in order to induce electronic currents in the system, we use a gauge transformation that allows us to include finite electric fields in the simulation. We have implemented this approach using time-dependent density functional theory (TDDFT). This implementation allows us to induce, measure and visualize the current density as a function of time, in simulations with thousands of electrons (hundreds and even thousands of atoms). We have found that real-time TDDFT can describe how currents naturally decay in metals. From this dissipation process we can directly calculate the frequency-dependent conductivity, including the direct current (DC) conductivity that is not accessible from linear-response approaches like Kubo-Greenwood.

**9:12AM K31.00005 Development of an ab-initio calculation method for 2D layered materials-based optoelectronic devices**, HAN SEUL KIM, YONG-HOON KIM, Korea Advanced Institute of Science and Technology — We report on the development of a novel first-principles method for the calculation of non-equilibrium nanoscale device operation process. Based on region-dependent  $\Delta$  self-consistent field method beyond the standard density functional theory (DFT), we will introduce a novel method to describe non-equilibrium situations such as external bias and simultaneous optical excitations. In particular, we will discuss the limitation of conventional method and advantage of our scheme in describing 2D layered materials-based devices operations. Then, we investigate atomistic mechanism of optoelectronic effects from 2D layered materials-based devices and suggest the optimal material and architecture for such devices.

**9:24AM K31.00006 The Time-Dependent Particle-Hole Map<sup>1</sup>**, CARSTEN ULLRICH, University of Missouri, YONGHUI LI, Vanderbilt University — The particle-hole map (PHM) is proposed as a new visualization tool to analyze electronic excitations in molecules in the time- or frequency domain, to be used in conjunction with TDDFT or other ab initio methods. The purpose of the PHM is to give detailed insight into electronic excitation processes which is not obtainable from local visualization methods such as transition densities, density differences, or natural transition orbitals. The PHM provides information on the origins, destinations, and coherences of charge fluctuations during an excitation process. In contrast with the transition density matrix, the PHM has a statistical interpretation involving joint probabilities of individual states and their transitions, and it is easier to read and interpret. We discuss and illustrate the properties of the PHM and give several examples and applications to excitations in one-dimensional model systems and in organic donor-acceptor systems.

<sup>1</sup>Work supported by NSF grant DMR-1408904

**9:36AM K31.00007 Exploiting initial-state dependence to improve the performance of adiabatic TDDFT**, JOHANNA I. FUKS, Hunter college City University of New York, SOEREN E.B. NIELSEN, MICHAEL RUGGENTHALER, Max-Planck-Institut für Struktur und Dynamik der Materie, Hamburg, NEEPA T. MAITRA, Hunter college City University of New York, HUNTER COLLEGE CITY UNIVERSITY OF NEW YORK COLLABORATION, MAX-PLANCK-INSTITUT FÜR STRUKTUR UND DYNAMIK DER MATERIE, HAMBURG COLLABORATION — Although time-dependent density functional theory (TDDFT) descriptions of dynamics in non-equilibrium situations have seen exciting successes recently, there have also been studies that throw into doubt the reliability of the approximate exchange-correlation functionals to accurately describe the dynamics. Here we study exact exchange-correlation potentials for few electron systems, found using the global fixed-point iteration method [NRL]. We find that the size of dynamical correlation features that are missing in the currently-used adiabatic approximations depend strongly on the choice of the initial Kohn-Sham wavefunction. With a judicious choice, the dynamical effects can be small over a finite time duration, but sometimes they can get large at longer times. We also examine different starting points, in particular an orbital-dependent potential directly obtained from the Kohn-Sham hole [LFSEM14], for approximate xc functionals: instead of building on an adiabatic approximation.

**9:48AM K31.00008 Studies of spuriously time-dependent resonances in TDDFT**, NEEPA MAITRA, Hunter College and the Graduate Center of the City University of New York, JOHANNA FUKS, Hunter College of the City University of New York — Recently the failure of some exchange-correlation functionals to accurately capture non-perturbative dynamics in time-dependent density functional theory (TDDFT) was shown to be correlated with their violation of an exact condition [1]: that the resonance positions of the system remain fixed during the evolution. Closely related is the inconsistent prediction of excitation frequencies in linear response when the reference state is an excited state of the system. We discuss this and the effect on dynamics in a range of molecular systems, exploring system-size dependence of the violation. [1] Time-resolved spectroscopy in time-dependent density functional theory: An exact condition, J. I. Fuchs, K. Luo, E. D. Sandoval, N. T. Maitra, Phys. Rev. Lett. **114**, 183002 (2015).

**10:00AM K31.00009 Open Quantum Transport and Non-Hermitian Real-Time Time-Dependent Density Functional Theory**, JUSTIN ELENEWSKI, Department of Chemistry, The George Washington University, YANXI-ANG ZHAO, Department of Mathematics, The George Washington University, HANNING CHEN, Department of Chemistry, The George Washington University — Sub-nanometer electronic devices are notoriously difficult to simulate, with the most widely adopted transport schemes predicting currents that diverge from experiment by several orders of magnitude. This deviation arises from numerous factors, including the inability of these methods to accommodate dynamic processes such as charge reorganization. A promising alternative entails the direct propagation of an electronic structure calculation, as exemplified by real-time time-dependent density functional theory (RT-TDDFT). Unfortunately this framework is inherently that of a closed system, and modifications must be made to handle incoming and outgoing particle fluxes. To this end, we establish a formal correspondence between the quantum master equation for an open, many-particle system and its description in terms of RT-TDDFT and non-Hermitian boundary potentials. By dynamically constraining the particle density within the boundary regions corresponding to the device leads, a simulation may be selectively converged to the non-equilibrium steady state associated with a given electrostatic bias. Our numerical tests demonstrate that this algorithm is both highly stable and readily integrated into existing electronic structure frameworks

**10:12AM K31.00010 TDDFT-based local control theory for chemical reactions**, IVANO TAVERNELLI, IBM Res Lab, BASILE F. E. CURCHOD, Department of Chemistry and the PULSE Institute, Stanford University, THOMAS J. PENFOLD, School of Chemistry, Newcastle University, Newcastle (UK) — In this talk I will describe the implementation of local control theory for laser pulse shaping within the framework of TDDFT-based nonadiabatic dynamics <sup>1</sup>. The method is based on a set of modified Tully's surface hopping equations and provides an efficient way to control the population of a selected reactive state of interest through the coupling with an external time-dependent electric field generated on-the-fly during the dynamics. This approach is applied to the investigation of the photoinduced intramolecular proton transfer reaction in 4-hydroxyacridine in gas phase and in solution <sup>2</sup>. The generated pulses reveal important information about the underlying excited-state nuclear dynamics highlighting the involvement of collective vibrational modes that would be neglected in studies performed on model systems. Finally, this approach can help to shed new light on the photophysics and photochemistry of complex molecular systems and guide the design of novel reaction paths.

<sup>1</sup>B. Curchod, T. Penfold, U. Rothlisberger, I. Tavernelli, Phys. Rev. A, **84**, 042507, 2011

<sup>2</sup>B.F.E. Curchod, T. J Penfold, U. Rothlisberger, I. Tavernelli, Chem. Phys. Chem., **16**, 2127, 2015

**10:24AM K31.00011 Mixed Quantum-Classical Dynamics Methods for Strong-Field Processes: Multiple-trajectory Ehrenfest dynamics + decoherence terms**, YASUMITSU SUZUKI, KAZUYUKI WATANABE, Tokyo University of Science, ALI ABEDI, Universidad del País Vasco, FEDERICA AGOSTINI, Max Planck Institute of Microstructure Physics, SEUNG KYU MIN, Ulsan National Institute of Science and Technology, NEEPA MAITRA, Hunter College of the City University of New York, E. K. U. GROSS, Max Planck Institute of Microstructure Physics — The exact factorization of the electron-nuclear wave function [1, 2, 3] allows to define the time-dependent potential energy surfaces (TDPEs) responsible for the nuclear dynamics and electron dynamics. Recently a novel coupled-trajectory mixed quantum-classical (CT-MQC) approach based on this TDPEs has been developed [4], which accurately reproduces both nuclear and electron dynamics. Here we study the TDPEs for laser-induced electron localization with a view to developing a MQC method for strong-field processes [5]. We show our recent progress in applying the CT-MQC approach to the systems with many degrees of freedom. [1] A. Abedi, N. T. Maitra, E. K. U. Gross, Phys. Rev. Lett. **105**, 123002 (2010). [2] Y. Suzuki, A. Abedi, N. T. Maitra, K. Yamashita, E. K. U. Gross, Phys. Rev. A, **89**, 040501(R) (2014). [3] A. Abedi, F. Agostini, Y. Suzuki, E. K. U. Gross, Phys. Rev. Lett. **110**, 263001 (2013); F. Agostini, A. Abedi, Y. Suzuki, S. K. Min, N. T. Maitra, E. K. U. Gross, J. Chem. Phys., **142**, 084303 (2015). [4] S. K. Min, F. Agostini, E. K. U. Gross, Phys. Rev. Lett., **115**, 073001, (2015). [5] Y. Suzuki, A. Abedi, N. T. Maitra, E. K. U. Gross, Phys. Chem. Chem. Phys., **17**, 29271 (2015).

**10:36AM K31.00012 Nuclear Quantum Effects in the Dynamics of Biologically Relevant Systems from First Principles**, MARIANA ROSSI, University of Oxford, UK, WEI FANG, ANGELOS MICHAELIDES, University College London, UK — Understanding the structure and dynamics of biomolecules is crucial for unveiling the physics behind biology-related processes. These molecules are very flexible and stabilized by a delicate balance of weak (quantum) interactions, thus requiring the inclusion of anharmonic entropic contributions and an accurate description of the electronic and nuclear structure from quantum mechanics. We here join state of the art density-functional theory (DFT) and path integral molecular dynamics (PIMD) to gain quantitative insight into biologically relevant systems. Our design of a better and more efficient approximation to quantum time correlation functions based on PIMD (TRPMD [1,2]) enables the calculation of ab initio TCFs with which we calculate IR/vibrational spectra and diffusion coefficients. In stacked polyglutamine strands (structures often related to amyloid diseases) a combination of NQE and H-bond cooperativity provides a small free energy stabilization that we connect to a softening of high frequency modes, enhanced by nuclear quantum anharmonicity [3]. [1] Rossi, Ceriotti, Manolopoulos, JCP **140**, 234116 (2014); [2] Rossi et al., JCP **141**, 181101 (2014); Rossi, Fang, Michaelides, JPCL **6**, 4233 (2015)

**10:48AM K31.00013 Properties of the Schrödinger Theory for Electrons in External Fields**, VIRAH SAHNI, CUNY-Brooklyn Coll, XIAO-YIN PAN, Ningbo University, China — We consider electrons in external electrostatic  $\mathcal{E}(\mathbf{r}) = -\nabla v(\mathbf{r})$  and magnetostatic  $\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$  fields. (The case of solely an electrostatic field constitutes a special case.) Via the ‘Quantal Newtonian’ first law for the individual electron we prove the following: (i) In addition to the external electric and Lorentz fields, each electron experiences an internal field representative of electron correlations due to the Pauli exclusion principle and Coulomb repulsion, the kinetic energy, the density, and the magnetic field; (ii) the scalar potential  $v(\mathbf{r})$  arises from a curl-free field and is thus path-independent; (iii) the magnetic field  $\mathbf{B}(\mathbf{r})$  appears explicitly in the Schrödinger equation in addition to the vector potential  $\mathbf{A}(\mathbf{r})$ ; (iv) The Schrödinger equation can be written to exhibit its intrinsic self-consistent form. (The generalization of the conclusions to time-dependent external fields via the ‘Quantal Newtonian’ second law follows.)

## Wednesday, March 16, 2016 8:00AM - 11:00AM –

**Session K32 DCP: Plasmonics and Beyond I: Resonant Coupling** 332 - David Nesbitt, JILA, University of Colorado

**8:00AM K32.00001 Coupling of Acoustic Vibrations to Plasmon Resonances in Metal Nanoparticles**, AFTAB AHMED, Argonne National Laboratory, MATTHEW PELTON, University of Maryland, Baltimore, JEFFREY GUEST, Argonne National Laboratory — Measurements of acoustic vibrations in nanoparticles provide a unique opportunity to study mechanical phenomena at nanometer length scales and picosecond time scales. Phonon vibrations of plasmonic nanoparticles are of particular interest, due to their large extinction efficiencies, and high sensitivity to surrounding medium. There are two mechanisms that transduce the mechanical oscillations into plasmon resonance shift: (1) changes in polarizability; and (2) changes in electron density. These mechanisms have been used to explain qualitatively the origin of the transient-absorption signals, however, a quantitative connection has not yet been made except for simple geometries. Here, we present a method to quantitatively determine the coupling between vibrational modes and plasmon modes in noble-metal nanoparticles including spheres, shells, rods and cubes. We separately determine the parts of the optical response that are due to shape changes and to changes in electron density, and we relate the optical signals to the symmetries of the vibrational and plasmon modes. These results clarify reported experimental results, and should help guide the optimization of future experiments.

**8:12AM K32.00002 Quantum effects in active linear and non-linear plasmonics.**, GARIKOITZ AGUIRRE-GABIRIA, JAVIER AIZPURUA, ANDREY K. KAZANSKY, PEDRO MIGUEL ECHENIQUE, Material Physics Center CSIC-UPV/EHU and Donostia International Physics Center DIPC, Paseo Manuel de Lardizabal 5 20018, Donostia-San Sebastian, Spain, MARIO ZAPATA, Departamento de Fisica, Universidad de los Andes, Bogot D.C., Colombia, PETER NORDLANDER, Department of Physics, MS61, Laboratory for Nanophotonics, Rice University, Houston, Texas 77005, USA, DANA CODRUTA MARINICA, ANDREI G. BORISSOV, Institut des Sciences Moléculaires d'Orsay - UMR 8214, CNRS-Université Paris Sud, Batiment 351, 91405 Orsay Cedex, France — The unique properties of localized surface plasmons have turned plasmonic nanoparticles into a suitable platform for novel and more efficient optoelectronic processes. Therefore, the development of practical approaches to actively control the plasmon excitations is a major fundamental and practical challenge. Using Time Dependent Density Functional Theory we explore the possibility of all electrical control of the optical properties of different plasmonic systems such as isolated nanoparticles as well as nanoparticle dimers, and core-shell nanoparticles with sub nm gaps. We demonstrate that for plasmonic systems with narrow gaps, the quantum regime owing to the electron tunneling offers the possibility of fast and reversible control of the plasmon resonances, by application of an external dc bias. Along with all-electrical control of the linear response, we also show that the external polarizing DC field can be used to actively control high-harmonic generation from plasmonic nanoparticles.

**8:24AM K32.00003 Plasmon-Induced Resonant Energy Transfer: a coherent dipole-dipole coupling mechanism**, ALAN D. BRISTOW, SCOTT K. CUSHING, JIANGTIAN LI, NIANQIANG WU, West Virginia University — Metal-insulator-semiconductor core-shell nanoparticles have been used to demonstrate a dipole-dipole coupling mechanism that is entirely dependent on the dephasing time of the localized plasmonic resonance [1]. Consequently, the short-time scale of the plasmons leads to broad energy uncertainty that allows for excitation of charge carriers in the semiconductor via stimulation of photons with energies below the energy band gap. In addition, this coherent energy transfer process overcomes interfacial losses often associated with direct charge transfer. This work explores the efficiency of the energy transfer process, the dipole-dipole coupling strength with dipole separation, shell thickness and plasmonic resonance overlap. We demonstrate limits where the coherent nature of the coupling is switched off and charge transfer processes can dominate. Experiments are performed using transient absorption spectroscopy. Results are compared to calculations using a quantum master equation. These nanostructures show strong potential for improving solar light-harvesting for power and fuel generation. [1] J. Li et al, Nature Photonics **9**, 601 (2015).

**8:36AM K32.00004 Nanoparticle Lasing Spasers.**, TERI ODOM, Northwestern University — Plasmon nanolasers, or spasers (surface plasmon amplification by stimulated emission of radiation) are devices based on plasmonic cavities and gain media that can compensate loss and achieve amplification of nano-localized electromagnetic fields. Several nanocavity architectures have been reported for spasers, such as a metal film-dielectric spacer-semiconductor nanowire configuration or arrays of plasmonic cavities, where the unit cells are nanoparticles or nanoholes. We will discuss two platforms based on nanoparticle arrays that support lattice plasmons for far-field directional emission that can achieve tunable lasing at room temperature. Also, we will describe competing and unique loss mechanisms in nanoparticle cavity arrays as well as the design principles for an optimized unidirectional lasing device by examining different plasmonic materials, unit cell shapes, and gain materials.

**9:12AM K32.00005 A Self-Consistent Scheme for Optical Response of large Hybrid Networks of Semiconductor Quantum Dots and Plasmonic Metal Nanoparticles**, BERNARDO BARBIELLINI, L. HAYATI, C. LANE, A. BANSIL, H. MOSALLAEI, Northeastern Univ. — We discuss a self-consistent scheme for treating the optical response of large, hybrid networks of semiconducting quantum dots (SQDs) and plasmonic metallic nanoparticles (MNPs). Our method is efficient and scalable and becomes exact in the limiting case of weakly interacting SQDs. The self-consistent equations obtained for the steady state are analogous to the Heisenberg equations of motion for the density matrix of a SQD placed in an effective electric field computed within the discrete dipole approximation (DDA). Illustrative applications of the theory to square and honeycomb SQD, MNP and hybrid SDQ/MNP lattices as well as SQD-MNP dimers are presented. Our results demonstrate that hybrid SQD-MNP lattices can provide flexible platforms for light manipulation with tunable resonant characteristics.

**9:24AM K32.00006 Colloidal aluminum nanoparticles with tunable localized surface plasmon resonances for energy applications**, YAN CHENG, KENNETH SMITH, EBUKA ARINZE, GABRIELLE NYIRJESY, ARTHUR BRAGG, SUSANNA THON, Johns Hopkins University — Localized surface plasmon resonances (LSPRs) of noble metal nanoparticles are of interest for energy applications due to their visible and near infrared wavelength sensitivity. However, application of these materials in optoelectronic devices is limited by their rarity and high cost. Earth-abundant, inexpensive and non-toxic aluminum is a promising alternative material with a plasmon resonance that can also be tuned via size-, shape- and surface-oxide-control. Here, we employ solution-processed methods to synthesize stable colloidal aluminum nanoparticles. We systematically investigate parameters in the synthesis that control size, shape and oxidation of the aluminum nanoparticles and tune their LSPRs over the ultraviolet and visible spectral regions. We optically characterize the nanoparticle solutions and evaluate their potential for future integration into photovoltaic, photocatalytic and photosensing systems.

**9:36AM K32.00007 Exciton-plasmon interactions in carbon nanotube arrays.**<sup>1</sup>, DAVID DROSDOFF, IGOR BONDAREV, North Carolina Central University — The response properties of semiconducting carbon nanotubes (CNs) allow for the excitation of both plasmons and excitons at optical frequencies, which can interact with each other to give rise to a variety of phenomena and applications [1-3]. If carbon nanotubes are aligned in a periodic array, then energy bands can be formed due to the array periodicity. Using a quantum electrodynamics approach, the energy dispersion relation for the coupled exciton and plasmon excitations in the CN array is theoretically analyzed. The predicted result is the formation of photonic bands, which may give rise to tunable optoelectronic devices and other applications. [1] I.V.Bondarev, L.M.Woods, and K.Tatur, PRB 80, 085407 (2009); [2] I.V.Bondarev, PRB 85, 035448 (2012); [3] I.V.Bondarev and A.V.Meliksetyan, PRB 89, 045414 (2014).

<sup>1</sup>Supported by NSF-ECCS-1306871

**9:48AM K32.00008 Quantum Beats from Entangled Localized Surface Plasmons**<sup>1</sup>, DAVID MASIELLO, University of Washington — Recent experiments report observations of quantum interference between plasmon resonances, inviting descriptions of plasmon-photon interaction using methods from quantum optics. Here we demonstrate, using a Heisenberg-Langevin approach, that the radiation emitted from the localized surface plasmon resonances of a mixed-metal heterodimer may exhibit observable, beat frequency interferences at a far-field detector, known as quantum beats. This prediction represents a correspondence between V-type atoms of quantum optics and the familiar heterodimer system of plasmonics. We explore this analogy in depth and find that although both systems support quantum beats, the heterodimer emits photons in bunches due to the bosonic nature of the plasmon. This highlights a significant difference between the properties of atomic and plasmonic systems.

<sup>1</sup>This work was supported by the National Science Foundations CAREER program under award number CHE-1253775 and NSF XSEDE resources under award number PHY-130045.

**10:24AM K32.00009 Toward Quantum Plasmonics with Plasmon Drag Effect. Theory and Experiment**, MAXIM DURACH, MATTHEW LEPAIN, ZOE MAPES, Georgia Southern University, VINCENT RONO, NATALIA NOGINOVA, Norfolk State University — Giant plasmon drag effect observed in plasmonic metal films and nanostructures brings new fundamental insights into ways in which light-matter interaction occurs. We demonstrate analytically, numerically and experimentally that rectified drag forces acting upon electrons in plasmonic metals are intimately related to the absorption of plasmonic excitations. The plasmon energy quanta absorbed by the metal plasma are associated with momentum quanta, which are also transferred to electrons upon energy absorption. We show that this picture directly applies to plasmon drag effect in a variety of systems, and, to our knowledge for the first time, is capable to explain and predict the magnitude of the effect not only qualitatively, but with close quantitative agreement. The plasmon drag effect opens new avenues for plasmonic-based electronics providing opportunities for incorporation of plasmonic circuits into electronic devices, and for optical sensing offering a new operational principle and an opportunity to substitute the bulky optical set-ups with diffraction limited sensing by electronics. Our work not only adds more clarity into the mechanism behind the plasmon drag effect but also contributes to the emerging field of quantum plasmonics.

**10:36AM K32.00010 Cavity-coupled molecular vibrational spectra and dynamics**<sup>1</sup>, JEFFREY OWRUTSKY, ADAM DUNKELBERGER, JAMES LONG, KENAN FEARS, Chemistry Division, Naval Research Lab, WALTER DRESSICK, Center for Biomolecular Sciences and Engineering, Naval Research Lab, RYAN COMPTON, BRYAN SPANN, BLAKE SIMPKINS, Chemistry Division, Naval Research Lab — Coherent coupling between an optical transition and confined optical mode, when sufficiently strong, gives rise to new modes separated by the vacuum Rabi splitting. Such systems have been investigated for electronic-state transitions, for quantum wells and dots, however, only very recently have vibrational transitions been explored. Both static and dynamic results are described for vibrational bands strongly coupled to optical cavities. First, we experimentally and numerically describe coupling between a Fabry-Perot cavity and carbonyl stretch ( $\sim 1730\text{ cm}^{-1}$ ) in poly-methylmethacrylate as a function of several parameters of the system including absorber strength and concentration as well as cavity length. Similar studies are carried out for anions both in solution and exchanged into cationic polymers. Ultrafast pump-probe studies are performed on  $\text{W}(\text{CO})_6$  in solution which reveals changes to the transient spectra and modified relaxation rates. We believe these modified relaxation rates are a consequence of the energy separation between the vibration-cavity polariton modes and excited state transitions. Cavity-modified vibrational states and energy transfer may provide a new avenue for systematic control of molecular processes and chemistry.

<sup>1</sup>The work supported by the Office of Naval Research through the Naval Research Laboratory

**10:48AM K32.00011 Non-adiabatic Dynamics of Molecules in Optical Cavities**<sup>1</sup>, MARKUS KOWALEWSKI, KOCHISE BENNETT, SHAUL MUKAMEL, Department of Chemistry, UC Irvine — Molecular systems coupled to optical cavities are promising candidates for a novel kind of photo chemistry. Strong coupling to the vacuum field of the cavity can modify the potential energy surfaces opening up new reaction pathways. We present a derivation of the non-adiabatic couplings for single molecules in the strong coupling regime. The possibilities for photo chemistry are demonstrated for a set of model systems representing typical situations found in molecules.

<sup>1</sup>Supported by the Alexander von Humboldt Foundation

**Wednesday, March 16, 2016 8:00AM - 10:48AM –**

**Session K33 DPOLY FIAP: Polymers for Solar Energy Conversion** 336 - Miriam Rafailovich, State University of New York, Stony Brook

**8:00AM K33.00001 Dynamic Covalent Functionalization as a route to Controlling Self Assembly of Organic Molecules**, EMILY PENTZER, Case Western Reserve University — Efforts to optimize the optoelectronic properties of conjugated organic materials are ongoing across many fields of science and engineering. For example, in bulk heterojunction polymer solar cells, researchers seek to optimize absorption of the solar spectrum by the active materials, form interpenetrating domains of p-type and n-type materials to facilitate exciton dissociation, and improve interactions between electrode, charge blocking layers, and active layers to ensure rapid charge transport. One advantage of organic polymers compared to inorganic materials (e.g., silicon), is the low cost and ability process the materials in solution. Moreover, assembly of conjugated organic materials in solution or in the solid state (i.e., films) can be used to optimize both a material's optoelectronic properties and its interface with surfaces and other materials, addressing many of the concerns listed above. Unfortunately, such solution processability requires appendage of insulating alkyl chains to the conjugated frameworks, which don solubility, but are also insulating and thus can hurt device performance. This presentation will report recent results from the Pentzer Lab from Case Western Reserve University on using functional alkyl chains that serve to control self-assembly, control interfaces with other materials, or can be removed by an external stimulus as a route to optimizing the materials for solar cell applications.

**8:36AM K33.00002 Control of Crystallization to Promote Microphase Separation in Fully Conjugated Block Copolymers**, YOUNGMIN LEE, THINH P. LE, Department of Chemical Engineering, The Pennsylvania State University, University Park, PA 16802, ZACH SEIBERS, S. MICHAEL KILBEY, II<sup>1</sup>, Department of Chemistry, University of Tennessee, Knoxville, TN 37996, QING WANG, Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA 16802, ENRIQUE D. GOMEZ<sup>2</sup>, Department of Chemical Engineering, The Pennsylvania State University, University Park, PA 16802 — Donor–acceptor fully conjugated block copolymers, where donor and acceptor conjugated polymers are covalently bonded together, are interesting as single-component active-layer materials for photovoltaics because it can adopt mesoscale microphase separated structures with length scales comparable to the exciton diffusion length. Nevertheless, due to the strong crystallization of poly(3-hexylthiophene-2,5-diyl) (P3HT), morphologies of fully conjugated block copolymers containing P3HT are predominantly driven by crystallization as opposed to microphase separation. We control the crystallization in block copolymers to promote microphase separation in fully conjugated block copolymers through the addition of small amounts of 3-octylthiophene to the polymerization of P3HT. Poly(3-hexylthiophene-2,5-diyl-*r*-3-octylthiophene-2,5-diyl)-*block*-poly((9,9-dioctylfluorene-2,7-diyl)-*alt*-(4,7-di(thiophene-2-yl)-2,1,3-benzothiadiazole)-5',5''-diyl) (P3HT-*b*-PFTBT) copolymers were prepared by Grignard metathesis for the alkylthiophene block followed by chain extension through a Suzuki-Miyaura polycondensation. We compare the crystallization, self-assembly and performance in devices of P3HT-*b*-PFTBT with a few mole percent of 3-octylthiophene in the P3HT block.

<sup>1</sup>Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831

<sup>2</sup>Materials Research Institute, The Pennsylvania State University, University Park, PA 16802

**8:48AM K33.00003 Spectral analysis of resonant scattering to quantify phase behavior in organic blends**, THOMAS FERRON, Washington State University, JON DOWNING, DEAN DELONGCHAMP, National Institute of Standards and Technology, BRIAN COLLINS, Washington State University — It is important in organic solar cells to understand how phase behavior and possible non-equilibrium states of device morphology relate to functionality. However, characterization of carbon based electronics can be a challenging endeavor due to low levels of crystallinity, anisotropic molecular structure leading to complex three dimensional morphologies, and low contrast that hamper traditional techniques such as electron microscopy or hard X-ray scattering. Recently, studies utilizing resonant x-rays have shown sensitivity to phase behavior but a quantitative characterization is vital to correlate device performance. Here we demonstrate a multi-domain analysis of spectrally resolved scattering using molecular optical constants to accurately calculate absolute domain volume fraction and composition of a model block co-polymer. Our methods address complex absorption and fluorescence that occur at the carbon edge in order to move current models beyond the Born approximation. Techniques developed have been applied to P3HT – PCBM solar cells to draw conclusions of device morphology.

**9:00AM K33.00004 Ternary blend polymer solar cells with self-assembled structure for enhancing power conversion efficiency**, ZHENHUA YANG, HONGFEI LI, State Univ of NY- Stony Brook, CHANG-YONG NAM, KIM KISSLINGER, Brookhaven National Lab, SUSHIL SATIJA, National Institute of Standards and Technology, MIRIAM RAFAILOVICH, State Univ of NY- Stony Brook — Bulk heterojunction (BHJ) polymer solar cells are an area of intense interest due to their advantages such as mechanical flexibility. The active layer is typically spin coated from the solution of polythiophene derivatives (donor) and fullerenes (acceptor) and interconnected domains are formed because of phase separation. However, the power conversion efficiency (PCE) of BHJ solar cell is restricted by the disordered inner structures in the active layer, donor or acceptor domains isolated from electrodes. Here we report a self-assembled columnar structure formed by phase separation between (PCDTBT) and polystyrene (PS) for the active layer morphology optimization. The BHJ solar cell device based on this structure is promising for exhibiting higher performance due to the shorter carrier transportation pathway and larger interfacial area between donor and acceptor. The surface morphology is investigated with atomic force microscopy (AFM) and the columnar structure is studied by investigation of cross-section of the blend thin film of PCDTBT and PS under the transmission electron microscopy (TEM). The different morphological structures formed via phase segregation are correlated with the performance of the BHJ solar cells.

**9:12AM K33.00005 Enhancing efficiency in polymer-blend solar cells: Structural insights through scattering**, VIKRAM KUPPA, University of Dayton — All-polymer solar cells that employ blends of semiconducting polymers are capable of harnessing a greater portion of the incident solar spectrum than singly sensitized devices. However, they invariably show poor performance when compared with small-molecule bulk heterojunction cells. Following our successful approach in adding very small quantities of pristine graphene to the active layer to boost performance in P3HT/PCBM cells, we have recently reported a three-fold enhancement in efficiency of all-polymer (a blend of P3HT and F8BT) photovoltaic devices. These new cells exhibit more balanced transport of electrons and holes, strong dependence of recombination behavior on graphene content, and up to two orders of magnitude increase in mobility, resulting in a peak improvement of over 200

**9:48AM K33.00006 Magnetic field effects in a polymer/fullerene blend photovoltaic cell**, HYUK-JAE JANG, JAMES I. BASHAM, DAVID J. GUNDLACH, CURT A. RICHTER, Engineering Physics Division, National Institute of Standards and Technology — Organic photovoltaic (OPV) systems based on blends of conjugated polymers and fullerene derivatives have shown great promise for low-cost and efficient photovoltaic applications. Recent findings suggest that a weak external magnetic field can disturb the spin configuration of excited states and subsequently change properties of OPV cells such as photocurrent. These changes are referred to as magnetic field effects (MFEs). In order to have a better understanding of the underlying mechanisms responsible for the MFEs in polymer/fullerene blend photovoltaic systems, we fabricated poly-3-hexylthiophene (P3HT):phenyl-C<sub>61</sub>-butyric acid methyl ester (PC<sub>61</sub>BM) cells and carried out photovoltaic device performance and impedance spectroscopy measurements with and without an externally applied magnetic field. A significant reduction in short circuit current ( $J_{SC}$ ) as well as open circuit voltage ( $V_{OC}$ ) was observed with an applied magnetic field of 0.1 tesla compared to those measured without a magnetic field under the same intensity of illumination. Impedance spectroscopy data gives insights into the influence of an external magnetic field on charge generation and recombination near normal photovoltaic operating conditions.

**10:00AM K33.00007 Conductivity Scaling Relationships of Nanostructured Membranes based on Hydrated Protic Polymerized Ionic Liquids: Effect of Domain Spacing**, GABRIEL SANOJA, University of California, Berkeley, BHOOSHAN PÖPERE, University of California, Santa Barbara, BRYAN BECKINGHAM, Joint Center for Artificial Photosynthesis, CHRISTOPHER EVANS, University of California, Santa Barbara, NATHANIEL LYND, University of Texas, Austin, RACHEL SEGALMAN, University of California, Santa Barbara — Elucidating the relationship between chemical structure, morphology, and ionic conductivity is essential for designing novel materials for electrochemical applications. In this work, the effect of lamellar domain spacing ( $d$ ) on ionic conductivity ( $\sigma$ ) is investigated for a model system of hydrated block copolymer based on a protic polymerized ionic liquid. We present a strategy that allows for the synthesis of a well-defined series of narrowly dispersed PS-*b*-PIL with constant volume fraction of ionic liquid moieties ( $f_{IL} \approx 0.39$ ). These materials self-assemble into ordered lamellar morphologies with variable domain spacing (23-59 nm) as demonstrated by SAXS. PS-*b*-PIL membranes exhibit ionic conductivities above  $10^{-4}$  S/cm at room temperature, which are independent of domain spacing. The conductivity scaling relationship demonstrated in this work suggests that a mechanically robust membrane can be designed without compromising its ability to transport ions. In addition, PIL-based membranes exhibit lower water uptake ( $\lambda = 10$ ) in comparison with many proton-conducting systems reported elsewhere. The low water content of these materials makes them promising candidates for solar-fuels electrochemical devices.

**10:12AM K33.00008 Electronic structure properties as signatures of morphological motifs in organic photovoltaics**, MATTHEW GOLDEY, GIULIA GALLI, University of Chicago — The effect of polymer morphologies upon the efficiency of organic solar cells is difficult to determine experimentally; however, theoretical models may directly probe how structural changes affect electronic properties, such as band locations and band gaps and hence provide key insight into solar energy conversion processes. Using density functional and many body perturbation theory (G0W0) calculations, we investigated the dependence of the electronic states on order parameters such as backbone dihedrals of organic donor polymers. We focused on the donor polymers PTB7 and PID2 and the acceptor PC71BM for which recent experiments[1] reported promising photoconversion efficiencies of 8.22% for ternary blend cells. Our results suggest that accurate predictions of the device performance must include a description of local disorder in the active layer. In particular, we found multiple possible configurations of the donor polymer with relative energies 0.06-0.3 eV/monomer above the lowest energy conformer whose electronic structure differ significantly. Using the lowest energy conformations found at zero T, calculated electronic energy levels are in good agreement with experimental values, with errors within 0.2 eV. [1] Lu, L., et. al. Nature Photon, 8(9), 716722 (2014).

**10:24AM K33.00009 Enhancing the performance of BHJ solar cell via self-assembly templates in active layer**, YING LIU, Stony Brook University, HONGFEI LI, ZHENHUA YANG, Stony Brook University, CHANG-YONG NAM, Brookhaven National Lab, SUSHIL SATIJA, National Institute of Standards and Technology, MIRIAM RAFAILOVICH, Stony Brook University — The bulk heterojunction (BHJ) solar cell is an important example of a polymer solar cell technology that has been proposed in recent years. However, due to the disordered inner structures in the active layer, control of the inner structure within the active layer is required to enhance the efficiency. In our approach, a self-assembly of tertiary polymer blend film is confined between the air and solid interfaces. The principal has been proved using a blend of PMMA: P3HT: PCBM where we showed that the PMMA phase formed a column structure in the P3HT, which template the PCBM phase between the electrodes. Neutron reflectometry was used to demonstrate the confinement of PCBM at the interface between P3HT and PMMA in the active layer. The columnar structured template is investigated under atomic force microscopy (AFM) and transmission electron microscopy (TEM). SCLC mobility measurement indicated an obvious improvement on both hole and electron mobility. The different morphological structures formed via phase segregation are correlated with the performance of the PEV cells fabricated at the BNL-CFN and significant enhancement for the efficiency is observed.

**10:36AM K33.00010 Electroabsorption spectroscopy of bulk heterojunction solar cells**, MARIAN TZOLOV, ZANE COHICK, CHRISTOPHER GREEN, Lock Haven University of PA — Bulk heterojunction solar cells were fabricated using PCPDTBT polymer and PCBM in inert atmosphere. Electroabsorption (EA) spectroscopy was performed in the spectral range 350-1000 nm. The first derivative of the optical absorbance spectra explains satisfactory most of the bands in the EA spectra. The only deviation is in the spectral range around 760 nm. Control experiments with devices containing only a PCPDTBT film confirm that the band at 760 nm is associated with the presence of PCBM, despite that pristine PCBM is not expected to have such band. Electrical DC bias strongly affects this band. Negative DC bias almost completely eliminates this band, while positive bias enhances it. We interpret the band at 760 nm as due to photogenerated charge carriers trapped at defect states or at interfaces within the composite PCPDTBT/PCBM film. The effective transfer of photogenerated charge carriers between PCPDTBT and PCBM is confirmed by the quenching of the photoluminescence in the composite film, while the emission of electroluminescence from the devices confirms that PCPDTBT is an effective medium for recombination of charges injected in it.

## Wednesday, March 16, 2016 8:00AM - 11:00AM – Session K34 GSOF: Rheology and Flow 337 - Paolo Arratia, University of Pennsylvania

**8:00AM K34.00001 A rheological signature of frictional interactions in shear thickening suspensions**, JOHN ROYER, NIST, DANIEL BLAIR, Georgetown University, STEVEN HUDSON, NIST — We elucidate the relative contributions from hydrodynamic lubrication and frictional contact forces to colloidal shear thickening by measuring both the viscosity  $\eta$  and first normal stress difference  $N_1$  in suspensions of silica spheres over a wide range of volume fractions. The first normal stress difference reveals a transition not apparent in the viscosity alone, from  $N_1 < 0$  at moderate volume fractions  $\phi \leq 0.52$  to  $N_1 > 0$  at larger values of  $\phi$ . While the  $N_1 < 0$  behavior is consistent with hydrodynamic models, the  $N_1 > 0$  behavior (dilation) is instead a characteristic of frictional 'granular' suspensions. Fitting our viscosity profiles  $\eta(\sigma, \phi)$  to a model for friction-driven shear thickening, we capture the shear thickening for  $\phi \geq 0.52$  but must adjust the maximum fraction of frictional contacts to fit at lower volume fractions. Our results bring together two contrasting theories for shear thickening; they show that friction drives shear thickening in concentrated colloidal suspensions, but also highlight the need to include hydrodynamic effects to fully describe the rheology at moderate concentrations.

**8:12AM K34.00002 Microstructure of Brownian Particles under Cyclic Shear<sup>1</sup>**, SOMAYEH FARHADI, University of Pennsylvania, NATHAN KEIM, California Polytechnic State University - San Luis Obispo, PAULO ARRATIA, University of Pennsylvania — We study the microstructure of a 2D colloidal system subject to cyclic shear. The system consists of  $1\mu\text{m}$  particles which are purely repulsive and are adsorbed at an oil-water interface. The particles, which exhibit Brownian motion, provide a model system for thermal glasses under external shear. Cyclic shear is induced by a magnetized needle which is also placed at the interface. The particles are tracked through consecutive images taken within each cycle. By measuring the non-affine stroboscopic displacement of the particles, we identify the spatial distribution of rearrangements. Similar to nonthermal colloids ( $4 - 6\mu\text{m}$ ), we observe localized regions of non-affine rearrangements. The number and size of these regions shrink as the Péclet number is increased. We also observe that similar to non-Brownian systems, a fraction of reversible cycles undergo plastic deformation. However, the spatial distribution of such Brownian particles is more homogeneous compared to non-Brownian system.

<sup>1</sup>Penn NSF MRSEC (DMR-1120901)

**8:24AM K34.00003 Forces acting in quasi 2d emulsions**, CARLOS ORELLANA, JANNA LOWENSOHN, ERIC WEEKS, Emory University — We study the forces in a quasi two dimensional emulsion system. Our samples are oil-in-water emulsions confined between two close-spaced parallel plates, so that the oil droplets are deformed into pancake shapes. By means of microscopy, we measure the droplet positions and their deformation, which we can relate to the contact forces due to surface tension. We improve over prior work in our lab, achieving a better force resolution. We use this result to measure and calibrate the viscous forces acting in our system, which fully determine all the forces on the droplets. Our results can be applied to study static configurations of emulsion, as well as faster flows.

**8:36AM K34.00004 Flow in Smectic Liquid Crystal Films: Examining the Flow Field of a Smectic Liquid Crystal Film due to Fluid Ejected From a Small Nozzle<sup>1</sup>**, KYLE FERGUSON, ZHIYUAN QI, CHEOL PARK, JOSPEH MACLENNAN, MATTHEW GLASER, NOEL CLARK, University of Colorado, Boulder — The rheological properties of 2D fluids are well-understood theoretically, but few experiments testing theoretical predictions have been carried out. We have used MX 12805, a smectic C liquid crystal at room temperature, to create quasi-2D films with which to study high-Reynolds number flow. We map the flow field as the fluid is ejected from a thin nozzle into a large reservoir, probing both laminar and turbulent flow. We also attempt to carry out the experiment in a vacuum to study the true 2D-regime; despite encountering experimental difficulties, some useful information can still be gleaned.

<sup>1</sup>This work was supported by NASA Grant NNX-13AQ81G, by the Soft Materials Research Center under NSF MRSEC Grants DMR-0820579 and DMR-1420736, by Department of Energy Grant DE-FG02-08ER54995, and by NSF Grant CBET-0854108.

**8:48AM K34.00005 Effect of Confinement on Suspension Rheology**, MEERA RAMASWAMY, BRIAN LEAHY, YEN-CHIH LIN, ITAI COHEN, Department of Physics, Cornell University — Confined systems are ubiquitous in nature and occur at widely separated length scales from the atomic to granular. While the flow properties of both atomic and granular systems has been well studied, examining the rheology of the intermediate length scale in colloidal suspensions is challenging. We use a confocal rheoscope to image the particle configuration in a suspension of silica microspheres while simultaneously measuring its stress responses. The confocal rheoscope has two precisely-aligned parallel plates that can confine the suspension with a variable gap size ranging from 3 to 30 particle diameters, allowing us to measure the response of the system as a function of the gap size. We find that the viscosity of the system decreases with confinement in sharp contrast to the increase reported in atomic and granular systems. The microscopy images indicate that this decrease in viscosity is due to the formation of particle layers in this shear regime where hydrodynamic forces dominate particle interactions. We discuss these results and their implications.

**9:00AM K34.00006 Orientation of dilute multi-walled carbon nanotube suspensions in shear and planar extensional flow**, BINBIN LUO, WESLEY BURGHARDT, Northwestern University — Small-angle x-ray scattering is used to study flow-induced orientation in suspensions of multi-walled carbon nanotubes in viscous, uncured epoxies. Shear flow studies are performed in an annular cone and plate shear cell in which fluid structure is probed in the flow-gradient (1-2) plane, allowing measures of both the degree and direction of nanotube orientation. General orientation behavior is consistent with expectations of Brownian dispersions of elongated particles. At high Peclet number, the degree of orientation saturates, and the orientation angle approaches the flow direction. Interestingly, otherwise identical suspensions in two different epoxies of different viscosity yield dramatically different degrees of orientation, even when compared at comparable Peclet number. The same suspensions are studied in planar extensional flow, using a cross-slot flow cell, in order to probe the relative effectiveness of shear and extensional flow at promoting nanotube orientation.

**9:12AM K34.00007 Alignment and rotation of anisotropic particles in complex flows**, GREG VOTH, Wesleyan University — Anisotropic particles in fluid flows develop orientational order that strongly affects both particle rotation statistics and rheology of multi-phase flows. We have measured the motion and rotation of non-brownian particles in chaotic and turbulent flows using video particle tracking to reconstruct 3D particle trajectories. The preferential alignment of particles of many different shapes can be understood using a simple picture that considers the stretching a particle has recently experienced. The stretching can be quantified using the Cauchy-Green strain tensors. Particle rotation statistics can be understood as a result of the preferential alignment of fluid vorticity and the particles by stretching. The Cauchy-Green eigenvalue fields have been widely used to identify Lagrangian coherent structures that affect fluid mixing. We show how their eigenvector fields can help understand the complex orientational order that occurs in these flows.

**9:24AM K34.00008 A unified description of the rheology of hard particles.**, MICHEL HERMES, BEN GUY, WILSON POON, The University of Edinburgh — The rheology of suspensions of Brownian, or colloidal, particles (diameter  $d \approx 1 \mu\text{m}$ ) differs markedly from that of larger grains ( $d \approx 50 \mu\text{m}$ ). Each of these two regimes has been separately studied, but the flow of suspensions with intermediate particle sizes ( $1 \mu\text{m} < d < 50 \mu\text{m}$ ), which occur ubiquitously in applications, remains poorly understood. By measuring the rheology of suspensions of hard spheres with a wide range of sizes, we show experimentally that shear thickening drives the transition from colloidal to granular flow across the intermediate size regime. This insight makes possible a unified description of the (non-inertial) rheology of hard spheres over the full size spectrum. Moreover, we are able to test a new theory of friction-induced shear thickening, showing that our data can be well fitted using expressions derived from it.

**9:36AM K34.00009 Flow Induced by an Oscillating Sphere in Probing Complex Viscosity of Nonadsorbing Polymer Solutions**, YANZHEN HE, TAI-HSI FAN, Mechanical Engineering, University of Connecticut, USA, REMCO TUINIER, Chemical Engineering and Chemistry, Eindhoven University of Technology, the Netherlands, TAKASHI TANIGUCHI, Chemical Engineering, Kyoto University, Japan — Theoretical investigation is presented for a linear viscoelastic flow induced by an oscillatory colloidal particle in nonadsorbing polymer solutions. The dilute to semi-dilute polymer solutions are treated as linear viscoelastic fluids. At small-amplitude oscillation, the polymer distribution is assumed at equilibrium and forms a depletion zone around the particle based on the mean field approximation. The analytical result based on the two-layer approximation is compared with numerical results using a continuous depletion profile to describe the nonuniform complex viscosity in the flow field. Depending on the polymer concentration, solution conditions and depletion thickness, the obtaining apparent complex viscosity or friction coefficient sensed by the particle could deviate significantly from the actual viscosity of the bulk polymer solution. The models developed can be applied, along with active and passive colloidal probing methods, for microrheological measurements of complex fluids that take depletion into account.

**9:48AM K34.00010 How does inertia affect the steady-shear rheology of disordered solids?**, JOERG ROTTLE, University of British Columbia, JEAN-LOUIS BARRAT, ALEXANDRE NICOLAS, LiPhy, Universit Grenoble-Alpes & CNRS — We study the finite-shear-rate rheology of disordered solids with molecular dynamics simulations in two dimensions. By systematically varying the damping strength  $\zeta$ , we identify two well defined flow regimes, separated by a thin crossover region. In the overdamped regime, the athermal rheology is governed by the competition between elastic forces and viscous forces, whose ratio gives the Weissenberg number  $Wi \propto \zeta\dot{\gamma}$ ; the macroscopic stress  $\Sigma$  follows the frequently encountered Herschel-Bulkley law  $\Sigma = \Sigma_0 + k\sqrt{Wi}$ , with yield stress  $\Sigma_0 > 0$ . In the underdamped (inertial) regime, dramatic changes in the rheology are observed for low damping: the flow curve becomes nonmonotonic. This change is not caused by longer-lived correlations in the particle dynamics at lower damping; instead, for weak dissipation, the sample heats up considerably and proportional to the driving. By thermostating more or less underdamped systems, we are able to link quantitatively the rheology to the kinetic temperature  $T_k$ , while the damping strength enters only indirectly by setting  $T_k$ .

**10:00AM K34.00011 The flow and fracture of concentrated colloidal suspensions**, MIKE SMITH, University of Nottingham — Concentrated colloidal suspensions display dramatic rises in viscosity, leading to jamming and granulation, with increasing shear rate. It has been proposed that these effects result from inter particle friction, as lubrication forces are overcome. This suggests the jamming of concentrated colloidal suspensions should exhibit some shared phenomenology with macroscopic granular systems where friction leads to two different types of jammed state. Here we show that transient rheological measurements can be used to probe the processes of granulation in concentrated colloidal suspensions [1]. Our results support the idea that frictional contacts are created between jammed particles. The jamming behaviour displays two qualitatively different regimes separated by a critical strain rate with qualitatively different types of fracture/break up behaviour. In the lower strain rate regime, it is found that vibrations can be used to control jamming and granulation, resulting in a flowable fluid. [1] Nature Sci. Rep. 5:14175 (2015)

**10:12AM K34.00012 Fragility in dense suspensions**, ROMAIN MARI, MIKE CATES, DAMTP - University of Cambridge — Dense suspensions can jam under shear when the volume fraction of solid material is large enough. In this work we investigate the mechanical properties of shear jammed suspensions with numerical simulations. In particular, we address the issue of the fragility of these systems, i.e., the type of mechanical response (elastic or plastic) they show when subject to a mechanical load differing from the one applied during their preparation history.

**10:24AM K34.00013 Role of inertia in the rheology of amorphous systems: a finite element based elasto plastic model**, KAMRAN KARIMI, JEAN-LOUIS BARRAT, Joseph Fourier University — A simple Finite Element analysis with varying damping strength is used to model the athermal shear rheology of densely packed glassy systems at a continuum level. We focus on the influence of dissipation mechanism on bulk rheological properties. Our numerical studies, done over a wide range of damping coefficients, identify two well-separated rheological regimes along with a cross-over region controlled by a critical damping. In the overdamped limit, inertial effects are negligible and the rheological response is well described by the commonly observed Herschel-Bulkley equation. In stark contrast, inertial vibrations in the underdamped regime prompt a significant drop in the mean-stress level, leading to a non-monotonic constitutive relation. The observed negative slope in the flow curve, which is a signature of mechanical instability and thus permanent shear-banding, arises from the sole influence of inertia, in qualitative agreement with the recent molecular dynamics study of Nicolas *et al.* (*arXiv preprint arXiv:1508.06067*, 2015).

**10:36AM K34.00014 Experimental Timescales of Fracture-Healing Rheological Behavior of Thermoreversible Gels**, TRAVIS L. THORNELL, KRITHIKA SUBRAMANIAM, KENDRA A. ERK, School of Materials Engineering, Purdue University — Acrylic thermoreversible physical gels were used as a model soft material system to investigate fracture-healing behavior by shear rheometry. By using shear start-up experiments, gels at various concentrations and temperatures were measured to determine shear stress responses, and fracture was indicated by a decrease in shear stress (confirmed with rheophysical flow visualization experiments). Fractured gels were allowed to recover in the rheometer for set periods of time and were tested again using the same shear start-up procedure to evaluate the recovery kinetics of network strength. Relationships between the network recovery and the normalized ratio of the resting times and characteristic relaxation times of the gels were determined. It was found that resting times for fully healed networks needed to be 2 or 3 orders of magnitude greater than the relaxation times. The extent of fracture was also investigated. Gels that were deformed to smaller total strain magnitudes were suspected to have incomplete (or partial) fracture as results showed various responses for given resting times.

**10:48AM K34.00015 Rich Janus Colloid Phase Behavior Under Steady Shear**, RONALD A. DELACRUZ-ARAUJO, Department of Chemical Engineering, University of Puerto Rico-Mayagüez, Mayagüez, PR 00681, USA, DANIEL J. BELTRAN-VILLEGAS, RONALD G. LARSON, Department of Chemical Engineering, University of Michigan, Ann Arbor, MI 48109, USA, UBALDO M. CORDOVA-FIGUEROA, Department of Chemical Engineering, University of Puerto Rico-Mayagüez, Mayagüez, PR 00681, USA — We study the assembly of single-patch Janus colloids under steady shear via Brownian dynamic simulations. Under quiescent conditions, varying the patch size, the range, and strength of the interaction potential we observe different aggregates such as micelles, wormlike clusters, vesicles and lamellae. Under shear conditions we observe rearrangement, deformation, and break-up of aggregates. At large Péclet (Pe) numbers the shear forces dominate over Brownian forces and aggregates dissociate in a gas for all structures studied. At small and intermediate Pe, the competition between rearrangement, deformation, and break-up favors the growth of micelles and vesicles with Pe, resulting in mean cluster size increases, consistent with a previous study of Janus particles under shear. After the initial shear-induced growth, micelles and vesicles dissociate into a gas. Wormlike aggregates initially break-up into micelles, and proceed to finally reach a gas phase. Lamellar structures initially break into smaller lamellae that align with the flow direction and finally dissociate into a gas. This work opens new actuation routes for re-configurable materials and applications where different types of aggregates will be present under quiescent conditions while others will form under shear.

## Wednesday, March 16, 2016 8:00AM - 10:48AM –

Session K35 DBIO: Physics of Sensorimotor Neural Circuits | 338 - Tatyana Sharpee, Salk Institute

**8:00AM K35.00001 Neural relativity principle**, ALEXEI KOULAKOV, Cold Spring Harbor Laboratory — Olfaction is the final frontier of our senses - the one that is still almost completely mysterious to us. Despite extensive genetic and perceptual data, and a strong push to solve the neural coding problem, fundamental questions about the sense of smell remain unresolved. Unlike vision and hearing, where relatively straightforward relationships between stimulus features and neural responses have been foundational to our understanding sensory processing, it has been difficult to quantify the properties of odorant molecules that lead to olfactory percepts. In a sense, we do not have olfactory analogs of "red", "green" and "blue". The seminal work of Linda Buck and Richard Axel identified a diverse family of about 1000 receptor molecules that serve as odorant sensors in the nose. However, the properties of smells that these receptors detect remain a mystery. I will review our current understanding of the molecular properties important to the olfactory system. I will also describe a theory that explains how odorant identity can be preserved despite substantial changes in the odorant concentration.

**8:36AM K35.00002 Molecular Cooperativity Governs Diverse and Monoallelic Olfactory Receptor Expression<sup>1</sup>**, JIANHUA XING, XIAOJUN TIAN, University of Pittsburgh, HANG ZHANG, Virginia Polytechnic Institute and State University, JENS SANNERUD, Brown University — Multiple-objective optimization is common in biological systems. In the mammalian olfactory system, each sensory neuron stochastically expresses only one out of up to thousands of olfactory receptor (OR) gene alleles; at organism level the types of expressed ORs need to be maximized. The molecular mechanism of this Nobel-Prize winning puzzle remains unresolved after decades of extensive studies. Existing models focus only on monoallele activation, and cannot explain recent observations in mutants, especially the reduced global diversity of expressed ORs in G9a/GLP knockouts. In this work we integrated existing information on OR expression, and proposed an evolutionarily optimized three-layer regulation mechanism, which includes zonal segregation, epigenetic and enhancer competition coupled to a negative feedback loop. This model not only recapitulates monoallelic OR expression, but also elucidates how the olfactory system maximizes and maintains the diversity of OR expression. The model is validated by several experimental results, and particularly underscores cooperativity and synergy as a general design principle of multi-objective optimization in biology.

<sup>1</sup>The work is supported by the NIGMS/DMS Mathematical Biology program

**8:48AM K35.00003 Derivation of Neural Circuits from the Similarity Matching Principle**, CENGIZ PEHLEVAN, DMITRI CHKLOVSKII, Simons Foundation — Our brains analyze high-dimensional datasets streamed by our sensory organs in multiple stages. Sensory cortices, for example, perform tasks like dimensionality reduction, sparse feature discovery and clustering. To model these tasks we pursue an approach analogous to use of action principles in physics and propose a new family of objective functions based on the principle of similarity matching. From these objective functions we derive online distributed algorithms that can be implemented by biological neural networks resembling cortical circuits. Our networks can adapt to changes in the number of latent dimensions or the number of clusters in the input dataset. Furthermore, we formulate minimax optimization problems from which we derive online algorithms with two classes of neurons identified with principal neurons and interneurons in biological circuits. In addition to bearing resemblance to biological circuits, our algorithms are competitive for Big Data applications.

**9:00AM K35.00004 The dynamics of neuronal redundancy in decision making**, BRYAN DANIELS, Arizona State University, JESSICA FLACK, DAVID KRAKAUER, Santa Fe Institute — We propose two temporal phases of collective computation in a visual motion direction discrimination task by analyzing recordings from 169 neural channels in the prefrontal cortex of macaque monkeys. Phase I is a distributed phase in which uncertainty is substantially reduced by pooling information from many cells. Phase II is a redundant phase in which numerous single cells contain all the information present at the population level in Phase I. A dynamic distributed model connects low redundancy to a slow timescale of information aggregation, and provides a common explanation for both behaviors that differs only in the degree of recurrent excitation. We attribute the slow timescale of information accumulation to critical slowing down near the transition to a memory-carrying collective state. We suggest that this dynamic of slow distributed accumulation followed by fast collective propagation is a generic feature of robust collective computing systems related to consensus formation.

**9:12AM K35.00005 Mathematical Relationships between Neuron Morphology and Neurite Growth Dynamics in *Drosophila melanogaster* Larva Class IV Sensory Neurons**, SUJOY GANGULY, Yale Univ, XIN LIANG, Tsinghua University, MICHAEL GRACE, DANIEL LEE, JONATHAN HOWARD, Yale Univ — The morphology of neurons is diverse and reflects the diversity of neuronal functions, yet the principles that govern neuronal morphogenesis are unclear. In an effort to better understand neuronal morphogenesis we will be focusing on the development of the dendrites of class IV sensory neuron in *Drosophila melanogaster*. In particular we attempt to determine how the total length, and the number of branches of dendrites are mathematically related to the dynamics of neurite growth and branching. By imaging class IV neurons during early embryogenesis we are able to measure the change in neurite length  $l(t)$  as a function of time  $v(t) = dl/dt$ . We found that the distribution of  $v(t)$  is well characterized by a hyperbolic secant distribution, and that the addition of new branches per unit time is well described by a Poisson process. Combining these measurements with the assumption that branching occurs with equal probability anywhere along the dendrite we were able to construct a mathematical model that provides reasonable agreement with the observed number of branches, and total length of the dendrites of the class IV sensory neuron.

**9:24AM K35.00006 An investigation into the induced electric fields from transcranial magnetic stimulation.**, RAVI HADIMANI, ERIK LEE, Iowa State University, WALTER DUFFY, MOHAMMED WARIS, WAQUAR SIDDIQUI, FAISAL ISLAM, MAHESH RAJAMANI, RYAN NATHAN, Premier Psychiatric Group, DAVID JILES, Iowa State University, DAVID C JILES TEAM, WALTER DUFFY COLLABORATION — Transcranial magnetic stimulation (TMS) is a promising tool for noninvasive brain stimulation that has been approved by the FDA for the treatment of major depressive disorder. To stimulate the brain, TMS uses large, transient pulses of magnetic field to induce an electric field in the head. This transient magnetic field is large enough to cause the depolarization of cortical neurons and initiate a synaptic signal transmission. For this study, 50 unique head models were created from MRI images. Previous simulation studies have primarily used a single head model, and thus give a limited image of the induced electric field from TMS. This study uses finite element analysis simulations on 50 unique, heterogeneous head models to better investigate the relationship between TMS and the electric field induced in brain tissues. Results showed a significant variation in the strength of the induced electric field in the brain, which can be reasonably predicted by the distance from the TMS coil to the stimulated brain. Further, it was seen that some models had high electric field intensities in over five times as much brain volume as other models.

**9:36AM K35.00007 A Robust Feedforward Model of the Olfactory System<sup>1</sup>**, YILUN ZHANG, TATYANA SHARPEE, Salk Institute for Biological Studies and University of California San Diego — Most natural odors have sparse molecular composition. This makes the principles of compressing sensing potentially relevant to the structure of the olfactory code. Yet, the largely feedforward organization of the olfactory system precludes reconstruction using standard compressed sensing algorithms. To resolve this problem, recent theoretical work has proposed that signal reconstruction could take place as a result of a low dimensional dynamical system converging to one of its attractor states. The dynamical aspects of optimization, however, would slow down odor recognition and were also found to be susceptible to noise. Here we describe a feedforward model of the olfactory system that achieves both strong compression and fast reconstruction that is also robust to noise. A key feature of the proposed model is a specific relationship between how odors are represented at the glomeruli stage, which corresponds to a compression, and the connections from glomeruli to Kenyon cells, which in the model corresponds to reconstruction. We show that provided this specific relationship holds true, the reconstruction will be both fast and robust to noise, and in particular to failure of glomeruli. The predicted connectivity rate from glomeruli to the Kenyon cells can be tested experimentally.

<sup>1</sup>This research was supported by James S. McDonnell Foundation, NSF CAREER award IIS-1254123, NSF Ideas Lab Collaborative Research IOS 1556388.

**9:48AM K35.00008 Animal-to-Animal Variation in Odor Preference and Neural Representation of Odors**, KYLE HONEGGER, MATTHEW SMITH, Harvard University, GLENN TURNER, HHMI, Janelia Farm Research Campus, BENJAMIN DE BIVORT, Harvard University — Across any population of animals, individuals exhibit diverse behaviors and reactions to sensory stimuli like tastes and odors. While idiosyncratic behavior is ubiquitous, its biological basis is poorly understood. In this talk, I will present evidence that individual fruit flies (*Drosophila melanogaster*) display idiosyncratic olfactory behaviors and discuss our ongoing efforts to map these behavioral differences to variation in neural circuits. Using a high-throughput, single-fly assay for odor preference, we have demonstrated that highly inbred flies display substantial animal-to-animal variability, beyond that expected from experimental error, and that these preferences persist over days. Using in vivo two-photon calcium imaging, we are beginning to examine the idiosyncrasy of neural coding in the fly olfactory pathway and find that the odor responses of individual processing channels in the antennal lobe can vary substantially from fly to fly. These results imply that individual differences in neural coding may be used to predict the idiosyncratic behavior of an individual - a hypothesis we are currently testing by imaging neural activity from flies after measuring their odor preferences.

**10:00AM K35.00009 Robust spatial memory maps in flickering neuronal networks: a topological model.**, YURI DABAGHIAN, ANDREY BABICHEV, Rice University, FACUNDO MEMOLI, SAMIR CHOWDHURY, Ohio State University, RICE UNIVERSITY COLLABORATION, OHIO STATE UNIVERSITY COLLABORATION — It is widely accepted that the hippocampal place cells provide a substrate of the neuronal representation of the environment—the “cognitive map”. However, hippocampal network, as any other network in the brain is transient: thousands of hippocampal neurons die every day and the connections formed by these cells constantly change due to various forms of synaptic plasticity. What then explains the remarkable reliability of our spatial memories? We propose a computational approach to answering this question based on a couple of insights. First, we propose that the hippocampal cognitive map is fundamentally topological, and hence it is amenable to analysis by topological methods. We then apply several novel methods from homology theory, to understand how dynamic connections between cells influences the speed and reliability of spatial learning. We simulate the rat’s exploratory movements through different environments and study how topological invariants of these environments arise in a network of simulated neurons with “flickering” connectivity. We find that despite transient connectivity the network of place cells produces a stable representation of the topology of the environment.

**10:12AM K35.00010 Efficient Signal Processing in Random Networks that Generate Variability: A Comparison of Internally Generated and Externally Induced Variability**, SAKYASINGHA DASGUPTA, RIKEN Brain Science Institute, ISAO NISHIKAWA, Institute of Industrial Science, The University of Tokyo, KAZUYUKI AIHARA, Department of Mathematical Informatics, The University of Tokyo, TARO TOYOIZUMI, RIKEN Brain Science Institute — Source of cortical variability and its influence on signal processing remain an open question. We address the latter, by studying two types of balanced randomly connected networks of quadratic I-F neurons, with irregular spontaneous activity: (a) a deterministic network with strong connections generating noise by chaotic dynamics (b) a stochastic network with weak connections receiving noisy input. They are analytically tractable in the limit of large network-size and channel time-constant. Despite different sources of noise, spontaneous activity of these networks are identical unless majority of neurons are simultaneously recorded. However, the two networks show remarkably different sensitivity to external stimuli. In the former, input reverberates internally and can be read out over long time, but in the latter, inputs rapidly decay. This is further enhanced with activity-dependent plasticity at input synapses producing marked difference in decoding inputs from neural activity. We show, this leads to distinct performance of the two networks to integrate temporally separate signals from multiple sources, with the deterministic chaotic network activity serving as reservoir for Monte Carlo sampling to perform near optimal Bayesian integration, unlike its stochastic counterpart.

**10:24AM K35.00011 Inference of pain stimulus level from stereotypical behavioral response of *C.elegans* allows quantification of effects of anesthesia and mutation**<sup>1</sup>, KAWAI LEUNG, Emory University, AYLIA MOHAMMADI, WILLIAM RYU, University of Toronto, ILYA NEMENMAN, Emory University — In animals, we must infer the pain level from experimental characterization of behavior. This is not trivial since behaviors are very complex and multidimensional. To establish *C.elegans* as a model for pain research, we propose for the first time a quantitative model that allows inference of a thermal nociceptive stimulus level from the behavior of an individual worm. We apply controlled levels of pain by locally heating worms with an infrared laser and capturing the subsequent behavior. We discover that the behavioral response is a product of stereotypical behavior and a nonlinear function of the strength of stimulus. The same stereotypical behavior is observed in normal, anesthetized and mutated worms. From this result we build a Bayesian model to infer the strength of laser stimulus from the behavior. This model allows us to measure the efficacy of anaesthetization and mutation by comparing the inferred strength of stimulus. Based on the measured nociceptive escape of over 200 worms, our model is able to significantly differentiate normal, anaesthetized and mutated worms with 40 worm samples.

<sup>1</sup>This work was partially supported by NSF grant No. IOS/1208126 and HFSP grant No. RGY0084/

**10:36AM K35.00012 *Drosophila* photo-taxis and odor-taxis are mediated by a shared computational pathway**, MIRNA MIHOVILOVIC SKANATA, RUBEN GEPNER, NATALIE BERNAT, MARGARITA KAPLOW, MARC GERSHOW, New York University — In natural environments, the *Drosophila* larva makes navigational decisions based on variable and conflicting sensory inputs. How larvae respond to multi-modal stimuli and how their neural circuits integrate and prioritize multi-sensory information remains unknown. To identify larval navigational computations we developed a high-throughput reverse-correlation assay. We provided larvae with visual and optogenetically induced fictive olfactory stimuli and measured the correlation between the presented stimulus and evoked turn decisions. We used this technique to fit parameters of a Linear-Nonlinear-Poisson model describing computations underlying turn decisions. For uni-modal inputs, the parameterized model allowed us to predict the behavior of populations of larvae responding to novel stimulus presentations. For multi-modal inputs, our assay showed that larvae linearly combine olfactory and visual signals upstream of the decision to turn. We verified this prediction using controlled combinations of stimuli. We studied other navigational decisions that determine the size and directions of turns and found that larvae integrated odor and light according to the same rule in all cases. These results suggest that photo-taxis and odor-taxis are mediated by a shared computational pathway.

**Wednesday, March 16, 2016 8:00AM - 11:00AM –**  
**Session K36 GSOF DPOLY DCOMP: Coarse-graining, Advanced Sampling and Multiscale Methods in Soft Matter** 339 - Gopinath Subramanian, University of Southern Mississippi

**8:00AM K36.00001 Long-time atomistic simulations with the Parallel Replica Dynamics method**<sup>1</sup>, DANNY PEREZ, Los Alamos National Laboratory — Molecular Dynamics (MD) — the numerical integration of atomistic equations of motion — is a workhorse of computational materials science. Indeed, MD can in principle be used to obtain any thermodynamic or kinetic quantity, without introducing any approximation or assumptions beyond the adequacy of the interaction potential. It is therefore an extremely powerful and flexible tool to study materials with atomistic spatio-temporal resolution. These enviable qualities however come at a steep computational price, hence limiting the system sizes and simulation times that can be achieved in practice. While the size limitation can be efficiently addressed with massively parallel implementations of MD based on spatial decomposition strategies, allowing for the simulation of trillions of atoms, the same approach usually cannot extend the timescales much beyond microseconds. In this article, we discuss an alternative parallel-in-time approach, the Parallel Replica Dynamics (ParRep) method, that aims at addressing the timescale limitation of MD for systems that evolve through rare state-to-state transitions. We review the formal underpinnings of the method and demonstrate that it can provide arbitrarily accurate results for any definition of the states. When an adequate definition of the states is available, ParRep can simulate trajectories with a parallel speedup approaching the number of replicas used. We demonstrate the usefulness of ParRep by presenting different examples of materials simulations where access to long timescales was essential to access the physical regime of interest and discuss practical considerations that must be addressed to carry out these simulations.

<sup>1</sup>Work supported by the United States Department of Energy (U.S. DOE), Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division.

**8:36AM K36.00002 Investigating the impact of representation upon coarse-grained models**<sup>1</sup>, THOMAS FOLEY<sup>2</sup>, Pennsylvania State University, M SCOTT SHELL<sup>3</sup>, University of California, Santa Barbara, WILLIAM NOID<sup>4</sup>, Pennsylvania State University — The first step in building a coarse-grained (CG) model is choosing a representation or 'mapping' of the original system at a reduced resolution. In practice, the mapping is often chosen on the basis of 'physical intuition.' Consequently this crucial step would greatly benefit from the development of systematic and principled methodologies. Accordingly, we have studied the relationship between the mapping and the resulting CG model. As a starting point, we have analytically derived, as a function of the CG mapping, the exact many-body potential of mean force (PMF) for the simple Gaussian Network Model (GNM) of protein fluctuations. We use this as a simple model for investigating the effect of the CG mapping upon the information loss and quality of the CG model. Moreover, by considering the GNM's for different proteins, we investigate the significance of high resolution structural features for the quality of the CG model.

<sup>1</sup>We acknowledge support from the NSF, Alfred P. Sloan Foundation, and KITP.

<sup>2</sup>Department of Physics and Chemistry

<sup>3</sup>Department of Chemical Engineering

<sup>4</sup>Department of Chemistry

**8:48AM K36.00003 Non-Markovian coarse-grained modeling of polymeric fluids based on the Mori-Zwanzig formalism<sup>1</sup>**, ZHEN LI, XIN BIAN, Brown University, XIANTAO LI, Pennsylvania State University, GEORGE KARNIADAKIS, Brown University — The Mori-Zwanzig formalism for coarse-graining a complex dynamical system typically introduces memory effects. The Markovian assumption of delta-correlated fluctuating forces is often employed to simplify the formulation of coarse-grained (CG) models and numerical implementations. However, when the time scales of a system are not clearly separated, the memory effects become strong and the Markovian assumption becomes inaccurate. To this end, we incorporate memory effects into CG modeling by preserving non-Markovian interactions between CG variables based on the Mori-Zwanzig formalism. For a specific example, molecular dynamics (MD) simulations of star polymer melts are performed while the corresponding CG system is defined by grouping many bonded atoms into single clusters. Then, the effective interactions between CG clusters as well as the memory kernel are obtained from the MD simulations. The constructed CG force field with a memory kernel leads to a non-Markovian dissipative particle dynamics (NM-DPD). Quantitative comparisons on both static and dynamic properties between the CG models with Markovian and non-Markovian approximations will be presented.

<sup>1</sup>Supported by the DOE Center on Mathematics for Mesoscopic Modeling of Materials (CM4) and an INCITE grant

**9:00AM K36.00004 A new graph-matching-based algorithm to study dynamical processes<sup>1</sup>**, FAUSTO MARTELLI, HSIN-YU KO, ROBERTO CAR, Princeton University — We present a new algorithm to identify and quantify the degree of local order in dynamical systems. To each particle site we associate a given number of neighboring sites the positions of which define the nodes of a pattern graph. We match this graph with a graph describing the geometry of an ordered reference system. The degree of overlap is obtained by recursively maximizing a score function having a value ranging from 0 (in the case of a completely disordered system) to 1 (in the case of a perfect crystal). While typically order parameters are tailored to specific cases, our approach is general and could be applied to different areas of condensed matter physics. Here we illustrate the approach with applications to atomic and molecular fluids, namely melting of Lennard Jones particles, direct crystallization of supercooled water and melting of Yukawa crystals.

<sup>1</sup>Scientific Discovery through Advanced Computing (SciDAC) program; the Department of Energy (DOE), grant number DESC0008626

**9:12AM K36.00005 HOMOGENOUS NUCLEATION AND CRYSTAL GROWTH IN A MODEL LIQUID FROM DIRECT ENERGY LANDSCAPE SAMPLING SIMULATION**, NATHAN WALTER, YANG ZHANG, University of Illinois at Champaign-Urbana — Nucleation and crystal growth are understood to be activated processes involving the crossing of free-energy barriers. Attempts to capture the entire crystallization process over long timescales with molecular dynamic simulations have met major obstacles because of molecular dynamics' temporal constraints. Herein, we circumvent this temporal limitation by using a brutal-force, metadynamics-like, adaptive basin-climbing algorithm and directly sample the free-energy landscape of a model liquid Argon. The algorithm biases the system to evolve from an amorphous liquid like structure towards an FCC crystal through inherent structure, and then traces back the energy barriers. Consequently, the sampled timescale is macroscopically long. We observe that the formation of a crystal involves two processes, each with a unique temperature-dependent energy barrier. One barrier corresponds to the crystal nucleus formation; the other barrier corresponds to the crystal growth. We find the two processes dominate in different temperature regimes. Compared to other computation techniques, our method requires no assumptions about the shape or chemical potential of the critical crystal nucleus. The success of this method is encouraging for studying the crystallization of more complex

**9:24AM K36.00006 Dynamical Density Functional Theory and Hydrodynamic Interactions in Confined Systems<sup>1</sup>**, BENJAMIN GODDARD, University of Edinburgh, SERAFIM KALLIADAKIS, ANDREAS NOLD, Imperial College London — Colloidal systems consist of nano-micrometer sized particles suspended in a bath of many more, much smaller and much lighter particles. When the colloidal particles move through the bath, e.g. when driven by external forces such as gravity, flows are induced in the bath. These flows in turn impart forces on the colloid particles. These bath-mediated forces, known as Hydrodynamic Interactions (HI) strongly influence the dynamics of the colloid particles. This is particularly true in confined systems, in which the presence of walls substantially modifies the HI compared to unbounded geometries. For many-particle systems, the number of degrees of freedom prohibit a direct solution of the underlying stochastic equations and a reduced model is necessary. We model such systems through Dynamical Density Functional Theory (DDFT), the computational complexity of which is independent of the number of particles. We include both inter-particle and particle-wall HI, demonstrating both their combined and relative effects.

<sup>1</sup>Funded by EPSRC grant no EP/L025159/1

**9:36AM K36.00007 Nondecaying hydrodynamic interactions along narrow channels**, KAROLIS MISIUNAS, STEFANO PAGLIARA, ERIC LAUGA, JOHN R LISTER, ULRICH KEYSER, University of Cambridge — Particle-particle interactions are of paramount importance in every multi-body system as they determine the collective behaviour and coupling strength. Many well-known interactions like electrostatic, van der Waals or screened Coulomb, decay exponentially or with negative powers of the particle spacing  $r$ . Similarly, hydrodynamic interactions between particles undergoing Brownian motion decay as  $1/r$  in bulk, and are assumed to decay in small channels. Such interactions are ubiquitous in biological and technological systems. Here we confine two particles undergoing Brownian motion in narrow, microfluidic channels and study their coupling through hydrodynamic interactions. Our experiments show that the hydrodynamic particle-particle interactions are distance-independent in these channels. This finding is of fundamental importance for the interpretation of experiments where dense mixtures of particles or molecules diffuse through finite length, water-filled channels or pore networks.

**9:48AM K36.00008 Topological properties and edge mode effects in classical thermal transport**, CHIHCHUN CHIEN, University of California, Merced, KIRILL VELIZHANIN, Los Alamos National Laboratory, YONATAN DUBI, Ben Gurion University, Israel, MICHAEL ZWOLAK, National Institute of Science and Technologies — Classical harmonic chains, with suitable parametrizations, can resemble quantum systems exhibiting interesting topological phases. By analytically solving the equations of motion of harmonic chains with alternating masses and coupling constants, the energy bands bear striking resemblance to topological electronic bands of the Su-Schrieffer-Heeger model. As a consequence, localized topological edge modes associated with topological invariants of the system arise in classical harmonic chains. Effects from topological properties on thermal transport through patterned harmonic chains are analyzed and the results are supported by molecular-dynamics simulations. We also found edge modes as a hindrance to achieving the maximal intrinsic thermal conductance. Possible applications in polymers will be discussed.

**10:00AM K36.00009 Durability of Long Equipartition Times In Anharmonic Oscillator Chains**, CHRISTOPHER WATENPOOL, DONALD PRIOUR, Youngstown State University — Vibrational modes, completely decoupled in the case of a purely harmonic chain do not interact, thereby preventing an even spread of energy over both low and high frequency states. The distribution of energy beyond a small set of initially excited modes, known as equipartition, proceeds over finite time scales with the admixture of an anharmonic term. However, in many cases (e.g.  $V(x) = \alpha x^2 + \beta x^4$ ), the transfer of energy from low to high frequency modes is hampered for an isolated chain, with equipartition times diverging with increasing system size. Using Molecular Dynamics simulations we relax the isolation condition, gradually coupling the ends of the chain to a thermal bath. Calculating equipartition times for various coupling strengths, we seek to determine if: (i) The bulk limit divergence persists for any coupling strength, (ii) Bulk equipartition times are finite beyond a coupling threshold, or (iii) Coupling to a thermal bath has a singular effect and yields finite equipartition times for any nonzero coupling strength.

**10:12AM K36.00010 Coarse-grained description of polymer blends as chains of interacting soft particles**, KEVIN WALTON, Department of Physics, University of Oregon, Eugene, Oregon 97403, MARINA GUENZA, Department of Chemistry, University of Oregon, Eugene, Oregon 97403 — We present an analytic pair potential in a coarse grain description of a polymer blend where each chain is represented as a chain of soft-colloidal particles. This coarse grain model is based on integral theory that can represent the chains at variable levels. The particles have soft repulsion at separation less than the size of each coarse grain unit and a long repulsive tail with small attractive portion. While the short range pieces of the potential dominates the liquid structure, the long range tail dominates the thermodynamics of the system. So an accurate potential in both the short and long range distances is needed to keep give correct structure and thermodynamical properties in the coarse grain description.

**10:24AM K36.00011 Langevin Equation for DNA Dynamics**, DAVID GRZYCH, JEREMY COPPERMAN, Univ of Oregon Dept. of Physics, MARINA GUENZA, Univ of Oregon Dept. of Chemistry — Under physiological conditions, DNA oligomers can contain well-ordered helical regions and also flexible single-stranded regions. We describe the site-specific motion of DNA with a modified Rouse-Zimm Langevin equation formalism that describes DNA as a coarse-grained polymeric chain with global structure and local flexibility. The approach has successfully described the protein dynamics in solution and has been extended to nucleic acids. Our approach provides diffusive mode analytical solutions for the dynamics of global rotational diffusion and internal motion. The internal DNA dynamics present a rich energy landscape that accounts for an interior where hydrogen bonds and base-stacking determine structure and experience limited solvent exposure. We have implemented several models incorporating different coarse-grained sites with anisotropic rotation, energy barrier crossing, and local friction coefficients that include a unique internal viscosity and our models reproduce dynamics predicted by atomistic simulations. The models reproduce bond autocorrelation along the sequence as compared to that directly calculated from atomistic molecular dynamics simulations. The Langevin equation approach captures the essence of DNA dynamics without a cumbersome atomistic representation.

**10:36AM K36.00012 Improving the kinetics from molecular simulations using biased Markov state models**, JOSEPH F RUDZINSKI, KURT KREMER, TRISTAN BERAUD, Max Planck Institute for Polymer Research — Molecular simulations can provide microscopic insight into the physical and chemical driving forces of complex molecular processes. Despite continued advancement of simulation methodology, model errors may lead to inconsistencies between simulated and experimentally-measured observables. This work presents a robust and systematic framework for reweighting the ensemble of dynamical paths sampled in a molecular simulation in order to ensure consistency with a set of given kinetic observables. The method employs the well-developed Markov state modeling framework in order to efficiently treat simulated dynamical paths. We demonstrate that, for two distinct coarse-grained peptide models, biasing the Markov state model to reproduce a small number of reference kinetic constraints significantly improves the dynamical properties of the model, while simultaneously refining the static equilibrium properties.

**10:48AM K36.00013 Multiscale Modeling of the Electrocaloric Effect in PVDF-based Polymers**, ALAN MCGAUGHEY, YING-JU YU, Carnegie Mellon University — We apply multi-scale modeling to explore the electrocaloric (EC) effect in PVDF-related ferroelectric polymers, which have application in active cooling of microsystems. The EC effect is the temperature rise and drop in some ferroelectric materials due to changes in the configurational entropy when an external electric field is applied and removed. The polymer is modeled as a series of bi-directional permanent dipoles and induced point dipoles distributed on its monomer sites. The flipping of these dipoles due to an applied electric field leads to polarization changes. Flipping the dipole moment of the polymer chain requires rotation of the individual monomers, each of which has its own energy barrier. This energy pathway is predicted from atomic-level nudged elastic band method calculations for a variety of chain environments. We then use first-passage time analysis to convert each energy pathway into an average transition rate for a full polymer chain rotation. The transition rates for all chains are integrated into a kinetic Monte Carlo algorithm in which the polarization change due to the application of an electric field is determined.

## Wednesday, March 16, 2016 8:00AM - 11:00AM —

Session K37 GSOF: Soft Matter at Interfaces (Particles) 340 - Michael Rubenstein, Univ. North Carolina

**8:00AM K37.00001 Soft particles at fluid interfaces: wetting, structure, and rheology.**<sup>1</sup>, LUCIO ISA, ETH Zurich — Most of our current knowledge concerning the behavior of colloidal particles at fluid interfaces is limited to model spherical, hard and uniform objects. Introducing additional complexity, in terms of shape, composition or surface chemistry or by introducing particle softness, opens up a vast range of possibilities to address new fundamental and applied questions in soft matter systems at fluid interfaces. In this talk I will focus on the role of particle softness, taking the case of core-shell microgels as a paradigmatic example. Microgels are highly swollen and cross-linked hydrogel particles that, in parallel with their practical applications, e.g. for emulsion stabilization and surface patterning, are increasingly used as model systems to capture fundamental properties of bulk materials. Most microgel particles develop a core-shell morphology during synthesis, with a more cross-linked core surrounded by a corona of loosely linked and dangling polymer chains. I will first discuss the difference between the wetting of a hard spherical colloid and a core-shell microgel at an oil-water interface, pinpointing the interplay between adsorption at the interface and particle deformation. I will then move on to discuss the interplay between particle morphology and the microstructure and rheological properties of the interface. In particular, I will demonstrate that synchronizing the compression of a core-shell microgel-laden fluid interface with the deposition of the interfacial monolayer makes it possible to transfer the 2D phase diagram of the particles onto a solid substrate, where different positions correspond to different values of the surface pressure and the specific area. Using atomic force microscopy, we analyzed the microstructure of the monolayer and discovered a phase transition between two crystalline phases with the same hexagonal symmetry, but with two different lattice constants. The two phases correspond to shell-shell or core-core inter-particle contacts, respectively, where with increasing surface pressure the former mechanically fail enabling the particle cores to come into contact. In the phase-transition region, clusters of particles in core-core contacts nucleate, melting the surrounding shell-shell crystal, until the whole monolayer moves into the second phase. We furthermore extended our analysis to measure the interfacial rheology of the monolayers as a function of the surface pressure using an interfacial microdisk rheometer; the interfaces always show a strong elastic response, with a dip in the elastic modulus in correspondence of the melting of the shell-shell phase, followed by a steep increase upon formation of a percolating network of the core-core contacts. The presented results highlight the complex interplay between the wetting and deformation of individual soft particles at fluid interfaces and the overall interface microstructure and mechanics. They show strong connections to fundamental studies on phase transitions in two-dimensional systems and pave the way for novel nanoscale surface patterning routes.

<sup>1</sup>The author acknowledges financial support from the Swiss National Science Foundation Grant PP00P2-144646/1

**8:36AM K37.00002 Sculpting Pickering Emulsion Droplets by Arrest and Jamming**<sup>1</sup>, CHRISTOPHER BURKE, Tufts Univ, ZENGYI WEI, University of New South Wales, MARCO CAGGIONI, Proctor & Gamble, PATRICK SPICER, University of New South Wales, TIM ATHERTON, Tufts Univ — Pickering emulsion droplets can be arrested into non-spherical shapes—useful for applications such as active delivery—through a general mechanism of deformation followed by absorption of additional colloidal particles onto the interface, relaxation of the droplet caused by surface tension and arrest at some point due to crowding of the particles. We perform simulations of the arrest process to clarify the relative importance of diffusive rearrangement of particles and collective forcing due to surface evolution. Experiment and theory are compared, giving insight into the stability of the resulting capsules and the robustness of the production process for higher-throughput production in, for example, microfluidic systems. We adapt theoretical tools from the jamming literature to better understand the arrested configurations and long timescale evolution of the system: using linear programming and a penalty function approach, we identify unjamming motions in kinetically arrested states. We propose a paradigm of metric jamming to describe the limiting behavior of this class of system: a structure is metric-jammed if it is stable with respect to collective motion of the particles as well as evolution of the hypersurface on which the packing is embedded.

<sup>1</sup>Supported by a Cottrell Award from the Research Corporation for Science Advancement

### 8:48AM K37.00003 Droplets on a deformable membrane with uniform and anisotropic tension

, RAFAEL SCHULMAN, McMaster University, RENÉ LEDESMA-ALONSO, THOMAS SALEZ, ELIE RAPHAËL, ESPCI, KARI DALNOKI-VERESS, McMaster University — We examine the deformation produced by micro-droplets atop thin elastomeric free-standing films. Under the action of surface tension, the droplets deform the membrane thereby forming a bulge. For films with isotropic tension, we measure the contact angles of the droplet and bulge relative to the planar film surrounding the droplet as a function of membrane tension. We find the measured contact angles to be in excellent agreement with a model which features a force balance at the contact line. Experiments are also performed on membranes with anisotropic tension and compared to theory. In this case, droplets are non-spherical and generate significant deformation of the surrounding film which becomes non-planar.

### 9:00AM K37.00004 Capillary Forces between Floating Objects: Superhydrophobic Surfaces Provide Mechanistic Insight

, MINCHAO ZHANG, THOMAS J. MCCARTHY, ALFRED J. CROSBY, Univ of Mass - Amherst — When two floating objects are close, they will either move towards or away from one another to minimize the energy caused by the overlap of the liquid/air interfacial deformations. Capillary forces cause these behaviors, but directly relating the interfacial deformations and the capillary interactions hasn't been explored experimentally. We choose a liquid marble, which has a superhydrophobic surface, as a free floating object and a fixed "wall" with carefully controlled contact angle as another object to generate two deformations at the interface. When the liquid marble is close to the wall, the two deformations interact, causing changes in the Laplace pressure at the interface and a reconfiguration of the interface. In response, the liquid marble moves either towards or away from the wall. Using image analysis of videos recording the liquid marble position as a function of time, we measured the liquid marble to wall distance and determine the spatio-temporal relationships. Furthermore, capillary forces were calculated from the velocities and accelerations. Based on this data, we present a new explanation for the capillary interactions from the perspective of Laplace pressure changing induced the reconfiguration of the interfacial deformations.

### 9:12AM K37.00005 Adsorption-desorption kinetics of soft particles onto surfaces

, BRENDAN OSBERG, ULRICH GERLAND, Technische Universität München — A broad range of physical, chemical, and biological systems feature processes in which particles randomly adsorb on a substrate. Theoretical models usually assume hard (mutually impenetrable) particles, but in soft matter physics the adsorbing particles can be effectively compressible, implying soft interaction potentials. We recently studied the kinetics of such soft particles adsorbing onto one-dimensional substrates, identifying three novel phenomena: (i) a gradual density increase, or "cramming", replaces the usual jamming behavior of hard particles, (ii) a density overshoot, can occur (only for soft particles) on a time scale set by the desorption rate, and (iii) relaxation rates of soft particles increase with particle size (on a lattice), while hard particles show the opposite trend. The latter occurs since unjamming requires desorption and many-bodied reorganization to equilibrate - a process that is generally very slow. Here we extend this analysis to a two-dimensional substrate, focusing on the question of whether the adsorption-desorption kinetics of particles in two dimensions is similarly enriched by the introduction of soft interactions. Application to experiments, for example the adsorption of fibrinogen on two-dimensional surfaces, will be discussed.

### 9:24AM K37.00006 Adsorption dynamics of colloidal ellipsoids at oil-water interfaces

, ANNA WANG, W. BENJAMIN ROGERS, VINOTHAN N. MANOHARAN, Harvard University — Nonspherical particles at immiscible fluid interfaces have strong interactions with each other and with the curvature of the host interface. However, the dynamics of nonspherical colloidal particles attaching to an interface have not yet been studied. We use digital holographic microscopy to image micron-sized polystyrene ellipsoids breaching an oil-water interface at hundreds of frames per second. We show that the particle height and polar angle have large fluctuations, but both change approximately logarithmically with time, likely due to contact line pinning on the surface of the particle. Equilibrium is reached on a timescale at least three orders of magnitude slower than that expected from Langevin dynamics simulations [1]. We also find that all the trajectories collapse into straight lines when we plot particle polar angle as a function of particle height, unlike the trajectories seen in simulation [1,2]. The differences between experiment and simulation suggest that contact line pinning and the shape of the three phase contact line may strongly influence the dynamics of particle adsorption. [1] The Journal of Chemical Physics 132 (16), 164902, (2010) [2] Soft Matter 10, 4977-4989 (2014)

### 9:36AM K37.00007 Phase Behavior of 2D Charged Hydrophobic Colloids in Flat and Curved

Space, COLM KELLEHER, RODRIGO GUERRA, PAUL CHAIKIN, Dept. of Physics, New York University — Charged hydrophobic colloids, when dispersed in oil with a relatively high dielectric constant, can become highly charged. In the presence of an interface with a conducting aqueous phase, particles bind strongly to the interface via image-charge attraction. At sufficiently high density, these charged interfacial particles self-organize into a 2D repulsive (Wigner) crystalline solid phase, while at lower densities, the particles form a 2D fluid. By observing samples prepared at different densities, we can probe various points in the phase diagram of this soft 2D material, and compare our results with applicable theory and simulations. In this talk, we present two sets of experiments we have performed on this system: first, we show how we can use gravity as an external force to create a controlled density gradient, and thereby directly measure the equation of state and other quantities of interest. Second, we discuss how, by observing particles which are bound to the surface of spherical droplets, we can explore how the presence of finite background curvature affects the phase behavior of the system.

### 9:48AM K37.00008 Bidispersed Sphere Packing on Spherical Surfaces<sup>1</sup>

, TIMOTHY ATHERTON, ANDREW MASCIOLI, CHRISTOPHER BURKE, Tufts University — Packing problems on spherical surfaces have a long history, originating in the classic Thompson problem of finding the ground state configuration of charges on a sphere. Such packings contain a minimal number of defects needed to accommodate the curvature; this is predictable using the Gauss-Bonnet theorem from knowledge of the topology of the surface and the local symmetry of the ordering. Famously, the packing of spherical particles on a sphere contains a 'scar' transition, where additional defects over those required by topology appear above a certain critical number of particles and self-organize into chains or scars. In this work, we study the packing of bidispersed packings on a sphere, and hence determine the interaction of bidispersity and curvature. The resultant configurations are nearly crystalline for low values of bidispersity and retain scar-like structures; these rapidly become disordered for intermediate values and approach a so-called Apollonian limit at the point where smaller particles can be entirely accommodated within the voids left by the larger particles. We connect our results with studies of bidispersed packings in the bulk and on flat surfaces from the literature on glassy systems and jamming.

<sup>1</sup>Supported by a Cottrell Award from the Research Corporation for Science Advancement

### 10:00AM K37.00009 Dynamics of particles and defects on spherical crystals

, RODRIGO GUERRA, COLM KELLEHER, PAUL CHAIKIN, New York Univ NYU — Repulsive particles confined to two dimensions can form nearly perfect crystals that melt via the well-known Kosterlitz-Thouless two-step process. By contrast, when identical particles are confined to the surface of a sphere, the curvature and topology of the surface distort the crystal lattice and forces it to accommodate point-like disclinations and chains of dislocations. Extensive numerical and theoretical investigation has shown that these extended scars are intrinsic to the ground-state-energy configuration of these packings, as they relieve some of the stress induced by the curvature of the surface. Nevertheless, the effect of these defects on the kinetics and phase behavior of spherical crystals is not at all well understood. Here we present results of computer simulations and experiments that suggest that these scars facilitate the motion of particles close to them and fundamentally alter the nature of the mobility and liquid-to-solid transition of packings of particles confined to spherical surfaces.

**10:12AM K37.00010 Phase nucleation in curved space**, LEOPOLDO GÓMEZ, NICOLÁS GARCÍA, Department of Physics, Universidad Nacional del Sur-CONICET. Argentina., VINCENZO VITELLI, Instituut-Lorentz, Universiteit Leiden, The Netherlands., JOS LORENZANA, Institute for Complex Systems, Consiglio Nazionale delle Ricerche, Italy, VEGA DANIEL, Department of Physics, Universidad Nacional del Sur-CONICET. Argentina. — Nucleation and growth is the dominant relaxation mechanism driving first-order phase transitions. In two-dimensional flat systems, nucleation has been applied to a wide range of problems in physics, chemistry and biology. Here we study nucleation and growth of two-dimensional phases lying on curved surfaces and show that curvature modifies both critical sizes of nuclei and paths towards the equilibrium phase. In curved space, nucleation and growth becomes inherently inhomogeneous and critical nuclei form faster on regions of positive Gaussian curvature. Substrates of varying shape display complex energy landscapes with several geometry-induced local minima, where initially propagating nuclei become stabilized and trapped by the underlying curvature (Gómez, L. R. et al. Phase nucleation in curved space. Nat. Commun. 6:6856 doi: 10.1038/ncomms7856 (2015).).

**10:24AM K37.00011 Clusters of polyhedra in spherical confinement**<sup>1</sup>, ERIN TEICH, GREG VAN ANDERS, DAPHNE KLOTSAS<sup>2</sup>, JULIA DSHEMUCHADSE, SHARON GLOTZER, University of Michigan — Dense particle packing in a confining volume is a rich, largely unexplored problem, with applications in blood clotting, plasmonics, industrial packaging and transport, colloidal molecule design, and information storage. We report simulation results for dense clusters of the Platonic solids in spherical confinement, for up to  $N = 60$  constituent particles. We discuss similarities between clusters in terms of symmetry, a connection to spherical codes, and generally the interplay between isotropic geometrical confinement and anisotropic particle shape. Our results showcase the structural diversity and experimental utility of families of solutions to the problem of packing in confinement.

<sup>1</sup>E.T. acknowledges support by the National Science Foundation Graduate Research Fellowship under Grant No. DGE 1256260.

<sup>2</sup>Current affiliation: University of North Carolina

**10:36AM K37.00012 Computer Simulation study of polyhedral nanoparticle self-assembly at interfaces.**, VIKRAM THAPAR, UNMUKT GUPTA, FERNANDO ESCOBEDO, Cornell University — The self-assembly of polyhedral particles confined to a fluid-fluid interface is studied using Monte Carlo simulations. Several polyhedral shapes are studied, which are selected from a family of truncated cubes which include cubes, cuboctahedra, and octahedra. First we studied the case of hard particles pinned to the interface by restricting their movement in the direction perpendicular to it while allowing their free rotations. Our results suggest that the known solid phases and mesophases of these shapes in the 3D bulk are "translated" into variants in 2D space. These insights on 2D entropic self-assembly of polyhedral particles is a first step toward understanding the self-assembly of particles at fluid-fluid interfaces, which is driven by a complex interplay of entropic and enthalpic forces. As a second step we hence studied the particle-surface and particle-particle interactions associated with a fluid-fluid interface using both continuum and polybead models to assess the role of enthalpic interactions in determining the particle orientation behavior with respect to interface. We find that the thickness of the interface can introduce non-trivial effects on the preferential particle orientations.

**10:48AM K37.00013 The Relationship between Self-Assembly and Conformal Mappings**, CARLOS DUQUE, CHRISTIAN SANTANGELO, University of Massachusetts Amherst — The isotropic growth of a thin sheet has been used as a way to generate programmed shapes through controlled buckling. We discuss how conformal mappings, which are transformations that locally preserve angles, provide a way to quantify the area growth needed to produce a particular shape. A discrete version of the conformal map can be constructed from circle packings, which are maps between packings of circles whose contact network is preserved. This provides a link to the self-assembly of particles on curved surfaces. We performed simulations of attractive particles on a curved surface using molecular dynamics. The resulting particle configurations were used to generate the corresponding discrete conformal map, allowing us to quantify the degree of area distortion required to produce a particular shape by finding particle configurations that minimize the area distortion.

## Wednesday, March 16, 2016 8:00AM - 11:00AM –

Session K38 DPOLY GSOF: Glasses Altered by Interfaces I 341 - Andrew Croll, North Dakota State University

**8:00AM K38.00001 Nanorheology of confined polymer films**, PAUL FOWLER, MARK ILTON, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON, Canada, JOSHUA D. MCGRAW, Dpartement de Physique, Ecole Normale Suprieure / PSL Research University, CNRS, 24 rue Lhomond, 75005 Paris, France, KARI DALNOKI-VERESS, Department of Physics & Astronomy and the Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON, Canada — Liquid films with a non-uniform thickness flatten in order minimize surface energy, a process driven by surface tension and mediated by viscosity. For a viscous thin film, the time evolution of the film height profile is accurately described by lubrication theory by the capillary-driven thin film equation. Previous experiments have successfully applied the thin film equation to measure the rheological properties of polymeric liquids. Here we probe confinement effects in thin polymer films. We measure the viscosity by tracking the levelling of surface perturbations with AFM. For films with thicknesses thinner than the end-to-end distance of the molecule we observe deviations from a thin film model with bulk viscosity.

**8:12AM K38.00002 Understanding the relationship between different measures of nanoconfinement effects on segmental dynamics and the glass transition.**<sup>1</sup>, DAVID SIMMONS, JAYACHANDRA HARI MANGALARA, WESTON MERLING, The University of Akron — Several decades of research have indicated that confinement of a polymer or other glass-forming material to a nanoscale domain can significantly alter its glass transition temperature and segmental dynamics. Such effects have been reported in thin films, nanolayered and block copolymers, ionomers, and semicrystalline polymers. These alterations in glass formation behavior have implications for applications ranging from microelectronics to water purification. Many of the major open questions in this field center on apparent differences in nanoconfinement effects as probed by different methods. Recent studies have reported substantial differences in the apparent magnitude, direction, and onset temperature of these effects as probed via ellipsometry, calorimetry, fluorescence, dielectric spectroscopy, neutron scattering, various measures of viscous relaxation, and simulation. Here we employ molecular dynamics simulations to elucidate relationships between different measures of nanoconfinement effects. Particular emphasis is placed on differences in the manner in which different metrologies average over interfacial gradients in dynamics and pseudothermodynamic properties.

<sup>1</sup>This material is based upon work supported by the National Science Foundation under Grant No. DMR1310433.

**8:24AM K38.00003 Length Scales of Local Glass Transition Temperature Gradients Near Soft and Hard Polymer-Polymer Interfaces**, ROMAN BAGLAY, CONNIE ROTH, Dept. of Physics, Emory University — Polymer-polymer interfaces are ubiquitous in polymer blends and block copolymers, while opening up another avenue for the study of interfacial perturbations to the local glass transition temperature  $T_g(z)$ . We have previously reported the full local  $T_g(z)$  profile across a glassy-rubbery polymer interface between polystyrene (PS) and poly(*n*-butyl methacrylate) (PnBMA), an 80 K difference in bulk  $T_g$  [Baglay & Roth, J Chem Phys 2015, 143, 111101]. By using local fluorescence measurements, we revealed how the  $T_g(z)$  profile extends hundreds of nanometers away from the interface showing an asymmetric behavior penetrating deeper into the glassy PS side relative to the composition profile. Here, we extend these measurements to investigate how the local  $T_g$  profile in PS varies when in contact with a variety of immiscible polymers whose  $T_g$ s vary between +90 K and -80 K relative to the bulk  $T_g$  of PS, so-called hard vs. soft confinement. The data reveal that the onset of local  $T_g$  deviation from bulk in PS occurs at two distinct length scales, which depend on whether PS is the low  $T_g$  component (hard confinement) or the high  $T_g$  component (soft confinement). In addition, we explore the influence of finite system size on the range of dynamics by the introduction of periodic boundary conditions, as is commonly encountered in computer simulations or block copolymer systems.

**8:36AM K38.00004 Glassy Dynamics Altered by a Free Surface**<sup>1</sup>, OPHELIA TSUI, Department of Physics and Division of Materials Science and Engineering, Boston University — Studies of polymer dynamics in thin films showed that a highly mobile region exists at the free surface of most if not all polymers. In this talk, I shall review some of these observations, with highlights given to the recent findings that chain flexibility and connectivity may on occasions be necessary for the free surface to exercise its influence. Afterward, I shall ponder on how the influence of the free surface may penetrate as far as several polymer radii of gyration into the inner region, as found both in experiments and simulations. Near the glass transition temperature, our MD simulations showed that the dynamics consist mainly of string-like particle hopping motions, as found by others. Importantly, as the temperature decreases, the hopping motions become increasingly repetitive and back-and-forth, contributing no structural relaxations. We propose that structural relaxations are then brought about by pair-interactions between strings. Near the free surface, however, similar repetitive hopping motions are only observed sufficiently far removed from the free surface. We propose that the free surface induces a penetrating surface mobile region by breaking the memory in the particle dynamics. A possible mechanism based on string interactions will be discussed.

<sup>1</sup>We are grateful to the support of NSF through project DMR-1310536 and Hong Kong GRF grant 15301014.

**9:12AM K38.00005 Understanding and characterizing the effect of nanoscale confinement on glass transition temperature and film dewetting of macrocyclic polystyrene**, LANHE ZHANG, Materials Science and Engineering, Northwestern University, RAVINDER ELUPULA, SCOTT GRAYSON, Department of Chemistry, Tulane University, JOHN TORKELOSON, Materials Science and Engineering, Department of Chemical and Biological Engineering, Northwestern University — There is a growing interest in the dynamics of different polymer topologies when confined to nanoscopic length scales. Macrocyclic polymers have attracted research interest because their lack of chain ends and cyclic topology has led to a range of unique physical properties. Cyclic polystyrene (*c*-PS) of well-defined molecular weight (MW) ranging from 2,300 to 8,700 g/mol was synthesized via click cyclization of dilute solutions of linear PS (*l*-PS) with azide and alkyne end functionalities. The click reaction enables nearly quantitative cyclization of *l*-PS. Differential scanning calorimetry was used to measure bulk glass transition temperature ( $T_g$ ) and fragility of *c*-PS, both of which exhibit less MW dependence compared to *l*-PS. Compared to thin *l*-PS films, thin *c*-PS films exhibited extraordinary stability against dewetting. 22-nm-thick *c*-PS films were nearly stable for up to 4 hr at bulk  $T_g + 45$  C; in contrast, 22-nm-thick *l*-PS films underwent severe dewetting. Nanoconfinement effects on  $T_g$  and fragility of *c*-PS are investigated using ellipsometry and/or fluorescence spectroscopy and compared to effects for *l*-PS precursors as well as commercial anionic *l*-PS standards.

**9:24AM K38.00006 The local segmental dynamics of polymer thin films.**<sup>1</sup>, C.M. ROLAND, RICCARDO CASALINI, Naval Research Laboratory, DANIELE PREVOSTO, MASSIMILIANO LABARDI, University of Pisa, LEI ZHU, ERIC BAER, Case Western University — The local segmental dynamics of poly(methyl methacrylate) (PMMA) in multi-layered films with polycarbonate was investigated using dielectric spectroscopy. The segmental relaxation time decreased with layer thickness down to 4 nm. However, two measures of the cooperativity of the dynamics, the breadth of the relaxation dispersion and the dynamic correlation volume, were unaffected by the film thickness. This absence of an effect of geometric confinement on the cooperativity, even when the confinement length scale approaches the correlation length scale, requires an asymmetric correlation volume; i.e., correlating regions having a string-like nature. To further probe the effect of layering on the segmental dynamics, we measured the segmental dynamics of poly(vinylacetate) thin films in contact with variously an aluminum interface, an incompatible polymer, and air (free surface). From local dielectric relaxation measurements using an AFM tip, the dynamics were observed to be faster in all thin film configurations compared to the bulk. However, no differences were observed for the various interfaces; capping the thin films with a rigid material accelerated the segmental motions equivalently to that for an air interface. This insensitivity of the dynamics to the nature of the interface affords a means to engineer thin films while maintaining desired mechanical properties.

<sup>1</sup>Work at NRL supported by the Office of Naval Research.

**9:36AM K38.00007 Synthesis and Characterization of Fluorescently Labeled Diblock Copolymers for Location-Specific Measurements of The Glass Transition Temperature**<sup>1</sup>, DANE CHRISTIE, RICHARD REGISTER, RODNEY PRIESTLEY, Princeton University — Interfaces play a determinant role in the size dependence of the glass transition temperature ( $T_g$ ) of polymers confined to nanometric length scales. Interfaces are intrinsic in diblock copolymers, which, depending on their molecular weight and composition, are periodically nanostructured in the bulk. As a result diblock copolymers are model systems for characterizing the effect of interfaces on  $T_g$  in bulk nanostructured materials. Investigating the effect of intrinsic interfaces on  $T_g$  in diblock copolymers has remained unexplored due to their small periodic length scale. By selectively incorporating trace amounts of a fluorescent probe into a diblock copolymer,  $T_g$  can be characterized relative to the diblock copolymer's intrinsic interface using fluorescence spectroscopy. Here, pyrene is selectively incorporated into the poly(methyl methacrylate) (PMMA) block of lamellar forming diblock copolymers of poly(butyl-*b*-methyl methacrylate) (PBMA-PMMA). Preliminary results show a correlation of  $T_g$  as measured by fluorescence with the onset of  $T_g$  as measured by calorimetry in labeled homopolymers of PMMA. This result is consistent with previous characterizations of  $T_g$  using fluorescence spectroscopy. In selectively labeled diblock copolymers  $T_g$  is found to vary systematically depending on the distance of the probe from the PBMA-PMMA interface.

<sup>1</sup>We acknowledge funding from the Princeton Center for Complex Materials, a MRSEC supported by NSF Grant DMR 1420541.

replacing MAR16-2015-001909

**9:48AM K38.00008 Glass Transition of Polystyrene Thin Films on Silicon Wafer Measured by Dynamic Mechanical Analysis and Ellipsometry**, CATHERYN JACKSON, Dow Chemical, Core RD, Collegeville, PA 19426, TIAN LAN, Departments of Chem. and Bio. Eng. and Mat. Sci. and Eng., Northwestern University, Evanston, Illinois 60208, STEFAN CAPORALE, Dow Chemical, Electronic Materials, Marlborough, MA 01752, JOHN TORKEKELSON, Departments of Chem. and Bio. Eng. and Mat. Sci. and Eng., Northwestern University, Evanston, Illinois 60208 — Measuring the glass transition temperature,  $T_g$ , of polymer films in the thickness range of 20-500 nm is non-routine but commercially important for polymer films used in applications such as membranes and electronic circuit boards. Various specialized methods have been used or developed to determine  $T_g$  in thin films, including thermal ellipsometry and many others. Differential scanning calorimetry (DSC) is a more conventional method that has been used to measure  $T_g$ , but since the thin films must be scraped from the wafer, consolidation and annealing can occur in the pan and may negate effects due to film thickness. Here we report results for polystyrene (PS) spin coated on silicon wafers in the range of 20-500 nm using a benchtop dynamic mechanical analyzer (DMA) in the 3-point bending mode. For the DMA, the peak  $\tan \delta$  temperature is related to the polymer  $T_g$  and effects due to confinement as a function of film thickness are compared to literature values. We use thermal ellipsometry as a control method to measure film thickness and  $T_g$  in parallel. Low level additives present in commercial PS were observed to strongly affect the results for thin films and are described.

**10:00AM K38.00009 Effects of Interfaces and Interactions on Stiffness-Confinement Behavior in Polymer Films: Characterization via Fluorescence and Nanoindentation**, SHADID ASKAR, MIN ZHANG, L BRINSON, JOHN TORKEKELSON, Northwestern Univ — Although stiffness-confinement effects in polymers have been well studied, disagreement exists regarding even the qualitative nature of such effects. With the exception of one experimental and several simulation studies that characterize stiffness gradients, all others report average stiffness-confinement behavior in polymers. These issues demonstrate the need for comparative studies that characterize stiffness gradients in polymers from interfaces. Here, we use a fluorescence technique that utilizes the sensitivity of pyrene dye fluorescence to local caging and nanoindentation to characterize stiffness gradients in the polymer model nanocomposites. Both techniques are in qualitative agreement that stiffness gradients extend a distance exceeding 100 nm from a substrate, and that stiffness-confinement effects are tunable via surface modification of the substrate. It is observed that PMMA supported on methylated cover glass exhibits less stiffening near the substrate compared to PMMA supported on cover glass with enhanced hydroxyl groups that can hydrogen bond with PMMA. PMMA supported on PDMS shows decreasing stiffness near the interface. These findings help address some of the inconsistencies observed in literature regarding stiffness-confinement effects.

**10:12AM K38.00010 Sidechain Dynamics Explain Dissimilar Strength of Nanoconfinement Effect in Polystyrene and Poly(methyl methacrylate) Free Standing Thin Films<sup>1</sup>**, DAVID HSU, WENJIE XIA, JAKE SONG, SINAN KETEN, Northwestern University — Despite substantially similar bulk glass transition temperature ( $T_g$ ) and other bulk properties, polystyrene (PS) and poly(methyl-methacrylate) (PMMA) exhibit characteristically different  $T_g$  depression in the free-standing ultrathin film configuration. The mechanism for this disparate  $T_g$ -nanoconfinement effect due to the free surfaces has not been fully explained. Here we utilize recently established chemically specific coarse grain (CG) models to qualitatively reproduce contrasting thickness dependent  $T_g$  and length scale of enhanced chain relaxation gradient in the interfacial layer. Vibrational mode analysis is utilized to uncover a relationship between the amplitude and frequency of sidechain fluctuations of reduced order models and the degree of  $T_g$ -nanoconfinement. By systematic variation of the distribution of mass in the sidechain versus the backbone, we demonstrate inertia-driven differences in sidechain fluctuations and  $T_g$ -nanoconfinement in the CG model. We hypothesize that mass distribution and sidechain flexibility are governing factors causing PS and PMMA free surface effect differences and also provide insight into broader nanoconfinement phenomena from past experiments.

<sup>1</sup>D.H., W.X., J.S., and S.K. acknowledge support by the University Partnership Initiative between Northwestern University and The Dow Chemical Company

**10:24AM K38.00011  $T_g$ -Confinement Effects in Polymer Thin Films, Nanotubes, and Nanospheres as Measured by DSC, Ellipsometry and Fluorescence**, JOHN TORKEKELSON, ANTHONY TAN, LAWRENCE CHEN, Northwestern Univ — The effect of nanoscale confinement on the glass transition temperature ( $T_g$ ) of supported and free-standing polymer films has been studied for two decades by various techniques. However, conventional DSC, which is the most common method for measuring  $T_g$  of bulk polymers, is not well suited for such measurements. Here, we demonstrate that  $T_g$ -confinement effects measured by conventional DSC in nanotubes of polymer supported in anodic aluminum oxide (AAO) templates compare well with  $T_g$ -confinement effects measured in supported polymer films by ellipsometry and fluorescence. We further show that  $T_g$ -confinement effect data for nanotubes obtained by fluorescence agree well with data obtained by DSC. Finally, we draw comparisons between the  $T_g$ -confinement behavior of nanoprecipitated polymer nanospheres as measured by fluorescence to  $T_g$ -confinement effects for both supported and free-standing polymer films. The roles, if any, of confinement dimensionality (1-D vs 2-D vs 3-D) and measurement technique on the observed  $T_g$ -confinement effect will be discussed.

**10:36AM K38.00012 Mechanophore activation in a crosslinked polymer matrix via instrumented indentation**, CHELSEA DAVIS, AARON FORSTER, JEREMIAH WOODCOCK, MUZHOU WANG, JEFFREY GILMAN, NIST - Natl Inst of Stds & Tech, MATERIAL MEASUREMENT LABORATORY TEAM — Recent advances in mechanically-activated fluorophores will enable a host of unique scientific challenges and opportunities to be addressed. Several mechanophores (MPs) in polymers have been reported, yet the specific deformation required to activate these molecules in a bulk polymer network has not been sufficiently specified. In an effort to develop the mechano-activation/deformation relationship of a spirolactam-based MP, scratches were applied to a MP-functionalized glassy crosslinked material at varying normal loads and lateral displacement rates. This experimental design allowed strain and strain rate effects to be decoupled. The fluorescence activation was then observed with a laser scanning confocal microscope. Areas of elastic and plastic deformation as well as brittle fracture were observed within each scratch as the normal loading of the indenter increased. The fluorescence intensity increased with increasing strain. Contact mechanics models are employed to demonstrate that relatively high degrees of strain are required to initiate the ring-opening activation transition within the spirolactam-based MP. These self-reporting damage sensors can be incorporated within polymeric coatings to allow real time structural health monitoring for a myriad of applications.

**10:48AM K38.00013 Why the Mechanical Properties of Cross-linked Polydimethylsiloxane Surface Enhance? — A First Principles Study**, ZHIFAN WANG, MENGTING JIN, YANNING ZHANG, Chengdu Green Energy and Green Manufacturing Technology RD Center, BEIJING COMPUTATIONAL SCIENCE RESEARCH CENTER COLLABORATION — Polydimethylsiloxane (PDMS) has been widely used in various areas due to its high flexibility, controllable mechanical properties, brilliant biocompatibility and low cost. Now more work on PDMS focus on tuning its surface physical and chemical properties. Our experimental group has shown that the top surface stiffness of PDMS is significantly enhanced after a surface treatment of hyperthermal hydrogen induced cross-linking (HHIC), without losing its inherent hydrophobicity. To understand why this, we investigated how the HHIC treatment changes the structure of PDMS molecules and chains, by using density functional theory (DFT) calculations with the nonlocal van der Waals interaction. The elastic and hydrophobic properties of PDMS, before and after the surface treatment, will be discussed then, providing deep understandings on the experimental observations. Our theoretical studies could give insights in the new development of HHIC tuning technology.

**Wednesday, March 16, 2016 8:00AM - 11:00AM — Session K39 DBIO: Evolutionary Design Principles of Bio-networks** 342 - Gabor Balazsi, Oleg Igoshin, Stony Brook University, Rice University

### **8:00AM K39.00001 Metabolic interactions and dynamics in microbial communities**, DANIEL SEGRE<sup>1</sup>,

Boston Univ — Metabolism, in addition to being the engine of every living cell, plays a major role in the cell-cell and cell-environment relations that shape the dynamics and evolution of microbial communities, e.g. by mediating competition and cross-feeding interactions between different species. Despite the increasing availability of metagenomic sequencing data for numerous microbial ecosystems, fundamental aspects of these communities, such as the unculturability of many isolates, and the conditions necessary for taxonomic or functional stability, are still poorly understood. We are developing mechanistic computational approaches for studying the interactions between different organisms based on the knowledge of their entire metabolic networks. In particular, we have recently built an open source platform for the Computation of Microbial Ecosystems in Time and Space (COMETS), which combines metabolic models with convection-diffusion equations to simulate the spatio-temporal dynamics of metabolism in microbial communities. COMETS has been experimentally tested on small artificial communities, and is scalable to hundreds of species in complex environments. I will discuss recent developments and challenges towards the implementation of models for microbiomes and synthetic microbial communities.

### **8:36AM K39.00002 Gene Expression Noise, Fitness Landscapes, and Evolution<sup>1</sup>**, DANIEL

CHARLEBOIS, Laufer Center for Physical and Quantitative Biology, Stony Brook University — The stochastic (or noisy) process of gene expression can have fitness consequences for living organisms. For example, gene expression noise facilitates the development of drug resistance by increasing the time scale at which beneficial phenotypic states can be maintained [1]. The present work investigates the relationship between gene expression noise and the fitness landscape [2]. By incorporating the costs and benefits of gene expression, we track how the fluctuation magnitude and timescale of expression noise evolve in simulations of cell populations under stress. We find that properties of expression noise evolve to maximize fitness on the fitness landscape, and that low levels of expression noise emerge when the fitness benefits of gene expression exceed the fitness costs (and that high levels of noise emerge when the costs of expression exceed the benefits). The findings from our theoretical/computational work offer new hypotheses on the development of drug resistance, some of which are now being investigated in evolution experiments in our laboratory using well-characterized synthetic gene regulatory networks in budding yeast. [1] D.A. Charlebois, N. Abdennur, M. Kaern, Gene expression noise facilitates adaptation and drug resistance independently of mutation, Physical Review Letters, 107, 218101 (2011). [2] D.A. Charlebois, Effect and Evolution of Gene Expression Noise on the Fitness Landscape, Physical Review E, 022713 (2015).

<sup>1</sup>NSERC Postdoctoral Fellowship (Grant No. PDF-453977-2014)

### **8:48AM K39.00003 Modularity Enhances the Rate of Evolution in a Rugged Fitness Landscape**

, DONG WANG, Rice University, JEONG-MAN PARK, Rice University and The Catholic University of Korea, MAN CHEN, MICHAEL DEEM, Rice University — Biological systems are modular, and this modularity affects the evolution of biological systems over time and in different environments. We here develop a theory for the dynamics of evolution in a rugged, modular fitness landscape. We show analytically how horizontal gene transfer couples to the modularity in the system and leads to more rapid rates of evolution at short times. The model, in general, analytically demonstrates a selective pressure for the prevalence of modularity in biology. We use this model to show how the evolution of the influenza virus is affected by the modularity of the proteins that are recognized by the human immune system. A modular model of the fitness landscape of the virus better fits the observed virus evolution data.

### **9:00AM K39.00004 In-silico studies of neutral drift for functional protein interaction networks**

, MD ZULFIKAR ALI, Clark University, NED S WINGREEN, Princeton University, RANJAN MUKHOPADHYAY, Clark University — We have developed a minimal physically-motivated model of protein-protein interaction networks. Our system consists of two classes of enzymes, activators (e.g. kinases) and deactivators (e.g. phosphatases), and the enzyme-mediated activation/deactivation rates are determined by sequence-dependent binding strengths between enzymes and their targets. The network is evolved by introducing random point mutations in the binding sequences where we assume that each new mutation is either fixed or entirely lost. We apply this model to studies of neutral drift in networks that yield oscillatory dynamics, where we start, for example, with a relatively simple network and allow it to evolve by adding nodes and connections while requiring that dynamics be conserved. Our studies demonstrate both the importance of employing a sequence-based evolutionary scheme and the relative rapidity (in evolutionary time) for the redistribution of function over new nodes via neutral drift. Surprisingly, in addition to this redistribution time we discovered another much slower timescale for network evolution, reflecting hidden order in sequence space that we interpret in terms of sparsely connected domains.

### **9:12AM K39.00005 Phase transitions in the evolution of gene regulatory networks**, ANTUN SKANATA,

EDO KUSSELL, New York Univ NYU — The role of gene regulatory networks is to respond to environmental conditions and optimize growth of the cell. A typical example is found in bacteria, where metabolic genes are activated in response to nutrient availability, and are subsequently turned off to conserve energy when their specific substrates are depleted. However, in fluctuating environmental conditions, regulatory networks could experience strong evolutionary pressures not only to turn the right genes on and off, but also to respond optimally under a wide spectrum of fluctuation timescales. The outcome of evolution is predicted by the long-term growth rate, which differentiates between optimal strategies. Here we present an analytic computation of the long-term growth rate in randomly fluctuating environments, by using mean-field and higher order expansion in the environmental history. We find that optimal strategies correspond to distinct regions in the phase space of fluctuations, separated by first and second order phase transitions. The statistics of environmental randomness are shown to dictate the possible evolutionary modes, which either change the structure of the regulatory network abruptly, or gradually modify and tune the interactions between its components.

### **9:24AM K39.00006 ABSTRACT MOVED TO C39.004 —**

### **9:36AM K39.00007 Shannon Entropy of the Canonical Genetic Code<sup>1</sup>**, LOUIS NEMZER, Nova Southeastern

University — The probability that a non-synonymous point mutation in DNA will adversely affect the functionality of the resultant protein is greatly reduced if the substitution is conservative. In that case, the amino acid coded by the mutated codon has similar physico-chemical properties to the original. Many simplified alphabets, which group the 20 common amino acids into families, have been proposed. To evaluate these schema objectively, we introduce a novel, quantitative method based on the inherent redundancy in the canonical genetic code. By calculating the Shannon information entropy carried by 1- or 2-bit messages, groupings that best leverage the robustness of the code are identified. The relative importance of properties related to protein folding - like hydrophathy and size - and function, including side-chain acidity, can also be estimated. In addition, this approach allows us to quantify the average information value of nucleotide codon positions, and explore the physiological basis for distinguishing between transition and transversion mutations.

<sup>1</sup>Supported by NSU PFRDG Grant 335347

### **9:48AM K39.00008 Genome-scale modeling of the evolutionary path to C4 photosynthesis**, CHRISTOPHER R. MYERS, Cornell University, ELI BOGART, Cornell University & Brigham and Women's Hospital — In C4 photosynthesis, plants maintain a high carbon dioxide level in specialized bundle sheath cells surrounding leaf veins and restrict CO<sub>2</sub> assimilation to those cells, favoring CO<sub>2</sub> over O<sub>2</sub> in competition for Rubisco active sites. In C3 plants, which do not possess such a carbon concentrating mechanism, CO<sub>2</sub> fixation is reduced due to this competition. Despite the complexity of the C4 system, it has evolved convergently from more than 60 independent origins in diverse families of plants around the world over the last 30 million years. We study the evolution of the C4 system in a genome-scale model of plant metabolism that describes interacting mesophyll and bundle sheath cells and enforces key nonlinear kinetic relationships. Adapting the zero-temperature string method for simulating transition paths in physics and chemistry, we find the highest-fitness paths connecting C3 and C4 positions in the model's high-dimensional parameter space, and show that they reproduce known aspects of the C3-C4 transition while making additional predictions about metabolic changes along the path. We explore the relationship between evolutionary history and C4 biochemical subtype, and the effects of atmospheric carbon dioxide levels.

**10:00AM K39.00009 Precision matters for position decoding in the early fly embryo** , MARIELA D PETKOVA, Harvard University, GASPER TKACIK, IST Austria, ERIC F WIESCHAUS, WILLIAM BIALEK, THOMAS GREGOR, Princeton University — Genetic networks can determine cell fates in multicellular organisms with precision that often reaches the physical limits of the system. However, it is unclear how the organism uses this precision and whether it has biological content. Here we address this question in the developing fly embryo, in which a genetic network of patterning genes reaches 1% precision in positioning cells along the embryo axis. The network consists of three interconnected layers: an input layer of maternal gradients, a processing layer of gap genes, and an output layer of pair-rule genes with seven-striped patterns. From measurements of gap gene protein expression in hundreds of wild-type embryos we construct a “decoder”, which is a look-up table that determines cellular positions from the concentration means, variances and co-variances. When we apply the decoder to measurements in mutant embryos lacking various combinations of the maternal inputs, we predict quantitative changes in the output layer such as missing, altered or displaced stripes. We confirm these predictions by measuring pair-rule expression in the mutant embryos. Our results thereby show that the precision of the patterning network is biologically meaningful and a necessary feature for decoding cell positions in the early fly embryo.

**10:12AM K39.00010 Enhancing Functional Robustness of Gene Regulatory Networks Based on Fitness Landscape Design<sup>1</sup>** , KYUNG KIM, University of Washington — We aim to develop design principles for enhancing functional robustness of engineered cells using gene-network topology. We observed the effect of genetic regulation types (inhibition and activation) on robustness. Inhibition was much more stable than activation in *E. coli*. In the case of activation, if the upstream activator expression is shutdown by mutation, then its downstream expression is shut down as well. Without activation, the activator shutdown due to mutation will make its downstream expression remains “turned off”. Thus, the change in the metabolic load is higher in the activation case. Therefore, the stronger activation, the less robust the circuits are. In the inhibition case, we found that the story becomes opposite. When an inhibitor expression is shut down by mutation, the downstream expression turns on because the inhibitor is not expressed. This compensates changes in the metabolic load that might have been decreased without the inhibition. This result presents potential significant roles of network topology on the robustness of engineered cellular networks. This also emphasizes that the concept of fitness landscape, where the local slope corresponds to the fitness difference between different genotypes, can be useful to design robust gene circuits.

<sup>1</sup>We acknowledge the support of the NSF (MCB Award 1515280).

**10:24AM K39.00011 The ecology and evolution of microbial behavior in complex communities** , ALVARO SANCHEZ, Harvard Univ — Microbes form complex ecological communities with multiple species coexisting and interacting with each other. Often, the ecological interactions among these species are mediated by molecules that the microbes actively secrete to the outside world. A large number of microbes are decomposers, and thus particularly relevant examples of these secreted molecules are the enzymes that microbes use to break down complex organic matter (e.g. dead tissue) and extract nutrients from it. In this talk, I will present an overview of the work that we have done to understand the ecology and evolution of the genes responsible for the expression of these enzymes. In particular, I will discuss how by regulating the amount of investment in the production of extracellular enzymes, microbes may modulate ecological interactions and change the number and stability of equilibria in ecosystems.

**Wednesday, March 16, 2016 8:00AM - 11:00AM —**  
**Session K40 GSNP GSOF: Mechanical Metamaterials and Origami II** 343 - Katia Bertoldi, Harvard University

**8:00AM K40.00001 Combinatorial Mechanical Metamaterials** , MARTIN VAN HECKE, Amolf Amsterdam & Leiden University — The structure of most mechanical metamaterials is periodic so that their design space is that of the unit cell. Here we introduce a combinatorial strategy to create a vast number of distinct mechanical metamaterials, each with a unique spatial texture and response. These are aperiodic stackings of anisotropic building blocks, and their functionality rests on both the block design and their stacking configuration which is governed by a tiling problem. We realize such metamaterials by 3D printing, and show that they act as soft machines, capable of pattern recognition and pattern analysis.

**8:12AM K40.00002 Geometry Driven Pathways in Hierarchical Mechanical Metamaterials** , CORENTIN COULAIS, Leiden University / AMOLF, ALBERICO SABBADINI, Leiden University, MARTIN VAN HECKE, Leiden University / AMOLF — Using exactly positioned vacancies in flexible tessellations of squares, we create novel hierarchical mechanical metamaterials that can exhibit multiple shape changes under mechanical actuation. By designing bending, buckling and self-contact interactions, we unravel the link between geometry and dynamical pathways and engineer 2D transformers, which explore complex sequences of symmetrical shapes.

**8:24AM K40.00003 Rigidity loss in disordered network materials** , WOUTER G. ELLENBROEK, Eindhoven University of Technology, VARDA F. HAGH, AVISHEK KUMAR, Arizona State University, M.F. THORPE, Arizona State University and University of Oxford, MARTIN VAN HECKE, Leiden University and AMOLF — Weakly jammed sphere packings show a very peculiar elasticity, with a ratio of compression modulus to shear modulus that diverges as the number of contacts approaches the minimum required for rigidity. Creating artificial isotropic network materials with this property is a challenge: so far, the least elaborate way to generate them is to actually simulate weakly compressed repulsive spheres. The next steps in designing such networks hinge upon a solid understanding of what properties of the sphere-packing derived network are essential for its elasticity. We elucidate the topological aspects of this question by comparing the rigidity transition in these networks to that in other random spring network models, including the common bond-diluted triangular net and a self-stress-free variant of that. We use the pebble game algorithm for identifying rigid clusters in mechanical networks to demonstrate that the marginally rigid state in sphere packings is perfectly isostatic everywhere, and the addition or removal of a single bond creates a globally stressed or globally floppy network, respectively. By contrast, the other classes of random network random networks show a more localized response to addition and removal of bonds, and, correspondingly, a more gradual rigidity transition.

**8:36AM K40.00004 Foam-like compression behavior of fibrin networks** , XIAOJUN LIANG, University of Pennsylvania, OLEG KIM, University of Notre Dame, RUSTEM LITVINOV, JOHN WEISEL, University of Pennsylvania, MARK ALBER, University of Notre Dame, PRASHANT PUROHIT, University of Pennsylvania — The rheological properties of fibrin networks have been of long-standing interest, especially shear and tensile responses. Their compressive behavior, however, remains unexplored. We show that the compressive behavior of fibrin networks consists of three regimes: 1) an initial linear regime, in which most fibers are straight, 2) a plateau regime, in which more and more fibers buckle and collapse, and 3) a markedly non-linear regime, in which network densification occurs by bending of buckled fibers and inter-fiber contacts. Importantly, the spatially non-uniform network deformation included formation of a moving phase boundary along the axis of strain, which segregated the fibrin network into two phases with different fiber densities and structure. The Young's modulus of the linear phase depends quadratically on the fibrin volume fraction while that in the densified phase depends cubically on it. The viscoelastic plateau regime corresponds to a change of volume fraction in mixture of these two phases. We model this regime using a continuum theory of phase transitions and analytically predict the storage and loss moduli. We show they are in good agreement with the experimental data. Our work shows that fibrin networks are a member of a broad class of natural cellular materials.

**8:48AM K40.00005 Topological boundary modes in jammed matter** , DANIEL SUSSMAN, OLAF STENULL, TOM LUBENSKY, University of Pennsylvania — Granular matter at the jamming transition is poised on the brink of mechanical stability, and hence it is possible that these random systems have topologically protected surface phonons. Studying two model systems for jammed matter, we find states that exhibit distinct mechanical topological classes, protected surface modes, and ubiquitous Weyl points. The detailed statistics of the boundary modes enable tests of a standard understanding of the detailed features of the jamming transition, and show that parts of this argument are invalid.

**9:00AM K40.00006 Rigidity Percolation in Mechanical Metamaterials** , LUUK LUBBERS, MARTIN VAN HECKE, Leiden University / AMOLF — We explore rigidity percolation of non-generic diluted tilings of rigid squares coupled by hinges. These compose the backbone of a range of mechanical metamaterials, and allow for a single degree of freedom motion even for full filling. We numerically study the onset and nature of additional floppy modes which arises when sufficient square tiles are removed.

**9:12AM K40.00007 to be determined by you** , JULIA GREER, California Institute of Technology — No abstract available.

**9:48AM K40.00008 Multistable Compliant Auxetic Metamaterials Inspired by Geometric Patterns in Islamic Arts** , AHMAD RAFSANJANI, DAMIANO PASINI, Mechanical Engineering Department, McGill University, PASINILAB TEAM — Beyond their aesthetic significance, geometric patterns in Islamic arts can offer a rich source of inspiration that can be used to create new mechanical metamaterials. In this work, we follow this route and present a new class of compliant mechanical metamaterials which simultaneously exhibit negative Poisson's ratio and structural bistability. Designed by finite element simulations, this multifunctional metamaterial is fabricated by perforating a symmetric cut pattern into a sheet of natural rubber. Its building blocks are rotating units with square or triangular shapes connected together with compliant flexure hinges. Under the action of uniaxial extension, the relative rotation between the adjacent members triggers snap-through instability and brings together auxeticity and structural bistability. As a result, this metamaterial can accomplish reversible reconfiguration between two stable arrangements.

**10:00AM K40.00009 The topology of gyroscopic metamaterials** , LISA M. NASH, University of Chicago, DUSTIN KLECKNER, University of California, Merced, ALISMARI READ, University of Chicago, VINCENZO VITELLI, Instituut-Lorentz, Leiden University, ARI M. TURNER, Johns Hopkins University, WILLIAM T.M. IRVINE, University of Chicago — Mechanical metamaterials can have topologically protected states, much like their electronic and optical counterparts. We recently demonstrated this in experiment by building a meta-material composed of coupled gyroscopes on a honeycomb lattice. This system breaks time-reversal symmetry and exhibits topologically protected one-way edge modes. In this talk we will explore the relationship between the topology of the band structure and the geometry of the lattice.

**10:12AM K40.00010 Modeling the Mechanical Metamaterials with Confinement Controlled Response.** , NITIN SINGH, CORENTIN COULAIS, BASTIAAN FLORIJN, MARTIN VAN HECKE, Univ of Leiden / AMOLF — Much of the physics of two dimensional mechanical metamaterials can be understood from tiling of rigid-polygons connected by hinges. Here we map recently introduced programmable mechanical metamaterials which are elastic slabs patterned with circular holes of two different sizes to a tiling of hinged rectangles. Torsional springs in the hinges and linear springs at the outside of this mechanism allow us to capture the experimentally observed mechanical response, and we connect the physical design parameters to the shape of the rectangles, and the strength of the torsional springs. We finally show that this soft mechanism provides us with an inverse design tool for metamaterials.

**10:24AM K40.00011 Taming the Exceptional Points of Parity-Time Symmetric Acoustics** , MARC DUBOIS, CHENGZHI SHI, Univ of California - Berkeley, YUN CHEN, LEI CHENG, Fudan University, HAMIDREZA RAMEZANI, YUAN WANG, XIANG ZHANG, Univ of California - Berkeley — Parity-time (PT) symmetric concept and development lead to a wide range of applications including coherent perfect absorbers, single mode lasers, unidirectional cloaking and sensing, and optical isolators. These new applications and devices emerge from the existence of a phase transition in PT symmetric complex-valued potential obtained by balancing gain and loss materials. However, the systematic extension of such devices is adjourned by the key challenge in the management of the complex scattering process within the structure in order to engineer PT phase and exceptional points. Here, based on active acoustic elements, we experimentally demonstrate the simultaneous control of complex-valued potentials and multiple interference inside the structure at any given frequency. This method broadens the scope of applications for PT symmetric devices in many fields including optics, microwaves, electronics, which are crucial for sensing, imaging, cloaking, lasing, absorbing, etc.

**10:36AM K40.00012 Overcoming dissipation with structure: Stable propagation of mechanical signals in soft mechanical metamaterials** , KATIA BERTOLDI, JORDAN RANEY, Harvard University, NEEL NADKARNI, California Institute of Technology, CHIARA DARAIO, ETH, DENNIS KOCHMANN, California Institute of Technology, JENNIFER LEWIS, Harvard University — Soft structures with rationally designed architectures capable of large, nonlinear deformation present opportunities for the design of unprecedented, highly-tunable devices and machines. However, the highly-dissipative nature of soft materials has inherently limited the way in which such systems can be used. Here we present an architected soft system comprised of elastomeric, bistable beam elements connected by elastomeric linear springs. The dissipative nature of the polymer readily damps linear waves, preventing propagation of any mechanical signal beyond a short distance, as expected. However, the unique architecture of the system enables propagation of stable, nonlinear solitary transition waves with constant velocity and pulse geometry over arbitrary distances. Since the high damping of the material removes all other linear, small amplitude excitations, the desired pulse propagates with high fidelity and controllability. This phenomenon can be used for control signals as we demonstrate through the design of soft diodes and soft mechanical logic gates.

**10:48AM K40.00013 Combinatorial Origami** , PETER DIELEMAN, SCOTT WAITUKAITIS, MARTIN VAN HECKE, Leiden University, FOM Institute AMOLF — To design rigidly foldable quadrilateral meshes one generally needs to solve a complicated set of constraints. Here we present a systematic, combinatorial approach to create rigidly foldable quadrilateral meshes with a limited number of different vertices. The number of discrete, 1 degree-of-freedom folding branches for some of these meshes scales exponentially with the number of vertices on the edge, whilst other meshes generated this way only have two discrete folding branches, regardless of mesh size. We show how these two different behaviours both emerge from the two folding branches present in a single generic 4-vertex. Furthermore, we model generic 4-vertices as a spherical linkage and exploit a previously overlooked symmetry to create non-developable origami patterns using the same combinatorial framework.

**Wednesday, March 16, 2016 8:00AM - 11:00AM —**

Session K41 DBIO DPOLY DCOMP: Physics of Proteins: Protein-Protein Interactions 344 - Wei Wang, Nanjing University

**8:00AM K41.00001 Random close packing in protein cores<sup>1</sup>**, COREY OHERN, Yale University — Shortly after the determination of the first protein x-ray crystal structures, researchers analyzed their cores and reported packing fractions  $\phi \approx 0.75$ , a value that is similar to close packing equal-sized spheres. A limitation of these analyses was the use of 'extended atom' models, rather than the more physically accurate 'explicit hydrogen' model. The validity of using the explicit hydrogen model is proved by its ability to predict the side chain dihedral angle distributions observed in proteins. We employ the explicit hydrogen model to calculate the packing fraction of the cores of over 200 high resolution protein structures. We find that these protein cores have  $\phi \approx 0.55$ , which is comparable to random close-packing of non-spherical particles. This result provides a deeper understanding of the physical basis of protein structure that will enable predictions of the effects of amino acid mutations and design of new functional proteins.

<sup>1</sup>We gratefully acknowledge the support of the Raymond and Beverly Sackler Institute for Biological, Physical, and Engineering Sciences, National Library of Medicine training grant T15LM00705628 (J.C.G.), and National Science Foundation DMR-1307712 (L.R.).

**8:36AM K41.00002 Predicting protein-peptide interactions from scratch<sup>1</sup>**, CHENGFEI YAN, XIANJIN XU, XIAOQIN ZOU, University of Missouri, ZOU LAB TEAM — Protein-peptide interactions play an important role in many cellular processes. The ability to predict protein-peptide complex structures is valuable for mechanistic investigation and therapeutic development. Due to the high flexibility of peptides and lack of templates for homologous modeling, predicting protein-peptide complex structures is extremely challenging. Recently, we have developed a novel docking framework for protein-peptide structure prediction. Specifically, given the sequence of a peptide and a 3D structure of the protein, initial conformations of the peptide are built through protein threading. Then, the peptide is globally and flexibly docked onto the protein using a novel iterative approach. Finally, the sampled modes are scored and ranked by a statistical potential-based energy scoring function that was derived for protein-peptide interactions from statistical mechanics principles. Our docking methodology has been tested on the Peptidb database and compared with other protein-peptide docking methods. Systematic analysis shows significantly improved results compared to the performances of the existing methods. Our method is computationally efficient and suitable for large-scale applications.

<sup>1</sup>NSF CAREER Award 0953839 (XZ) NIH R01GM109980 (XZ)

**8:48AM K41.00003 Computational Studies of Protein-Protein Interface Designs**, JENNIFER GAINES, COREY O'HERN, LYNNE REGAN, Yale University — We implement a hard-sphere model for amino acid structure to study natural and designed protein-protein interfaces. Current computational methods have found limited success in designing novel interfaces and resorted to implementing several rounds of experimental mutation and selection to achieve successful designs. Here, we show that the hard-sphere model can recapitulate the side chain dihedral angle distributions for amino acids at natural protein-protein interfaces. In addition, we calculate the packing fraction in naturally occurring interfaces and find that it is comparable to dense random packing in protein cores. We then evaluate a number of successful and unsuccessful prior computational designs in terms of the number of allowed side chain dihedral angle conformations and the packing fraction of residues at the interface.

**9:00AM K41.00004 Characterizing the statistical properties of protein surfaces<sup>1</sup>**, JI HYUN BAK, ANNE-FLORENCE BITBOL, WILLIAM BIALEK, Princeton University — Proteins and their interactions form the body of the signaling transduction pathway in many living systems. In order to ensure the accuracy as well as the specificity of signaling, it is crucial that proteins recognize their correct interaction partners. How difficult, then, is it for a protein to discriminate its correct interaction partner(s) from the possibly large set of other proteins it may encounter in the cell? An important ingredient of recognition is shape complementarity. The ensemble of protein shapes should be constrained by the need for maintaining functional interactions while avoiding spurious ones. To address this aspect of protein recognition, we consider the ensemble of proteins in terms of the shapes of their surfaces. We take into account the high-resolution structures of E.coli non-DNA-binding cytoplasmic proteins, retrieved from the Protein Data Bank. We aim to characterize the statistical properties of the protein surfaces at two levels: First, we study the intrinsic dimensionality at the level of the ensemble of the surface objects. Second, at the level of the individual surfaces, we determine the scale of shape variation. We further discuss how the dimensionality of the shape space is linked to the statistical properties of individual protein surfaces.

<sup>1</sup>JHB and WB acknowledge support from National Science Foundation Grants PHY-1305525 and PHY-1521553. AFB acknowledges support from the Human Frontier Science Program.

**9:12AM K41.00005 Difference in aggregation between functional and toxic amyloids studied by atomistic simulations**, MARTIN CARBALLO PACHECO, Research Center Juelich and RWTH Aachen University, AHMED E. ISMAIL, RWTH Aachen University, BIRGIT STRODEL, Research Center Juelich and Heinrich Heine University Duesseldorf — Amyloids are highly structured protein aggregates, normally associated with neurodegenerative diseases such as Alzheimer's disease. In recent years, a number of nontoxic amyloids with physiologically normal functions, called functional amyloids, have been found. It is known that soluble small oligomers are more toxic than large fibrils. Thus, we study with atomistic explicit-solvent molecular dynamics simulations the oligomer formation of the amyloid- $\beta$  peptide A $\beta_{25-35}$ , associated with Alzheimer's disease, and two functional amyloid-forming tachykinin peptides: kassinin and neuromedin K. Our simulations show that monomeric peptides in extended conformations aggregate faster than those in collapsed hairpin-like conformations. In addition, we observe faster aggregation by functional amyloids than toxic amyloids, which could explain their lack of toxicity.

**9:24AM K41.00006 Oligomer stability of Amyloid- $\beta$  (A $\beta$ ) 25-35 : A Dissipative Particle Dynamics study**, IGOR PIVKIN, EMANUEL PETER, University of Lugano — Alzheimer's disease is strongly associated with an accumulation of Amyloid- $\beta$  (A $\beta$ ) peptide plaques in the human brain. A $\beta$  is a 43 residues long intrinsically disordered peptide and has a strong tendency to form aggregates. Evidence accumulates that A $\beta$  acts toxic to the neurons in the brain through the formation of small soluble oligomers. A $\beta$  25-35 is the smallest fragment of A $\beta$  which still retains its toxicity and its ability to form extended fibrils. In this talk we will present the results from simulations of aggregation of up to 100 A $\beta$  25-35 peptides using a novel polarizable coarse-grained protein model in combination with Dissipative Particle Dynamics.

**9:36AM K41.00007 A thermodynamic study of Abeta(16-21) dissociation from a fibril using computer simulations.**, CRISTIANO DIAS, FARBOD MAHMOUDINOBAR, ZHAOQIAN SU, New Jersey Institute of Technology — Here, I will discuss recent all-atom molecular dynamics simulations with explicit water in which we studied the thermodynamic properties of Abeta(16-21) dissociation from an amyloid fibril. Changes in thermodynamics quantities, e.g., entropy, enthalpy, and volume, are computed from the temperature dependence of the free-energy computed using the umbrella sampling method. We find similarities and differences between the thermodynamics of peptide dissociation and protein unfolding. Similarly to protein unfolding, Abeta(16-21) dissociation is characterized by an unfavorable change in enthalpy, a favorable change in the entropic energy, and an increase in the heat capacity. A main difference is that peptide dissociation is characterized by a weak enthalpy-entropy compensation. We characterize dock and lock states of the peptide based on the solvent accessible surface area. The Lennard-Jones energy of the system is observed to increase continuously in lock and dock states as the peptide dissociates. The electrostatic energy increases in the lock state and it decreases in the dock state as the peptide dissociates. These results will be discussed as well as their implication for fibril growth.

## 9:48AM K41.00008 Role of mutation on fibril formation in small peptides by REMD , FARBOD

MAHMOUDINOBAR<sup>1</sup>, CRISTIANO DIAS<sup>2</sup>, New Jersey Inst of Tech — Amyloid fibrils are now recognized as a common form of protein structure. They have wide implications for neurological diseases and entities involved in the survival of living organisms, e.g., silkworm eggshells. Biological functions of these entities are often related to the superior mechanical strength of fibrils that persists over a broad range of chemical and thermal conditions desirable for various biotechnological applications, e.g., to encapsulate drugs. Mechanical properties of fibrils was shown to depend strongly on the amino acid sequence of its constituent peptides whereby bending rigidities can vary by two orders of magnitude. Therefore, the rational design of new fibril-prone peptides with tailored properties depends on our understanding of the relation between amino acid sequence and its propensity to fibrillize. In this presentation I will show results from extensive Replica Exchange Molecular Dynamics (REMD) simulations of a 12-residue peptide containing the fibril-prone motif KFFE and its mutants. Simulations are performed on monomers, dimers, and tetramers. I will discuss effects of side chain packing, hydrophobicity, charges and beta-sheet propensity on fibril formation.

<sup>1</sup>Physics Department, University Heights, Newark, New Jersey, 07102-1982, USA

<sup>2</sup>Physics Department, University Heights, Newark, New Jersey, 07102-1982, USA

## 10:00AM K41.00009 Oligomerization of the protein tau in the Alzheimer's disease , LUCA LARINI,

Rutgers University - Camden — The Alzheimer's disease is characterized by the formation of protein aggregates both within and outside of the brain's cells, the neurons. Within the neurons, the aggregation of the microtubule associated protein tau leads to the destruction of the microtubules in the axon of the neuron. Tau is extremely flexible and is classified as an intrinsically disordered protein due to its low propensity to form secondary structure. Tau promotes tubulin assembly into microtubules, which are an essential component of the cytoskeleton of the axon. The microtubule binding region of tau consists of 4 pseudo-repeats that are critical for aggregation as well. In this study, we focus on the aggregation propensity of different segments of the microtubule binding region as well as post-translational modifications that can alter tau dynamics and structure. We have performed replica exchange molecular dynamics simulations to characterize the ensemble of conformations of the monomer and small oligomers as well as how these structures are stabilized or destabilized by mutations and post-translational modifications.

## 10:12AM K41.00010 Stability of ALS-related Superoxide Dismutase Protein variants , DANIEL

LUSEBRINK, STEVEN PLOTKIN, Department of Physics and Astronomy, University of British Columbia — Superoxide dismutase (SOD1) is a metal binding, homodimeric protein, whose misfolding is implicated in the neurodegenerative disease amyotrophic lateral sclerosis (ALS). Monomerization is believed to be a key step in the propagation of the disease. The dimer stability is often difficult to measure experimentally however, because it is entangled with protein unfolding and metal loss. We thus computationally investigate the dimer stability of mutants of SOD1 known to be associated with ALS. We report on systematic trends in dimer stability, as well as intriguing allosteric communication between mutations and the dimer interface. We study the dimer stabilities in molecular dynamics simulations and obtain the binding free energies of the dimers from pulling essays. Mutations are applied *in silico* and we compare the differences of binding free energies compared to the wild type.

## 10:24AM K41.00011 Nuclear magnetic resonance studies of bovine $\gamma$ B-crystallin<sup>1</sup> , GEORGE

THURSTON, JEFFREY MILLS, LEA MICHEL, KAYLEE MATHEWS, JOHN ZANET, ANGEL PAYAN, KEITH VAN NOSTRAND, MICHAEL KOTLARCHYK, DAVID ROSS, Rochester Institute of Technology, CHRISTOPHER WAHLE, University of Findlay, JOHN HAMILTON, Rochester Institute of Technology — Anisotropy of shape and/or interactions play an important role in determining the properties of concentrated solutions of the eye lens protein,  $\gamma$ B-crystallin, including its liquid-liquid phase transition. We are studying  $\gamma$ B anisotropic interactions with use of nuclear magnetic resonance (NMR) concentration- and temperature-dependent chemical shift perturbations (CSPs). We analyze two-dimensional heteronuclear spin quantum coherence (HSQC) spectra on backbone nitrogen and attached hydrogen nuclei for CSPs, up to 3 percent volume fraction. Cumulative distribution functions of the CSPs show a concentration and temperature-dependent spread. Many peaks that are highly shifted with either concentration or temperature are close (i) crystal intermolecular contacts (ii) locations of cataractogenic point mutations of a homologous human protein, human  $\gamma$ D-crystallin, and (iii) charged amino-acid residues. We also discuss the concentration- and temperature-dependence of NMR and quasielastic light scattering measurements of rotational and translational diffusion of  $\gamma$ B crystallin in solution, affected by interprotein attractions.

<sup>1</sup>Supported by NIH EY018249

## 10:36AM K41.00012 Membrane Pore Formation by Amyloid beta (25-35) Peptide , NABIN KANDEL,

SUREN TATULIAN, University of Central Florida — Amyloid (A $\beta$ ) peptide contributes to Alzheimer's disease by a yet unidentified mechanism. One of the possible mechanisms of A $\beta$  toxicity is formation of pores in cellular membranes. We have characterized the formation of pores in phospholipid membranes by the A $\beta$ <sub>25–35</sub> peptide (GSNKGAIIGLM) using fluorescence, Fourier transform infrared spectroscopy (FTIR) and circular dichroism (CD) techniques. CD and FTIR identified formation of  $\beta$ -sheet structure upon incubation of the peptide in aqueous buffer for 2 hours. Unilamellar vesicles composed of a zwitterionic lipid, 1-palmitoyl-2-oleoyl-phosphatidylcholine (POPC), and 70% POPC plus 30% of an acidic lipid, 1-palmitoyl-2-oleoyl-phosphatidylglycerol (POPG), are made in 30 mM CaCl<sub>2</sub>. Quin-2, a fluorophore that displays increased fluorescence upon Ca<sup>2+</sup> binding, is added to the vesicles externally. Peptide addition results in increased Quin-2 fluorescence, which is interpreted by binding of the peptide to the vesicles, pore formation, and Ca<sup>2+</sup> leakage. The positive and negative control measurements involve addition of a detergent, Triton X-100, which causes vesicle rupture and release of total calcium, and blank buffer, respectively.

## 10:48AM K41.00013 Holographic characterization of protein aggregates<sup>1</sup> , CHEN WANG, XIAO ZHONG,

New York University, DAVID RUFFNER, Spheryx, Inc., ALEXANDRA STUTT, Packer Collegiate Institute, LAURA PHILIPS, Spheryx, Inc., MICHAEL WARD, DAVID GRIER, New York University — Holographic characterization directly measures the size distribution of subvisible protein aggregates in suspension and offers insights into their morphology. Based on holographic video microscopy, this analytical technique records and interprets holograms of individual aggregates in protein solutions as they flow down a microfluidic channel, without requiring labeling or other exceptional sample preparation. The hologram of an individual protein aggregate is analyzed in real time with the Lorenz-Mie theory of light scattering to measure that aggregates size and optical properties. Detecting, counting and characterizing subvisible aggregates proceeds fast enough for time-resolved studies, and lends itself to tracking trends in protein aggregation arising from changing environmental factors. No other analytical technique provides such a wealth of particle-resolved characterization data in situ. Holographic characterization promises accelerated development of therapeutic protein formulations, improved process control during manufacturing, and streamlined quality assurance during storage and at the point of use.

<sup>1</sup>MRSEC and MRI program of the NSF, Spheryx Inc.

# Wednesday, March 16, 2016 8:00AM - 10:48AM –

## Session K42 DPOLY: Polymer Dynamics - Insight from In-Situ Scattering 345 - Lilin He, Oak Ridge

National Laboratory

**8:00AM K42.00001 Local Dynamics of Acid- and Ion-containing Copolymer Melts.** , KAREN WINEY, ROBERT MIDDLETON, University of Pennsylvania, JACOB TARVER, MADHUSUDAN TYAGI, CHRISTOPHER SOLES, NIST, AMALIE FRISCHKNECHT, Sandia National Laboratory — Interest in acid- and ion-containing polymers arises in part from applications as single-ion conductors for selectively transporting a counter ion for battery applications. Structurally, the low dielectric constant of organic polymers and strong ionic interactions leads to ionic aggregation. Here the polymer backbone motion was investigated through quasi-elastic neutron scattering measurements (QENS) and compared with fully atomistic molecular dynamic simulations of precise poly(ethylene-acrylic acid) copolymers and their ionomers (pAA-y%Li). The effect of carbon spacer length ( $x=9, 15, 21$ ) between the acid groups and the degree of neutralization ( $y$ ) with Li on PE backbone dynamics were considered. Systematic slowing in chain dynamics were observed with increasing neutralization where polymer dynamics appear constrained due to anchoring effects. Simulations provide complementary viewpoints indicating a gradient in chain dynamics as a distance away from acid groups. These results indicate that the addition of pendant acid groups inhibit typical PE backbone motion and the neutralized forms strongly suppress the fraction of mobile PE chain.

**8:12AM K42.00002 Effect of Increasing Molecular Weight on the A and B blocks of a Single-ion-conducting Block Copolymer Electrolyte for Lithium Batteries** , ADRIANA ROJAS, University of California, Berkeley, SEBNEM INCEOGLU, Lawrence Berkeley National Laboratory, KANAV THAKKER, NIKOLAUS MACKAY, NITASH BALSARA, University of California, Berkeley — Single-ion-conducting block copolymer electrolytes are desirable for lithium metal batteries due to their ability to eliminate salt concentration gradients across the electrolyte; i.e., the lithium ion transference number is approximately unity. A series of poly(ethylene oxide)-*b*-poly(styrenesulfonyllithium(trifluoromethylsulfonyl)imide) (PEO-*b*-PSLiTFSI) copolymers was studied wherein the molecular weights of both blocks were varied. Small angle x-ray scattering and ac impedance spectroscopy were used to probe the dependence of ionic conductivity on morphology. Preliminary work suggests that increasing the molecular weights of the blocks results in increased disorder and lower conductivity.

**8:24AM K42.00003 SUPERCOOLED WATER IN SUPRAMOLECULAR HYDROGELS** , CLINTON WIENER, BRYAN VOGT, R.A. WEISS, University of Akron — The suppression of water crystallization with appreciable water supercooling is challenging due to its large enthalpy of fusion. A common theme to supercool water is to confine the water in the pores of microporous/mesoporous solids where mechanical confinement prevents water crystallization. Nature takes a different approach with crystallization suppression through a combination of preferential adsorption on ice nuclei and confinement between hydrophobic residues using organic components only. Here, we demonstrate that mechanically robust confinement within a hard material is not necessary to significantly supercool water. In this case, a supramolecular hydrogel, based on a random amphiphilic copolymer, is used to provide soft confinement of water between the hydrophobic aggregates with an interdomain spacing  $<8$  nm. Small angle neutron scattering (SANS) provides insight into the structural evolution of the supramolecular structure of the hydrogel on supercooling. The structural changes are sensitive to the composition of the copolymer as determined by contrast variation SANS. Similarly, the dynamics of both the copolymer and water are probed using quasielastic neutron scattering (QENS). Using QENS, a highly mobile water phase ( $\tau \approx 23$  ps) is identified to be present even when slowly cooling to as low as 220K.

**8:36AM K42.00004 Segmental chain dynamics of ABA triblock copolymer micelles in aqueous solution**<sup>1</sup> , VIVEK PRABHU, GUANGMIN WEI, NIST Material Measurement Laboratory, MICHIOHITO NAGAO, NIST Center for Neutron Research, SHRINIVAS VENKATARAMAN, YI YAN YANG, AStar-Singapore, Institute of Bioengineering and Nanotechnology, JAMES HEDRICK, IBM Almaden Research Center — The polymer physics of hierarchical, aqueous self-assembled ABA block copolymers is an active area of research for both advanced materials and biomaterial applications [1]. Scattering-based techniques provide a direct measure of the correlations and structure across multiple length and time scales. Hierarchical clusters of micelles are formed by well-defined poly(ethylene glycol) triblock copolymers with oligo-fluorene hydrophobic end-groups in aqueous solutions. The structure and dynamics of this system was studied by small-angle neutron scattering (SANS), and static and dynamic light scattering [2]. We will present new neutron spin-echo spectroscopy (NSE) results that provides direct insight into the segmental chain dynamics constrained by the  $\pi$ - $\pi$  stacking of the oligo-fluorene end groups. The dilute cluster regime within the temperature-composition phase diagram is of current interest. [1] S. Venkataraman, A.L. Lee, H.T. Maune, J.L. Hedrick, V.M. Prabhu, and Y.Y. Yang, *Macromolecules* 46, 4839 (2013). [2] V.M. Prabhu et al. "Equilibrium self-assembly, structure and dynamics of clusters of star-like micelles," *ACS Macro Letters*, 4, 1128 (2015).

<sup>1</sup>NIST Materials Genome Program

**8:48AM K42.00005 Viscoelastic hydrodynamic interactions and anomalous CM diffusion in polymer melts**<sup>1</sup> , HENDRIK MEYER, Institut Charles Sadron, CNRS Strasbourg, France — We have recently discovered that anomalous center-of-mass (CM) diffusion occurring on intermediate time scales in polymer melts can be explained by the interplay of viscoelastic and hydrodynamic interactions (VHI). The theory has been solved for unentangled melts in 3D [1] and 2D [2] and excellent agreement between theory and simulation is found, also for alkanes with a force field optimized from neutron scattering [3]. The physical mechanism considers that hydrodynamic interactions are not screened: they are time dependent because of increasing viscosity before the terminal relaxation time. The VHI are generally active in melts of any topology. They are most important at early times well before the terminal relaxation time and thus affect the nanosecond time range typically observable in dynamic neutron scattering experiments [1,3]. We illustrate the effects with recent molecular dynamics simulations of linear, ring and star polymers. [1] PRL 107, 178301 (2011); PRE 85, 051807 (2012). [2] PRL 109, 248304 (2012); Soft Matter 9, 4249 (2013). [3] PRL 111, 173003 (2013).

<sup>1</sup>Work performed with A.N. Semenov and J. Farago

**9:00AM K42.00006 Nanostructures and dynamics of macromolecules bound to attractive filler surfaces**<sup>1</sup> , TAD KOGA, DEBORAH BARKLEY, NAISHENG JIANG, MAYA ENDOH, Stony Brook University, TOMOMI MASUI, HIROYUKI KISHIMOTO, Sumitomo Rubber Industries Ltd., MICHIOHITO NAGAO, SUSHIL SATIJA, NIST Center for Neutron Research, TAKASHI TANIGUCHI, Kyoto University — We report in-situ nanostructures and dynamics of polybutadiene (PB) chains bound to carbon black (CB) fillers (the so-called "bound polymer layer (BPL)") in a good solvent. The BPL on the CB fillers were extracted by solvent leaching of a CB-filled PB compound and subsequently dispersed in deuterated toluene to label the BPL for small-angle neutron scattering and neutron spin echo techniques. Intriguingly, the results demonstrate that the BPL is composed of two regions regardless of molecular weights of PB: the inner unswollen region of  $\approx 0.5$  nm thick and outer swollen region where the polymer chains display a parabolic profile with a diffuse tail. This two-layer formation on the filler surface is similar to that reported for polymer chains adsorbed on planar substrates from melts [1]. In addition, the results show that the dynamics of the swollen bound chains can be explained by the so-called "breathing mode" and is generalized with the thickness of the swollen BPL. Furthermore, we will discuss how the breathing collective dynamics is affected by the presence of polymer chains in a matrix solution. [1] Gin et al., *Phys. Rev. Lett.*, (2012), 109, 265501.

<sup>1</sup>We acknowledge the financial support from NSF Grant No. CMMI-1332499.

**9:12AM K42.00007 SAXS/WAXS studies of shear-induced crystallization of poly(1-butene)** , MU SUNG KWEON, BINBIN LUO, WESLEY BURGHARDT, Northwestern University — Flow-induced crystallization of poly(1-butene) was studied in shear flow. Flow was produced using a Linkam shear cell that has been modified to allow x-ray access for in situ studies of polymer structure using synchrotron x-ray scattering techniques. After loading in the shear cell, samples were first heated well into the melt, and then cooled to a crystallization temperature selected such that negligible quiescent crystallization would occur on reasonable time scales. A short burst of shear flow was then applied at various rates, after which simultaneous wide- and small-angle x-ray scattering (WAXS and SAXS, respectively) data were collected to study the impact of both deformation rate and total applied strain on accelerated crystallization kinetics as well as the morphology of the resulting crystallites (e.g. degree of crystallite orientation). SAXS and WAXS data generally showed qualitative agreement in measures of the extent of crystallization and the degree of crystallite orientation. Average crystallite orientation was found to decrease over the course of crystallization. The crystalline volume fraction in the sample was calculated from the (i) SAXS invariant and (ii) integrated WAXS intensity profile to quantify the extent to which the sample crystallized at various flow c

**9:24AM K42.00008 Leveraging intrinsic chain anisotropy to align coil-coil block copolymers with magnetic fields** , YEKATERINA ROKHLENKO, KAI ZHANG, MANESH GOPINADHAN, Yale University, STEVE LARSON, University of WisconsinMadison, PAWEL MAJEWSKI, KEVIN YAGER, Brookhaven National Lab, PADMA GOPALAN, University of WisconsinMadison, COREY O'HERN, CHINEDUM OSUJI, Yale University — Magnetic field alignment of block copolymers (BCPs) has typically relied on the presence of liquid crystalline or crystalline assemblies to provide sufficient magnetic anisotropy to drive alignment. Recent experiments however show that alignment is also possible in simple coil-coil BCPs. In particular, alignment of lamellae was observed in poly(styrene-*b*-4-vinylpyridine) (PS-P4VP) on cooling across the order-disorder transition at field strengths as low as 1 T, with alignment improving markedly with increasing field strength and decreasing cooling rate. Here we discuss the intrinsic chain anisotropy which drives the observed alignment, and its display as a net microdomain anisotropy due to chain tethering at the block interface. We use in-situ X-ray scattering to study the phase behavior and temperature-, time-, and field- dependent dynamics of magnetic alignment in coil-coil BCPs, highlighting the important roles of chain anisotropy and grain size in alignment. For the right combination of field strength and grain size, we can leverage intrinsic chain anisotropy to magnetically direct self-assembly in other coil-coil systems, including cylinder-forming poly(styrene-*b*-dimethylsiloxane). Field alignment of PS-P4VP with PEO and other blends provides a route to form functional materials such as nanoporous films and ion conducting polymers.

**9:36AM K42.00009 Elucidating the Molecular Deformation Mechanism of Entangled Polymers in Fast Flow by Small Angle Neutron Scattering** , YANGYANG WANG, LUIS SANCHEZ-DIAZ, SHIWANG CHENG, KUNLUN HONG, WEI-REN CHEN, Oak Ridge National Laboratory, JIANNING LIU, PANPAN LIN, SHI-QING WANG, University of Akron — Understanding the viscoelastic properties of polymers is of fundamental and practical importance because of the vast and ever expanding demand of polymeric materials in daily life. Our current theoretical framework for describing the nonlinear flow behavior of entangled polymers is built upon the tube model pioneered by de Gennes, Doi, and Edwards. In this work, we critically examine the central hypothesis of the tube model for nonlinear rheology using small angle neutron scattering (SANS). While the tube model envisions a unique non-affine elastic deformation mechanism for entangled polymers, our SANS measurements show that the evolution of chain conformation of a well-entangled polystyrene melt closely follows the affine deformation mechanism in uniaxial extension, even when the Rouse Weissenberg number is much smaller than unity. This result provides a key clue for understanding the molecular deformation mechanism of entangled polymers in fast flow. Several implications from our analysis will be discussed in this talk.

**9:48AM K42.00010 Insights into the Dynamics of Polymers and Nanocomposites via Quasi-elastic Neutron Scattering** , MADHU SUDAN TYAGI, NIST Center for Neutron Research — Neutron scattering is a powerful technique to study polymer dynamics. In particular, its angular momentum (*Q*) dependence provide a unique opportunity to study polymer motions at different length scales of interest. This is particularly important when examining some of the crucial aspects related with glass transitions and in particular chain behavior under confinement. Of particular interests are the examples of nanocomposites and ionomers. The interactions between polymer chain and nanoparticle in nanocomposites can cause significant heterogeneities in the polymer dynamics and strongly affect its properties. Dynamical perturbations are generally expected to be limited to interfacial polymer segments. However, composites with highly anisotropic nanoparticles usually exhibit very low percolation threshold and in such systems a complex polymer relaxation behavior can be observed that is not anticipated from dilute nanoparticle dispersions in polymer matrix. A lot of progress has been made over the last decade, however, the effect of chemical binding, physical adsorption and inclusion of nanoparticles in polymer matrix on the local and global dynamics of chain molecules still remains controversial subject. In this talk I will present some examples of our recent work where neutron scattering has been able to make some important breakthroughs in these topics.

**10:24AM K42.00011 SAXS studies of the structure of a BCC-ordered block copolymer melt subjected to uniaxial extensional flow** , WESLEY BURGHARDT, ERICA MCCREADY, Northwestern University — We report in situ small-angle x-ray scattering (SAXS) investigations of a spherically-ordered block copolymer melt with a low styrene content (13%) resulting in spherical polystyrene microdomains ordered in BCC lattice. Melt annealing after clearing above the ODT produces ordered samples that have a macroscopically random orientation distribution of BCC 'grains'. Melt samples are subjected to uniaxial extensional flow in a counter-rotating drum extensional flow fixture housed in an oven with synchrotron x-ray access. During flow, initially isotropic diffraction rings in SAXS patterns become deformed, reflecting distortion of the BCC lattice. Diffracted intensity also concentrates azimuthally, indicating macroscopic alignment of the BCC lattice. There is evidence that extensional flow leads to progressive disordering of the BCC structure, with loss of higher order peaks and the emergence of a diffuse 'halo' of scattering. While the primary diffraction peak is visible in directions parallel and perpendicular to the stretching direction, the deformation of the lattice d-spacing follows affine deformation. Indications of ordering persist to higher strains in samples stretched at higher extension rates, and evidence of affine lattice deformation persists to very high strains (Hencky

**10:36AM K42.00012 Neutron Reflectivity Measurement for Polymer Dynamics near Graphene Oxide Monolayers.** , JASEUNG KOO, Korea Atomic Energy Research Institute — We investigated the diffusion dynamics of polymer chains confined between graphene oxide layers using neutron reflectivity (NR). The bilayers of polymethylmethacrylate (PMMA)/ deuterated PMMA (d-PMMA) films and polystyrene (PS)/d-PS films with various film thickness sandwiched between Langmuir-Blodgett (LB) monolayers of graphene oxide (GO) were prepared. From the NR results, we found that PMMA diffusion dynamics was reduced near the GO surface while the PS diffusion was not significantly changed. This is due to the different strength of GO-polymer interaction. In this talk, these diffusion results will be compared with dewetting dynamics of polymer thin films on the GO monolayers. This has given us the basis for development of graphene-based nanoelectronics with high efficiency, such as heterojunction devices for polymer photovoltaic (OPV) applications.

**Wednesday, March 16, 2016 8:00AM - 10:36AM –**  
**Session K43 GSNP: Complex Networks and their Applications I** 346 - Flaviano Morone, City College of New York

### 8:00AM K43.00001 Influence maximization in complex networks through optimal percolation

, FLAVIANO MORONE, HERNAN MAKSE, City College of New York, CUNY COLLABORATION, CUNY COLLABORATION — The whole frame of interconnections in complex networks hinges on a specific set of structural nodes, much smaller than the total size, which, if activated, would cause the spread of information to the whole network, or, if immunized, would prevent the diffusion of a large scale epidemic. Localizing this optimal, that is, minimal, set of structural nodes, called influencers, is one of the most important problems in network science. Here we map the problem onto optimal percolation in random networks to identify the minimal set of influencers, which arises by minimizing the energy of a many-body system, where the form of the interactions is fixed by the non-backtracking matrix of the network. Big data analyses reveal that the set of optimal influencers is much smaller than the one predicted by previous heuristic centralities. Remarkably, a large number of previously neglected weakly connected nodes emerges among the optimal influencers. Reference: F. Morone, H. A. Makse, Nature 524,65-68 (2015)

### 8:12AM K43.00002 Collective opinion formation on fluctuating networks

, VUDTIWAT NGAM-PRUETIKORN, Okinawa Institute of Science and Technology, GREG STEPHENS, Vrije Universiteit Amsterdam & Okinawa Institute of Science and Technology — Thanks to the advent of online social networks, not only are we more connected than ever but we are also able to design and maintain our own social networks. An insight into this phenomenon will be key to understanding modern societies. To this end, we argue that active network maintenance exposes individuals to selective exposure (preference for agreeing information sources) and we explore how this could affect the structure of social networks and collective opinion formation. More technically, we investigate opinion dynamics on a complex network with fast stochastic rewiring. We show that selective exposure while inducing segregation of agents with different opinions, stabilises consensus state regardless of opinion update rules. We argue further that selective exposure can lead to a shorter time to consensus. The time to consensus has non-trivial dependence on the magnitude of selective exposure. Moreover, we find for some opinion updating rules, selective exposure can increase the lifetime of opinion segregation (polarisation of opinions).

### 8:24AM K43.00003 Choice Shift in Opinion Network Dynamics<sup>1</sup>

, MICHAEL GABBAY, University of Washington — Choice shift is a phenomenon associated with small group dynamics whereby group discussion causes group members to shift their opinions in a more extreme direction so that the mean post-discussion opinion exceeds the mean pre-discussion opinion. Also known as group polarization, choice shift is a robust experimental phenomenon and has been well-studied within social psychology. In opinion network models, shifts toward extremism are typically produced by the presence of stubborn agents at the extremes of the opinion axis, whose opinions are much more resistant to change than moderate agents. However, we present a model in which choice shift can arise without the assumption of stubborn agents; the model evolves member opinions and uncertainties using coupled nonlinear differential equations. In addition, we briefly describe the results of a recent experiment conducted involving online group discussion concerning the outcome of National Football League games are described. The model predictions concerning the effects of network structure, disagreement level, and team choice (favorite or underdog) are in accord with the experimental results.

<sup>1</sup>This research was funded by the Office of Naval Research and the Defense Threat Reduction Agency.

### 8:36AM K43.00004 Social Network Influence and Personal Financial Status

, SHAOJUN LUO, FLAVIANO MORONE, City College of CUNY, CARLOS SARRAUTE, Grandata, Buenos Aires, Argentina, HERNAN MAKSE, City College of CUNY — Networks of social ties emerging from individual economic needs display a highly structured architecture. In response to socio-economic demands, people reshape their circle of contacts for maximizing their social status, and ipso facto, the pattern of their interconnections is strongly correlates with their personal financial situation. In this work we transform this qualitative and verbal statement into an operative definition, which allows us to quantify the economic wellness of individuals through a measure of their collective influence. We consider the network of mobile phone calls made by the Mexican population during three months, in order to study the correlation of person's economic situation with her network location. Notably, we find that rich people tend to be also the most influential nodes, i.e., they self-organize to optimally position themselves in the network. This finding may be also raised at the level of a principle, a fact that would explain the emergence of the phenomenon of collective influence itself as the result of the local optimization of socio-economic interactions. Our method represents a powerful and efficient indicator of socio-economic robustness, which may be applied to maximize the effect of large scale economic intervention and stimulus policies

### 8:48AM K43.00005 More Opportunities than Wealth: Inequality and Emergent Social Classes in a Network of Power and Frustration

, CRISTIANO NISOLI, Los Alamos National Laboratory, BENOIT MAHAULT, Service de Physique de l'Etat Condense, CNRS UMR 3680, CEA-Saclay, 91191 Gif-sur-Yvette, France, AVADH SAXENA, Los Alamos National Laboratory — We introduce a minimal agent-based model to qualitatively conceptualize the allocation of limited wealth among more abundant opportunities. There the interplay of power, satisfaction and frustration determines the distribution, concentration, and inequality of wealth. Our framework allows us to compare subjective measures of frustration and satisfaction to collective measures of fairness in wealth distribution, such as the Lorenz curve and the Gini index. We find that a completely libertarian, law-of-the-jungle setting, where every agent can acquire wealth from, or lose wealth to, anybody else invariably leads to large inequality. The picture is however dramatically modified when hard constraints are imposed over agents, and they are limited to share wealth with neighbors on a network. We address dynamical societies via an out of equilibrium coevolution of the network, driven by a competition between power and frustration. The ratio between power and frustration controls different dynamical regimes separated by kinetic transitions and characterized by drastically different values of the indices of equality. In particular, it leads to the emergence of three self-organized social classes, lower, middle, and upper class, whose interactions drive a cyclical regime.

### 9:00AM K43.00006 Dynamic networks community detection via low rank component recovery of adjacency matrices

, WEI BAO, GEORGE MICHAILIDIS, University of Michigan, Ann Arbor — Dynamic community detection in networks has been of high interest due to its various applications. In this work, we apply low rank extraction technique on adjacency matrices to approximate the community structures. Not only can we accurately identify the phase transition time points where significant changes in the community structures occur, but also we can increase the accuracy of the core community structures recovered in the peace time ranges by averaging the low rank components. A systematic methodology has been proposed as how to accomplish the target. Factor model, and stochastic block model (including weighted scenario) have been tested for the robustness of our model. Besides, applications on both Kuramoto model and US Senate Roll Call data are also carried out and interesting results are obtained.

### 9:12AM K43.00007 Multiway spectral community detection in networks

, XIAO ZHANG, MARK NEWMAN, Univ of Michigan - Ann Arbor — Spectral methods are widely used for community detection in networks because of their high efficiency and amenability to formal analysis. However, spectral algorithms have been limited to the division of networks into only two or three communities. Here we present a spectral algorithm that can directly divide a network into any number of communities. The algorithm makes use of a mapping from modularity maximization to a vector partitioning problem, combined with a fast heuristic for vector partitioning. We compare the performance of this spectral algorithm with previous approaches and find it to give superior results. We also give demonstrative applications of the algorithm to real-world networks and find that it produces results in good agreement with expectations for the networks studied.

**9:24AM K43.00008 Utilizing Maximal Independent Sets as Dominating Sets in Scale-Free Networks<sup>1</sup>** , N. DERZSY, Rensselaer Polytechnic Institute, F. MOLNAR JR., Northwestern University, B. K. SZYMANSKI, G. KORNISS, Rensselaer Polytechnic Institute — Dominating sets provide key solution to various critical problems in networked systems, such as detecting, monitoring, or controlling the behavior of nodes. Motivated by graph theory literature [Erdos, *Israel J. Math.* **4**, 233 (1966)], we studied *maximal independent sets* (MIS) as dominating sets in scale-free networks. We investigated the scaling behavior of the size of MIS in artificial scale-free networks with respect to multiple topological properties (size, average degree, power-law exponent, assortativity), evaluated its resilience to network damage resulting from random failure or targeted attack [Molnar et al., *Sci. Rep.* **5**, 8321 (2015)], and compared its efficiency to previously proposed dominating set selection strategies. We showed that, despite its small set size, MIS provides very high resilience against network damage. Using extensive numerical analysis on both synthetic and real-world (social, biological, technological) network samples, we demonstrate that our method effectively satisfies four essential requirements of dominating sets for their practical applicability on large-scale real-world systems: 1.) small set size, 2.) minimal network information required for their construction scheme, 3.) fast and easy computational implementation, and 4.) resiliency to network damage.

<sup>1</sup>Supported by DARPA, DTRA, and NSF.

**9:36AM K43.00009 Growing Networks with Positive and Negative Links** , CORYNNE DECH, SHADRACK ANTWI, LEAH SHAW, College of William and Mary — Scale-free networks grown via preferential attachment have been used to model real-world networks such as the Internet, citation networks, and social networks. Here we investigate signed scale-free networks where an edge represents a positive or negative connection. We present analytic results and simulation for a growing signed network model. We compare the signed network to an unsigned scale-free network. We discuss several options for preferential attachment in a signed network that could be further adapted to model the accumulation of links over time in real-world signed networks.

**9:48AM K43.00010 Robustness of networks of networks with degree-degree correlation** , BYUNGJOON MIN, City College of New York, SANTIAGO CANALS, Instituto de Neurociencias, HERNAN MAKSE, City College of New York — Many real-world complex systems ranging from critical infrastructure and transportation networks to living systems including brain and cellular networks are not formed by an isolated network but by a network of networks. Randomly coupled networks with interdependency between different networks may easily result in abrupt collapse. Here, we seek a possible explanation of stable functioning in natural networks of networks including functional brain networks. Specifically, we analyze the robustness of networks of networks focused on one-to-many interconnections between different networks and degree-degree correlation. Implication of the network robustness on functional brain networks of rats is also discussed.

**10:00AM K43.00011 Degree distributions of bipartite networks and their projections** , DEMIVAL VASQUES FILHO, DION O'NEALE, University of Auckland — Bipartite networks play an important role in the analysis of social and economic systems as they explicitly show the conceptual links between different types of entities. As an example, it is possible to build networks to investigate interactions regarding scientific and technological innovation that are well represented by a natural bipartite structure. Since we are often most interested in only one of the node types (e.g. the authors in an author-publication network), it is common to end up working with a projected version of the underlying bipartite network. The topology of projections and the dynamics that take place on it are highly dependent on the probability distribution of nodes degrees. We use the formalism of generating functions to infer how the degree distributions of the original bipartite network affect the distribution in the projected version. Moreover, we create artificial bipartite graphs by arbitrarily choosing degree distributions for the sets of nodes and construct the projection to analyze the resulting probability distribution. Our findings show that when projecting onto a particular set of nodes, the resulting degree distribution follows the behavior of the probability distribution of such nodes, subject, however, to the tail of the opposite distribution.

**10:12AM K43.00012 Spectra of Adjacency Matrices in Networks with Extreme Introverts and Extroverts<sup>1</sup>** , KEVIN E. BASSLER, Department of Physics, University of Houston, ROYCE K.P. ZIA, Department of Physics and Astronomy, Iowa State University, and Department of Physics, Virginia Tech — In recent studies of networks with preferred degrees (suitable for describing social networks in which individuals tend to prefer a certain number of contacts), the XIE model of extreme introverts and extroverts was found to display remarkable collective behavior and to raise interesting theoretical issues. Though this system is defined through its dynamics, i.e., introverts/extroverts always cut/add links, the steady state turns out to be a Boltzmann-like distribution. While the intra-group links are static, the cross-links are dynamic and lead to an ensemble of bipartite graphs, with extraordinary long-ranged correlations between elements of the incidence matrix (details in JSTAT P07013, 2015). Here, we report simulation studies of a different perspective of networks, namely, the spectra associated with this ensemble of adjacency matrices. As a baseline, we first consider the spectra associated with (the adjacency matrices of) a simple random (Erdős-Rényi) ensemble of bipartite graphs, where simulation results can be understood analytically.

<sup>1</sup>Work supported by the NSF through grants DMR-1206839 and DMR-1507371.

**10:24AM K43.00013 Complex root networks of Chinese characters** , PO-HAN LEE, Affiliated Senior High School of National Taiwan Normal University, Taipei, Taiwan, JIA-LING CHEN, Chinese Department, National Taiwan Normal University, Taipei, Taiwan, PO-CHENG WANG, Institute of Physics, Academia Sinica, Nankang, Taipei, Taiwan, TING-TING CHI, Chinese Department, National Taiwan Normal University, Taipei, Taiwan, ZHI-REN XIAO, ZIH-JIAN JHANG, Physics Department, National Taiwan University, Taipei, Taiwan, YEONG-NAN YEH, Institute of Mathematics, Academia Sinica, Nankang, Taipei, Taiwan, YIH-YUH CHEN, Physics Department, National Taiwan University, Taipei, Taiwan, CHIN-KUN HU, Institute of Physics, Academia Sinica, Taipei, Taiwan — There are several sets of Chinese characters still available today, including Oracle Bone Inscriptions (OBI) in Shang Dynasty, Chu characters (CC) used in Chu of Warring State Period, Small Seal Script in dictionary Shuowen Jiezi (SJ) in Eastern Han Dynasty, and Kangxi Dictionary (KD) in Qing Dynasty. Such as Chinese characters were all constructed via combinations of meaningful patterns, called roots. Our studies for the complex networks of all roots indicate that the roots of the characters in OBI, CC, SJ and KD have characteristics of small world networks and scale-free networks.

**Wednesday, March 16, 2016 8:00AM - 11:00AM —**  
**Session K44 GQI: Quantum Error Correction, Control & Simulation** 347 - Todd Brun, University of Southern California

**8:00AM K44.00001 Hamiltonian Engineering for High Fidelity Quantum Operations**, HUGO RIBEIRO, ALEXANDRE BAKSIC, AASHISH CLERK, McGill University — High-fidelity gates and operations are crucial to almost every aspect of quantum information processing. In recent experiments [1], fidelity is mostly limited by unwanted couplings with states living out of the logical subspace. This results in both leakage and phase errors. Here, we present a general method to deal simultaneously with both these issues and improve the fidelity of quantum gates and operations. Our method is applicable to a wide variety of systems. As an example, we can correct gates for superconducting qubits [1], improve coherent state transfer between a single NV centre electronic spin and a single nitrogen nuclear spin [2], improve control over a nuclear spin ensemble [3], etc. Our method is intimately linked to the Magnus expansion. By modifying the Magnus expansion of an initially given Hamiltonian  $H_i$ , we find analytically additional control Hamiltonians  $H_{\text{ctrl}}$  such that  $H_i + H_{\text{ctrl}}$  leads to the desired gate while minimizing both leakage and phase errors. [1] Zijun Chen, *et al.*, arXiv:1509.05470. [2] G. D. Fuchs, *et al.*, Nat. Phys. 7, 789793 (2011). [3] Mathieu Munsch, *et al.*, Nat. Nano. 9, 671675 (2014).

**8:12AM K44.00002 Method for generating all uniform  $\pi$ -pulse sequences used in deterministic dynamical decoupling<sup>1</sup>**, HAOYU QI<sup>2</sup>, JONATHAN DOWLING<sup>3</sup>, Department of Physics & Astronomy, Louisiana State University — Dynamical decoupling has been actively investigated since Viola first suggested using a pulse sequence to protect a qubit from decoherence. Since then, many schemes of dynamical decoupling have been proposed to achieve high-order suppression, both analytically and numerically. However, hitherto, there has not been a systematic framework to understand all existing uniform  $\pi$ -pulse dynamical decoupling schemes. In this report, we use the projection pulse sequences as basic building blocks and concatenation as a way to combine them. We derived a concatenated-projection dynamical decoupling, a framework in which we can systematically construct pulse sequences to achieve arbitrary high suppression order. All previously known uniform dynamical decoupling sequences using  $\pi$  pulse can be fit into this framework. Understanding uniform dynamical decoupling as successive projections on the Hamiltonian will also give insights on how to invent new ways to construct better pulse sequences.

<sup>1</sup>This work is supported by AirForce Office of Scientific Research, the US Army Research Office, and the National Science Foundation

<sup>2</sup>Quantum Sciences & Technologies Group Horace C. Hearne Jr. Institute for Theoretical Physics

<sup>3</sup>Quantum Sciences & Technologies Group Horace C. Hearne Jr. Institute for Theoretical Physics

**8:24AM K44.00003 Quantum gates with optimal bandwidth in noisy environments**, GUANG HAO LOW, YODER THEODORE, ISAAC CHUANG, Massachusetts Inst of Tech-MIT — The traditional approach of open-loop quantum error correction suppresses certain systematic imperfections  $\epsilon$  in quantum control to higher orders  $\epsilon^{\mathcal{O}(L)}$  by a well-designed sequence of  $L$  imperfect quantum gates. However, this philosophy of maximal flatness leads to an  $\epsilon$ -bandwidth that scales poorly with length and a residual that is easily overwhelmed by unaccounted sources of noise. We advance the paradigm of eiripple compensated gates that directly optimize for bandwidth given the limitations imposed by noise of magnitude  $\delta$ , leading to dramatically improved performance. Where  $\epsilon$  represent amplitude errors, we provide a formalism that generalizes both approaches and is effective at finding such gates. With it, we provide in closed-form the phase angles for an optimal family of population inversion gates with an  $\bar{\epsilon}$ -bandwidth of  $\mathcal{O}(\frac{\log \delta^{-1}}{L})$  — a quadratic improvement over optimal maximally flat variants. We also construct optimal NOT gates and discuss extensions to other gates and error models.

**8:36AM K44.00004 Engineering autonomous error correction in stabilizer codes at finite temperature**, C. DANIEL FREEMAN, University of California - Berkeley, CHRIS HERDMAN, University of Waterloo, BIRGITTA WHALEY, University of California - Berkeley — We present an error correcting protocol that enhances the lifetime of stabilizer code based qubits which are susceptible to string-like error modes at finite temperature, such as the toric code. The primary tool employed is dynamic application of the CSWAP operator, a local, unitary operator which exchanges defects and thereby translates quasiparticles. Crucially, the protocol does not require any information about the locations of quasiparticles, and can be used to enhance the lifetime of an encoded qubit in the absence of stabilizer measurement. This work was supported by the NSF grant DGE-1106400.

**8:48AM K44.00005 New class of photonic quantum error correction codes**, MATTI SILVERI, MARIOS MICHAEL, R. T. BRIERLEY, JUHA SALMILEHTO, VICTOR V. ALBERT, LIANG JIANG, S. M. GIRVIN, Departments of Physics and Applied Physics, Yale University — We present a new class of quantum error correction codes for applications in quantum memories, communication and scalable computation. These codes are constructed from a finite superposition of Fock states and can exactly correct errors that are polynomial up to a specified degree in creation and destruction operators. Equivalently, they can perform approximate quantum error correction to any given order in time step for the continuous-time dissipative evolution under these errors. The codes are related to two-mode photonic codes[1] but offer the advantage of requiring only a single photon mode to correct loss (amplitude damping), as well as the ability to correct other errors, e.g. dephasing. Our codes are also similar in spirit to photonic "cat codes" but have several advantages including smaller mean occupation number and exact rather than approximate orthogonality of the code words. We analyze how the rate of uncorrectable errors scales with the code complexity and discuss the unitary control for the recovery process. These codes are realizable with current superconducting qubit technology[2] and can increase the fidelity of photonic quantum communication and memories. [1] I.Chuang et al., Phys. Rev. A 56, 1114 (1997).[2] R.Heeres et al., Phys. Rev. Lett. 115, 137002 (2015).

**9:00AM K44.00006 Non-commuting two-local Hamiltonians for quantum error suppression**, ELEANOR RIEFFEL, NASA Ames Research Center, ZHANG JIANG, Stinger Ghaffarian Technologies Inc., NASA Ames Research Center, QUAIL TEAM — Physical constraints make it challenging to implement and control multi-body interactions. Designing quantum information processes with Hamiltonians consisting of only one- and two-local terms is a worthwhile challenge. A common approach to robust storage of quantum information is to encode in the ground subspace of a Hamiltonian. Even allowing particles with high Hilbert-space dimension, it is not possible to protect quantum information from single-site errors by encoding in the ground subspace of any Hamiltonian containing only commuting two-local terms [1]. We demonstrate how to get around this no-go result by encoding in the ground subspace of a Hamiltonian consisting of non-commuting two-local terms arising from the gauge operators of a subsystem code. Specifically, we show how to protect stored quantum information against single-qubit errors using a Hamiltonian consisting of sums of the gauge generators from Bacon-Shor codes [2] and generalized-Bacon-Shor code [3]. Thus, non-commuting two-local Hamiltonians have more error-suppressing power than commuting two-local Hamiltonians. Finally, we comment briefly on the robustness of the whole scheme. [1] I. Marvian and D. A. Lidar, PRL 113, 260504 (2014) [2] D. Bacon, PRA 73, 012340 (2006) [3] S. Bravyi, PRA 83, 012320 (2011)

**9:12AM K44.00007 Error threshold for the surface code in a superohmic environment<sup>1</sup>**, DANIEL A. LOPEZ-DELGADO, Universidade Estadual de Campinas - Brazil, E. NOVAIS, Universidade Federal do ABC - Brazil, EDUARDO R. MUCCILO, University of Central Florida, AMIR O. CALDEIRA, Universidade Estadual de Campinas - Brazil — Using the Keldysh formalism, we study the fidelity of a quantum memory over multiple quantum error correction cycles when the physical qubits interact with a bosonic bath at zero temperature. For encoding, we employ the surface code, which has one of the highest error thresholds in the case of stochastic and uncorrelated errors. The time evolution of the fidelity of the resulting two-dimensional system is cast into a statistical mechanics phase transition problem on a three-dimensional spin lattice, and the error threshold is determined by the critical temperature of the spin model. For superohmic baths, we find that time does not affect the error threshold: its value is the same for one or an arbitrary number of quantum error correction cycles.

<sup>1</sup>Financial support Fapesp, and CNPq (Brazil).

**9:24AM K44.00008 Fidelity of a quantum state protected by the surface code in the presence of a finite-temperature bosonic bath<sup>1</sup>**, E. NOVAIS, Federal University of ABC (SP-BRAZIL), A. J. STANFORTH, EDUARDO R. MUCCIOLO, University of Central Florida — We evaluate the fidelity of a multi-qubit quantum state protected by the surface code during a single quantum error correction cycle when qubits couple to a gapless bosonic environment. We discuss the protection of the state for different spectral functions and bath temperatures. Analytical results are supported by finite-size scaling analyses based on Monte Carlo and exact numerical calculations. Our results demonstrate a finite threshold that explicitly depends on the bath-mediated qubit-qubit interaction range and bath spectral function and temperature.

<sup>1</sup>This work was supported by the NSF grant CCF 1117241 and by Fapesp(Brazil) grant 2014/26356-9.

**9:36AM K44.00009 Repeated quantum error correction by real-time feedback on continuously encoded qubits**, JULIA CRAMER, NORBERT KALB, M. ADRIAAN ROL, BAS HENSEN, MACHIEL S. BLOK, QuTech and Kavli Institute of Nanoscience Delft, MATTHEW MARKHAM, DANIEL J. TWITCHEN, Element Six Innovation, RONALD HANSON, TIM H. TAMINIAU, QuTech and Kavli Institute of Nanoscience Delft — Because quantum information is extremely fragile, large-scale quantum information processing requires constant error correction. To be compatible with universal fault-tolerant computations, it is essential that quantum states remain encoded at all times and that errors are actively corrected. I will present such active quantum error correction in a hybrid quantum system based on the nitrogen vacancy (NV) center in diamond [1]. We encode a logical qubit in three long-lived nuclear spins, detect errors by multiple non-destructive measurements using the optically active NV electron spin and correct them by real-time feedback. By combining these new capabilities with recent advances in spin control, multiple cycles of error correction can be performed within the dephasing time. We investigate both coherent and incoherent errors and show that the error-corrected logical qubit can indeed store quantum states longer than the best spin used in the encoding [1]. Furthermore, I will present our latest results on increasing the number of qubits in the encoding, required for quantum error correction for both phase- and bit-flip. [1] J. Cramer et al. 2015; arXiv:1508.01388v1

**9:48AM K44.00010 Serialized Quantum Error Correction Protocol for High-Bandwidth Quantum Repeaters**, ANDREW GLAUDELL, Univ. of Maryland, National Institute of Standards and Technology, EDO WAKS, Univ. of Maryland and the National Institute of Standards and Technology, JACOB TAYLOR, Univ. of Maryland, National Institute of Standards and Technology — Advances in single-photon creation, transmission, and detection suggest that sending quantum information over optical fibers may have low enough losses to be overcome using quantum error correction. Such error-corrected communication is equivalent to a novel quantum repeater scheme, but crucial questions regarding implementation and system requirements remain open. In this talk, I will show that long-range entangled bit generation with rates approaching  $10^8$  entangled bits per second may be possible using a completely serialized protocol, in which photons are generated, entangled, and error corrected via sequential, one-way interactions with as few matter qubits as possible. Provided loss and error rates of the required elements are below the threshold for quantum error correction, this scheme demonstrates improved performance over transmission of single photons. We find improvement in entangled bit rates at large distances using this serial protocol and various quantum error correcting codes.

**10:00AM K44.00011 Spectroscopy of cross-correlations of environmental noises with two qubits<sup>1</sup>**, LUKASZ CYWINSKI, Institute of Physics, Polish Academy of Sciences, PIOTR SZANKOWSKI, MAREK TRIPPENBACH, Faculty of Physics, University of Warsaw, — A single qubit driven by an appropriate sequence of control pulses can serve as a spectrometer of local noise affecting its energy splitting. We show that by driving and observing two spatially separated qubits, it is possible to reconstruct the spectrum of cross-correlations of noises acting at various locations. When the qubits are driven by the same sequence of pulses, real part of cross-correlation spectrum can be reconstructed, while applying two distinct sequence to the two qubits allows for reconstruction of imaginary part of this spectrum [1]. The latter quantity contains information on either causal correlations between environmental dynamics at distinct locations, or on the occurrence of propagation of noisy signals through the environment. While entanglement between the qubits is not necessary, its presence enhances the signal from which the spectroscopic information is reconstructed. [1] P. Szankowski, M. Trippenbach, and L. Cywinski, arXiv:1507.03897.

<sup>1</sup>This work is supported by funds of Polish National Science Center (NCN) under decision no. DEC- 2012/07/B/ST3/03616

**10:12AM K44.00012 1D quantum simulation using a solid state platform<sup>1</sup>**, MEGAN KIRKENDALL, PATRICK IRVIN, MENGCHEN HUANG, JEREMY LEVY, University of Pittsburgh, HYUNGWOO LEE, CHANG-BEOM EOM, University of Wisconsin - Madison — Understanding the properties of large quantum systems can be challenging both theoretically and numerically. One experimental approach—quantum simulation—involves mapping a quantum system of interest onto a physical system that is programmable and experimentally accessible. A tremendous amount of work has been performed with quantum simulators formed from optical lattices; by contrast, solid-state platforms have had only limited success. Our experimental approach to quantum simulation takes advantage of nanoscale control of a metal-insulator transition at the interface between two insulating complex oxide materials<sup>2</sup>. This system naturally exhibits a wide variety of ground states (e.g., ferromagnetic, superconducting) and can be configured into a variety of complex geometries. We will describe initial experiments that explore the magnetotransport properties of one-dimensional superlattices with spatial periods as small as 4 nm, comparable to the Fermi wavelength. The results demonstrate the potential of this solid-state quantum simulation approach, and also provide empirical constraints for physical models that describe the underlying oxide material properties.

<sup>1</sup>We gratefully acknowledge financial support from AFOSR (FA9550-12-1- 0057 (JL), FA9550-10-1-0524 (JL) and FA9550-12-1-0342 (CBE)), ONR N00014-15-1-2847 (JL), and NSF DMR-1234096 (CBE)

<sup>2</sup>C. Cen *et al.*, Nat. Mater. **7**, 298 (2008)

**10:24AM K44.00013 Classical Emulation of a Two-Qubit Quantum Computer with Analog Electronics<sup>1</sup>**, BRIAN LA COUR, COREY OSTROVE, GRANVILLE OTT, MICHAEL STARKEY, GARY WILSON, Applied Research Laboratories, The University of Texas at Austin — Abstract: The Hilbert space mathematical structure of a gate-based quantum computer may be reproduced by mapping the computational basis states to corresponding functions in the space of complex exponentials and identifying an inner product between any two such functions. The span of these complex basis exponentials may then identified with the finite-dimensional Hilbert space of a gate-based quantum computer. By using classical analog electronic components, such as four-quadrant multipliers and operational amplifiers, voltage signals representing arbitrary four-dimensional quantum states, along with the equivalent gate and measurement operations of a quantum computer have been physically realized through the corresponding circuitry. The fidelity of the emulation is measured using both a direct evaluation of the signal as well as through an emulation of quantum state tomography to infer the quantum state. We demonstrate that for both state synthesis and gate operations, our quantum emulation device is capable of achieving over 99% fidelity.

<sup>1</sup>This work was supported by the Office of Naval Research under Grant No. N00014-14-1-0323.

**10:36AM K44.00014 Fourth-order master equation for a charged harmonic oscillator coupled to an electromagnetic field**, ARZU KURT<sup>1</sup>, RESUL ERYIGIT<sup>2</sup>, Abant İzzet Baysal University — Using Krylov averaging method, we have derived a fourth-order master equation for a charged harmonic oscillator weakly coupled to an electromagnetic field. Interaction is assumed to be of velocity coupling type which also takes into account the diamagnetic term. Exact analytical expressions have been obtained for the second, the third and the fourth-order corrections to the diffusion and the drift terms of the master equation. We examined the validity range of the second order master equation in terms of the coupling constant and the bath cutoff frequency and found that for the most values of those parameters, the contribution from the third and the fourth order terms have opposite signs and cancel each other. Inclusion of the third and the fourth-order terms is found to not change the structure of the master equation.

<sup>1</sup>Bolu, Turkey

<sup>2</sup>Bolu, Turkey

**10:48AM K44.00015 A Numerical Study of Entanglement Entropy of the Heisenberg Model on a Bethe Cluster**, BARRY FRIEDMAN, Physics, Sam Houston State University, GREG LEVINE, Physics and Astronomy, Hofstra University — Numerical evidence is presented for a nearest neighbor Heisenberg spin model on a Bethe cluster, that by bisecting the cluster, the generalized Renyi entropy scales as the number of sites in the cluster. This disagrees with spin wave calculations and a naive application of the area law but agrees with previous results for non interacting fermions on the Bethe cluster. It seems this scaling is not an artifact of non interacting particles. As a consequence, the area law in greater than one dimension is more subtle than generally thought and applications of the density matrix renormalization group to Bethe clusters face difficulties at least as a matter of principle.

**Wednesday, March 16, 2016 8:00AM - 11:00AM –**

**Session K45 GQI DAMOP: Hybrid Quantum Systems II** 348 - Mark Friesen, University of Wisconsin - Madison

**8:00AM K45.00001 Hamiltonian simulation for improved state transfer and readout in cavity QED**, FÉLIX BEAUDOIN, McGill University, ALEXANDRE BLAIS, Université de Sherbrooke, WILLIAM A. COISH, McGill University — Quantum state transfer into a memory, state shuttling over long distances via a quantum bus, and high-fidelity readout are important tasks for quantum technology. Generating the Hamiltonians that realize these tasks is challenging in the presence of realistic couplings to an environment. Here, we use average Hamiltonian theory to design the desired Hamiltonians in cavity QED. In particular, we present a protocol for state transfer between a qubit and a cavity. This approach makes use of a controllable qubit-cavity coupling strength to achieve a high fidelity even in the presence of inhomogeneous broadening that is stronger than the qubit-cavity coupling strength. In addition, we design a time-averaged interaction that allows for an improved quantum nondemolition readout. These ideas can be applied directly to propel novel systems coupling single spins to a microwave cavity into the strong coupling regime [Viennot et al, Science 349, 408 (2015)]. The approach can also be employed to improve quantum operations with spin ensembles.

**8:12AM K45.00002 Quantum efficiency of a double quantum dot microwave photon detector<sup>1</sup>**, CLEMENT WONG, MAXIM VAVILOV, Univ of Wisconsin-Madison — Motivated by recent interest in implementing circuit quantum electrodynamics with semiconducting quantum dots, we study charge transfer through a double quantum dot (DQD) capacitively coupled to a superconducting cavity subject to a microwave field. We analyze the DQD current response using input-output theory and determine the optimal parameter regime for complete absorption of radiation and efficient conversion of microwave photons to electric current. For experimentally available DQD systems, we show that the cavity-coupled DQD operates as a photon-to-charge converter with quantum efficiencies up to 80%

<sup>1</sup>C.W. acknowledges support by the Intelligence Community Postdoctoral Research Fellowship Program

**8:24AM K45.00003 Optical-Fiber-Illuminated Response of a Superconducting Microwave Resonator Below 1 K**, KRISTEN VOIGT, J. B. HERTZBERG, S. K. DUTTA, J. E. HOFFMAN, J. A. GROVER, J. LEE, P. SOLANO, R. P. BUDYO, C. BALLARD, J. R. ANDERSON, C. J. LOBB, S. L. ROLSTON, F. C. WELLSTOOD, JQI and CNAM, Dept. of Physics, University of Maryland — As a step towards building a hybrid quantum system that couples superconducting elements to neutral atoms trapped on a tapered optical nanofiber, we have studied how the presence of the fiber dielectric and light scattered from a fiber affect the response of a translatable thin-film lumped-element superconducting Al microwave resonator that is cooled to 15 mK. The resonator has a resonance frequency of about 6 GHz, a quality factor  $Q \approx 2 \times 10^5$ , and is mounted inside a 3D Al superconducting cavity. An optical fiber is tapered to a 60  $\mu\text{m}$  diameter and passes through two small holes in the 3D cavity such that it sits near the resonator. The 3D cavity is mounted on an x-z piezo-translation stage that allows us to change the relative position of the thin-film resonator and fiber. When the resonator is brought closer to the fiber, the resonance frequency decreases slightly due to the presence of the fiber dielectric. When 200  $\mu\text{W}$  of 780 nm light is sent through the fiber, about 100 pW/mm is Rayleigh-scattered from the fiber. This causes a position-dependent illumination of the resonator, affecting its resonance frequency and Q. We compare our results to a model of the resonator response that includes the generation, diffusion, and recombination of quasiparticles in the resonator and find that the frequency response allows us to track the position of the fiber to within 10  $\mu\text{m}$ .

**8:36AM K45.00004 Connecting trapped ions and quantum dots with photons**, MICHAEL KOEHL, University of Bonn — Coupling individual quantum systems lies at the heart of building scalable quantum networks. Here, we report the first direct photonic coupling between a semiconductor quantum dot and a trapped ion and we demonstrate that single photons generated by a quantum dot controllably change the internal state of an  $\text{Yb}^+$  ion. We ameliorate the effect of the sixty-fold mismatch of the radiative linewidths with coherent photon generation and a high-finesse fiber-based optical cavity enhancing the coupling between the single photon and the ion. The transfer of information presented here via the classical correlations between the  $\sigma_z$  projection of the quantum-dot spin and the internal state of the ion provides a promising step towards quantum state-transfer in a hybrid photonic network.

**9:12AM K45.00005 Encoding a Qubit into a Cavity Mode in Circuit-QED using Phase Estimation**, BARBARA TERHAL, DANIEL WEIGAND, RWTH - Aachen — Gottesman, Kitaev and Preskill have formulated a way of encoding a qubit into an oscillator such that the qubit is protected against small shifts (translations) in phase space. The idea underlying this encoding is that error processes of low rate can be expanded into small shift errors. The qubit space is defined as an eigenspace of two mutually commuting displacement operators which act as large shifts/translations in phase space. We propose and analyze the approximate creation of these qubit states by coupling the oscillator to a sequence of ancilla qubits realizing the protocol of approximate phase estimation for a displacement operator. We analyze the performance of repeated and adaptive phase estimation as the experimentally most viable schemes given a realistic upper limit on the number of photons in the oscillator. We propose a physical implementation of the protocol using the dispersive coupling between an ancilla transmon qubit and a cavity mode in circuit-QED. We estimate that in a current experimental set-up one can prepare a good code state from a squeezed vacuum state using 8 rounds of adaptive phase estimation lasting in total about 4  $\mu\text{sec}$ , with at least 80

### 9:24AM K45.00006 Long-distance entanglement of spin qubits via quantum Hall edge states

, GUANG YANG, CHEN-HSUAN HSU, PETER STANO, RIKEN Center for Emergent Matter Science, Wako, Japan, JELENA KLINOVAJA, DANIEL LOSS, Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — The implementation of a functional quantum computer involves entangling and coherent manipulation of a large number of qubits. For qubits based on electron spins confined in quantum dots, which are among the most investigated solid-state qubits at present, architectural challenges are often encountered in the design of quantum circuits attempting to assemble the qubits within the very limited space available. Here, we provide a solution to such challenges based on an approach to realizing entanglement of spin qubits over long distances. We show that long-range Ruderman-Kittel-Kasuya-Yosida interaction of confined electron spins can be established by quantum Hall edge states, leading to an exchange coupling of spin qubits. The coupling is anisotropic and can be either Ising-type or XY-type, depending on the spin polarization of the edge state. Such a property, combined with the dependence of the electron-spin susceptibility on the chirality of the edge state, can be utilized to gain valuable insights into the topological nature of various quantum Hall states.

### 9:36AM K45.00007 Entangling distant resonant exchange qubits via circuit quantum electrodynamics

, VANITA SRINIVASA, Laboratory for Physical Sciences/University of Maryland, College Park, MD, JACOB M. TAYLOR, Joint Center for Quantum Information and Computer Science/Joint Quantum Institute/National Institute of Standards and Technology, Gaithersburg, MD, CHARLES TAHAN, Laboratory for Physical Sciences, College Park, MD — Enabling modularity within a quantum information processing device relies on robust entanglement of coherent qubits at macroscopic distances. To address this challenge, we investigate theoretically a hybrid quantum system consisting of spatially separated resonant exchange qubits, defined in three-electron semiconductor triple quantum dots, that are coupled via a superconducting transmission line resonator. By analyzing three specific approaches drawn from circuit quantum electrodynamics and Hartmann-Hahn double resonance techniques for implementing resonator-mediated two-qubit entangling gates in both dispersive and resonant regimes, we show that methods for entangling superconducting qubits map directly to resonant exchange qubits. We also calculate the rate of relaxation via phonons for resonant exchange qubits in silicon triple dots and show that such an implementation is particularly well-suited to achieving the strong coupling regime. Our approach combines the robustness of encoded spin qubits in silicon with the rapid and robust long-range entanglement provided by circuit QED systems.

### 9:48AM K45.00008 Long distance coupling of resonant exchange qubits

, MAXIMILIAN RUSS, GUIDO BURKARD, Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — We investigate the effectiveness of a microwave cavity as a mediator of interactions between two resonant exchange (RX) qubits<sup>1,2</sup> in semiconductor quantum dots (QDs) over long distances<sup>3</sup>, limited only by the extension of the cavity. Our interaction model includes the orthonormalized Wannier orbitals constructed from Fock-Darwin states under the assumption of a harmonic QD confinement potential. We calculate the qubit-cavity coupling strength  $g_r$  in a Jaynes-Cummings Hamiltonian, and find that dipole transitions between two states with an asymmetric charge configuration constitute the relevant RX qubit-cavity coupling mechanism. The effective coupling between two RX qubits in a shared cavity yields a universal two-qubit iSWAP-gate with gate times on the order of nanoseconds over distances on the order of up to a millimeter. Funded by ARO through grant No. W911NF-15-1-0149.

<sup>1</sup>J. Medford et al., Phys. Rev. Lett. 111, 050501 (2013)

<sup>2</sup>J. M. Taylor et al., Phys. Rev. Lett. 111, 050502 (2013)

<sup>3</sup>M. Russ and G. Burkard, arXiv: 1508.07122 (2015)

### 10:00AM K45.00009 Injection locking of a semiconductor double-quantum-dot micromaser<sup>1</sup>

, Y.-Y. LIU, J. STEHLIK, Department of Physics, Princeton University, M. J. GULLANS, J. M. TAYLOR, Joint Quantum Institute/NIST, J. R. PETTA, Department of Physics, Princeton University — Narrow linewidth lasers and masers are desirable for applications such as frequency standards and low-noise amplifiers. Recently we have demonstrated a double-quantum-dot (DQD) micromaser, which generates photons through single electron tunneling events.<sup>2</sup> Charge noise couples to the DQD energy levels and results in a maser linewidth that is 100 times larger than the Schawlow-Townes prediction. We demonstrate linewidth narrowing by more than a factor of 10 using injection locking. The injection locking range is measured as a function of input power and shown to be in excellent agreement with the Adler equation. The position and amplitude of distortion sidebands that appear outside of the injection locking range are quantitatively examined. Our results show that this unconventional maser, which is impacted by strong charge noise and electron-phonon coupling, is well described by standard laser models.<sup>3</sup>

<sup>1</sup>Supported by the National Science Foundation and the Gordon and Betty Moore Foundation's EPiQS initiative through grant no. GBMF4535.

<sup>2</sup>Y.-Y. Liu, J. Stehlik, C. Eichler, M. J. Gullans, J. M. Taylor, and J. R. Petta, Science **347**, 285 (2015).

<sup>3</sup>Y.-Y. Liu, J. Stehlik, M. J. Gullans, J. M. Taylor, and J. R. Petta, Phys. Rev. A (in press).

### 10:12AM K45.00010 Real-time tuning of a double quantum dot using a Josephson parametric amplifier<sup>1</sup>

, J. STEHLIK, Y.-Y. LIU, Department of Physics, Princeton University, C. M. QUINTANA, Department of Physics, UC Santa Barbara, C. EICHLER, T. R. HARTKE, J. R. PETTA, Department of Physics, Princeton University — Josephson parametric amplifiers (JPAs)<sup>2</sup> have enabled advances in readout of quantum systems. Here we demonstrate JPA-assisted readout of a cavity-coupled double quantum dot (DQD).<sup>3</sup> Utilizing a JPA we improve the signal-to-noise ratio (SNR) by a factor of 2000 compared to the situation with the parametric amplifier turned off. At an interdot charge transition we achieve a SNR of 76 (19 dB) with an integration time  $\tau = 400$  ns, which is limited by the linewidth of our cavity. By measuring the SNR as a function of  $\tau$  we extract an equivalent charge sensitivity of  $8 \times 10^{-5} e/\sqrt{\text{Hz}}$ . We develop a dual-gate-voltage rastering scheme that allows us to acquire a DQD charge stability diagram in just 20 ms. Such rapid data acquisition rates enable device tuning in live "video-mode," where the results of parameter changes are immediately displayed. Live tuning allows the DQD confinement potential to be rapidly tuned, a capability that will become increasingly important as semiconductor spin qubits are scaled to a larger number of dots.

<sup>1</sup>Research is supported by the Packard Foundation, ARO Grant No. W911NF-15-1-0149, DARPA QuEST Grant No. HR0011-09-1-0007, and the NSF (Grants No. DMR-1409556 and DMR-1420541).

<sup>2</sup>B. Yurke, J. Opt. Soc. Am. B, **4** 1551 (1987).

<sup>3</sup>J. Stehlik *et al.*, Phys. Rev. Appl., **4** 014018 (2015).

**10:24AM K45.00011 Investigating the level broadening of a semiconductor charge qubit in microwave emission measurements**, A. STOCKKLAUSER, N. HEDRICH, V. F. MAISI, J. BASSET, K. CUJIA, C. REICHL, W. WEGSCHEIDER, T. IHN, K. ENSSLIN, A. WALLRAFF, ETH Zurich — We investigate a hybrid circuit quantum electrodynamics architecture in which a double quantum dot charge qubit is coupled to a nearby microwave cavity. The discussed experiments explore the emission of microwave radiation from a voltage-biased GaAs double dot similar to Ref. [1]. A superconducting coplanar waveguide resonator serves as a tool to study aspects of the quantum dot level structure that are difficult to access in transport measurements. We explore resonances in microwave emission that arise from inelastic interdot transitions resonant with the cavity [2]. In particular, the line width of the emission resonances is investigated and linked to the level broadening of the double dot charge qubit. We study the dependence of the emission line width on the tunnel rates to the leads and identify this as the dominant contribution to the broadening of the qubit levels. For the explored bias conditions qubit decoherence is low in comparison. We extract the tunnel rates to the leads from the linewidth of the emission signal and compare it with the tunnel rates extracted from current measurements.

[1] Y.-Y. Liu *et al.*, Phys. Rev. Lett. **113**, 036801 (2014).

[2] A. Stockklauser *et al.*, Phys. Rev. Lett. **115**, 046802 (2015).

**10:36AM K45.00012 Observation of magnon number states in a superconducting qubit spectrum**, DANY LACHANCE-QUIRION, Université de Sherbrooke, YUTAKA TABUCHI, SEIICHIRO ISHINO, ATSUSHI NOGUCHI, TOYOFUMI ISHIKAWA, REKISHU YAMAZAKI, KOJI USAMI, RCAST, The University of Tokyo, YASUNOBU NAKAMURA, RCAST, The University of Tokyo, CEMS, RIKEN — A quantum transducer interfacing qubits in the microwave domain to optical light requires a quantum system interacting with photons of both frequency domains. Coherent interaction between collective excitations (magnons) in the ferrimagnetic insulator yttrium iron garnet (YIG) and a superconducting qubit through virtual microwave photons has recently been demonstrated [1]. In this talk, we present results on the observation of magnon number states in a superconducting qubit spectrum when creating a coherent state in a magnetostatic mode of a YIG sphere interacting dispersively with the qubit. The dispersive interaction strength of 1.2 MHz measured in the straddling regime is in good agreement with numerical simulations. Furthermore the probability distribution of magnon number states, recovered from the qubit spectrum, is compared with the Poisson distribution expected for a coherent state. Resolving magnon number states constitutes a first step toward encoding quantum information into a quantum state of a magnetostatic mode [2].

[1] Y. Tabuchi, S. Ishino, A. Noguchi, T. Ishikawa, R. Yamazaki, K. Usami, and Y. Nakamura, Science **349**, 405 (2015).

[2] Z. Leghtas, G. Kirchmair, B. Vlastakis, M. Devoret, R. Schoelkopf, and M. Mirrahimi, Phys. Rev. A **87**, 042315 (2013).

**10:48AM K45.00013 Emergent Curved space induced by adiabatic approximation<sup>1</sup>**, RAN CHENG, XIAOCHUAN WU, DI XIAO, Carnegie Mellon University — Berry curvature, serving as the imaginary part of quantum geometric tensor (QGT), gives rise to an effective Lorentz force to the dynamics of the adiabatic parameter. However, it is not clear whether the real part of QGT, the quantum metric, has any dynamical consequence as the Berry gauge force. We show in a general way that during an adiabatic process, the particle in a hybrid quantum system governed by an equation of motion second order in time is subject to an induced gravitational force. The adiabatic dynamics can be described by a geodesic equation as if the spacetime is curved by the quantum metric. As an example, we demonstrate the above result in a simple toy model.

<sup>1</sup>This work is supported by DOE BES (No. DE-SC0012509) and AFOSR (No. FA9550-12-1-0479)

## Wednesday, March 16, 2016 8:00AM - 10:48AM —

Session K46 GIMS: Advances in Scanning Probe Microscopy III: Scanning Probe Spectroscopic Techniques 311 - Jeonghoon Ha, National Magnet Laboratory

**8:00AM K46.00001 The influence of deformation rate on polymer nanomechanical properties as measured by Atomic Force Microscopy.**, BEDE PITTENGER, THOMAS MUELLER, Bruker Nano, AFM UNIT TEAM — Polymeric composites often have heterogeneities at the nanometer length scale. AFM based mechanical property measurements have the sensitivity and resolution necessary to visualize these features and better understand their influence on bulk properties. In the past few years, AFM mechanical property mapping has evolved from slow force volume to faster, but conceptually very similar, PeakForce Tapping. Currently, the time scale of tip-sample interaction spans from microseconds to seconds, tip sample forces can be controlled from piconewtons to micronewtons, and spatial resolution can reach sub-nanometer. AFM has become a unique mechanical measurement tool having large dynamic range (1kPa to >100GPa in modulus) with the flexibility to integrate with other physical property characterization techniques in versatile environments. In particular, researchers have begun to take advantage of the wide range of deformation rates accessible to AFM in order to study time dependent properties of materials such as viscoelasticity. This presentation will review this recent progress, providing examples that demonstrate the dynamic range of the measurements and the resolution with which they were obtained. Additionally, the effect of time dependent material properties on the types of measurements will be explored.

**8:12AM K46.00002 Atomic Force Tomography of a Nonplanar Molecule: Role of Lateral and Chemical Sample-Tip Interactions<sup>1</sup>**, XIANGHUA KONG, Ph. D candidate, WEI JI, Professor, PHYSICS DEPARTMENT, MCGILL TEAM, PHYSICS DEPARTMENT, RENMIN UNIVERSITY OF CHINA TEAM — Atomically identification of the molecular geometric structures is an important prerequisite to understand their chemical and electrical properties. TiOPc, a steric structure, gives rise to two adsorption configurations of TiOPc on Cu(111), namely O-dn and O-up. The roles of chemical specific interactions of different intramolecular atoms with the AFM tips were discussed at the submolecular level. For O-up, the molecular backbone of TiOPc is only visible out of a certain range from the center of the molecule, accompanied with significant dissipation signal. Theoretical calculation identifies such dissipation signal as the chemical attraction between the out-of-plane O in TiOPc and the Cu atoms behind the CO of a tip at a certain range of lateral distance between them. When they approach closer, the sample O repulses another O in the CO tip making it tilting strongly, which softens the tip and thus leads to even stronger O (sample) – Cu (tip) attraction. A direct demonstration of sample-tip electronic hybridization was manifested in the simpler O-dn case where an explicit wavefunction overlap between the tip O atom and the sample Ti atom. Given these results presented here, we anticipate that this method might be developed further generally useful in single-molecule chemistry and physics.

<sup>1</sup>X.K. thanks the Chinese Scholarship Council for support

**8:24AM K46.00003 Scanning Ion Conductance Microscopy for living cell membrane potential measurement**, NAMUNA PANDAY, Florida Intl Univ — Recently, the existence of multiple micro-domains of extracellular potential around individual cells have been revealed by voltage reporter dye using fluorescence microscopy. One hypothesis is that these long lasting potential patterns play a vital role in regulating important cell activities such as embryonic patterning, regenerative repair and reduction of cancerous disorganization. We used multifunctional Scanning Ion Conductance Microscopy (SICM) to study these extracellular potential patterns of single cell with higher spatial resolution. To validate this novel technique, we compared the extracellular potential distribution on the fixed HeLa cell surface and Polydimethylsiloxane (PDMS) surface and found significant difference. We then measured the extracellular potential distributions of living melanocytes and melanoma cells and found both the mean magnitude and spatial variation of extracellular potential of the melanoma cells are bigger than those of melanocytes. As compared to the voltage reporter dye based fluorescence microscope method, SICM can achieve quantitative potential measurements of non-labeled living cell membranes with higher spatial resolution.

**8:36AM K46.00004 Local Imaging of Conductance Evolution in Ion-Gel-Gated Transitional Metal Dichalcogenide Transistors**, XIAOYU WU, DI WU, Univ of Texas, Austin, HONGTAO YUAN, HAROLD HWANG, YI CUI, Stanford University, KEJI LAI, Univ of Texas, Austin — Electrolyte-gated electric double layer transistors (EDLTs) have demonstrated carrier density modulation in a remarkably wide range in systems ranging from complex oxides to layered metal chalcogenides. Cryogenic microwave impedance microscopy (MIM) has been used to perform real-space mapping of nanoscale conductance evolution in oxide EDLT gated with an ultrathin ionic gel layer. However, such microwave imaging was previously only possible at temperatures lower than the glass transition temperature (frozen temperature) of the gel because of the contact-mode scanning. Here, we report in-situ imaging of conductance evolution in  $\text{WSe}_2$  transistors using a MIM based on the frequency-modulated atomic force microscopy (FM-AFM) mode. With a typical tip-sample distance of 30nm, the  $\text{WSe}_2$  EDLT can be simultaneously gate-modulated and imaged at 220K, which is above the frozen temperature of the gel. The microwave images vividly show the spatial evolution of channel conductance in  $\text{WSe}_2$  during the metal-insulator transition and mesoscopic electronic inhomogeneity with different configurations of source/drain/gate voltages. Such in-situ microwave imaging provides new opportunities to correlate the macroscopic transport results and microscopic conductivity distribution in both equilibrium and non-equilibrium states of the EDLTs.

**8:48AM K46.00005 Resolving local voltage variations in opto-electronic devices with Kelvin probe force microscopy**, ELIZABETH TENNYSON, University of Maryland College Park - Department of Materials Science and Engineering, JOSEPH GARRETT, University of Maryland College Park - Department of Physics, JEREMY MUNDAY, University of Maryland College Park - Department of Electrical and Computer, MARINA LEITE, University of Maryland College Park - Department of Materials Science and Engineering — We employ illuminated Kelvin probe force microscopy (KPFM) to spatially resolve the open-circuit voltage ( $V_{oc}$ ) of optoelectronic devices with nanoscale spatial resolution, >5 orders of magnitude better than previous methods. In illuminated-KPFM, we measure the difference in work function between the sample surface and the probe, termed the contact potential difference (CPD). By grounding the bottom contact of the solar cell to the AFM probe, the difference between the illuminated and the dark signals is proportional to quasi-Fermi level splitting and, therefore, the  $V_{oc}$ . We apply our scanning probe technique to a variety of solar cell materials, including polycrystalline CIGS, where we resolve local variations in  $V_{oc} > 150$  mV [1]. We use heterodyne-KPFM (where we map  $1 \mu\text{m}^2$  in 16 seconds) to probe hybrid perovskites solar cells, and quantify in real-time the voltage changes upon material relaxation after illumination. This metrology yields new insights into the local electrical properties of solar cells, and can be expanded to any optoelectronic device. [1] E.M. Tennyson et al., Adv. Energy Mat., **5** (2015) in press, front cover.

**9:00AM K46.00006 Multi-step atomic interchange mechanism for atom manipulation on semiconductor surfaces.**, BATNYAM ENKHTAIVAN, ATSUSHI OSHIYAMA, Department of Applied Physics, The University of Tokyo — We report on our total-energy electronic-structure calculations based on the density-functional theory that clarify atom-scale mechanisms of atom-manipulation recently realized on semiconductor surfaces [1]. We focus on Ge(111) and Si(111) surfaces and identify reaction pathways and corresponding reaction energy barriers. Considering the atom manipulation of Pb and Sn atoms on Ge(111) surfaces, we find that the substitutional Sn (Pb) diffuses to neighboring Ge adatom, and forms a dimer with Ge spontaneously. Then the Sn (Pb) and the Ge adatom exchange their position concertedly with the dimer structure kept. These diffusion and exchange processes are multi-step atomic processes consisting of multiple metastable states. For the case of Sb manipulation on the Si(111) surface, the dimer structure does not form spontaneously when the AFM tip is absent. We find that the roles of the AFM tip during the atom manipulation are the lowering of the diffusion energy barrier and stabilization of the dimer structure. [1] Y. Sugimoto et al., e-J. Surf. Sci. Nanotech. **4**, 376-383 (2006).

**9:12AM K46.00007 Measuring electron-phonon coupling with Scanning Tunneling Microscopy**, VIDYA MADHAVAN, University of Illinois, Urbana-Champaign — Electron-boson interactions are ubiquitous in systems ranging from simple metals to novel materials such as graphene, high-temperature superconductors and topological insulators. Of particular interest is the coupling between electrons and phonons. In general, electron-phonon coupling gives rise to quasiparticles of decreased mobility and increased effective mass. Nearly all information about electron-phonon coupling is contained in the Eliashberg function ( $\alpha^2 F(\omega; k, E)$ ) of the material. In this talk I discuss the various methods by which the effects of electron-phonon coupling can be measured by scanning tunneling microscopy. I will present STM data on a variety of systems ranging from metals to topological insulators and discuss the signatures of electron-phonon interactions in different types of STM data. In particular I discuss how high resolution measurements allow us to measure the dispersion and obtain the real part of the self-energy, which can in principle be inverted to obtain the Eliashberg function.

**9:48AM K46.00008 Lateral manipulation and interplay of local Kondo resonances in a two-impurity Kondo system.**, HAIMING GUO, Institute of Physics, Chinese Academy of Sciences — The control of a single spin of an atom is of great interest in Kondo physics and a potential application in spin based electronics. Low-temperature scanning tunneling microscopy and spectroscopy (LT-STM/STS) is a powerful tool to probe the single spin and its Kondo effect at the atomic scale on surfaces. I am going to present the modulation of magnetic properties and Kondo effect of Co adatoms on graphene layer. This is also the first discovery of a Kondo effect caused from a magnetic impurities doped in graphene layer in experiment. The tiny diverse interaction between magnetic impurity and graphene host further modulates the Kondo effect. Next, the atomic-scale spatial relationship of a two-impurity Kondo system at varying lateral distance will be reported. A notable interplay is determined between two individual Kondo singlet states, which are formed by the localized spins of two cobalt magnetic adatoms that are placed on different electrodes of an STM. The  $dI/dV$  spectra show the continuous changes of the resonance peak feature when approaching the Kondo tip laterally to the local sample-Kondo impurity on the surface.

**10:00AM K46.00009 Local Force Interactions and Image Contrast Reversal on Graphite Observed with Noncontact Atomic Force Microscopy**, OMUR DAGDEVIREN, JAN GOETZEN, ERIC ALTMAN, UDO SCHWARZ, Yale University — Surface interactions of graphene-based nanostructures remain a topic of considerable interest in nanotechnology. Similarly, tip-dependent imaging contrasts have attracted attention as they allow conclusions to be made about the surface's chemical structure and local reactivity. In this talk, we present noncontact atomic force microscopy data recorded in the attractive regime on highly oriented pyrolytic graphite that reveals image contrast reversal for the first time. While larger tip-sample separations feature bright spots on atomic sites, the maximum of the tip-sample interaction flips to the hollow site positions upon further approach, which represents the contrast predominantly observed in previous studies during attractive-mode imaging. This cross over of the local chemical interaction is confirmed in force spectroscopy experiments. The results will be discussed in light of recent theoretical simulations that have predicted the occurrence of such contrast reversal for specific tip terminations.

**10:12AM K46.00010 Theoretical model of the tunneling current between a metallic tip and a ferroelectric material.**<sup>1</sup>, RAVI NEUPANE, ANDREW YOST, TEYU CHIEN, Univ of Wyoming — We present a model to calculate the tunneling current for a ferroelectric (FE) material in a metal/vacuum/Ferroelectric tunneling junction. Using this model, we try to explore the effect of the FE dipole orientation's direction on  $I - V$  spectrum using scanning tunneling spectroscopy (STS). The STM tunneling current for non-FE materials depends upon various factors such as tip-sample distance (vacuum gap), temperature, density of states (DOS) of tip and of sample, and tip-sample bias. FE materials have internal electric dipoles giving rise to internal and external electric fields. The electric field induced by these dipoles will distort the Fermi level as a function of depth in the material. In our model, the Fermi level is assumed to be inclined with a slope as a function of the depth. The slope depends upon the orientation and the strength of the electric dipole moment. In this model we use the WKB method accounting for the slope of the Fermi level to calculate the tunneling probability from tip to different depths then summing all contributions to obtain the total current as a function of tip-sample bias, i.e.  $I - V$  curves.

<sup>1</sup>School of Energy Resources, University of Wyoming

**10:24AM K46.00011 The power laws of nanoscale forces in ambient conditions**, MATTEO CHIESA, SERGIO SANTOS, CHIA-YUN LAI, Laboratory for Energy and NanoScience, Masdar Institute — Power laws are ubiquitous in the physical sciences and indispensable to qualitatively and quantitatively describe physical phenomena. A nanoscale force law that accurately describes the phenomena observed in ambient conditions at several nm or fractions of a nm above a surface however is still lacking. Here we report a power law derived from experimental data and describing the interaction between an atomic force microscope AFM tip modelled as a sphere and a surface in ambient conditions. By employing a graphite surface as a model system the resulting effective power is found to be a function of the tip radius and the distance. The data suggest a nano to mesoscale transition in the power law that results in relative agreement with the distance-dependencies predicted by the Hamaker and Lifshitz theories for van der Waals forces for the larger tip radii only

**10:36AM K46.00012 Development of tip Scanning High Speed AFM operating at 1,000 Lines/s & 15m**, UMIT CELIK, Material Science and Engineering, Istanbul Technical University, Turkey, IHSAN KEHRIBAR, NanoMagnetics Instruments, Turkey, KUBRA CELIK, Material Science and Engineering, Istanbul Technical University, Turkey, H. ZGR ZER, Physics Department, Istanbul Technical University, Turkey, AHMET ORAL, Physics Department, Middle East Technical University, Turkey — High speed atomic force microscope allows imaging dynamic processes on the surfaces. We have developed a very high speed tip scanning atomic force microscope (HS-AFM). We designed the tip scanning system to overcome the sample size limits, with a beam tracking capability to follow the cantilever motion. A high resonance frequency flexure scanner developed which has 15m scan range in XY and 3m in Z axis. A novel FPGA based high speed scanning and data acquisition system was developed. The scanner is driven by sine wave in X-axis to avoid resonances and data were captured at equal sample intervals. 1 KHz line scan rate is achieved at 15m scan range with the HS-AFM.

**Wednesday, March 16, 2016 8:00AM - 11:00AM –**

**Session K47 DCP: Bulk Water: Experiment and Theory** 312 - David Chandler, Sandia National Laboratory

**8:00AM K47.00001 Accurate path integral molecular dynamics simulation of ab-initio water at near-zero added cost<sup>1</sup>**, DANIEL ELTON, Stony Brook University, MICHELLE FRITZ, JOS SOLER, Universidad Autonoma de Madrid, MARIVI FERNANDEZ-SERRA, Stony Brook University — It is now established that nuclear quantum motion plays an important role in determining waters structure and dynamics. These effects are important to consider when evaluating DFT functionals and attempting to develop better ones for water. The standard way of treating nuclear quantum effects, path integral molecular dynamics (PIMD), multiplies the number of energy/force calculations by the number of beads, which is typically 32. Here we introduce a method whereby PIMD can be incorporated into a DFT molecular dynamics simulation at virtually zero cost. The method is based on the cluster (many body) expansion of the energy. We first subtract the DFT monomer energies, using a custom DFT-based monomer potential energy surface. The evolution of the PIMD beads is then performed using only the more-accurate Partridge-Schwenke monomer energy surface. The DFT calculations are done using the centroid positions. Various bead thermostats can be employed to speed up the sampling of the quantum ensemble. The method bears some resemblance to multiple timestep algorithms and other schemes used to speed up PIMD with classical force fields. We show that our method correctly captures some of key effects of nuclear quantum motion on both the structure and dynamics of water.

<sup>1</sup>We acknowledge support from DOE Award No. DE-FG02-09ER16052 (D.E.) and DOE Early Career Award No. DE-SC0003871 (M.V.F.S.)

**8:12AM K47.00002 ABSTRACT WITHDRAWN –**

**8:24AM K47.00003 X-ray absorption of liquid water studied by advanced *ab initio* methods<sup>1</sup>**, ZHAORU SUN, JIANPING WANG, Temple University, WEI KANG, Peking University, ROBERTO CAR, Princeton University, XIFAN WU, Temple University — Oxygen K-edge X-ray absorption spectra (XAS) provide a sensitive local probe of the H-bond structure of liquid water. Based on the static COHSEX approach, we computed the XAS spectra of liquid water from molecular structures generated by *ab initio* molecular dynamics (AIMD) simulations using a van der Waals (vdW) inclusive hybrid functional (PBE0) that gives ambient water structure in quantitative agreement with experiment [JCP 141, 084502 (2014)]. We find that good agreement between experimental and theoretical XAS requires both improved molecular modeling and excitation treatment. In our simulation the over-structured H-bond network resulting from GGA-AIMD is systematically reduced as the directional H-bond strength is lowered by the mitigated self-interaction error in PBE0 and the increased population of interstitial water molecules promoted by vdW interactions. The better H-bond structure in turn gives improved XAS spectra. Moreover, we find that the orbitals obtained from the self-consistent diagonalization of the self-energy are crucial in obtaining spectra that compare well with experiment.

<sup>1</sup>DOE SciDAC: DE-SC0008626 and DE-SC0008726

**8:36AM K47.00004 Why does hydronium diffuse faster than hydroxide in liquid water?<sup>1</sup>**, LIXIN ZHENG, Temple University, BISWAJIT SANTRA, Princeton University, ROBERT DISTASIO, Cornell University, MICHAEL KLEIN, Temple University, ROBERTO CAR, Princeton University, XIFAN WU, Temple University — Experiments show that the hydronium ion ( $\text{H}_3\text{O}^+$ ) diffuses much faster than the hydroxide ion ( $\text{OH}^-$ ) in liquid water. *ab initio* molecular dynamics (AIMD) simulations correctly associated the diffusion mechanism to proton transfer (PT) but have been unable so far to clearly identify the reason for the faster diffusion of hydronium compared to hydroxide, as the diffusion rate was found to depend sensitively on the adopted functional approximation. We carried out AIMD simulations of the solvated water ions using a van der Waals (vdW) inclusive PBE0 hybrid density functional. It is found that not only hydronium diffuses faster than hydroxide but also the absolute rates agree with experiment. The fast diffusion of  $\text{H}_3\text{O}^+$  occurs via concerted PT that enables the ion to jump across several H-bonded molecules in successful transfer events; in contrast, such concerted motion is significantly hindered in  $\text{OH}^-$  where the ion is easily trapped in a hyper-coordination configuration (a local solvation structure that forbids PT). As a result multiple PT events are rare and the diffusion of  $\text{OH}^-$  is significantly slowed down. Such a clear difference between the two ions results from the combined effect of vdW interactions and self-interaction correction.

<sup>1</sup>DOE SciDac: DE-SC0008626 and DE-SC0008726

**8:48AM K47.00005 Electrical Mobility of Protons and Proton-Holes in Pure Water Characterized by Physics-Based Water Model.**, BINBIN JIE, CHIHTANG SAH, Department of Physics, Xiamen University, China — Pure water has been characterized empirically for nearly a century, as dissociation into hydronium ( $\text{H}_3\text{O}^+$ )<sup>1+</sup> and hydroxide ( $\text{OH}^-$ )<sup>1-</sup> ions. Last March, we reported that the ~40 year experimental industrial standard of chemical equilibrium reaction constant, the ion product, can be accounted for by a statistical-physics-based concentration product of two electrical charge carriers, the positively charged protons,  $\text{p}^+$ , and the negatively charged proton holes or proholes,  $\text{p}^-$ , with a thermal activation energy or proton trapping well depth of  $E_{\text{p}^+/\text{p}^-} = 576$  meV, in the 0-100°C pure liquid water. We now report that the empirically fitted industrial standard experimental data (1985, 1987, 2005) of the two dc ion mobilities in liquid water, can also be accounted for by trapping-limited drift of protons and proholes through proton channels of lower proton electrical potential valleys,  $E_{\text{p}^+/\text{p}^-} \leq E_{\text{p}^+/\text{p}^-} < (E_{\text{p}^+/\text{p}^-}/3)$ , in the tetrahedrally-directed electron-pair-bonded oxygen ions,  $\text{O}^{2-}$ , in hexagonal lattice based on the 1935 Pauling statistical model using the 1933 Bernal-Fowler water rule.

**9:00AM K47.00006 Nuclear Quantum Effects in Different Ice Phases<sup>1</sup>** , MARIVI FERNANDEZ-SERRA, Stony Brook University, BETUL PAMUK, CNRS and Université Pierre et Marie Curie, PHILIP B. ALLEN, Stony Brook University — We have previously explained that the anomalous isotope effect in hexagonal ices is linked to the anticorrelation between the covalent OH bond and the hydrogen bond by using the quasiharmonic approximation combined with *ab initio* density functional theory. [1] In this study, we show that similar physics plays a role in the isotope effect on temperature of the proton-order/disorder phase transition between ice XI and ice<sub>lh</sub>. By using a van der Waals density functional, we calculate a temperature difference between heavy and light ices of 6 K as compared to the experimental value of 4 K. [2] Furthermore, we extend our study to analyze the zero-point effects in different ice phases and ice-like structures with different densities and crystal structures to understand how this can be linked to the anomalous isotope effect in liquid water. [3] [1] B. Pamuk, *et al.* Phys. Rev. Lett. **108**, 193003 (2012). [2] B. Pamuk, P. B. Allen, M-V. Fernandez-Serra Phys. Rev. B **92**, 124105 (2015). [3] B. Pamuk, *et al.* in preparation.

<sup>1</sup>This work is supported by DOE Grants No. DE-FG02-09ER16052, No. DE-SC0003871 (M.V.F.S.), and No. DE-FG02-08ER46550 (P.B.A.) and the grant FIS2012-37549-C05 from the Spanish Ministry of Economy and Competitiveness.

**9:12AM K47.00007 Electron Traps at the Ice Surface** , MICHEL BOCKSTEDTE, PHILIPP AUBURGER, ANJA MICHL, Theor. Festkörperphysik, FAU Erlangen-Nuernberg, Erlangen, Germany — Water, water clusters and ice possess the fascinating ability to solvate electrons. On the surface of water cluster<sup>1</sup> and thin crystalline ice structures on a metal substrate<sup>2</sup> long-living solvated electron states were observed that evolve from pre-existing surface traps. The identification of such traps provides important insight into the electronic structure of the water or ice surface, and the dissociative interaction of electrons with adsorbates. Models<sup>2,3</sup> based on the bilayer terminated Ih-(0001) surface related such traps to orientational defects or vacancies. So far, the understanding of the electronic structure of the ice surface with the electron traps is incomplete. Here we address this issue including also water ad-structures<sup>4</sup> within hybrid density functional theory and many-body perturbation theory ( $G_0W_0$ ). We identify a hierarchy of traps with increasing vertical electron affinity, ranging from hexagonal adrows to clusters of orientational defects and vacancies with dangling OH-groups. Siefermann and Abel, Angew. Chem. Int. Ed. **50**, 5264 (2011). Bovensiepen *et al.*, J. Chem. Phys. C **113**, 979 (2013). Hermann *et al.*, J. Phys.: cond. matter **20**, 225003 (2008). Mehlhorn and Morgenstern, Phys. Rev. Lett. **99**, 246101 (2007)

**9:24AM K47.00008 Quantum Water Ice** , NIC SHANNON, OWEN BENTON, Okinawa Institute of Science and Technology Graduate University, OLGA SIKORA, Jagiellonian University, Krakow — There is now a growing body of evidence, from both simulation [1] and experiment [2], that the protons in common, hexagonal water ice are not merely disordered, but mobile, collectively tunnelling from one configuration to another. In this talk we revisit the theory of proton correlations in hexagonal water ice, showing how the disordered state selected by the ice rules changes, once collective quantum tunnelling is taken into account [3]. We find that correlations are governed by a lattice-gauge theory with exactly the same structure as electromagnetism, in which the low-energy excitations of protons have the character of “photons”. The predictions of the quantum theory are shown to be in quantitative agreement with the results of quantum Monte Carlo simulations of hexagonal water ice, and to reproduce the “wings” of incoherent inelastic neutron scattering observed by Bove *et al.* [2]. These results raise the intriguing possibility that the protons in hexagonal water ice could form a quantum liquid with many of the same properties as the quantum spin liquids sought in frustrated magnets. [1] C. Drechsel-Grau and D. Marx, Phys. Rev. Lett. **112**, 148302 (2014). [2] L. Bove *et al.*, Phys. Rev. Lett. **103**, 165901 (2009). [3] O. Benton, O. Sikora and N. Shannon, arXiv:1504.04158.

**9:36AM K47.00009 Role of Inter-molecular Charge Transfer in Simulating Concentration Dependent Water Diffusivity of Aqueous Salt Solutions** , YI YAO, MAX BERKOWITZ, YOSUKE KANAI, Univ of NC - Chapel Hill — The translational diffusivity of water in solutions of alkali halide salts depends on the identity of ions, exhibiting dramatically different behavior even in solutions of similar salts of NaCl and KCl. The water diffusion coefficient decreases as the salt concentration increases in NaCl. Yet, in KCl solution it slightly increases and remains above bulk value as salt concentration increases. Previous classical molecular dynamics simulations have failed to describe this important behavior even with polarizable models. Here we show that the missing physical effect in previous simulations was charge transfer; its inclusion produces results in a quantitative agreement with experiments. We found that the concentration-dependent diffusivity reflects the importance of many-body effects among the water molecules when the ions are present. Explicit inclusion of charge transfer allows us to model accurately the difference in the concentration-dependent water diffusivity between Na<sup>+</sup> and K<sup>+</sup> ions in simulations, and it is likely to impact modeling of a wide range of systems.

**9:48AM K47.00010 Ab initio Determination of Formation Energies and Charge Transfer Levels of Charged Ions in Water.** , ANOOP KISHORE VATTI, MIRA TODOROVA, JOERG NEUGEBAUER, Department for Computational Materials Design, Max-Planck-Institut fuer Eisenforschung GmbH, Duesseldorf, Germany — The ability to describe the complex atomic and electronic structure of liquid water and hydrated ions on a microscopic level is a key requirement to understand and simulate electro-chemical and biological processes. Identifying theoretical concepts which enable us to achieve an accurate description in a computationally efficient way is thereby of central importance. Aiming to unravel the importance and influence of different contributions on the hydration energy of ions we perform extensive ab-initio molecular dynamics simulations for charged and neutral cations (Zn, Mg) and anions (Cl, Br, I) in water. The structural correlations and electronic properties of the studied ions are analysed and compared to experimental observations. Following an approach inspired by the defect chemistry in semiconductors [1] and aligning the water band edges on an absolute scale allows us to benchmark the calculated formation energies, identify transition states and compare the results to experiment. Based on these results we discuss the performance of various DFT xc-functionals to predict charge transfer levels and photo-emission experiments [2]. [1] M. Todorova and J. Neugebauer, Phys. Rev. Applied **1**, 014001 (2014). [2] B. Winter *et al.*, JACS **127**, 7203 (2005).

**10:00AM K47.00011 Orientational relaxation of OH-bond in water over short to intermediate timescales** , PING-HAN TANG, SUAN-JEN LIN, TEN-MING WU, Natl Chiao Tung Univ — By simulating the rigid simple point charge extended model at 300K, the orientational relaxation of the OH-bond in water was investigated over short to intermediate timescales, within which molecules undergo inertial rotation and libration and then enter the rotational diffusion regime. Simulated molecules were classified into subensembles according to their H-bond connections. For global molecules and classified subensembles of molecules, the simulation results of the orientational time correlation functions (TCFs) were compared with the second-cumulant predictions obtained using the rotational stable instantaneous-normal-mode (INM) spectra and the power spectra of angular velocity autocorrelation functions (AVAFs). On short timescales, the OH-bond in water behaves similar to an inertial rotor and its anisotropy is lower than that of a water molecule. For molecules connected with three or more H-bonds, the OH-bond orientational TCFs are characterized by a recurrence, which is an indication for OH-bond libration. By contrast, the OH-bond orientational TCFs of molecules initially connected with one or two H-bonds decay monotonically or exhibit a weak recurrence, indicating rapid relaxation into the rotational diffusion regime after the initial Gaussian decay.

**10:12AM K47.00012 What is the effective molecular polarizability of water in condensed phases?**<sup>1</sup> , XIAOCHUAN GE, DEYU LU, Brookhaven National Laboratory — Electronic polarization plays a crucial role in determining the structural and dynamical properties of water with different boundary conditions. Although it is well known that the molecular polarization in condensed phases behaves substantially differently from that in the vacuum due to the intermolecular interaction, these environmental effects have not been fully understood from first principles methods. As a result, how to rigorously define and calculate the effective molecular polarizability of a water molecule in different chemical environments remains an open question. The answer to this question not only improves our fundamental understanding of water, but also has immediate practical impact on computational modeling of water, e.g. through an accurate polarizable force field model. A main challenge to this puzzle arises from the intrinsic non-local nature of the electronic susceptibility. Recently we developed an ab initio local dielectric response theory [arxiv 1508.03563] that partitions dielectric response in real space based on a Wannier representation. In this work we apply this method to compute the effective molecular polarizability of water in the condensed phase, and discuss how the effective molecular polarizability evolves from gas phase to the condensed phase.

<sup>1</sup>This research used resources of the Center for Functional Nanomaterials, which is a U.S. DOE Office of Science Facility, at Brookhaven National Laboratory under Contract No. DE-SC0012704.

**10:24AM K47.00013 Metastable liquid-liquid phase separation and criticality in water-like models** , RAKESH SINGH, Princeton University, JOHN BIDDLE, University of Maryland, PABLO DEBENEDETTI, Princeton University, MIKHAIL ANISIMOV, University of Maryland — Water shows intriguing thermodynamic and dynamic anomalies in the supercooled liquid state. A possible explanation of the origin of these anomalies lies in the existence of a metastable first order liquid-liquid phase transition (LLPT) between two (high and low density) forms of liquid water. Unambiguous experimental proof of existence of LLPT in bulk supercooled water is so far hampered by ultra-fast ice crystallization. Computer simulations of water models are therefore crucial for exploring the possibility of LLPT in deeply supercooled water. We present computer simulation results that elucidate the possibility of a metastable LLPT in one of the most accurate atomistic models of water, TIP4P/2005. To describe the computed properties, we have applied two-state thermodynamics, viewing water as a non-ideal mixture of two inter-convertible states. The thermodynamic behavior of the model in the one-phase region suggests the existence of energy-driven LLPT. We compare the behavior of TIP4P/2005 with other popular water models, and with real water, all of which are well-described by two-state thermodynamics. Additionally, we also elucidate the relation between the phenomenological order parameter of the two-state thermodynamics and the microscopic nature of the low-density structure.

**10:36AM K47.00014 Structure Evolution of Metal Nanoparticles in Water Environment.** , YI GAO, BEIEN ZHU, Shanghai Institute of Applied Physics, Chinese Academy of Sciences — Metal nanoparticles have drawn extensive attentions in materials science due to their widespread applications in electronics, engineering and catalysis. A very fundamental question is their structure evolution and surface segregation. Many recent observations have shown that reactive gases or supports may have strong effects on the morphology change and surface segregation. However, the effect of water—the most common solvent and environment—has not received enough attention. Here, we will give two examples to show water adsorption could induce the morphology change and strong surface segregation tendencies for the metal nanoparticles. This finding not only prompts us to re-examine the potential effects of water on metal nanoparticles, but would be also very helpful as a guide for the further theoretical and experimental studies in this field.

**10:48AM K47.00015 Ionic structure in electrolyte confined by dielectric interfaces** , YUFEI JING, Northwestern University, VIKRAM JADHAO, Johns Hopkins University, JOS W. ZWANIKKEN, University of Massachusetts, Lowell, MONICA OLVERA DE LA CRUZ, Northwestern University — The behavior of ions in liquids confined between macromolecules determines the outcome of many nanoscale assembly processes in synthetic and biological materials. To model these systems, both the macromolecules and the surrounding solvent are treated as continuous media characterized with different dielectric permittivities. As the macromolecule-liquid boundary is modeled as a dielectric interface, an important quantity of interest is the ionic structure in a liquid confined between two such interfaces. We compute the ionic structure in a model system of electrolyte confined by two planar dielectric interfaces using molecular dynamics simulations and liquid state theory. We give a comprehensive description of the effects of high electrolyte concentrations, multivalent ions, dielectric contrasts, and external electric field on the ionic distributions. We observe novel features in ionic structure near polarizable/unpolarizable macromolecules which is attributed to the competition between electrostatic and steric (entropic) interactions. We argue that the combined effect of ionic correlations and inhomogeneous dielectric permittivity significantly changes the character of the effective interaction between the two macromolecules.

## Wednesday, March 16, 2016 8:00AM - 11:00AM –

Session K48 GQI: Novel Superconducting Qubits & Architectures 349 - John Martinis, Google, Inc.

**8:00AM K48.00001 The gatemon: a transmon with a voltage-variable superconductor-semiconductor junction**<sup>1</sup> , KARL PETERSSON, Center for Quantum Devices and Station Q Copenhagen, Niels Bohr Institute, University of Copenhagen, Denmark — We have developed a superconducting transmon qubit with a semiconductor-based Josephson junction element.<sup>2,3</sup> The junction is made from an InAs nanowire with *in situ* molecular beam epitaxy-grown superconducting Al contacts. This gate-controlled transmon, or gatemon, allows simple tuning of the qubit transition frequency using a gate voltage to vary the density of carriers in the semiconductor region. In the first generations of devices we have measured coherence times up to  $\sim 10 \mu\text{s}$ . These coherence times, combined with stable qubit operation, permit single qubit rotations with fidelities of  $\sim 99.5\%$  for all gates including voltage-controlled  $Z$  rotations. Towards multi-qubit operation we have also implemented a two qubit voltage-controlled cPhase gate. In contrast to flux-tuned transmons, voltage-tunable gatemons may simplify the task of scaling to multi-qubit circuits and enable new means of control for many qubit architectures.

<sup>1</sup>In collaboration with T.W. Larsen, L. Casparis, M.S. Olsen, F. Kuemmeth, T.S. Jespersen, P. Krogstrup, J. Nygard and C.M. Marcus. Research was supported by Microsoft Project Q, Danish National Research Foundation and a Marie Curie Fellowship.

<sup>2</sup>T.W. Larsen *et al.*, Phys. Rev. Lett. **115**, 127001 (2015).

<sup>3</sup>G. de Lange *et al.*, Phys. Rev. Lett. **115**, 127002 (2015),

**8:36AM K48.00002 Progress toward coupled flux qubits with high connectivity and long coherence times** , STEVEN WEBER, DAVID HOVER, DANNA ROSENBERG, GABRIEL SAMACH, JONILYN YODER, ANDREW KERMAN, WILLIAM OLIVER, MIT Lincoln Laboratory — The ability to engineer interactions between qubits is essential to all areas of quantum information science. The capability to tune qubit-qubit couplings *in situ* is desirable for gate-based quantum computing and analog quantum simulation and necessary for quantum annealing. Consequently, tunable coupling has been the subject of several experimental efforts using both transmon qubits and flux qubits. Recently, our group has demonstrated robust and long-lived capacitively shunted (C-shunt) flux qubits. Here, we discuss our efforts to develop architectures for tunably coupling these qubits. In particular, we focus on optimizing the RF SQUID coupler to achieve high connectivity. This research was funded by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA) and by the Assistant Secretary of Defense for Research & Engineering under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of ODNI, IARPA, or the US Government.

**8:48AM K48.00003 Three coupled qubits in a single superconducting quantum circuit<sup>1</sup>**, MADHAVI CHAND, SUMAN KUNDU, N. NEHRA, COSMIC RAJ, TANAY ROY, A. RANADIVE, MEGHAN P. PATANKAR, R. VIJAY, Tata Institute of Fundamental Research, Mumbai 400005 — We propose a new design for a 3-qubit system in the 3D circuit QED architecture. Our design exploits the geometrical symmetry of a single superconducting circuit with three degrees of freedom to generate three coupled qubits. However, only one of these is strongly coupled to the environment while the other two are protected from the Purcell effect. Nevertheless, all three qubits can be measured using the standard dispersive technique. We will present preliminary data on this circuit showing evidence of three distinct qubits that retain the essential properties of a 3D transmon, namely insensitivity to charge noise, sufficient anharmonicity and good coherence times. We will also characterize the coupling of the three qubits to each other, to the environment and to a neighboring transmon qubit. Finally, we will compare our design to previous multi-qubit circuits and discuss possible applications in quantum computing and quantum simulations.

<sup>1</sup>Funding: Department of Atomic Energy, Govt. of India; Department of Science and Technology, Govt. of India

**9:00AM K48.00004 Analog approaches to quantum computation using highly-controllable superconducting qubits**, C. NEILL, UCSB, P. ROUSHAN, R. BARENDSE, Google Inc., B. CAMPBELL, UCSB, Y. CHEN, Google Inc., Z. CHEN, B. CHIARO, A. DUNSWORTH, UCSB, A. FOWLER, E. JEFFREY, J. KELLY, E. LUCERO, A. MEGRANT, J. MUTUS, M. NEELEY, Google Inc., P. O'MALLEY, C. QUINTANA, UCSB, D. SANK, Google Inc., J. WENNER, UCSB, T. WHITE, J. MARTINIS, Google Inc. — The first generation of quantum hardware that outperforms classical computers will likely be analog in nature. In an effort to realize such a platform, we have built a one-dimensional chain of 9 superconducting qubits. This device provides individual time-dependent control over all nearest-neighbor couplings and local fields (X, Y, Z) in the multi-qubit Hamiltonian. In this talk, I will focus on open problems in non-equilibrium statistical mechanics where dynamical properties become impossible to compute for only a few 10s of qubits. In particular, I will review device performance and the scaling of analog errors with system size. By studying how errors scale during practical applications, we aim to predict if otherwise-intractable computations could be carried out with 30 to 40 qubits.

**9:12AM K48.00005 Concentric transmon qubit featuring fast tunability and site-selective Z coupling**, MARTIN WEIDES, JOCHEN BRAUMUELLER, Karlsruhe Institute of Technology, MARTIN SANDBERG, MICHAEL VISSERS, National Institute of Standards and Technology, ANDRE SCHNEIDER, STEFFEN SCHLOER, LUKAS GRUENHAUPT, HANNES ROTZINGER, MICHAEL MARTHALER, ALEXANDER LUKASHENKO, AMADEUS DIETER, ALEXEY USTINOV, Karlsruhe Institute of Technology, DAVID PAPPAS, National Institute of Standards and Technology — We present a planar qubit design based on a superconducting circuit that we call concentric transmon. While employing a simple fabrication process using Al evaporation and lift-off lithography, we observe qubit lifetimes and coherence times in the order of 10  $\mu$ s. We systematically characterize loss channels such as incoherent dielectric loss, Purcell decay and radiative losses. The implementation of a gradiometric SQUID loop allows for a fast tuning of the qubit transition frequency and therefore for full tomographic control of the quantum circuit. The presented qubit design features a passive direct Z coupling between neighboring qubits, being a pending quest in the field of quantum simulation.

**9:24AM K48.00006 Blackbox quantization and numerical simulation of a concentric transmon superconducting qubit**, ALIREZA NAJAFI-YAZDI, KEVIN LALUMIERE, Anyon Systems Inc., J. BRAUMÜLLER, MARTIN WEIDES, KIT — We present a blackbox quantization [1] and numerical study of a planar concentric transmon superconducting qubit. This architecture has been recently proposed and experimentally investigated by Braumüller et al [2]. The device involves a gradiometric SQUID loop for a fast tuning of the qubit transition frequency. This allows for full tomographic control of the quantum circuit. A fully automatized numerical package for quantization of superconducting qubits is developed and used for the study of the concentric transmon. A systematic characterization of loss channels such as Purcell decay and radiative losses are also studied. Numerical results are in close agreement with experimental data and suggest the platform to be a useful tool in the design of superconducting circuits. References: [1] Firat, S., DiVincenzo, D. W., David, P., Physical Review B, Vol. 90, No. 13, pp. 134-504, 2014. [2] J. Braumüller et al., arXiv:1509.08014

**9:36AM K48.00007 Weakly-tunable transmon qubits in a multi-qubit architecture**, JARED HERTZBERG, NICHOLAS BRONN, ANTONIO CORCOLES, MARKUS BRINK, GEORGE KEEFE, MAIKA TAKITA, IBM T J Watson Res Ctr, M. HUTCHINGS, B. L. T. PLOURDE, Syracuse University, JAY GAMBETTA, JERRY CHOW, IBM T J Watson Res Ctr — Quantum error-correction employing a 2D lattice of qubits requires a strong coupling between adjacent qubits and consistently high gate fidelity among them. In such a system, all-microwave cross-resonance gates offer simplicity of setup and operation. [1] However, the relative frequencies of adjacent qubits must be carefully arranged in order to optimize gate rates and eliminate unwanted couplings. [2] We discuss the incorporation of weakly-flux-tunable transmon qubits into such an architecture. Using DC tuning through filtered flux-bias lines, we adjust qubit frequencies while minimizing the effects of flux noise on decoherence. [1] J.M. Chow et al, Nat Comm 5, 4015 (2014). [2] A.D. Corcoles et al, Nat Comm 6, 6979 (2015).

**9:48AM K48.00008 Semiconductor-inspired superconducting quantum computing**, YUN-PIL SHIM, Laboratory for Physical Sciences — Superconducting circuits offer tremendous design flexibility in the quantum regime culminating most recently in the demonstration of few qubit systems supposedly approaching the threshold for fault-tolerant quantum information processing. Competition in the solid-state comes from semiconductor qubits, where nature has bestowed some very useful properties which can be utilized for spin qubit based quantum computing. Here we present an architecture for superconducting quantum computing based on selective design principles deduced from spin-based systems [1]. We propose an encoded qubit approach realizable with state-of-the-art tunable Josephson junction qubits. Our results show that this design philosophy holds promise, enables microwave-free control, and offers a pathway to future qubit designs with new capabilities such as with higher fidelity or, perhaps, operation at higher temperature. The approach is especially suited to qubits based on variable super-semi junctions. [1] Yun-Pil Shim and Charles Tahan, arXiv:1507.07923

**10:24AM K48.00009 Coupling a Transmon Qubit to a Superconducting Metamaterial Resonator**, HAOZHI WANG, M. HUTCHINGS, SAGER INDRAJEET, FRANCISCO ROUXINOL, MATTHEW LAHAYE, B.L.T. PLOURDE, Syracuse Univ, BRUNO G. TAKETANI, FRANK K. WILHELM, Saarland University — Arrays of lumped circuit elements can be used to form metamaterial resonant structures that exhibit significantly different mode structures compared to resonators made from conventional distributed transmission lines. In particular, it is possible to produce a high density of modes in the microwave regime where a superconducting qubit can be operated and coupled to the various modes. We will present our low-temperature measurements of such a superconducting metamaterial resonator coupled to a tunable transmon qubit. By tuning the magnetic flux biasing the qubit, we observe vacuum Rabi splittings in the modes that the qubit transition passes through. We will also discuss our measurements of an interaction between neighboring modes of the metamaterial system that is mediated by the qubit. Because of the dispersive coupling of the qubit to the various modes of the system, driving a microwave tone near one mode of the system can have a significant influence on the transmission through another mode, with a strong dependence on the bias point of the qubit. We will compare these measurements with a theoretical model of the system.

**10:36AM K48.00010 Coplanar waveguide flux qubit suitable for quantum annealing<sup>1</sup>**, CHRIS QUINTANA, UC Santa Barbara, YU CHEN, D. SANK, D. KAFRI, A. MEGRANT, T. C. WHITE, A. SHABANI, R. BARENDTS, Google, Santa Barbara, B. CAMPBELL, Z. CHEN, B. CHIARO, A. DUNSWORTH, UC Santa Barbara, A. FOWLER, E. JEFFREY, J. KELLY, E. LUCERO, J. Y. MUTUS, M. NEELEY, Google, Santa Barbara, C. NEILL, P. J. J. O'MALLEY, UC Santa Barbara, P. ROUSHAN, Google, Santa Barbara, A. VAINSENER, J. WENNER, UC Santa Barbara, J. M. MARTINIS, University of California and Google, Santa Barbara — We introduce the "fluxmon" flux qubit, designed with the goal of practical quantum annealing. The qubit's capacitance and linear inductance are provided by a coplanar waveguide on a low loss substrate, minimizing dielectric dissipation and in principle allowing for GHz-scale inter-qubit coupling in a highly connected tunable architecture. Utilizing a dispersive microwave readout scheme, we characterize single-qubit noise and dissipation, and present a simple tunable inter-qubit coupler. We discuss tradeoffs between coherence and coupling in a quantum annealing architecture.

<sup>1</sup>This work was supported by Google Inc. and by the NSF GRFP

**10:48AM K48.00011 Proposal for a cavity based superconducting qubit**, ANDREI VRAJITOAREA, Princeton University, JENS KOCH, Northwestern University, ANDREW HOUCK, Princeton University — Various technological challenges need to be resolved in order to demonstrate a working cQED network of superconducting qubits. For single Josephson junction devices important factors include improving coherence times and reducing fluctuations in junction critical current that ultimately lead to dephasing and unwanted frequency collisions. Superconducting microwave resonators show great potential for storing and manipulating quantum states and are known for their accurate reproducibility. We propose the direct addressability of a two level cavity state by dispersively coupling a fluxonium qubit to a coplanar lumped element resonator. We report preliminary experimental results that point towards an induced cavity anharmonicity due to the large dispersive shifts of the fluxonium system.

**Wednesday, March 16, 2016 8:00AM - 11:00AM –**  
**Session K50 DAMOP: Spin-Orbit Coupling and Artificial Gauge Fields** Hilton Baltimore Holiday Ballroom  
1 - Lauren Aycock, Joint Quantum Institute, University of Maryland

**8:00AM K50.00001 Magnetic phases of spin-1 spin-orbit coupled Bose gases<sup>1</sup>**, DANIEL CAMPBELL, RYAN PRICE, ANDIKA PUTRA, ANA VALDÉS-CURIEL, DIMITRIOS TRYPOGEORGOS, IAN SPIELMAN, Joint Quantum Institute, University of Maryland, College Park, Maryland, 20742, USA, SPIELMAN TEAM — We experimentally explore the magnetic phases present in a near-zero temperature spin-1 spin-orbit coupled atomic Bose gas. We observe ferromagnetic and unpolarized phases which are stabilized by the spin-orbit couplings explicit locking between spin and motion. In the limit of weak spin-orbit coupling, these phases are separated by a critical curve of 1st order quantum phase transitions, with an observed width as small as  $\hbar \times 4Hz$ . These phase transitions give rise to long-lived metastable states.

<sup>1</sup>This work was partially supported by the ARO's atomtronics MURI, by the AFOSR's Quantum Matter MURI, NIST, and the NSF through the PFC at the JQI

**8:12AM K50.00002 Quantum double-exchange physics with ultracold atoms and synthetic gauge potentials<sup>1</sup>**, JOHANNES SCHACHENMAYER, LEONID ISAEV, ANA MARIA REY, JILA, NIST and Dept. of Physics, University of Colorado Boulder — We study an interplay between local spin exchange and Néel antiferromagnetism in a two-band optical lattice. The lowest narrow band is half-filled and implements the magnetic background, while a higher band contains mobile atoms. When the local spins are locked in a Néel state, the motion of itinerant atoms is hindered by exchange energy barriers and the system is a flat-band insulator. As we show, this picture breaks down when exchange interaction between local and mobile spins is comparable to an energy scale of the Néel state. In this regime, formation of singlets between local and itinerant spins gives rise to a metallic phase of mobile atoms dressed by the spin fluctuations. This state is characterized by coupled spin-charge excitations whose spin is transverse to the Néel vector. Our predictions can be realized with ultracold alkaline-earth fermionic atoms coupled to a laser-induced staggered magnetic field, which stabilizes the Néel order and controls the amount of quantum fluctuations of local spins. By tuning the strength of this laser coupling relative to the exchange interaction, one can either adiabatically drive the crossover between the flat-band insulator and correlated metal phases, or explore non-equilibrium spin-charge dynamics in quench experiments.

<sup>1</sup>This work was supported by the NSF (PIF-1211914 and PFC-1125844), AFOSR, AFOSR-MURI, NIST and ARO individual investigator awards

**8:24AM K50.00003 Interaction effects in cold gases in synthetic gauge fields<sup>1</sup>**, THOMAS BILITEWSKI, NIGEL COOPER, T.C.M. Group, Cavendish Laboratory, J.J. Thomson Avenue, Cambridge CB3 0HE, United Kingdom — There has been a long-standing goal to find ways to cause neutral atoms to experience synthetic gauge fields, extending the capabilities of ultracold gases as simulators of quantum many-body systems. Such gauge fields can mimic the effect of magnetic fields and generate topological energy bands. Recent proposals to generate synthetic gauge fields rely on time-dependent periodic forcing of the quantum system.

Interactions are of particular interest in these systems, as the interplay of time dependence and interactions can lead to inelastic scattering and the combined effect of synthetic gauge fields and strong correlations could lead to a variety of novel many body phases of degenerate fermionic or bosonic atoms.

In the framework of Floquet Theory we study the effects of inelastic scattering induced by the intrinsic time dependence of the eigenstates and the elastic two-body interactions [1]. Specifically, we discuss this mechanism as a potential explanation of heating and band population dynamics in current experimental setups.

[1] T. Bilitewski and N. R. Cooper, *Phys. Rev. A* 91, 033601 (2015) & *Phys. Rev. A* 91, 063611 (2015)

<sup>1</sup>EPSRC Grant No. EP/K030094/1

**8:36AM K50.00004 Spin-Orbit Coupled Fermions in Harmonic Trap**, DOGA MURAT KURKCUOGLU, Georgia Southern University, Georgia Inst of Tech — After the realization of artificial spin-orbit coupling in ultracold atoms experimentally, there is an interest in spin-orbit coupled systems in ultracold atoms. In this abstract, I will discuss the emergence of two-body bound states between two Fermi atoms in the presence of spin-orbit coupling and Zeeman fields. The fermions are assumed to have only two internal states and to have attractive contact (zero-ranged) interactions. We also add an isotropic three-dimensional harmonic trap to the system, since it is the experimentally relevant case. For such a system, I will describe the few-body solutions and the effective masses of the bound-states as a function of spin-orbit and Zeeman fields.

**8:48AM K50.00005 Thermodynamics of interacting cold atomic Fermi gases with spin-orbit coupling<sup>1</sup>**, SCOTT JENSEN, YORAM ALHASSID, CHRISTOPHER GILBRETH, Center for Theoretical Physics, Yale University — New physics is suggested with the prediction of novel phases in cold atom systems when a synthetic spin-orbit coupling is introduced. In particular, recent studies show that a new type of Bose-Einstein condensate, termed Rashbon-BEC, is formed when a generalized Rashba spin-orbit term is present [1]. The Rashbon-BEC phase can be obtained by tuning the spin-orbit coupling strength even in the case of finite negative scattering length. This stands in contrast to the BCS-BEC crossover in the absence of spin-orbit coupling where a negative scattering length is associated with BCS physics, and its divergence signals the crossover. In our work we apply finite-temperature quantum Monte Carlo methods to a spherical Rashba spin-orbit coupled two-species Fermi gas with contact s-wave interaction in three dimensions. We will discuss the phase diagram for this system, and its crossover behavior from BCS to Rashbon-BEC.  
[1] See for example in J. P. Vyasanakere, S. Zhang and V. B. Shenoy, Phys. Rev. B 84, 14512 (2011).

<sup>1</sup>This work was supported in part by the Department of Energy grant No. DE-FG-0291-ER-40608

**9:00AM K50.00006 Spin-orbit coupling in the strongly interacting Fermi gas: an exact quantum Monte Carlo study<sup>1</sup>**, PETER ROSENBERG, HAO SHI, SIMONE CHIESA, SHIWEI ZHANG, College of William and Mary — Spin-orbit coupling (SOC) plays an essential role in a variety of intriguing condensed matter phenomena, including the quantum Hall effect, and topological insulators and superconductors. The recent experimental realization of spin-orbit coupled Fermi gases provides a unique opportunity to study the effects of SOC in a tunable, disorder-free system. Motivated by this experimental progress, we present here the first exact numerical results on the two-dimensional, unpolarized, uniform Fermi gas with attractive interactions and Rashba SOC. Using auxiliary-field quantum Monte Carlo and incorporating recent algorithmic advances, we carry out exact calculations on sufficiently large system sizes to provide accurate results systematically as a function of experimental parameters. We obtain the equation of state, study the spin behavior and momentum distribution, and examine the interplay of SOC and pairing in real and momentum space. Our results help illuminate the rich pairing structure induced by SOC, and provide important guidance to future experimental efforts.

<sup>1</sup>Supported by DOE SciDAC and NSF

**9:12AM K50.00007 Melting of phase-strips in Bose-Einstein condensates with synthetic spin-orbit coupling<sup>1</sup>**, ASLE SUDBO, PEDER GALTELAND, Norwegian Univ Tech (NTNU), EGOR BABAEV, Royal Institute of Technology, Stockholm, Sweden — We study a two-component, density imbalanced Bose-Einstein condensate with density-density interactions and synthetic spin-orbit coupling, focusing on the impact of thermal fluctuations and density-density interactions on spin-orbit induced effects. We find that for intermediate density imbalance and small intercomponent density-density interactions, the ground state is non-uniform, represented by a striped state of modulated phases of the individual complex order parameter components. By using mean-field stability arguments, we calculate a critical value for the intercomponent density-density interaction, above which the non-uniform ground state collapses into a uniform single-component state. This is reproduced in Monte-Carlo simulations for intermediate values of the spin-orbit coupling. We also find that the non-uniform ground state is disordered by thermal fluctuations when heated, through a Berizinskii-Kosterlitz-Thouless unbinding of dislocation pairs. We argue that, to lowest order, the spin-orbit coupling can be seen as an effective Josephson-type locking of the phase difference  $\theta_1 - \theta_2$  while simultaneously allowing the system to gain energy by modulating the phase sum  $\theta_1 + \theta_2$ .

<sup>1</sup>Work supported by the Norwegian Research Council, the Swedish Research Council, and the National Science Foundation

**9:24AM K50.00008 Pairing of fermions with unequal charges in an artificial magnetic field**, NUR UNAL, Cornell Univ, M. O. OKTEL, Bilkent Univ — Artificial magnetic fields (AMFs) created for ultra cold systems depend sensitively on the internal structure of the atoms. In a mixture, each component couples to the AMF with a different charge. This enables the study of Bardeen-Cooper-Schrieffer pairing of fermions with unequal charges. We investigate the superconducting (SC) transition of a system formed by such pairs as a function of the field strength. We consider a homogeneous two-component Fermi gas of unequal charges but equal densities with attractive interactions. We find that the phase diagram is altered drastically compared to the usual equal charge case. First, for some AMFs there is no SC transition and isolated SC phases are formed, reflecting the discrete Landau level (LL) structure. SC phases become reentrant both in AMF and temperature. For extremely high fields where both components are confined to their lowest LLs, the effect of the charge imbalance is suppressed. Charge asymmetry reduces the critical temperature even in the low-field semiclassical regime. We discuss a pair breaking mechanism due to the unequal Lorentz forces acting on the components of the Cooper pairs to identify the underlying physics.

**9:36AM K50.00009 SPECTRUM OF THE RASHBA SPIN-ORBIT COUPLED HAMILTONIAN WITH SPIN-DEPENDENT CONTACT INTERACTION IN DIMENSION THREE**, RYTIS JURSENAS, Vilnius University, Institute of Theoretical Physics and Astronomy — The presentation provides functional analytic interpretation for the spectrum of the Rashba spin-orbit coupled Hamiltonian considered in the presence of the out-of-plane magnetic field. The impurity scattering is treated by means of a spin-dependent contact interaction. The research was inspired by a recently proposed technique [1, 2, 3] for producing the Rashba-type spin-orbit coupling for a three-dimensional ultracold atom. The analysis of the resolvent formula shows that, for nonzero spin-orbit coupling, the eigenvalues solve the transcendental equation. For small spin-orbit-coupling strength  $\alpha$ , the eigenvalues are derived analytically with the accuracy up to  $O(\alpha^4)$ . It is shown that there are no eigenvalues above the threshold no matter the form of a nonzero coupling parameter of contact interaction. When the lower branch of dispersion relation attains two minima, the eigenvalues are situated only below the threshold or above the minimum of the upper branch of dispersion relation; the upper bound of discrete states is also obtained. [1] B. M. Anderson et al, Phys. Rev. Lett. 111 (2013), 125301. [2] D. L. Campbell et al, Phys. Rev. A 84 (2011), 025602. [3] F. Jendrzejewski et al, Nature Physics 8 (2012), 398.

**9:48AM K50.00010 Vortex line of spin-orbit coupled Fermi superfluid through BCS to BEC Crossover<sup>1</sup>**, JUAN YAO, SHIZHONG ZHANG, The Univ of Hong Kong — Superfluid Fermi gases with spin-orbit interaction provides a unique opportunity to investigate possible effects of strong interaction in a topological superfluid. It has been suggested that with addition of Rashba-type spin-orbit coupling, a two-component Fermi gas with strong s-wave interaction can become a topological superfluid with zero-energy bound state at the core of the vortex. In this talk, I discuss the evolution of vortex structure in a spin-orbit coupled Fermi gas through the BCS-BEC crossover within Bogoliubov-de Gennes formalism. We find that the largest critical current occurs in the BEC side of the resonance, in contradiction to the usual crossover without spin-orbit coupling where it occurs at unitarity. Furthermore, we discuss the core structure of the vortex by calculating the spin and density distribution around the vortex.

<sup>1</sup>Department of Physics and Centre of Theoretical and Computational Physics, The University of Hong Kong, Hong Kong, China

**10:00AM K50.00011 Stripe phase and double-roton excitations in interacting spin-orbit-coupled spin-1 Bose-Einstein condensates**, KUEI SUN, The University of Texas at Dallas, Richardson, Texas, USA, CHUNLEI QU, The University of Texas at Dallas, Richardson, Texas, USA and Università di Trento, Povo, Italy, YONG XU, The University of Texas at Dallas, Richardson, Texas, USA, YONGPING ZHANG, OIST Graduate University, Onna, Okinawa, Japan, CHUANWEI ZHANG, The University of Texas at Dallas, Richardson, Texas, USA — Spin-orbit (SO) coupling plays a major role in many important phenomena in condensed matter physics. However, the SO coupling physics in high-spin systems, especially with superfluids, has not been well explored because of the spin half of electrons in solids. In this context, the recent experimental realization of spin-orbit coupling in spin-1 Bose-Einstein condensates (BECs) has opened a completely new avenue for exploring SO-coupled high-spin superfluids. Nevertheless, the experiment has only revealed the single-particle physics of the system. Here, we study the effects of interactions between atoms on the ground states and collective excitations of SO-coupled spin-1 BECs in the presence of a spin-tensor potential. We find that ferromagnetic interaction between atoms can induce a stripe phase exhibiting two modulating patterns. We characterize the phase transitions between different phases using the spin-tensor density as well as the collective dipole motion of the BEC. We show that there exists a new type of double maxon-roton structure in the Bogoliubov-excitation spectrum, attributing to the three band minima of the SO-coupled spin-1 BEC. Our work could motivate further theoretical and experimental study along this direction.

**10:12AM K50.00012 Finite temperature theory of spin-orbit coupled fermions in three dimensions in the presence of external Zeeman fields and tunable s-wave interactions**, PHILIP POWELL, Lawrence Livermore National Laboratory, GORDON BAYM, University of Illinois at Urbana-Champaign, CARLOS SA DE MELO, Georgia Institute of Technology, Joint Quantum Institute — We develop a finite temperature theory of ultracold three-dimensional Fermi gases in the presence of artificial spin-orbit coupling, Zeeman fields, and tunable s-wave interactions. With the inclusion of quadratic fluctuations, we compute both the critical temperature for superfluidity and the population of bound and unbound fermions throughout the evolution from the Bardeen-Cooper-Schrieffer (BCS) to Bose-Einstein condensate (BEC) regimes. In particular, we show that in the BEC regime, spin-orbit coupling is capable of increasing the critical temperature relative to the no-field case, by inducing a triplet component to the superfluid order parameter, while decreasing the many-body effective mass. We also derive the time-dependent Ginzburg-Landau equation to sixth-order in the superfluid order parameter, and obtain explicit expressions for the coefficients of the effective theory valid across the entire evolution from BCS to BEC superfluidity.

**10:24AM K50.00013 Entanglement of Vortex Lattices for Ultracold Bose Gases in a Non-Abelian Gauge Potential**, SZU-CHENG CHENG, Department of Optoelectric Physics, Chinese Culture University, Taiwan, ROC, T. F. JIANG, SHIH-DA JHENG, Institute of Physics, National Chiao Tung University, Taiwan, ROC, ATOMIC AND MOLECULAR PHYSICS TEAM, ATOMIC AND MOLECULAR PHYSICS TEAM — We develop a theory, referred to as the von Neumann lattice in a higher Landau level, for vortex lattices labelled by an integral number of flux quanta per unit cell in a higher Landau level. Using this lattice theory, we study the vortex lattice states of a pseudospin-1/2 ultracold Bose gas with contact interactions in a non-Abelian gauge potential. In addition to a uniform magnetic field, the Bose gas is also subjected to a non-Abelian gauge field, which creates an effect of the spin-orbit coupling to lift the spin degeneracy of the Landau levels. Because of interactions from the spin-orbit coupling, there are new degenerate points of the single particle spectrum due to the crossings of two Landau levels at certain coupling strengths. We show that interactions from the spin-orbit coupling force the nature and structure of the vortex lattice changing dramatically if the strength of the non-Abelian gauge field is increasing. We also find that the ground state of the vortex lattice at a degenerate point exhibits strong correlation and entanglement involving vortex lattices from different Landau levels. This entangled state builds the connection between two phases of vortex lattices during the first order phase transition of the adiabatic evolution.

**10:36AM K50.00014 Baryon squishing in synthetic dimensions by effective  $SU(M)$  gauge fields<sup>1</sup>**, SUDEEP KUMAR GHOSH, UMESH K. YADAV, VIJAY B. SHENOY, Indian Institute of Science Bangalore — We investigate the physics of  $SU(M)$  symmetric interactions in the “synthetic dimensions” (Celi et al., PRL 112, 043001 (2014)) that provides a cold atom realization of the Hofstadter model. We show that this system is equivalent to particles (with  $SU(M)$  symmetric interactions) experiencing an  $SU(M)$  Zeeman field at each lattice site *and* a non-Abelian  $SU(M)$  gauge potential that affects their hopping. This equivalence brings out the possibility of generating *non-local* interactions between particles at different sites of the optical lattice. In addition, the gauge field induces a *flavor-orbital coupling*, which mitigates the “baryon breaking” effect of the Zeeman field. For  $M$  particles, concomitantly, the  $SU(M)$  singlet baryon which is site localized in the usual 1d optical lattice, is deformed to a non-local object (“squished baryon”). We conclusively demonstrate this effect by analytical arguments and exact (numerical) diagonalization studies. Our study promises a rich many-body phase diagram for this system. It also uncovers the possibility of using the synthetic dimension system to laboratory realize condensed matter models such as the  $SU(M)$  random flux model, inconceivable in conventional experimental systems. Reference: arXiv:1503.02301

<sup>1</sup>Work supported by CSIR, DST and DAE

**10:48AM K50.00015 Cavity-Assisted Spin Orbit Coupling**, CHUANZHOU ZHU, LIN DONG, HAN PU, Rice University — We consider a single ultracold atom trapped inside a single-mode optical cavity, where a two-photon Raman process induces an effective coupling between atom's pseudo-spin and external center-of-mass (COM) motion. Without the COM motion, this system is described by the Jaynes-Cummings (JC) model. We show how the atomic COM motion dramatically modifies the predictions based on the JC model. We also investigated the situation when cavity pumping and decay are taken into account. We take a quantum Master equation approach to study this open system and again show how the cavity-induced spin-orbit coupling affects the properties of the system.

## Wednesday, March 16, 2016 8:00AM - 11:00AM –

**Session K51 FIAP: Fractional QHE: Topological, Non-Abelian, and 5/2 States** Hilton Baltimore Holiday Ballroom 2 - John Cumings, University of Maryland

**8:00AM K51.00001 Possibility of topological order in partially flat band systems**, ABOLHASSAN VAEZI, Stanford University — In this talk, we discuss the possibility of topological order in two-dimensional partially flat bands. We first consider a tight-binding model whose valence band is (nearly) flat only in some regions of the Brillouin zone, where the Berry curvature is mostly concentrated, and dispersive otherwise. We then investigate the ground-states of these systems when the flat regions are fractionally filled. We argue that under certain conditions spontaneous symmetry breaking orders such as charge density wave (CDW) can emerge. The resulting CDW enlarges the unit cell and separates the flat regions from the rest of the valence band by a finite energy gap. Interestingly, the broken symmetry state can exhibit fractional Chern insulator phase with quantized Hall conductivity. Finally, we present our numerical results for the phase diagram of such systems.

**8:12AM K51.00002 Measurement of 2D topological invariants from anomalous edge spectral flow**, SRIRAM GANESHAN, Simons center of geometry and physics, Stony Brook University, SUNIL MITTAL, JINGYUN FAN, Joint Quantum Institute, NIST/University of Maryland, College Park, ABOLHASSAN VAEZI, Stanford University, MOHAMMAD HAFEZI, Joint Quantum Institute, NIST/University of Maryland, College Park MD — A hallmark example of a TQFT is the 2+1 D Chern-Simons (CS) theory, which describes topological properties of both integer and fractional quantum Hall effects. The gauge invariant form of the CS theory with boundaries, encompassing both edge and bulk terms, provides an unambiguous way to relate bulk topological invariants to the edge dynamics. This bulk-edge correspondence is manifested as a gauge anomaly in the bulk and chiral anomaly at the edge, and provides a direct insight into the bulk topological order. In this work, we experimentally implement the integer quantum Hall model in a photonic system where the edge modes are described by the anomalous chiral conformal field theory. By selectively manipulating and probing the edge, we exploit the chiral anomaly of the edge theory, for the first time. The associated spectral edge flow associated to the chiral anomaly allows us to unambiguously measure topological invariants, i.e., the winding number of the edge states. This experiment provides a new approach for direct measurement of topological invariants, independent of the microscopic details, and thus could be extended to probe strongly-correlated topological orders.

**8:24AM K51.00003 Bose condensation in topologically ordered quantum liquids**, TITUS NEUPERT, HUAN HE, CURT VON KEYSERLINGK, Princeton University, GERMAN SIERRA, UAM-CSIC Madrid, ANDREI BERNEVIG, Princeton University — The condensation of bosons can induce transitions between topological quantum field theories (TQFTs). This has been previously investigated through the formalism of Frobenius algebras and with the use of Vertex lifting coefficients. We discuss an alternative, algebraic approach to boson condensation in TQFTs that is physically motivated and computationally efficient. With a minimal set of assumptions, such as commutativity of the condensation with the fusion of anyons, we can prove a number of theorems linking boson condensation in TQFTs with algebra extensions in conformal field theories and with the problem of factorization of completely positive matrices over the positive integers. We propose an algorithm for obtaining a condensed theory fusion algebra and its modular matrices. For example, this formalism can be used to build multi-layer TQFTs which could be a starting point to build three-dimensional topologically ordered phases. Using this formalism, we also give examples of bosons that cannot undergo a condensation transition due to topological obstructions.

**8:36AM K51.00004 Fermion Parity Flips and Majorana Defects in Superconducting Fractional Topological Phases**, MAYUKH KHAN, University of Illinois at Urbana-Champaign, JEFFREY TEO, University of Virginia, TAYLOR HUGHES, SMITHA VISHVESHWARA, University of Illinois at Urbana-Champaign — We consider layered heterojunctions of s-wave superconductors and Abelian topologically ordered (TO) phases. We derive the emergent theories for a wide variety of fractional quantum Hall states promoted by a  $Z_2$  gauge theory. The theory always carries an anyonic symmetry (AS) which effects a fermion parity flip. The associated twist defects, which flip the parities of some types of orbiting quasiparticles, trap ordinary zero energy Majorana bound states (MBS), and can bind fractional charge. For example, an  $h/2e$  flux vortex of the superconductor that circulates around the MBS undergoes a fermion parity flip and is accompanied by a level crossing in the vortex energy spectrum. We show numerical evidence of the level crossing in the simplest examples: a Chern insulator and a normal insulator/topological insulator/superconductor junction. Finally, we briefly describe the resulting twist liquid theory after gauging the AS where the twist defects become deconfined anyonic excitations.

**8:48AM K51.00005 A New Kind of Topological Quantum Order: A Dimensional Hierarchy of Quasiparticles Built from Stationary Excitations**, S. VIJAY, JEONGWAN HAAH, LIANG FU, Massachusetts Inst of Tech-MIT — We introduce exactly solvable models of interacting (Majorana) fermions in  $d \geq 3$  spatial dimensions that realize a new kind of topological quantum order, building on a model presented in ref. [1]. These models have extensive topological ground-state degeneracy and a hierarchy of point-like, topological excitations that are only free to move within sub-manifolds of the lattice. In particular, one of our models has fundamental excitations that are completely stationary. To demonstrate these results, we introduce a powerful polynomial representation of commuting Majorana Hamiltonians. Remarkably, the physical properties of the topologically-ordered state are encoded in an algebraic variety, defined by the common zeros of a set of polynomials over a finite field. This provides a “geometric” framework for the emergence of topological order. [1] S. Vijay, T. H. Hsieh and L. Fu, arXiv:1504.01724 (2015).

**9:00AM K51.00006 Particle-vortex duality of 2d Dirac fermion from electric-magnetic duality of 3d topological insulators**, MAX METLITSKI, Perimeter Institute for Theoretical Physics, ASHVIN VISHWANATH, University of California, Berkeley — Particle-vortex duality is a powerful theoretical tool that has been used to study systems of bosons. In arXiv:1505.05142, we propose an analogous duality for Dirac fermions in 2+1 dimensions. The physics of a single Dirac cone is proposed to be described by a dual theory, QED3 with a dual Dirac fermion coupled to a  $u(1)$  gauge field. This duality is established by considering two alternate descriptions of the 3d topological insulator (TI) surface. The first description is the usual Dirac cone surface state. The second description is accessed via an electric-magnetic duality of the bulk TI coupled to a gauge field, which maps it to a gauged topological superconductor. This alternate description ultimately leads to a new surface theory - dual QED3. The dual theory provides an explicit derivation of the T-Pfaffian state, a proposed surface topological order of the TI, which is simply the paired superfluid state of the dual fermions. The roles of time reversal and particle-hole symmetry are exchanged by the duality, which connects some of our results to a recent conjecture by Son on particle-hole symmetric quantum Hall states at  $\nu = 1/2$ .

**9:12AM K51.00007 Half-filled topological flat bands, dualities and SPT surface states**, ANDREW POTTER, Univ of California - Berkeley, MAX METLITSKI, Perimeter Institute, ASHVIN VISHWANATH, Univ of California - Berkeley — The surface states of 3D symmetry protected topological phases are impossible to realize in pure 2D systems with a local implementation of symmetry. However, systems with non-local symmetries, e.g. associated with filling or emptying a topological flat band, can circumvent this limitation. A well studied recent example is that of the  $1/2$ -filled Landau level, which effectively realizes the physics of a particular type of time-reversal invariant topological superconductor. In this talk, I will generalize these concepts to other classes of 2D topological flat bands with non-local symmetries, that are related to 3D SPT surface states with local implementations of the same symmetry. This generalization reveals new dualities between strongly interacting gapless phases. In addition, physical implications for new gapless and topologically ordered states in multicomponent quantum Hall systems will be mentioned.

**9:24AM K51.00008 Non-Abelian states in Fractional Quantum Hall effect in charge carrier hole systems<sup>1</sup>**, GEORGE SIMION, YULI LYANDA-GELLER, Department of Physics and Astronomy, Purdue University — Quasiparticle excitations obeying non-Abelian statistics represent the key element of topological quantum computing. Crossing of levels and strong coupling between angular momentum and orbital motion, described by Luttinger Hamiltonian, make properties of charge carrier holes different from those of electrons. Peculiarities of hole spectrum in magnetic field provide an opportunity for controlling Landau level mixing in charge carrier hole systems. In order to describe Fractional Quantum Hall effect for holes, we propose a method to map hole spectrum and wavefunctions using a spherical shell. We investigate the experimentally observed  $\nu = 1/2$  state in spherical geometry. Haldane pseudopotentials are computed and the effect of Landau level mixing is evaluated. Exact diagonalization of Coulomb interaction in systems with eight to fourteen holes is performed. We determine that the ground state superposition with Abelian 331 state is very small and the overlap with Moore-Read state is significant. The quasihole and quasielectron excitations are discussed.

<sup>1</sup>Research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-SC0010544.

**9:36AM K51.00009 The Fractional Quantum Hall States at  $\nu = 13/5$  and  $12/5$  and their Non-Abelian Nature<sup>1</sup>**, W. ZHU, Cal State Univ - Northridge, S. S. GONG, National High Magnetic Field Lab, D. N. SHENG, Cal State Univ - Northridge — Topological quantum states with non-Abelian Fibonacci anyonic excitations are widely sought after for their exotic fundamental physics and potential applications in universal quantum computing. The fractional quantum Hall (FQH) state at filling factor  $\nu = 12/5$  is such a promising candidate, however, its precise nature is still under debate and no consensus has been achieved so far. Here, we investigate the nature of the FQH  $\nu = 13/5$  state and its particle-hole conjugate state at  $12/5$  with the Coulomb interaction, and address the issue of possible competing states. Based on a large-scale density-matrix renormalization group (DMRG) calculation in spherical geometry, we present evidence that the essential physics of the Coulomb ground state (GS) at  $\nu = 13/5$  and  $12/5$  is captured by the  $k = 3$  parafermion Read-Rezayi state ( $RR_3$ ), including a robust excitation gap and the topological fingerprint from entanglement spectrum and topological entanglement entropy. Furthermore, by considering the infinite-cylinder geometry (topologically equivalent to torus geometry), we expose the non-Abelian GS sector corresponding to a Fibonacci anyonic quasiparticle, which serves as a signature of the  $RR_3$  state at  $13/5$  and  $12/5$  filling numbers.

<sup>1</sup>This work is supported by the DOE grants No. DE-FG02-06ER46305, DE-SC0002140, and the NSF grant No. DMR-1408560.

**9:48AM K51.00010 Interferometric measurements to test non-Abelian properties of  $e/4$  charges in the fractional quantum Hall state at  $5/2$** , ROBERT WILLETT, Alcatel-Lucent/Bell Labs, MICHAEL MANFRA, Purdue University, LOREN PFEIFFER, Princeton University, KIRILL SHTENGEL, University of California, Riverside, CHETAN NAYAK, University of California, Santa Barbara, and Microsoft Q — The excitations of charge  $e/4$  at  $5/2$  filling factor are proposed to obey non-Abelian statistics. To test this, interferometry at fractional quantum Hall states can be performed that controllably braids edge currents around localized charges. We have conducted these measurements in a large number of interferometers of different sizes, also using multiple designs of high quality 2D electron heterostructures. We observe properties of the interference measurements at  $5/2$  that are specifically consistent with non-Abelian  $e/4$ . In particular, magnetic field sweeps around  $5/2$  show interference oscillations with frequency spectra that are consistent in detail with non-Abelian  $e/4$  properties. Four frequency spectra peaks are observed corresponding to both  $e/4$  and  $e/2$  charges; importantly a rapid non-Abelian  $e/4$  component is seen that is split due to beating between the two  $e/4$  braiding processes. We review these results and their observation in a range of interferometer dimensions and in different heterostructure designs.

**10:00AM K51.00011 Abelian and non-Abelian states in  $\nu = 2/3$  bilayer fractional quantum Hall systems<sup>1</sup>**, MICHAEL PETERSON, Cal State Univ- Long Beach, YANG-LE WU, Joint Quantum Institute, University of Maryland, MENG CHENG, MAISSAM BARKESHLI, Microsoft, ZHENGHAN WANG, Microsoft, University of California Santa Barbara — There are several possible theoretically allowed non-Abelian fractional quantum Hall (FQH) states that could potentially be realized in one- and two-component FQH systems at total filling fraction  $\nu = n + 2/3$ , for integer  $n$ . Some of these states even possess quasiparticles with non-Abelian statistics that are powerful enough for universal topological quantum computation, and are thus of particular interest. Here we initiate a systematic numerical study, using both exact diagonalization and variational Monte Carlo, to investigate the phase diagram of FQH systems at total filling fraction  $\nu = n + 2/3$ , including in particular the possibility of the non-Abelian  $Z_4$  parafermion state. In  $\nu = 2/3$  bilayers we determine the phase diagram as a function of interlayer tunneling and repulsion, finding only three competing Abelian states, without the  $Z_4$  state. On the other hand, in single-component systems at  $\nu = 8/3$ , we find that the  $Z_4$  parafermion state has significantly higher overlap with the exact ground state than the Laughlin state, together with a larger gap, suggesting that the experimentally observed  $\nu = 8/3$  state may be non-Abelian. Our results from the two complementary numerical techniques agree well with each other qualitatively.

<sup>1</sup>We acknowledge the Office of Research and Sponsored Programs at California State University Long Beach and Microsoft Station Q.

**10:12AM K51.00012 Particle-hole symmetry without particle-hole symmetry in the quantum Hall effect at  $\nu = 5/2$ .<sup>1</sup>**, DMITRI FELDMAN, PHILIP ZUCKER, Brown Univ — Numerical results suggest that the quantum Hall effect at  $\nu = 5/2$  is described by the Pfaffian or anti-Pfaffian state in the absence of disorder and Landau level mixing. In realistic samples both disorder and Landau level mixing are strong on the  $5/2$  plateau. The experimental observation of the upstream neutral mode on the sample edge is incompatible with the Pfaffian state. Tunneling experiments give an upper bound on the universal exponent  $g$  in the zero bias conductance  $G \sim T^{2g-2}$ . That bound is inconsistent with the anti-Pfaffian state. We show that a recent proposal of the PH-Pfaffian topological order by Son is compatible with the tunneling experiments and the observation of the upstream mode. The quasiparticle statistics of the PH-Pfaffian state is similar to the statistics in the Pfaffian and anti-Pfaffian states and its interferometric signatures are also similar to those of the Pfaffian and anti-Pfaffian topological orders. The absence of the particle-hole symmetry at  $\nu = 5/2$  is not an obstacle to the existence of the PH-Pfaffian order since the order is robust to symmetry breaking.

<sup>1</sup> We acknowledge support by the NSF under Grant No. DMR-1205715.

**10:24AM K51.00013 Electric Fields in the  $5/2$  fractional quantum Hall effect<sup>1</sup>**, ANTHONY TYLANTYLER, Univ of Pittsburgh, YULI LYANDA-GELLER, Purdue University — The potential for non-Abelian quasiholes in the  $5/2$  fractional quantum Hall effect makes the state of interest theoretically and experimentally. The presence of such features in the ground state of the system would allow for the implementation of a topological quantum computation scheme. In order to probe the system for these features, a small measuring voltage, i.e. an electric field, is applied. In Corbino geometries, these electric fields are applied radially. This breaks the Galilean invariance, which in an infinite planar geometry allows us to transform to a moving frame of reference, eliminating the electric field. To study the effects of these fields, we carry out exact diagonalization calculations in a disk geometry. We find that application of small fields can lead to an improvement in the overlap with the Moore-Read Pfaffian long before the state is destroyed by the field. Additionally, we find that the coherence length of quasiholes travelling along the edge of the sample increases significantly when compared to the case with no applied field.

<sup>1</sup>This research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-SC0010544.

**10:36AM K51.00014 Probing bulk physics in the 5/2 fractional quantum Hall effect using the Corbino geometry**, BENJAMIN SCHMIDT, McGill University, KEYAN BENNACEUR, Sherbrooke University, SIMON BILODEAU, SAMUEL GAUCHER, McGill University, MICHAEL LILLY, JOHN RENO, Sandia National Laboratories, LOREN PFEIFFER, KEN WEST, Princeton University, BERTRAND REULET, Sherbrooke University, GUILLAUME GERVAIS, McGill University — We present two- and four-point Corbino geometry transport measurements in the second Landau level in GaAs/AlGaAs heterostructures. By avoiding edge transport, we are able to directly probe the physics of the bulk quasiparticles in fractional quantum Hall (FQH) states including 5/2. Our highest-quality sample shows stripe and bubble phases in high Landau levels, and most importantly well-resolved FQH minima in the second Landau level. We report Arrhenius-type fits to the activated conductance, and find that  $\sigma_0$  agrees well with theory and existing Hall geometry data in the first Landau level, but not in the second Landau level. We will discuss the advantages the Corbino geometry could bring to various experiments designed to detect the non-Abelian entropy at 5/2, and our progress towards realizing those schemes. The results of these experiments could complement interferometry and other edge-based measurements by providing direct evidence for non-Abelian behaviour of the bulk quasiparticles. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL8500.

**10:48AM K51.00015 Discovery of competing 5/2 fractional quantum Hall states<sup>1</sup>**, XI LIN, HAILONG FU, PENGJIE WANG, PUJIA SHAN, LIN XIONG, Peking University, LOREN PFEIFFER, KEN WEST, Princeton University, MARC KASTNER, MIT & Science Philanthropy Alliance — With an even denominator,  $\nu = 5/2$  fractional quantum Hall state (FQH) is different from most of the other FQH states. Some of its proposed wave functions may exhibit novel non-Abelian statistics, which is related to topological quantum computation. We carried out tunneling measurements within a quantum point contact (QPC) at the 5/2 state and we were able to match the QPC's density to the two-dimensional electron gas bulk density. Such a density match guarantees the uniform filling factor inside and outside the QPC. The interaction parameter  $g$  and the effective charge  $e^*$  can be extracted through the weak tunneling theory [1]. We found  $g$  and  $e^*$  similar to what people believed to be the Abelian 331 state [2, 3]. By tuning the confinement, we observed another region where the experimental data agree well with the weak tunneling theory, which leads to  $e^*=0.25$  and  $g=0.52$ , implying non-Abelian wavefunctions such as anti-Pfaffian or  $U(1)SU(2)$ . Our discovery suggests that there are competing 5/2 fractional quantum Hall ground states depending on the confinement. [1] Science 320, 899 (2008). [2] Phys. Rev. B 85, 165321 (2012). [3] Phys. Rev. B 90, 075403 (2014).

<sup>1</sup>The work at PKU was funded by NSFC and NBRPC. The work at Princeton University was funded by the Gordon and Betty Moore Foundation through the EPiQS initiative Grant GBMF4420, and by the National Science Foundation MRSEC Grant DMR-1420541.

## Wednesday, March 16, 2016 8:00AM - 10:36AM –

Session K52 GERA DPOLY: Nanostructured Photovoltaics Hilton Baltimore Holiday Ballroom 3 -

**8:00AM K52.00001 Ligand engineering of lead chalcogenide nanoparticle solar cells<sup>1</sup>**, MARTON VOROS, Materials Science Division, Argonne National Laboratory, NICHOLAS BRAWAND, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago — Semiconductor nanoparticles (NP) are promising materials to build cheap and efficient solar cells. One of the key challenges in their utilization for solar energy conversion is the control of ligand-NP interfaces. Recent experiments have shown that by carefully choosing the ligands terminating the NPs, one can tailor electronic and optical absorption properties of NP assemblies, along with their transport properties.[1] By using density functional theory based methods, we investigated how the opto-electronic properties of lead chalcogenide NPs may be tuned by using diverse organic and inorganic ligands. We interpreted experiments, and we showed that an essential prerequisite to avoid detrimental trap states is to ensure charge balance at the ligand-NP interface, possibly with the help of hydrogen treatment. [1] Ryan Crisp et al., Scientific Reports 5, 9945 (2015); Carlo Giansante et al., J. Am. Chem. Soc. 137, 1875 (2015).

<sup>1</sup>Work supported by the Center for Advanced Solar Photophysics, an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Office of Basic Energy Sciences.

**8:12AM K52.00002 Verifying field-effect passivation of a SiN<sub>x</sub> layer on a silicon nanopillar array using surface photovoltage characterization**, EUNAH KIM, YUNAE CHO, AHRUM SOHN, DONG-WOOK KIM, Ewha Womans University, HYEONG-HO PARK, Korea Advanced Nanofab Center, JOONDONG KIM, Incheon National University — In silicon (Si) wafer based photovoltaic (PV) devices, light-trapping strategies to improve optical absorption are very important due to the indirect bandgap of Si. Surface nano-patterned Si enable omnidirectional broadband antireflection (AR) effects with the help of graded refractive index, multiple scattering, diffraction, and Mie resonance. In this work, the surface photovoltage (SPV) of periodic nanopillar (NP) arrays were investigated using Kelvin probe force microscopy (KPFM). The SPV characteristics clearly revealed that positive fixed charges in SiN<sub>x</sub> layers induced downward band bending at the Si surface and increased SPV at the NP top surface. The similar SPV value of NPs and planar counterpart suggests that field effect passivation by the dielectric layer coating could help improve PV performance of nanostructure-based Si solar cells and that KPFM measurements are useful tool for quantitative investigation of surface electrical properties of Si nanostructures.

**8:24AM K52.00003 Ultra-dense silicon nanowire array solar cells by nanoimprint lithography<sup>1</sup>**, PENG ZHANG, PEI LIU, STYLIANOS SIONTAS, ALEXANDER ZASLAVSKY, DOMENICO PACIFICI, Brown Univ, JONG-YOON HA, SERGIY KRYLYUK, Univ of Maryland & National Institute of Standards and Technology, ALBERT DAVYDOV, National Institute of Standards and Technology — Nanowire (NW) solar cells have been attracting increasing interest due to their potentially superior light absorption compared to thin bulk films. In order to improve light trapping, we have used nanoimprint lithography (NIL) to fabricate high-density NW arrays with deep sub-micron pitch (P) and diameter (D). We have grown dense vertical arrays of Si axial  $p-i-n$  junction NWs of  $D = 170$  nm and  $P = 500$  nm by vapor-liquid-solid epitaxy on seed arrays produced by NIL. The NWs were 9  $\mu$ m length long with a 5  $\mu$ m intrinsic section. The NW arrays were planarized using SU-8 photoresist, followed by reactive ion etching to expose the NW tips. Top  $n$ -contact was realized by sputter deposition of a transparent 200 nm IZO layer. The nanoimprinted NW array samples measured under AM 1.5 G illumination showed a peak external quantum efficiency of  $\sim 8\%$  and internal quantum efficiency of  $\sim 90\%$  in the visible spectral range. Three-dimensional finite-difference time-domain simulations of Si NW periodic arrays with varying P confirm the importance of high NW density. Specifically, due to diffractive scattering and light trapping, absorption efficiency close to 100% in the 400–650 nm spectral range is predicted for a Si NW array with an even smaller  $P = 250$  nm, significantly outperforming a blanket Si film of the same thickness. Such pitch values are accessible to NIL and work on such arrays is in progress.

<sup>1</sup>National Science Foundation

**8:36AM K52.00004 High Efficiency InP Solar Cells Through Nanostructuring**, DANIEL GOLDMAN, JOSEPH MURRAY, JEREMY MUNDAY, University of Maryland, College Park — We describe high efficiency InP solar cells which utilize a periodic array of optically designed TiO<sub>2</sub> nanocylinders. Optical and electronic simulations were performed to determine the spectrally resolved reflectivity and I-V characteristics of potential devices under AM1.5G illumination. The reflectivity of InP solar cells with these nanocylinders is found to have an average value of 2% over the visible and near-IR spectral range, which outperforms traditional antireflection coatings. Coupling between Mie scattering resonances and thin film interference effects is found to accurately describe the optical enhancement provided by the nanocylinders. These nanostructured solar cells have power conversion efficiencies greater than 23%, which is comparable to the highest quoted efficiencies for InP solar cells.

**8:48AM K52.00005 Roles of SiN<sub>x</sub> layers in light trapping and carrier collection of nanostructured crystalline Si solar cells**, YUNAE CHO, EUNAH KIM, MINJI GWON, DONG-WOOK KIM, Ewha Womans University, HYEONG-HO PARK, Korea Advanced Nanofab Center, JOONDONG KIM, Incheon National University — We investigated optical properties and photovoltaic (PV) performance of nanostructured Si solar cells with and without SiN<sub>x</sub> dielectric layers. The SiN<sub>x</sub> layer contributed to the enhancement of internal quantum efficiency of the nanostructured cells at both short and long wavelengths. In contrast, the surface passivation of SiN<sub>x</sub> layers on flat cells helped the carrier collection mainly at short wavelength. The surface nanopatterned array enhanced the optical absorption and also concentrated incoming light near the surface in broad wavelength range, revealed by experimental data and optical simulation results. As a result, the nanostructured cells had high density of photo-generated carriers near the surface. This could lead to significant recombination loss of the cells without SiN<sub>x</sub> layers. Our work suggested that the SiN<sub>x</sub> layer played a crucial role in the improved carrier collection of the nanostructured Si PV devices.

**9:00AM K52.00006 Gold Nanoparticles Assisted Photocurrent Enhancement in Hybrid Nanostructures Based Heterojunction Solar Cell Device<sup>1</sup>**, GEN LONG, MICHAEL BEATTIE, HUIZHONG XU, MOSTAFA SADOQI, Department of Physics, St John's University — In this presentation, we report a first hand study of plasmon enhanced photocurrent observed in hybrid nanostructures based heterojunction solar cell. The heterojunction solar cell was fabricated, using chemically synthesized narrow gap, IV-VI group semiconductor nanoparticles (PbS and PbSe), wide gap semiconductor ZnO nanowires, and gold nanoparticles, by spin-coating onto FTO glasses, in ambient conditions (25C, 1atm). The synthesized nanostructures were characterized by XRD, UV-VIS absorption, SEM, AFM, TEM, solar simulator, etc. Nanostructures of variant sizes were integrated in to the heterojunction devices to study the effects on photocurrent and solar cell performance. The architecture of film stack, i.e., the positions of Au nanoparticles and PbS, PbSe nanoparticles were also studied. We believe that introducing Au nanoparticles with proper size will lead to increase of photocurrent as well as solar cell devices.

<sup>1</sup>The authors thank Center for Functional Nanomaterials of DOE for providing facilities access.

**9:12AM K52.00007 Dielectric micro-resonator arrays for optical coupling to solar cells**, DONGHEON HA, CHEN GONG, MARINA S. LEITE, JEREMY N. MUNDAY, Univ of Maryland-College Park, MUNDAY LAB TEAM, LEITE LAB COLLABORATION — Reflection occurs at the interface of a semiconductor and air as a result of the index of refraction contrast between the two media. In order to increase the coupling efficiency of free-space light to the modes of a solar cell, single- or double-layer dielectric thin-film anti-reflection coatings (ARC) are typically used. As an alternative approach, we introduce a new anti-reflection coating based on silicon dioxide (SiO<sub>2</sub>) nanospheres that enable high absorption and low-cost photovoltaic devices through a combination of effects including scattering, thin-film interference, and sphere-sphere coupling. From experiments and Finite Difference Time Domain (FDTD) simulations, we show that there is ~15-20% enhancement in light absorption within the substrate (Si), which ultimately leads to increased spectral current density. We also show the enhancement of the optoelectronic properties via photo-response measurement on multi-crystalline Si solar cells with SiO<sub>2</sub> nanosphere arrays on top. Because the layer can be made with an easy, inexpensive, and scalable process, this proposed ARC is an excellent candidate for substituting conventional ARC technologies relying on complicated, high temperature and expensive processes.

**9:24AM K52.00008 Importance of Depletion Width on Charge Transport and Interfacial Recombination in Extremely Thin Absorber Solar Cells**, MICHAEL EDLEY, TREAVOR JONES, JASON BAXTER, Drexel University — The dynamics of charge carrier transport and recombination and their dependence on physical and electrochemical length scales in extremely thin absorber (ETA) solar cells is vital to cell design. We used J-V characterization, transient photocurrent / photovoltage, and electrochemical impedance spectroscopy to study electron transport and interfacial recombination in ETA cell. ETA cells were composed of ZnO nanowires coated with an ultrathin (5 nm) CdS buffer layer and CdSe absorbers with thicknesses of 10 – 40 nm, with polysulfide electrolyte. In thinner absorbers near short circuit, the depletion region can extend radially into the nanowire, inhibiting interfacial recombination rate. However, depleting the periphery of the nanowire reduces the cross sectional area for charge transport, resulting in longer characteristic collection times. Thicker absorbers suffered more significant bias-dependent collection, and we conclude that slight radial penetration of the depletion region into the nanowires enhances charge collection. This work highlights the importance of considering the impact of depletion width on charge transport and interfacial recombination in the design of liquid junction, semiconductor-sensitized solar cells.

**9:36AM K52.00009 MOVED ABSTRACT TO R26.011 —**

**9:48AM K52.00010 Exciton Transfer in Carbon Nanotube Aggregates for Energy Harvesting Applications<sup>1</sup>**, AMIRHOSSEIN DAVOODY, FARHAD KARIMI, IRENA KNEZEVIC, Univ of Wisconsin, Madison — Carbon nanotubes (CNTs) are promising building blocks for organic photovoltaic devices, owing to their tunable band gap, mechanical and chemical stability. We study intertube excitonic energy transfer between pairs of CNTs with different orientations and band gaps. The optically bright and dark excitonic states in CNTs are calculated by solving the Bethe-Salpeter equation. We calculate the exciton transfer rates due to the direct and exchange Coulomb interactions, as well as the second-order phonon-assisted processes. We show the importance of phonons in calculating the transfer rates that match the measurements. In addition, we discuss the contribution of optically inactive excited states in the exciton transfer process, which is difficult to determine experimentally. Furthermore, we study the effects of sample inhomogeneity, impurities, and temperature on the exciton transfer rate. The inhomogeneity in the CNT sample dielectric function can increase the transfer rate by about a factor of two. We show that the exciton confinement by impurities has a detrimental effect on the transfer rate between pairs of similar CNTs. The exciton transfer rate increases monotonically with increasing temperature.

<sup>1</sup>Support by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-SC0008712

**10:00AM K52.00011 Ultrafast Spectroscopy Reveals Frenkel-CT Mixed Excitonic States in Copper Phthalocyanine**, ROBERT YOUNTS, TERRY MCAFEE, BHOJ GAUTAM, DANIEL DOUGHERTY, HARALD ADE, KENAN GUNDOGU, North Carolina State University — In organic semiconducting systems, intermolecular charge transport and energy diffusion take place along the  $\pi$ - $\pi$  stacking direction, which is beneficial for opto-electronic devices. Therefore it is essential to study electronic state structure in the  $\pi$ - $\pi$  stacking direction in organic solids. We studied a model quasi-one-dimensional molecular crystal copper phthalocyanine, which has strong intermolecular coupling along the  $\pi$ - $\pi$  stack. In this work, we used polarization resolved transient absorption spectroscopy and identified the coupling of low-lying singlet Frenkel (intramolecular) excitons with CT (intermolecular) excitons. Our study shows an evolution between localized and delocalized excitations which can be utilized to tune charge transport properties in molecular crystals. These studies provide fundamental understanding of electronic state structures, which will be essential for tailoring electronic properties of desired applications.

**10:12AM K52.00012 Investigation of transport properties of ZnO/PbS heterojunction solar cells<sup>1</sup>**, YANG CHENG, MICHAEL D. C. WHITAKER, VINCENT R. WHITESIDE, LLOYD A. BUMM, IAN R. SELLERS, Department of Physics & Astronomy, University of Oklahoma, Norman OK 73019 — Lead sulfide (PbS) and lead selenide (PbSe) colloidal quantum dots (CQDs) are considered as a potential candidate material for solar cell applications due to their large band gap tunability range (0.5 to 1.7 eV) and cost-effective solution based processing. A series of Glass/ITO/ZnO/PbS/MoO<sub>3</sub>/Au heterojunction solar cells were processed and analyzed. A stable (reproducible) 2% conversion efficiency under 1-sun is achieved based on the result of  $J - V$  measurements. Absorbance and external quantum efficiency (EQE) measurements clearly show photo-generated carrier extraction from PbS active layers in the solar cell. However, a non-ideal  $J - V$  behavior is observed in current-voltage measurements. This behavior may be attributed to a high density of trap states at the QD surface or defect states at the PbS/ZnO or ITO/ZnO interfaces. C-V and Impedance spectroscopy measurements are used to study this unusual behavior. These techniques could also help probe the transport properties and limitation of these heterojunction solar cells.

<sup>1</sup>This research is funded through NASA EPSCoR program award # NNX13AN101A

**10:24AM K52.00013 Limits of Plasmonic Nanoparticle Enhancement in Solution-Processed Solar Cells**, EBUKA ARINZE, BOTONG QIU, GABRIELLE NYIRJESY, SUSANNA THON, Johns Hopkins Univ — Solution-processed solar cells are particularly suited to benefit from plasmonic absorption enhancement due to their transport-limited film thicknesses, and the favorable compatibility of material integration. To date, experimental demonstrations of device enhancements via plasmonic nanoparticle-based strategies have achieved photocurrents that still fall below the theoretical predicted limits. We critically evaluate the prospects for plasmonic enhancements in solution-processed thin-film solar cells. We develop an effective medium model for embedded plasmonic nanostructures in photovoltaic thin films, evaluate the model in the context of previous results achieved in the field, and use the model as a framework for identifying the most promising avenues to realizing plasmonic performance enhancements in practical photovoltaic devices. Our model results indicate that further plasmonic enhancement gains may be possible in organic photovoltaic cells. For achieving maximum photocurrent potential, we identify fine-tuning of the concentration of embedded plasmonic enhancers within the absorbing medium as the crucial factor in achieving a balance between useful scattering and detrimental parasitic absorption losses.

## **Wednesday, March 16, 2016 8:00AM - 11:00AM —**

**Session K53 DFD GSOF GSNP: Granular and Multiphase Flows** Hilton Baltimore Holiday Ballroom 4 -

**8:00AM K53.00001 Ferrofluid-based Diamagnetic Particle Separation in U-shaped Microchannels.<sup>1</sup>**, YILONG ZHOU, XIANGCHUN XUAN, Clemson University — We demonstrate in this talk a continuous-flow sheath-free separation method of diamagnetic particles in ferrofluids through U-shaped microchannels. Due to the action of a size-dependent magnetic force, diamagnetic particles are focused into a single stream in the inlet branch of the U-turn and then continuously separated into two streams in its outlet branch. We also develop a 3D numerical model to predict and understand the diamagnetic particle transport during the separation process. The numerical predictions are found to agree well with the experimental observations in a systematic study of multiple parameter effects including ferrofluid flow rate, concentration and magnet-channel distance.

<sup>1</sup>This work was supported by NSF.

**8:12AM K53.00002 Smart microgels for controlling two-phase fluid structure in porous media<sup>1</sup>**, JING FAN, DAVID WEITZ, Harvard University — Understanding the transport of microgels in porous media directly benefits the conformance improvement technique using preformed gels in the oil industry. We develop a new type of microgels that can swell in response to specific stimuli in an aqueous environment. From a practical point of view, this enables us to deliver the microgels to the deep reservoir formation and control the permeability profile more effectively. With confocal microscopy imaging, we show that we can deliver such smart microgels to the high-permeability region in a stratified porous medium, which subsequently changes the two-phase fluid structure in the medium. From a scientific point of view, this allows for characterizing the permeability change due to homogeneous pore-clogging by soft particles instead of surface clogging; using the typical microgels this can hardly be done because we cannot place gel particles with comparable size to the pore uniformly into a porous medium. This study may shed light on understanding many other processes involving the transport of soft particles in porous structures.

<sup>1</sup>The authors acknowledge the financial support from Advanced Energy Consortium, BEG08-27.

**8:24AM K53.00003 Effect of Microstructural Geometry for Computing Closure Models in Multiscale Modeling of Shocked Particle Laden Flow**, OISHIK SEN, H.S. UDAYKUMAR, Univ of Iowa, GUSTAAF JACOBS, San Diego State University — Interaction of a shock wave with dust particles is a complex physical phenomenon. A computational model for studying this two-phase system is the Particle-Source in Cell (PSIC) approach. In this method, the dust particles are tracked as point particles in a Lagrangian frame of reference immersed in a compressible fluid. Two-way interaction between the carrier and the dispersed phases is ensured by coupling the momentum and energy transfer between the two phases as source terms in the respective governing equations. These source terms (e.g. drag force on particles) may be computed from resolved numerical simulations by treating each macroscopic point particle as an ensemble of cylinders immersed in a compressed fluid. However the drag so computed must be independent of the geometry of the mesoscale. In this work, the effect of the stochasticity of the microstructural geometry in construction of drag laws from resolved mesoscale computations is studied. Several different arrangement of cylinders are considered and the mean drag law as a function of Mach Number and Volume Fraction for each arrangement is computed using the Dynamic Kriging Method. The uncertainty in the drag forces arising because of the arrangement of the cylinders for a given volume fraction is quantified as 90% credible sets and the effect of the uncertainty on PSIC computations is studied.

**8:36AM K53.00004 Time dependent behavior of impact angle in turbulent pipe flows experience erosion.**<sup>1</sup>, AMADOR GUZMAN, Pontificia Universidad Catolica de Chile, DIEGO OYARZUN<sup>2</sup>, Universidad de Santiago de Chile, MAGDALENA WALCZAK<sup>3</sup>, JAVIERA AGUIRRE<sup>4</sup>, Pontificia Universidad Catolica de Chile — Erosion-corrosion in pipe systems transporting slurry turbulent flows is of a great importance in industrial and mining applications, where large volumes of suspended solids are sent up to hundreds of kilometers, to be further processed. The slurry is typically sent over large diameter steel pipes, which not always have an anti-abrasion coating. During the transport, the thickness of the pipe diminishes and eventually leaks and breaks, due to the combined effects of wear and corrosion. The processes of pipe degradation are further enhanced by the content of the slurry electrolytes that might switch from neutral to aggressive. The understanding of these processes in terms of operational parameters is critical for anticipating and mitigating a catastrophic outcome. This paper describes turbulent flow numerical simulations in a slurry transporting steel pipe with an emphasis on the correlation between the time dependent impact angle in the vicinity of the steel pipe and the rate of material loss. Full numerical simulations in a 3D long domain by using an Eulerian –Eulerian two phase flow approach coupled to a  $\kappa$ -epsilon turbulent model are performed for different solid particle concentration and flow velocity and compared to existing experimental and numerical results for validation with and without gravity. Time-dependent axisymmetric turbulent flow simulations are performed for determining both the time dependent behavior of the axial and radial velocities near the pipe wall and the impact angle.

<sup>1</sup>Financial support from Conicyt through the Fondecyt proposal 1141107 is acknowledged

<sup>2</sup>Assistant Professor of Mechanical Engineering

<sup>3</sup>Associate Professor of Mechanical Engineering

<sup>4</sup>Doctoral student and research assistant

**8:48AM K53.00005 Caustics and the growth of droplets**<sup>1</sup>, RAMA GOVINDARAJAN, S RAVICHANDRAN, TIFR Centre for Interdisciplinary Sciences, Hyderabad, India, SAMRIDDHI RAY, International Centre for Theoretical Sciences, TIFR, Bangalore, P DEEPU, TIFR Centre for Interdisciplinary Sciences, Hyderabad, India — Caustics are formed when inertial particles of very different velocities collide in a flow, and are a consequence of the dissipative nature of particle motion in a suspension. Using a model vortex-dominated flow with heavy droplets in a saturated environment, we suggest that sling caustics form only within a neighbourhood around a vortex, the square of whose radius is proportional to the product of circulation and particle inertia. Droplets starting close to this critical radius congregate very close together, resulting in large spikes in (Lagrangian) number density. Allowing for merger when droplets collide, we show that droplets starting out close to the critical radius display a much more rapid growth in size than those starting elsewhere, and a large fraction of the large droplets are those that originate within the caustics-forming region. We test these predictions in a two-dimensional simulation of turbulent flow. We hope that our study will be of interest in long-standing problems of physical interest such as the mechanism of broadening of droplet spectra in a turbulent flow.

<sup>1</sup>Support from the Ministry of Earth Sciences, Government of India for the project Coupled physical processes in the Bay of Bengal and monsoon air-sea interaction under OMM is gratefully acknowledged

**9:00AM K53.00006 Soft Sphere Suspensions: Flow and Relaxation**, MARCEL WORKAMP, JOSHUA A. DIJKSMAN, Physical Chemistry and Soft Matter, Wageningen University — We experimentally study the role of particle elasticity on the rheology of soft sphere suspensions. Experiments consist of custom designed particles with tuneable stiffness. These particles allow us to probe the role of elastic timescales, relaxation and anisotropy in a custom 3D printed shear cell. We find robust rheological features, such as a flow instability, that are not well captured by existing models for suspension flows. In addition, we find relaxation effects after shear even in the absence of shear or thermal fluctuations. We aim to integrate these findings in the emerging unified framework for structured fluids.

**9:12AM K53.00007 Impact cratering on granular beds: From the impact of raindrops to the strike of hailstones**<sup>1</sup>, LEONARDO GORDILLO, JUNPING WANG, FRED JAPARDI, WARREN TEDDY, MING GAO, XIANG CHENG, CEMS - University of Minnesota — Impact craters generated by the impact of a spherical object onto a granular bed strongly depend on the material properties of impactors. As an example, impact cratering by liquid drops and by solid spheres exhibits qualitatively different power-law scalings for the size of resulting impact craters. While the basic energy conservation and dimensional analysis provide simple guiding rules, the detailed dynamics governing the relation between these power-law scalings is still far from clear. To analyze the transition between liquid-drop and solid-sphere impact cratering, we investigate impact cratering by liquid drops for a wide range of viscosities over 7 decades. Using high-speed photography and laser profilometry, we delineate the liquid-to-solid transition and show the emergence of the two asymptotic behaviors and their respective power laws. We find that granular avalanches triggered by impacts are crucial in understanding the energy partition between impacted surfaces and impactors, which directly determines the observed scaling relations. A simple model is constructed for the initial stage of the impact that explains the energy partition during crater formation.

<sup>1</sup>We acknowledge the support of NSF CAREER DMR-1452180. LG acknowledges fundings from CONICYT/BECAS CHILE 74160007.

**9:24AM K53.00008 Scaling of liquid-drop impact craters in granular media**<sup>1</sup>, RUNCHEN ZHAO, QIANYUN ZHANG, HENDRO TJUGITO, MING GAO, XIANG CHENG, University of Minnesota — Granular impact cratering by liquid drops is a ubiquitous phenomenon, directly relevant to many important natural and industrial processes such as soil erosion, drip irrigation, and dispersion of micro-organisms in soil. Here, by combining the high-speed photography with high precision laser profilometry, we investigate the liquid-drop impact dynamics on granular surfaces and monitor the morphology of resulting craters. Our experiments reveal novel scaling relations between the size of granular impact craters and important control parameters including the impact energy, the size of impinging drops and the degree of liquid saturation in a granular bed. Interestingly, we find that the scaling for liquid-drop impact cratering in dry granular media can be quantitatively described by the Schmidt-Holsapple scaling originally proposed for asteroid impact cratering. On the other hand, the scaling for impact craters in wet granular media can be understood by balancing the inertia of impinging drops and the strength of impacted surface. Our study sheds light on the mechanism governing liquid-drop impacts on dry/wet granular surfaces and reveals a remarkable analogy between familiar phenomena of raining and catastrophic asteroid strikes.

<sup>1</sup>Scaling of liquid-drop impact craters in granular media

**9:36AM K53.00009 Scaling of granular convective velocity and timescale of asteroidal resurfacing**, TOMOYA YAMADA, KOUSUKE ANDO, TOMOKATSU MOROTA, HIROAKI KATSURAGI, Department of Earth and Environmental Sciences, Nagoya University — Granular convection is one of the well-known phenomena observed in a vertically vibrated granular bed. Recently, the possible relation between granular convection and asteroidal surface processes has been discussed. The granular convection on the surface of small asteroids might be induced by seismic vibration resulting from meteorite impacts. To quantitatively evaluate the timescale of asteroidal resurfacing by granular convection, the granular convective velocity under various conditions must be revealed. As a first step to approach this problem, we experimentally study the velocity scaling of granular convection using a vertically vibrated glass-beads layer. By systematic experiments, a scaling form of granular convective velocity has been obtained. The obtained scaling form implies that the granular convective velocity can be written by a power-law product of two characteristic velocity components: vibrational and gravitational velocities. In addition, the system size dependence is also scaled. According to the scaling form, the granular convective velocity is almost proportional to gravitational acceleration. Using this scaling form, we have estimated the resurfacing timescale on small asteroid surface.

**9:48AM K53.00010 The Larger the Viscosity, the Higher the Bounce**, MENACHEM STERN, MARTIN KLEIN SCHAARSBERG, IVO PETERS, KEVIN DODGE, WENDY ZHANG, HEINRICH JAEGER, The Physics Department and the James Franck Institute, The University of Chicago — A low-viscosity liquid drop can bounce upon impact onto a solid. A high-viscosity drop typically just flattens, i.e., it splats. Surprisingly, our experiments with a droplet made of densely packed glass beads in silicone oil display the opposite behavior: the low-viscosity oil suspension drop splats. The high-viscosity oil suspension bounces. Increasing solvent viscosity *increases* the rebound energy. To gain insight into the underlying mechanism, we model the suspension as densely packed elastic spheres experiencing viscous lubrication drag between neighbors. The model reproduces the observed trends. Plots of elastic compression and drag experienced by the particles show that rebounds are made possible by (1) a fraction of the impact energy being stored during initial contact via elastic compression, (2) a rapid broadening of local lubrication drag interactions at the initial impact site into a spatially uniform upward force throughout the drop. Including finite wall drag due to the presence of ambient air into the numerical model diminishes and eventually cuts off the rebound.

**10:00AM K53.00011 Percolation velocity dependence on local concentration in bidisperse granular flows<sup>1</sup>**, RYAN P. JONES, HONGYI XIAO, ZHEKAI DENG, PAUL B. UMBANHOWAR, RICHARD M. LUEPTOW, Northwestern University — The percolation velocity,  $u_p$ , of granular material in size or density bidisperse mixtures depends on the local concentration, particle size ratio, particle density ratio, and shear rate,  $\dot{\gamma}$ . Discrete element method computational results were obtained for bounded heap flows with size ratios between 1 and 3 and for density ratios between 1 and 4. The results indicate that small particles percolate downward faster when surrounded by large particles than large particles percolate upward when surrounded by small particles, as was recently observed in shear-box experiments. Likewise, heavy particles percolate downward faster when surrounded by light particles than light particles percolate upward when surrounded by heavy particles. The dependence of  $u_p/\dot{\gamma}$  on local concentration results in larger percolation flux magnitudes at high concentrations of large (or light) particles compared to high concentrations of small (or heavy) particles, while local volumetric flux is conserved. The dependence of  $u_p/\dot{\gamma}$  on local concentration can be incorporated into a continuum model, but the impact on global segregation patterns is usually minimal.

<sup>1</sup>Partially funded by Dow Chemical Company and NSF Grant No. CBET-1511450

**10:12AM K53.00012 Impact of Overburden on Segregation in Sheared Granular Flow**, ALEXANDER M. FRY, PAUL B. UMBANHOWAR, RICHARD M. LUEPTOW, Northwestern University — Dense granular materials tend to segregate into size or density graded regions when subjected to shear. Previous experiments demonstrated that overburden – normal confining pressure on a granular system – can slow the rate of size segregation in an annular shear cell. Here, we explore the effects of overburden on sheared granular material through Discrete Element Method (DEM) simulations in a planar shear cell geometry in which shear is applied by a moving bottom wall, while a massive upper wall provides the overburden. Segregation decreases with increasing overburden, but the picture is complicated by concurrent changes in the streamwise velocity profile. To decouple these effects, we also test an idealized system in which a desired streamwise velocity profile – and therefore shear rate – is imposed by applying additional horizontal forces to each particle. Based on this approach, we link the effect of overburden on segregation to the grain-scale behavior of the system. Partially funded by Procter & Gamble.

**10:24AM K53.00013 Impact of a hydrophobic granular stream in water<sup>1</sup>**, BRIAN UTTER, Bucknell University, HARRY MANDELES, JACOB PARKHOUSE, James Madison University — We experimentally investigate the flow of a stream of hydrophobic granular particles impacting a water surface from above. The granular sample is composed of a mixture of hydrophobic and hydrophilic grains and the concentration, stream diameter, and drop height are independently controlled. While granular flows are common in nature and industry, effects of surface chemistry on flow behavior have received relatively little attention. The present experiment complements rheological measurements performed in parallel and aims to elucidate prior experiments on hydrophobic samples in a rotating drum. The present experimental geometry allows us to compare the behavior of granular streams to prior work on impacts of solids and fluid streams. Sequential images of the granular stream in water are taken and analyzed. We present data on the size, length, and shape of the aggregate streams with variations in concentration, entering stream diameter, and drop height. We find that increased hydrophobic grain concentration leads to increased aggregation due to an effectively cohesive interaction mediated by entrained air. At lower concentrations, the stream exhibits a lateral instability. Finally, we will make connections to rheology and rotating drum results.

<sup>1</sup>This work was supported by NSF CBET award 1067598.

**10:36AM K53.00014 Numerical Simulation and Performance Optimization of a Magnetophoretic Bio-separation chip.**, MATIN GOLOZAR, JEFF DARABI, MAJID MOLKI, Southern Illinois University Edwardsville — Separation of micro/nanoparticles is important in biomedicine and biotechnology. This research presents the modeling and optimization of a magnetophoretic bio-separation chip for the isolation of biomaterials, such as circulating tumor cells (CTCs) from the peripheral blood. The chip consists of a continuous flow through microfluidic channels that contains locally engineered magnetic field gradients. The high gradient magnetic field produced by the magnets is spatially non-uniform and gives rise to an attractive force on magnetic particles that move through the flow channel. The computational model takes into account the magnetic and fluidic forces as well as the effect of the volume fraction of particles on the continuous phase. The model is used to investigate the effect of two-way particle-fluid coupling on both the capture efficiency and the flow pattern in the separation chip. The results show that the microfluidic device has the capability of separating CTCs from their native environment. Additionally, a parametric study is performed to investigate the effects of the channel height, substrate thickness, magnetic bead size, bioparticle size, and the number of beads per cell on the cell separation performance.

Dept of Chemical Engineering  
Lamar University, Beaumont, TX 77710  
Cameron Corporation  
4901 West Sam Houston Parkway North  
Houston, Texas 77041  
USA  
Dept of Chemical Engineering

**10:48AM K53.00015 A Statistical investigation of sloshing parameters in offshore separators**, MD MAHMUD, Lamar University, RAFIQUK KHAN, Cameron Corporation, QIANG XU, Lamar University — Offshore separators have been the subject of intense investigations for last several decades both by experiments and numerical simulations. However, some others have developed new methods to describe sloshing phenomenon. Mathematical models are developed to characterize sloshing phenomenon. However, a comprehensive statistical analysis is not yet been studied. In this study, statistical approach will be considered to determine the significant parameters for liquid sloshing. Principal component analysis techniques are considered to identify the significant parameters for liquid sloshing. Computation Fluid Dynamics (CFD) technique using ANSYS Fluent software. The input parameters considered are wave acceleration, wave frequencies, amplitudes in various sea state conditions. The measured variables include hydrodynamic pressure, kinetic energy, height of the free surface, vorticity. Mathematical correlations may be developed from the data.

Lamar University, Beaumont, TX 77710

## Wednesday, March 16, 2016 8:00AM - 9:30AM –

Session K54 APS: Tutorial for Authors and Referees Hilton Baltimore Holiday Ballroom 5 -

### 8:00AM K54.00001 TUTORIAL FOR AUTHORS AND REFEREES

— Editors from Physical Review Letters and Physical Review will provide information and tips for our less experienced referees and authors. This session is aimed at anyone looking to submit to or review for any of the APS journals, as well as anyone who would like to learn more about the authoring and refereeing processes. Topics for discussion will include advice on how to write good manuscripts, similarities and differences in writing referee reports for PRL and PR, and other ways in which authors, referees, and editors can work together productively. Following a short presentation from the editors, there will be a moderated discussion.

## Wednesday, March 16, 2016 8:00AM - 11:00AM –

Session K55 DBIO GSOF: Physics of Cancer Metastasis Hilton Baltimore Holiday Ballroom 6 - Michael Espey, National Institute of Health

8:00AM K55.00001 Why do tumor cells spread? , KENNETH PIENTA, Johns Hopkins Univ — No abstract available.

### 8:36AM K55.00002 Mechanical induction of transitions into mesenchymal and amoeboid states

, JAN LIPHARDT, Stanford University — One of the fundamental mysteries of biology lies in the ability of cells to convert from one phenotype to another in response to external control inputs. We have been studying the Epithelial-to-Mesenchymal Transition (EMT), which allows organized assemblies of epithelial cells to scatter into lone mesenchymal cells. EMT is critical for normal development and wound healing, and may be important for cancer metastasis. I'll present recent data on disorganizing mammary epithelial structures. We have used CRISPR to insert fluorescent tags directly into eight EMT-related genes (such as E-cadherin and Vimentin), which allows us to monitor the dynamics of the transition in real time, subject only to delays imposed by fluorophore folding/maturation times. With this information, we can begin to order events in time (temporal resolution ~30 minutes), starting with external signal inputs and proceeding through a secession of intracellular changes of gene expression on the path to the mesenchymal state.

### 9:12AM K55.00003 The Genetics and Biophysics of the Epithelial-Mesenchymal Transition (EMT): Can Theoretical Physics Help Cancer Biology

, HERBERT LEVINE, Rice University — In order to spread from the primary tumor to distant sites, cancer cells must undergo a coordinated change in their phenotypic properties referred to as the "epithelial-to-mesenchymal" transition. We have studied the nonlinear genetic circuits that are responsible for this cellular decision-making process and propose that the transition actually goes through a series of intermediate states. At the same time, we have formulated motility models which allow for the correlation of the state of this network and the cell's biophysical capabilities. Hopefully, these thereby efforts will help us better understand the transition to metastatic disease and possible treatments thereof.

### 9:48AM K55.00004 Critical high-dimensional state transitions in cell populations or why cancers follow the principle "What does not kill me makes me stronger"<sup>1</sup>

, SUI HUANG, Institute for Systems Biology — Transitions between high-dimensional attractor states in the quasi-potential landscape of the gene regulatory network, induced by environmental perturbations and/or facilitated by mutational rewiring of the network, underlie cell phenotype switching in development as well as in cancer progression, including acquisition of drug-resistant phenotypes. Considering heterogeneous cell populations as statistical ensembles of cells, and single-cell resolution gene expression profiling of cell populations undergoing a cell phenotype shift allow us now to map the topography of the landscape and its distortion. From snapshots of single-cell expression patterns of a cell population measured during major transitions we compute a quantity that identifies symmetry-breaking destabilization of attractors (bifurcation) and concomitant dimension-reduction of the state space manifold (landscape distortion) which precede critical transitions to new attractor states. The model predicts, and we show experimentally, the almost inevitable generation of aberrant cells associated with such critical transitions in multi-attractor landscapes: therapeutic perturbations which seek to push cancer cells to the apoptotic state, almost always produce "rebellious" cells which move in the "opposite direction": instead of dying they become more stem-cell-like and malignant. We show experimentally that the inadvertent generation of more malignant cancer cells by therapy indeed results from transition of surviving (but stressed) cells into unforeseen attractor states and not simply from selection of inherently more resistant cells. Thus, cancer cells follow not so much Darwin, as generally thought (survival of the fittest), but rather Nietzsche (What does not kill me makes me stronger).

<sup>1</sup>Supported by NIH (NCI, NIGMS), Alberta Innovates

### 10:24AM K55.00005 Cell-ECM Interactions During Cancer Invasion<sup>1</sup>

, YI JIANG, Georgia State University — The extracellular matrix (ECM), a fibrous material that forms a network in a tissue, significantly affects many aspects of cellular behavior, including cell movement and proliferation. Transgenic mouse tumor studies indicate that excess collagen, a major component of ECM, enhances tumor formation and invasiveness. Clinically, tumor associated collagen signatures are strong markers for breast cancer survival. However, the underlying mechanisms are unclear since the properties of ECM are complex, with diverse structural and mechanical properties depending on various biophysical parameters. We have developed a three-dimensional elastic fiber network model, and parameterized it with in vitro collagen mechanics. Using this model, we study ECM remodeling as a result of local deformation and cell migration through the ECM as a network percolation problem. We have also developed a three-dimensional, multiscale model of cell migration and interaction with ECM. Our model reproduces quantitative single cell migration experiments. This model is a first step toward a fully biomechanical cell-matrix interaction model and may shed light on tumor associated collagen signatures in breast cancer.

<sup>1</sup>This work was partially supported by NIH-U01CA143069.

## Wednesday, March 16, 2016 11:15AM - 2:15PM –

Session L1 DCMP: Design and Control of the Superconducting Order Parameter in Low Dimensions Ballroom I - Trivedi Nandini, Ohio State University

**11:15AM L1.00001 Gate tunability and collapse of superconductivity in hybrid tin-graphene Josephson junction arrays**, VINCENT BOUCHIAT, NEEL Institute, CNRS-Grenoble — The accessible and surface-exposed 2D electron gas offered by graphene provides indeed an ideal platform on which to tune, via application of an electrostatic gate, the coupling between adsorbates deposited on its surface. We have experimentally studied the case of graphene transistors which channel is decorated with an array of superconducting tin nanoparticles. They induce via percolation of proximity effect a global 2D superconducting state which critical temperature  $T_c$  can be tuned by gate voltage. When the Graphene show strong disorder, it is possible to tune via the applied gate voltage the system towards an insulating state, demonstrating the possibility to trigger a superconducting to insulator transition [1], which features resembles those found in granular superconductors. In this work, graphene monolayers are surface-conjugated to regular arrays of superconducting disk-shaped metal islands, whose inter-island distances were patterned to be in the quasi-ballistic limit of the underlying 2D electron gas. Arrays can be made on a large range of geometry and density, up to the highly diluted limit with less than 5% surface coverage and few micrometers in between islands. In the lower temperature limit ( $<100$  mK), despite of the long distance (2 microns) in between islands, a supercurrent was observed among the whole graphene sheet. Interestingly, the superconducting state vanishes exponentially in gate voltage and rests in a metallic state [2], caused by quantum fluctuations of phase is found for diluted and regular arrays. This peculiar behaviour provides evidence for recently developed theory, and may provide a hint to the understanding of long-standing issue of "zero-temperature" bosonic metallic state. [1] A. Allain, et al. Nat. Mat., **11**, 590, (2012). [2] Z. Han et al., Nat. Phys. **10**, 380 (2014).

**11:51AM L1.00002 The Emergence of Superconductivity in Inhomogeneous, Mesoscopic Systems<sup>1</sup>**, NADYA MASON, Univ of Illinois - Urbana — Although low-dimensional, inhomogeneous superconductors have been intensely studied, the nature of the onset of superconductivity in these systems is still largely unknown. In this talk we present transport measurements on mesoscopic disks of granular, inhomogeneous Nb, where we determine the superconducting transition temperature as a function of disk diameter. We observe an unexpected suppression of superconductivity at micron diameters, length scales that are considerably longer than the coherence length of Nb. This suppression does not appear in large-scale films, and cannot be explained by single-grain small-size effects. By considering the diameter-dependence of the transition, as well as observations of strong fluctuations in the transition temperature as disk diameters decrease, we are able to explain this long length scale dependence by an extremal-grain model, where superconducting order first appears in unusually large grains and, due to proximity coupling, spreads to other grains. The extremal-grain onset of superconductivity has not previously been observed experimentally, and explains how superconductivity can emerge in granular or inhomogeneous superconductors.

<sup>1</sup>This work is funded by DOE-BES under Award DE-SC0012649

**12:27PM L1.00003 Cooper Pair Insulators<sup>1</sup>**, JAMES VALLES, Brown University — One of the recent advances in the field of the Superconductor to Insulator Transition (SIT) has been the discovery and characterization of the Cooper Pair Insulator phase. This bosonic insulator, which consists of localized Cooper pairs, exhibits activated transport and a giant magneto-resistance peak. These features differ markedly from the weakly localized transport that emerges as pairs break at a "fermionic" SIT. I will describe how our experiments on films nano-patterned with a nearly triangular array of holes have enabled us to 1) distinguish bosonic insulators from fermionic insulators, 2) show that Cooper pairs, rather than quasi-particles dominate the transport in the Cooper Pair insulator phase, 3) demonstrate that very weak, sub nano-meter thickness inhomogeneities control whether a bosonic or fermionic insulator forms at an SIT and 4) reveal that Cooper pairs disintegrate rather than becoming more tightly bound deep in the localized phase. We have also developed a method, using a magnetic field, to tune flux disorder reversibly in these films. I will present our latest results on the influence of magnetic flux disorder and random gauge fields on phenomena near bosonic SITs.

<sup>1</sup>This work was performed in collaboration with M. D. Stewart, Jr., Hung Q. Nguyen, Shawna M. Hollen, Jimmy Joy, Xue Zhang, Gustavo Fernandez, Jeffrey Shainline and Jimmy Xu. It was supported by NSF Grants DMR 1307290 and DMR-0907357.

**1:03PM L1.00004 Designing Quantum Matter with Superconducting Nanowires<sup>1</sup>**, NINA MARKOVIC, Goucher College — Superconducting nanowires are an experimental realization of a model quantum system that features collective degrees of freedom and exhibits a host of non-equilibrium and non-local phenomena. The nature of the quantum states in nanowires is particularly sensitive to size and shape quantization, coupling with the environment and proximity effects. I will demonstrate how we can utilize these features to tailor the quantum states in nanowires in desirable ways. Specifically for this purpose, we have developed a unique nanoprinting method for fabrication of ultranarrow nanowires with unprecedented control over their physical texture and their transport properties. I will show how short nanowires exhibit a tunable vortex-in-a-box blockade phenomenon, and how tunable interfaces with graphene and topological insulators lead to unusual properties. Finally, I will discuss the bigger picture for how the texture of the superconducting wavefunction can be precisely controlled by the size, shape, magnetic field and tunable interfaces with materials that exhibit unconventional order, spin texture or topological properties.

<sup>1</sup>This work is supported by NSF DMR-1507782.

**1:39PM L1.00005 Proximity and Anti-proximity effects in nanowires<sup>1</sup>**, MOSES CHAN, Penn State University — Near a superconductor/normal-metal interface, the leakage of Cooper pairs extends superconducting behavior into the metal. The spatial range of this proximity effect in a normal metal can be as long as 1  $\mu$ m. However, when a ferromagnet is placed in contact with a superconductor, the Cooper pairs from the superconductor are not expected to survive beyond at most a few nanometers into the ferromagnet. Surprisingly we find when a cobalt nanowire as long as 600 nm is sandwiched between superconducting electrodes, it attains zero resistance at low temperature. For even longer wires, the transition to incomplete superconductivity via this (long range) proximity effect is foreshadowed by a large resistance peak (1). On the other hand when Zn nanowires of 40 nm diameter are contacted by superconducting electrodes, their superconductivity is unexpectedly suppressed (2). 1. Wang et al., PRL **102**, 247003(2009); Nature Phys. **6**, 389 (2010) 2. Tian et al., PRL **95**, 076802 (2005); PRB **88**, 064511 (2013)

<sup>1</sup>worked supported by Penn State MRSEC.

**Wednesday, March 16, 2016 11:15AM - 2:15PM —**  
**Session L2 DCMP: Physics of Interacting Particles in Two Dimensional Electron Systems at Half-Filling** Ballroom II - Mansour Shayegan, Princeton University

**11:15AM L2.00001 Do composite fermions satisfy Luttinger's area rule?**<sup>1</sup>, JAINENDRA JAIN, Pennsylvania State Univ — While an ordinary Fermi sea is perturbatively robust to interactions, the paradigmatic composite-fermion Fermi sea [1] arises as a non-perturbative consequence of emergent gauge fields in a system where there was no Fermi sea to begin with. A mean-field picture suggests two Fermi seas, of composite fermions made from electrons or holes in the lowest Landau level, which occupy different areas away from half filling and thus appear to represent distinct states. We show [2] that in the microscopic theory of composite fermions, which satisfies particle-hole symmetry in the lowest Landau level to an excellent degree, the Fermi wave vectors at filling factors  $\nu$  and  $1 - \nu$  are the same, and are generally consistent with the experimental findings of Kamburov *et al.* [3]. Our calculations [2] suggest that the area of the CF Fermi sea may slightly violate the Luttinger area rule. We further determine the area of the spin unpolarized composite-fermion Fermi sea, for which the Fermi seas at  $\nu$  and  $1 - \nu$  are not related by particle hole symmetry. [1] B.I. Halperin, P.A. Lee, N. Read, PRB 47, 7312 (1993). [2] A. C. Balram, C. Töke, J. K. Jain, Phys. Rev. Lett. 115, 186805 (2015). [3] D. Kamburov *et al.* Phys. Rev. Lett. 113, 196801 (2014).

<sup>1</sup>Supported by the DOE.

**11:51AM L2.00002 Spontaneous time reversal symmetry breaking in atomically confined two-dimensional impurity bands in silicon and germanium**<sup>1</sup>, ARINDAM GHOSH, Indian Inst of Science — Three-dimensional bulk-doped semiconductors, in particular phosphorus (P)-doped silicon (Si) and germanium (Ge), are among the best studied systems for many fundamental concepts in solid state physics, ranging from the Anderson metal-insulator transition to the many-body Coulomb interaction effects on quantum transport. Recent advances in material engineering have led to vertically confined doping of phosphorus (P) atoms inside bulk crystalline silicon and germanium, where the electron transport occurs through one or very few atomic layers, constituting a new and unique platform to investigate many of these phenomena at reduced dimensions. In this talk I shall present results of extensive quantum transport experiments in delta-doped silicon and germanium epilayers, over a wide range of doping density that allow independent tuning of the on-site Coulomb interaction and hopping energy scales. We find that low-frequency flicker noise, or the  $1/f$  noise, in the electrical conductance of these systems is exceptionally low, and in fact among the lowest when compared with other low-dimensional materials. This is attributed to the physical separation of the conduction electrons, embedded inside the crystalline semiconductor matrix, from the charged fluctuators at the surface. Most importantly, we find a remarkable suppression of weak localization effects, including the quantum correction to conductivity and universal conductance fluctuations, with decreasing doping density or, equivalently, increasing effective on-site Coulomb interaction. In-plane magneto-transport measurements indicate the presence of intrinsic local spin fluctuations at low doping although no signatures of long range magnetic order could be identified. We argue that these results indicate a spontaneous breakdown of time reversal symmetry, which is one of the most fundamental and robust symmetries of nonmagnetic quantum systems. While the microscopic origin of this spontaneous time reversal symmetry breaking remains unknown, we believe this indicates a new many-body electronic phase in two-dimensionally doped silicon and germanium with a half-filled impurity band.

<sup>1</sup>We acknowledge financial support from Department of Science and Technology, Government of India, and Australia-India Strategic Research Fund (AISRF)

**12:27PM L2.00003 The half-filled Landau level and topological insulator surfaces**, T SENTHIL, Massachusetts Institute of Technology — The metallic state of the half-filled Landau level - described originally in pioneering work by Halperin, Lee, and Read as a liquid of composite fermions - was proposed recently by Son to be described by a particle-hole symmetric effective field theory distinct from that in the prior literature. This talk will develop a simple picture of the particle-hole symmetric composite fermion through a modification of older pictures as electrically neutral "dipolar" particles. This picture, and the proposed particle-hole symmetric theory, will be further substantiated through a recently developed deep connection between the half-filled Landau level and correlated surface states of certain three dimensional topological insulators. The phenomenology of composite fermi liquids (with or without particle-hole symmetry) will be revisited. It will be shown that their heat/electrical transport dramatically violates the conventional Wiedemann-Franz law but satisfies a modified one. References: 1. Chong Wang and T. Senthil, Half-filled Landau Level, Topological Insulator Surfaces, and Three Dimensional Quantum Spin Liquids, cond-mat arXiv:1507.08290 (2015).

**1:03PM L2.00004 Experimental Observations of Particle-hole Asymmetry for Composite Fermions**<sup>1</sup>, YANG LIU, Electrical engineering, Princeton University — In this talk, I will present our experimental study of the breaking of particle-hole symmetry for composite fermions (CFs), quasi-particles formed by attaching two flux quanta to each electron at large perpendicular magnetic fields. We measure the Fermi contour of the spin-polarized CFs near  $\nu = 1/2$  via commensurability oscillations, and find an asymmetry of the Fermi wave vector for  $\nu < 1/2$  and  $> 1/2$ . In particular, we find that the deduced wave vector is smaller for  $\nu > 1/2$  compared to  $\nu < 1/2$ , and on both sides consistent with the density of minority carriers in the lowest Landau level. We also study the spin-polarization transitions of fractional quantum Hall states near  $\nu = 3/2$  and  $1/2$ ; these states are particle-hole conjugates of each other and are expected to have the same polarization energies. Our systematic results clearly show the transition energies are about three times larger for states near  $\nu = 3/2$  compared to those near  $\nu = 1/2$ . Work done in collaboration with D. Kamburov, M. A. Mueed, S. Hasdemir, A. Wojs, J.K. Jain, L.N. Pfeiffer, K.W. West, K.W. Baldwin, and M. Shayegan.

<sup>1</sup>We acknowledge support from the DOE, NSF, the Gordon and Betty Moore Foundation and the Keck Foundation. The experiments were partly performed at the National High Magnetic Field Laboratory.

**1:39PM L2.00005 A model wavefunction for the composite Fermi liquid: its geometry and entanglement.**<sup>1</sup>, F. D. M. HALDANE, Princeton University — I will describe a model wavefunction for the composite Fermi liquid in a partially-filled Landau level, recently formulated in a torus geometry (Shao *et al.*, Phys. Rev. Lett. 114, 206402 (2015)), that allows a manifold of gapless composite Fermi-liquid states to be characterized, parametrized by an analog of the "occupation number" that defines the Fermi surface in a free-electron gas. Unlike incompressible FQHE states, which only occur in an inversion-symmetric momentum sector, these CFL states occur in each distinct momentum sector allowed by the periodic boundary condition. The fundamental wavefunction of this type describes a system with  $\nu = 1/2$ , but multiplication by (or division by) a Vandermonde factor describes states at  $\nu = 1/m$ . The CFL states are characterized by an "intrinsic metric" which determines the shape of the Fermi surface, and corresponds to the shape of the "flux-attachment" that forms the composite fermion. The wavefunction is well-suited for Monte-Carlo calculations, as it is analogous to a determinant form used by Jain in spherical geometry. The violation of "area-law" (perimeter-law) entanglement found in Monte-Carlo calculations will be described.

<sup>1</sup>supported in part by DOE DE-SC0002140 and W. M. Keck Foundation

**Wednesday, March 16, 2016 11:15AM - 2:15PM –**  
**Session L3 DCMP GSNP GSOF: Buckley, Lilienfeld and Onsager Prize Session** Ballroom III - Sharon Glotzer, University of Michigan

**11:15AM L3.00001 Photonic Crystals-Inhibited Spontaneous Emission: Optical Antennas-Enhanced Spontaneous Emission** , ELI YABLONOVITCH, UC Berkeley Electrical Engineering and Computer Sciences Dept. — Photonic crystals are also part of everyday technological life in opto-electronic telecommunication devices that provide us with internet, cloud storage, and email. But photonic crystals have also been identified in nature, in the coloration of peacocks, parrots, chameleons, butterflies and many other species.

In spite of its broad applicability, the original motivation of photonic crystals was to create a “bandgap” in which the spontaneous emission of light would be inhibited. Conversely, the opposite is now possible. The “optical antenna” can accelerate spontaneous emission. Over 100 years after the radio antenna, we finally have tiny “optical antennas” which can act on molecules and quantum dots. Employing optical antennas, spontaneous light emission can become faster than stimulated emission.

**11:51AM L3.00002 Julius Edgar Lilienfeld Prize: Lilienfeld Prize Lecture: Emergent Behavior in Quantum Matter** , DAVID PINES, Physics Dept., U C Davis and UIUC, Santa Fe Institute — We live in an **emergent universe** in which interactions between the basic building blocks of matter and their environment give rise to unpredicted and unexpected **emergent** behavior at every scale. As physicists we seek to identify the organizing principles responsible for that behavior, construct soluble models that incorporate these, and explain experiment. In this lecture, I illustrate this approach to understanding emergent behavior in quantum matter through three examples: collective modes in electron, helium, and nuclear liquids; the emergence of superconductivity in conventional and unconventional superconductors, nuclei, and neutron stars; and the emergence of heavy electrons in Kondo lattice materials.

**12:27PM L3.00003 Lars Onsager Prize: Phase transitions in massive data acquisition** , MARC MEZARD, Ecole normale supérieure - PSL Research University — The rapid increase in the amount of data that is presently being generated, acquired and processed opens new perspectives in many branches of science. In order to take full advantage of this data revolution, and to turn it into a major tool for scientific discoveries, new concepts and methods need to be developed, thus allowing us to focus on the extraction of significant information. Referring to the case of compressed sensing, the talk will show how ideas and methods in statistical physics -from spin glass theory to crystal nucleation - can help design faster, less destructive, and more efficient signal acquisition protocols, with possible applications in numerous fields -from magnetic resonance imaging to astronomy, tomography, or gene interaction network reconstruction.

**1:03PM L3.00004 Lars Onsager Prize: The mean field solution for Hard Sphere Jamming and a new scenario for the low temperature landscape of glasses.** , GIORGIO PARISI, University of Rome, “La Sapienza”, Italy — In a hard spheres system particles cannot overlap. Increasing the density we reach a point where most of the particles are blocked and the density cannot be increased any more: this is the jamming point. The jamming point separates the phase, where all the constraints can be satisfied, from an unsatisfiable phase, where spheres do have to overlap. A scaling theory of the behavior around the jamming critical point has been formulated and a few critical exponents have been introduced. The exponents are apparently super-universal, as far as they do seem to be independent from the space dimensions. The mean field version of the model (i.e. the infinite dimensions limit) has been solved analytically using broken replica symmetry techniques and the computed critical exponents have been found in a remarkable agreement with three-dimensional and two-dimensional numerical results and experiments. The theory predicts in hard spheres (in glasses) a new transition (the Gardner transition) from the replica symmetric phase to the replica broken phase at high density (at low temperature), in agreement with simulations on hard sphere systems. I will briefly discuss the possible consequences of this new picture on the very low temperature behavior of glasses in the quantum regime.

**1:39PM L3.00005 Lars Onsager Prize: Optimization and learning algorithms from the theory of disordered systems** , RICCARDO ZECCHINA, Politecnico di Torino — The extraction of information from large amounts of data is one of the prominent cross disciplinary challenges in contemporary science. Solving inverse and learning problems over large scale data sets requires the design of efficient optimization algorithms over very large scale networks of constraints. In such a setting, critical phenomena of the type studied in statistical physics of disordered systems often play a crucial role. This observation has led in the last decade to a cross fertilization between statistical physics, information theory and computer science, with applications in a variety of fields. In particular a deeper geometrical understanding of the ground state structure of random computational problems and novel classes of probabilistic algorithms have emerged. In this talk I will give a brief overview of these conceptual advances and I will discuss the role that subdominant states play in the design of algorithms for large scale optimization problems. I will conclude by showing how these ideas can lead to novel applications in computational neuroscience.

**Wednesday, March 16, 2016 11:15AM - 2:15PM –**

**Session L4 DMP: Physics for Everyone** Ballroom IV - Daniel Dessau, University of Colorado, Boulder

**11:15AM L4.00001 Nanoscience and Reminiscences of a Woman in Physics** , MILDRED DRESSELHAUS, Massachusetts Inst of Tech-MIT — My entry into carbon science and nanoscience at an early stage in my career occurred in part because I was a woman in physics. In these reminiscences I will relate why working on carbon science started because I was a woman interested in working on a topic that interested me greatly, but was unpopular at the time; carbon science and thermoelectricity are two examples. I will elaborate on how our research system allows safe study of unpopular topics so that both the researcher and research sponsor are satisfied with outcomes. I also learned a lot from my family and acknowledge their contributions as well as those of sponsors who supported high-risk projects.

**11:51AM L4.00002 Physics Behind Optical Fiber Communications: Technologies that Drive the Internet Capacity Growth** , ALAN WILLNER, Univ. of Southern California — Optical fiber communications forms the backbone for global communications, especially as it relates to the Internet. Indeed, the Internet as we know it today would not exist without optical communications. The data transmission capacity through an optical fiber has undergone an exponential growth increase for decades, progressing from Megabits/sec to now Petabits/sec in just the past 40 years. This growth came about due to many physics advances in the field of optical fiber communications, dating back to 1966 when Sir Charles Kao proposed the idea of a communication system based on low-loss optical glass fiber. This presentation will explore the past and present physics-based crucial innovations needed for this continuing story. Specific topics to be highlighted include: (a) ultra-pure fiber that decreased the attenuation losses through glass by many orders of magnitude, (b) single-frequency lasers that defined a specific data channel that could propagate with low signal distortion, (c) Erbium-doped fiber amplifiers that had high gain and low additive noise allowing for amplifier cascades and conquering enormous distances, (d) the simultaneous transmission of multiple wavelength-division-multiplexing data channels down the optical fiber, and (e) the tackling of various dispersive and nonlinear effects that are introduced by the optical fiber itself, cause the data to degrade, and necessitate some form of compensation or management.

**12:27PM L4.00003 Computational Social Science: Exciting Progress and Future Challenges**, DUNCAN WATTS, Microsoft Research, NYC — The past 15 years have witnessed a remarkable increase in both the scale and scope of social and behavioral data available to researchers, leading some to herald the emergence of a new field: computational social science. Against these exciting developments stands a stubborn fact: that in spite of many thousands of published papers, there has been surprisingly little progress on the big questions that motivated the field in the first place: questions concerning systemic risk in financial systems, problem solving in complex organizations, and the dynamics of epidemics or social movements, among others. In this talk I highlight some examples of research that would not have been possible just a handful of years ago and that illustrate the promise of CSS. At the same time, they illustrate its limitations. I then conclude with some thoughts on how CSS can bridge the gap between its current state and its potential.

**1:03PM L4.00004 Are There Two Forms of Liquid Water?**, H. E. STANLEY, Departments of Physics, Chemistry, Physiology, & Biomedical Engineering: Boston University — We will introduce some of the 73 documented anomalies of the most complex of liquids, water, focusing on recent progress in understanding these anomalies by combining information provided by recent experiments and simulations on water in bulk, nanoconfined and biological environments designed to test the hypothesis that liquid water has behavior consistent with the novel phenomenon of liquid polymorphism in that water can exist in two distinct phases [1]. We will also discuss very recent work on nanoconfined water anomalies as well as the apparently related, and highly unusual, behavior of water in biological environments. Finally, we will discuss how the general concept of liquid polymorphism is proving useful in understanding anomalies in other liquids, such as silicon, silica, and carbon, as well as metallic glasses, which have in common that they are characterized by two characteristic length scales in their interactions.

This work has been supported by the NSF Chemistry Division grant CHE-1213217 and was performed in collaboration with, among others, C. A. Angell, S. V. Buldyrev, S.-H. Chen, D. Corradini, P. G. Debenedetti, G. Franzese, P. Kumar, E. Lascaris, F. Mallamace, O. Mishima, P. H. Poole, S. Sastry, F. Sciortino, and L. Xu.

[1] H. E. Stanley, Editor, Liquid Polymorphism, Vol. 152 in Advances in Chemical Physics, S. A. Rice, Series Editor (Wiley, New York, 2013).

**1:39PM L4.00005 Is the Choice Bad Science or No Science?**, RUSH HOLT, American Association for the Advancement of Science — In our efforts to teach good scientists we leave everyone else with the impression that they cannot do science or appreciate it and should not even try. Should we be surprised when many in the public adopt unscientific beliefs?

## Wednesday, March 16, 2016 11:15AM - 2:15PM —

**Session L5 GMAG DMP: Frustrated Magnetism: Artificial Spin Ice** 301 - Jayasimha Atulasimha, Virginia Commonwealth University

**11:15AM L5.00001 Nearest neighbor correlations in perpendicular artificial spin ice arrays in the presence of an applied field**, SUSAN KEMPINGER, ROBERT FRALEIGH, PAUL LAMMERT, VINCENT CRESPI, NITIN SAMARTH, Pennsylvania State University, PETER SCHIFFER, University of Illinois — By studying the field dependent magnetization switching process in perpendicular artificial spin ice arrays, we hope to gain insight into the dynamical properties of interacting spin systems. To this end, we have used diffraction-limited Kerr imaging to study lithographically patterned arrays of single domain, nanoscale islands of Co/Pt multilayers. We can tune the interaction strength and introduce geometric frustration in to the patterned systems by changing the lattice spacing and geometry of the arrays. Using MOKE microscopy we are able to optically resolve, spatially isolate, and extract the switching field of each island in an array in the presence of an external field. These switching fields allow us to calculate the magnetization and nearest neighbor spin-spin correlation throughout a hysteresis loop. These quantities help us determine the effect of increased interactions and geometric frustration on the switching process of dipole coupled arrays. Funded by DOE.

**11:27AM L5.00002 Dimensionality Reduction in Artificial Spin Ice<sup>1</sup>**, IAN GILBERT<sup>2</sup>, YUYANG LAO, ISAAC CARRASQUILLO, University of Illinois at Urbana-Champaign, LIAM O'BRIEN<sup>3</sup>, JUSTIN WATTS, MICHAEL MANNO, CHRIS LEIGHTON, University of Minnesota, ANDREAS SCHOLL, Lawrence Berkeley National Laboratory, CRISTIANO NISOLI, Los Alamos National Laboratory, PETER SCHIFFER, University of Illinois at Urbana-Champaign — Over the past ten years, square and hexagonal arrays of single-domain nanomagnets, known as artificial spin ice, have been used to study the microscopic properties of geometrical frustration. Here we describe the fabrication of a new type of artificial spin ice, the tetris lattice. The ground state configuration of the nanomagnets' moments was determined with photoemission electron microscopy. This lattice is designed such that its vertices (small clusters of nanomagnets) cannot all simultaneously achieve their ground state. As a consequence, the lattice decomposes into alternating ordered and disordered one-dimensional bands of moments. The disordered bands can be described by a thermal one-dimensional Ising model, underscoring the emergent dimensionality reduction found in this lattice.

<sup>1</sup>This work was primarily supported by the US DOE. Work at UMN was supported by NSF MRSEC.

<sup>2</sup>Present affiliation: National Institute of Standards and Technology

<sup>3</sup>Also University of Cambridge

**11:39AM L5.00003 DC Magnetization and FMR results of Fibonacci Distortions on the Honeycomb Artificial Spin Ice**, JUSTIN WOODS, BARRY FARMER, TODD HASTINGS, JUSTIN VISAK, LANCE DE LONG, Univ of Kentucky — Nanofabrication techniques allow magnetic thin films to be lithographically-patterned into arrays of interacting macro-spins that can be designed to study emergent physical properties. Here we discuss the effects of continuous symmetry breaking on the equilibrium and dynamic magnetic properties of frustrated magnetic metamaterials. We have patterned five Permalloy ( $\text{Ni}_{0.80}\text{Fe}_{0.20}$ ) samples of distorted Kagome ASI arrays that are generated by repeated application of a substitution algorithm. This algorithm employs an aperiodic Fibonacci sequence of binary digits that can be mapped into short ( $d_1$ ) and long ( $d_2$ ) distances. This distorts film segment lengths while the width (nominally 70 nm) and thickness (25 nm) remain constant. Additionally, the coordination of each three-fold Kagome vertex is continuously modified via these distortions. Micromagnetic simulations predict the Fibonacci distortions causes jamming of Dirac String propagation. We report DC magnetization and FMR dispersion for different magnitudes of distortion, and compare these results to simulation. Research at University of Kentucky supported by U.S. National Science Foundation grant no. DMR-1506979.

**11:51AM L5.00004 Beller Lecture: Artificial Ferroic Systems**, LAURA HEYDERMAN, ETH Zurich - Paul Scherrer Institute — In artificial ferroic systems [1], novel functionality is engineered through the combination of structured ferroic materials and the control of the interactions between the different components. I will present two classes of these systems, beginning with hybrid mesoscopic structures incorporating two different ferromagnetic layers whose static and dynamic behaviour result from the mutual imprint of the magnetic domain configurations [2]. Here we have demonstrated a new vortex core reversal mechanism [3], which occurs when it is displaced across domain boundaries with a magnetic field. I will then describe our progress on artificial spin ice, consisting of arrays of dipolar-coupled nanomagnets arranged in frustrated geometries. We have employed photoemission electron microscopy to observe the behaviour of emergent magnetic monopoles in an array of nanomagnets placed on the kagome lattice [4]. We have also created artificial spin ice with fluctuating magnetic moments and observed the evolution of magnetic configurations with time. This has provided a means to study relaxation processes with a controlled route to the lowest-energy state [5]. Recently, we have demonstrated with muon spin relaxation that these magnetic metamaterials can support thermodynamic phase transitions [6], and future directions include the incorporation of novel magnetic materials such as ultrathin magnetic films [7], the investigation of 3D structures [8], as well as the implementation of x-ray resonant magnetic scattering to study magnetic correlations in smaller nanomagnets and at faster timescales [9]. [1] L.J. Heyderman and R.L. Stamps, JPCM (2013); [2] G. Heldt et al., APL (2014); [3] P. Wohlhuter et al., Nature Comms (2015); [4] E. Mengotti et al., Nature Phys. (2011); [5] A. Farhan et al., Nature Phys. and PRL (2013); [6] L. Anghinolfi et al., Nature Comms (2015); [7] V. Kapaklis et al., Nature Nanotech. (2014); [8] C. Donnelly et al., PRL (2015); [9] J. Perron et al., PRB (2013)

**12:27PM L5.00005 Doped Artificial Spin Ice**, CYNTHIA OLSON REICHHARDT, Theoretical Division, Los Alamos National Laboratory, ANDRAS LIBAL, Faculty of Mathematics and Computer Science, Babes-Bolyai University, CHARLES REICHHARDT, Theoretical Division, Los Alamos National Laboratory — We examine square and kagome artificial spin ice for colloids confined in arrays of double-well traps. Unlike magnetic artificial spin ices, colloidal and vortex artificial spin ice realizations allow creation of doping sites through double occupation of individual traps. We find that doping square and kagome ice geometries produces opposite effects. For square ice, doping creates local excitations in the ground state configuration that produce a local melting effect as the temperature is raised. In contrast, the kagome ice ground state can absorb the doping charge without generating non-ground-state excitations, while at elevated temperatures the hopping of individual colloids is suppressed near the doping sites. These results indicate that in the square ice, doping adds degeneracy to the ordered ground state and creates local weak spots, while in the kagome ice, which has a highly degenerate ground state, doping locally decreases the degeneracy and creates local hard regions.

**12:39PM L5.00006 Systematic Angular Study of Magnetoresistance in Permalloy Connected Kagome Artificial Spin Ice**, JUNGSIK PARK, BRIAN LE, Univ of Illinois - Urbana, JUSTIN WATTS, CHRIS LEIGHTON, University of Minnesota, NITIN SAMARTH, Pennsylvania State University, PETER SCHIFFER, Univ of Illinois - Urbana — Artificial spin ices are nanostructured two-dimensional arrays of ferromagnetic elements, where frustrated interactions lead to unusual collective magnetic behavior. Here we report a room-temperature magnetoresistance study of connected permalloy ( $\text{Ni}_{81}\text{Fe}_{19}$ ) kagome artificial spin ice networks, wherein the direction of the applied in-plane magnetic field is systematically varied. We measure both the longitudinal and transverse magnetoresistance in these structures, and we find certain transport geometries of the network show strong angular sensitivity – even small variations in the applied field angle lead to dramatic changes of the magnetoresistance response. We also investigate the magnetization reversal of the networks using magnetic force microscopy (MFM), demonstrating avalanche behavior in the magnetization reversal. The magnetoresistance features are analyzed using an anisotropic magnetoresistance (AMR) model. Supported by the US Department of Energy. Work at the University of Minnesota was supported by Seagate Technology, NSF MRSEC, and a Marie Curie International Outgoing Fellowship within the 7th European Community Framework Programme.

**12:51PM L5.00007 Spin wave band structure of artificial square ices<sup>1</sup>**, EZIO IACocca, University of Colorado - Boulder, Co, USA; Chalmers University of Technology, Sweden, SEBASTIAN GLIGA, ETZ, Switzerland; PSI, Switzerland, ROBERT STAMPS, University of Glasgow, UK, OLLE HEINONEN, Argonne National Laboratory, IL, USA — Artificial square spin ices are structures composed of magnetic elements located on the sites of a geometrically frustrated, two-dimensional square lattice. Using a semi-analytical approach, we show that square spin ices exhibit a rich spin wave band structure that is tunable both by external magnetic fields and the magnetic state of individual elements. Internal degrees of freedom can give rise to equilibrium states with bent magnetization at the edges of each element, leading to characteristic excitations; in the presence of magnetostatic interactions these form separate bands analogous to impurity bands in semiconductors. Full-scale micromagnetic simulations corroborate our semi-analytical approach. This study shows that the magnon spectra, and therefore group and phase velocities and band gap, can be manipulated by external fields, temperature, or more sophisticated techniques such as using spin torque on individual elements, and suggesting that artificial square spin ices can be used as metamaterials for spin waves. Our results close the gap between the research fields of artificial spin ices and magnonics.

<sup>1</sup>E.I. acknowledges the Swedish Research Council, Reg.No. 637-2014-6863. The work by O.H. was funded by the Department of Energy Office of Science, Materials Sciences and Engineering Division. The work by R.L.S. was funded by EPSRC EP/L002922/1.

**1:03PM L5.00008 Lithography patterns and data analysis for topologically frustrated artificial spin ice**, THOMAS MARSH, JASPER DRISKO, JOHN CUMINGS, University of Maryland, College Park — Artificial spin ices (ASIs), lattices composed of nanoscale single-domain magnetic islands, have been studied extensively for their insights on frustrated systems. Recently, the square and kagome geometries have received the most attention. We study a variation of the square lattice, where we include one or more edge dislocations in an otherwise perfect arrangement, resulting in topological frustration of the system. We create lithography patterns using a MATLAB script that models the system as a lattice of connected nodes and starts by removing partial rows or columns of elements. We then allow the system to relax, reshaping these patterns with an algorithm that attempts to equalize the angles of the elements at each node and also maintain identical island lengths throughout the lattice. We then analyze experimental Lorentz Transmission Electron Microscopy (TEM) images of these lattices using another program, which manipulates the images in order to find and index all of the individual magnetic islands, and then uses the Lorentz contrast of the element to determine the direction of each island's magnetic moment. These moment directions are then combined to determine the type of each lattice vertex, using the traditional type I-IV notation for square lattices. The script then marks the TEM images to reflect the vertex classification, which allows us to clearly identify chains of type II & III vertices in the Lorentz images. The chains carry net magnetic moment, in a direction defined by the type II vertices, which may then reverse at the type III vertices.

**1:15PM L5.00009 Topological frustration of artificial spin ice**, JASPER DRISKO, THOMAS MARSH, JOHN CUMINGS, University of Maryland, College Park — Dislocations are topological defects ubiquitous in crystalline materials, although they are often neglected in experimental and theoretical studies due to their complexity. Artificial spin ices (ASIs), lithographically patterned arrays of ferromagnetic nanostructures, are highly tunable systems that allow for detailed investigations of frustration by providing exquisite control and insight at the single-spin level. Here, we introduce controlled topological defects into thermally active square ASI lattices and directly observe the resulting spin configurations upon annealing. Whereas a canonical square ASI lattice can support perfect ground state ordering, we find the presence of a dislocation results in extended frustration within the system. Locally, the magnets are unfrustrated, but frustration of the lattice persists due to its topology. A chain of higher energy vertices always originates from each dislocation point and either extends to an edge of our finite crystal, or rarely, to a second dislocation point if it is present in the same crystal. We also simulate our work using a kinetic Monte Carlo technique and find remarkably similar behavior between the simulations and our experiments, with the same types of domain walls and domain patterns as in our experimental samples. Our results indicate that topological defects have non-trivial consequences and should receive more attention in investigations of three dimensional crystals with  $\mathbf{q} \neq \mathbf{0}$  order parameters.

**1:27PM L5.00010 Nanomagnetic field-driven thermal mobility of emergent monopoles in artificial spin ice.** , SOPHIE MORLEY, MARK C. ROSAMOND, University of Leeds, DIEGO ALBA VENERO, ISIS, ALES HRABEC, Université Paris Sud, JOSE MARIA PORRO, ISIS, MI-YOUNG IM, CXRO, LBNL and DGIST, PETER FISCHER, UC Santa Cruz, SEAN LANGRIDGE, ISIS, CHRISTOPHER H. MARROWS, University of Leeds — Artificial spin ices are nanomagnetic islands confined in 2D and their size means they can be considered as single domain and Ising-like. In the square geometry, each vertex has four nanomagnets which can point either in or out. The lowest energy arrangement consists of two-in and two-out and obeys the so-called 'ice-rule'. It is possible to construct an ordered state by tiling such vertices, above which it is possible to have ice-rule-violating excitations known as emergent magnetic monopoles. It is their propagation which has been imaged with a transmission X-ray microscope and, due to a novel on-membrane heater, elevated temperatures applied up to 700 K. Square ice arrays were fabricated on a SiN membrane, the CoFeB islands were 80x250 nm, 10nm thick and had lattice spacings in the 350-500nm. Increased avalanche length and faster string velocities were observed for both stronger interaction and increased temperature. We have also been able to define a magnetic mobility in our systems and observed increased mobility in more interacting systems or elevated temperature. The largest change in the magnetic mobility was found for the most strongly interacting array, increasing by  $1.7 \pm 0.7 \text{ mm}^2 \text{ A}^{-1} \text{ s}^{-1}$  for  $\Delta T \approx 30 \text{ K}$ .

**1:39PM L5.00011 Macroscopic Artificial Magnetic Honeycomb Lattice of Thermally Controlled Ultra-Small Bonds** , BROCK SUMMERS, ASHUTOSH DAHAL, Univ of Missouri - Columbia, LISA DEBEER-SCHITT, Oak Ridge National Lab , JAGATH GUNASEKERA, DEEPAK SINGH , Univ of Missouri - Columbia — The two-dimensional artificial magnetic honeycomb lattice system is evolving into a new research arena to explore a plethora of novel magnetism that are predicted to occur as functions of temperature and magnetic field: a long-range spin ice, spin liquid, an entropy-driven magnetic charge-ordered state involving topological vortex pairs and a spin-order due to the spin chirality. We have created macroscopic samples of artificial magnetic honeycomb lattices of Cobalt and Permalloy having connected ultra-small elements (bonds), with length scales of sub-10 nm to 30 nm, which have never before been possible. The equivalent energy of the resulting systems is 10-100 K and is thus amenable to both temperature- and field-dependent exploration of novel magnetic phenomena. We have performed detailed magnetic and small angle neutron scattering measurements (SANS) on the newly fabricated honeycomb lattice of Permalloy that show the thermal character of the system. Furthermore, the experimental data reveals the onset of magnetic ordered regimes in temperature that are consistent with the predicted novel phase diagram in artificial honeycomb lattice. Research is supported by U.S. Department of Energy, Office of Basic Energy Sciences under Grant No. DE-SC0014461.

**1:51PM L5.00012 Real time dynamic behavior of vertex frustrated artificial spin ice.** , YUYANG LAO, JOSEPH SKLENAR, University of Illinois at Urbana-Champaign, IAN GILBERT, National Institute of Standards and Technology, ISAAC CARRASQUILLO, University of Illinois at Urbana-Champaign, ANDREAS SCHOLL, ANTHONY YOUNG, Lawrence Berkeley National Laboratory, CRISTIANO NISOLI, Los Alamos National Laboratory, PETER SCHIFFER, University of Illinois at Urbana-Champaign — Artificial spin ice systems comprise two dimensional arrays of nanoscale single domain ferromagnets designed to have frustrated interactions among the moments. By decimating islands from the common square artificial spin ice, one can design lattices with so called 'vertex frustration'. In such lattices, the geometry prevents all vertices from occupying local ground states simultaneously. Using Photoemission Electron Microscopy (PEEM), we access the real time thermally induced dynamics of the moment behavior in those lattices. Operating at a proper temperature, the moment direction of each island fluctuates with a sufficiently slow frequency that it can be resolvable by acquiring successive PEEM images. We can extract information regarding the collective excitations of the moments and understand how they reflect the frustration of lattice. Supported by the US Department of Energy, Office of Basic Energy Sciences, Materials Science and Engineering Division under grant no. DE-SC0010778. The work of C.N. was carried out under the auspices of the US Department of Energy at LANL under contract no. DE-AC52-06NA253962. The ALS is supported by the Director, Office of Science, Office of Basic Energy Sciences, of the US Department of Energy under contract no. DE-AC02-05CH11231.

**2:03PM L5.00013 Monte Carlo simulations of kagome lattices with magnetic dipolar interactions** , MARTIN PLUMER, Memorial University Newfoundland, MARK HOLDEN, University of Waterloo, ANDREW WAY, Memorial University of Newfoundland, IVAN SAIKA-VOIVOD, Memorial University Newfoundland, BYRON SOUTHERN, University of Manitoba — Monte Carlo simulations of classical spins on the two-dimensional kagome lattice with only dipolar interactions are presented [1]. In addition to revealing the sixfold-degenerate ground state, the nature of the finite-temperature phase transition to long-range magnetic order is discussed. Low-temperature states consisting of mixtures of degenerate ground-state configurations separated by domain walls can be explained as a result of competing exchange-like and shape-anisotropy-like terms in the dipolar coupling. Fluctuations between pairs of degenerate spin configurations are found to persist well into the ordered state as the temperature is lowered until locking in to a low-energy state. Results suggest that the system undergoes a continuous phase transition at  $T \approx 0.43$  in agreement with previous MC simulations [2] but the nature of the ordering process differs [3]. Preliminary results which extend this analysis to the 3D fcc ABC-stacked kagome systems will be presented [4].

1. M. S. Holden, M. L. Plumer, I. Saika-Voivod, and B. W. Southern, Phys. Rev. B 91, 224425 (2015).
2. M. Maksymenko, V. R. Chandra, and R. Moessner, Phys. Rev. B 91, 184407 (2015).
3. Y. Tomita, J. Phys. Soc. Jpn. 78, 114004 (2009).
4. V. Hemmati, et al., Phys. Rev. B 86, 104419 (2012)

**Wednesday, March 16, 2016 11:15AM - 2:15PM –**

**Session L6 GMAG DMP FIAP: Spin-Transport Phenomena: Oscillators and Spin-Injections I**  
302 - Lihui Bai, University of Manitoba

**11:15AM L6.00001 Mutual synchronization of two spin transfer oscillators coupled through their self-emitted microwave currents** , V. CROS, R. LEBRUN, Unit Mixte CNRS/Thales, Univ. Paris-Sud, Univ. Paris-Saclay, Palaiseau, France, S. TSUNEGI, Spintronic Research Center, AIST, Tsukuba, Japan, P. BORTOLOTTI, Unit Mixte CNRS/Thales, Univ. Paris-Sud, Univ. Paris-Saclay, Palaiseau, France, H. KUBOTA, Spintronic Research Center, AIST, Tsukuba, Japan, M. ROMERA, Unit Mixte CNRS/Thales, Univ. Paris-Sud, Univ. Paris-Saclay, Palaiseau, France, K. YAKUSHIJI, A. FUKUSHIMA, Spintronic Research Center, AIST, Tsukuba, Japan, J. GROLLIER, Unit Mixte CNRS/Thales, Univ. Paris-Sud, Univ. Paris-Saclay, Palaiseau, France, S. YUASA, Spintronic Research Center, AIST, Tsukuba, Japan, UNIT MIXTE DE PHYSIQUE CNRS/THALES COLLABORATION, SPINTRONICS RESEARCH CENTER, AIST COLLABORATION — Here, we demonstrate the mutual synchronization of two vortex STOs through electrical coupling. We describe how in using a delay line, we can optimize the locking range of the synchronization. We also evidence that the coupling efficiency is tuned by the nonlinear parameters of STOs but also more originally through the ratio between the two components of spin transfer torques. This represents a definite advantage of our vortex-STNOs for their future implementation in large arrays of synchronized STOs. We find that the linewidth of the two synchronized STOs decreases by a factor 2 and the output power increases by factor 4 ( $\sim 1.6 \text{ W}$ ) compared to non-interacting STOs. These results provide a solid basis towards the efficient synchronization of multiple STOs. EU FP7 grant (MOSAIC No. ICT-FP7-317950 is acknowledged).

**11:27AM L6.00002 Toggling synchronization of nano-contact spin torque oscillators with spin wave beams<sup>1</sup>**, RANDY DUMAS, AFSHIN HOUSHANG, PHILIPP DURRENFELD, JOHAN AKERMAN, University of Gothenburg-Physics — The synchronization of multiple nano-contact spin torque oscillators (NC-STOs) [1-3] is mediated by propagating spin waves (SWs) [4]. Furthermore, it has been shown that the Oersted field in the vicinity of the NC can induce highly directional SW beams [5, 6]. Not only have we recently demonstrated the robust synchronization between two oscillators separated by over 1 micron, but also the driven synchronization of up to five oscillators by purposefully taking advantage of such SW beams [7]. Here, we demonstrate that when the NC diameters differ by a significant amount, the Oersted field scale in such a way as to promote or block synchronization depending on the SW propagation direction, allowing one to easily toggle between synchronized and un-synchronized states by simply altering the applied field direction. [1] S. Kaka, *et al.*, *Nature* **437**, 389 (2005). [2] F.B. Mancoff, *et al.*, *Nature* **437**, 393 (2005). [3] S.R. Sani, *et al.*, *Nat. Comm.* **4**, 2731 (2013). [4] M.R. Pufall, *et al.*, *Phys. Rev. Lett.* **97**, 087206 (2006). [5] R.K. Dumas, *et al.*, *Phys. Rev. Lett.* **110**, 257202 (2013). [6] M.A. Hoefer, *et al.*, *Phys. Rev. B*, **77**, 144401 (2008). [7] A. Houshang, *et al.*, *Nature Nanotechnol.*, in press.

<sup>1</sup>This work was supported by the European Commission FP7-ICT-2011 contract No. 317950 MOSAIC, ERC grant 307144 MUSTANG, VR, SSF, and the Knut and Alice Wallenberg Foundation.

**11:39AM L6.00003 Theory of mode coupling in spin torque oscillators coupled to a thermal bath of magnons**, YAN ZHOU<sup>1</sup>, University of Hong Kong, SHULEI ZHANG<sup>2</sup>, University of Missouri, DONG LI, Hong Kong Baptist University, OLLE HEINONEN<sup>3</sup>, Argonne National Lab and Northwestern University — Recently, numerous experimental investigations have shown that the dynamics of a single spin torque oscillator (STO) exhibits complex behavior stemming from interactions between two or more modes of the oscillator. Examples are the observed mode-hopping and mode coexistence. There has been some initial work indicating how the theory for a single-mode (macro-spin) spin torque oscillator should be generalized to include several modes and the interactions between them. In this work, we rigorously derive such a theory starting with the generalized Landau-Lifshitz-Gilbert equation in the presence of the current-driven spin transfer torques. We will first show, in general, that how a linear mode coupling would arise through the coupling of the system to a thermal bath of magnons, which implies that the manifold of orbits and fixed points may shift with temperature. We then apply our theory to two experimentally interesting systems: 1) a STO patterned into nano-pillar with circular or elliptical cross-sections and 2) a nano-contact STO. For both cases, we found that in order to get mode coupling, it would be necessary to have either a finite in-plane component of the external field or an Oersted field. We will also discuss the temperature dependence of the linear mode coupling.

<sup>1</sup>Y. Zhou acknowledges the support by the Seed Funding Program for Basic Research from the University of Hong Kong, and University Grants Committee of Hong Kong (Contract No. AoE/P-04/08).

<sup>2</sup>S. Zhang was supported by NSF Grants DMR-1406568.

<sup>3</sup>Work by O.Heinonen was supported by the U.S. Department of Energy.

**11:51AM L6.00004 Nonlocal spin-transfer with low-resistance  $\text{AlO}_x$  spin injection interface and ohmic spin absorption interface**, YUNJIAO CAI, CHUAN QIN, SHUHAN CHEN, YI JI, Univ of Delaware — Mesoscopic nonlocal spin valves are fabricated for the purpose of spin-transfer with pure spin current. The device consists of a 300 nm wide Py (NiFe alloy) spin injector (F1), an 80 nm wide Py spin detector (F2) and an 80 nm wide Cu channel. The thickness of F1, F2, and Cu is 15 nm, 3 nm, and 110 nm, respectively. A 3 nm layer of low-resistance  $\text{AlO}_x$  is placed at the F1/Cu interface to mitigate the spin resistance mismatch between Py and Cu and to provide substantial injection spin polarization. The F1 injector and the F1/ $\text{AlO}_x$ /Cu interface are robust enough to sustain a d.c. injection current up to 6 mA. The F2/Cu interface remains ohmic to facilitate an efficient absorption of the pure spin current from the Cu channel into the F2. A nanoscale magnetic domain in F2 underneath the F2/Cu interface can be reversibly switched between 5 K and 150 K via spin-transfer by the pure spin current. The critical injection current for the reversal at 100 K is ~1.5 mA, which is significantly lower than those in previous studies for nonlocal spin-transfer.

**12:03PM L6.00005 Spin current valve effect in normal metal/magnetic insulator/normal metal sandwiches<sup>1</sup>**, JUNXUE LI, YADONG XU<sup>2</sup>, MOHAMMED ALDOSARY, CHI TANG, ZHISHENG LIN, UC Riverside, SHUFENG ZHANG, University of Arizona, ROGER LAKE, JING SHI, UC Riverside, SHINES COLLABORATION — Pure spin current is generated in two common ways. One makes use of the spin Hall effect in normal metals (NM), the other utilizes spin waves with the quasi-particle excitations called magnons. A popular material for the latter is yttrium iron garnet (YIG), a magnetic insulator (MI). Here we demonstrate in NM/MI/NM sandwiches that these two types of spin current are interconvertible, which allows transmitting an electrical signal across the MI, predicted as the magnon-mediated current drag phenomenon. We show experimentally that the spin current can be switched on or off by controlling the magnetization orientation of MI, analogous to conventional spin valves for spin-polarized charge current. The transmitted current drag signal scales linearly with the driving current without any threshold and follows the power-law  $T^n$  with  $n$  ranging from 1.5 to 2.5. Our results indicate that the NM/MI/NM sandwich structure can serve as a scalable pure spin current valve device which is an essential ingredient in spintronics.

<sup>1</sup>As part of the SHINES, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award SC0012670.

<sup>2</sup>The first two authors contributed equally.

**12:15PM L6.00006 Comparison of spin transfer mechanisms in three terminal spin-torque-oscillators**, EMILIE JUE, WILLIAM RIPPARD, MATTHEW PUFALL, ERIC R. EVARTS, NIST - Boulder, QUANTUM ELECTROMAGNETICS DIVISION TEAM — The manipulation of magnetization by electric current is one of the most active field of spintronics due to its interests for memory and logic applications. This control can be achieved through the transfer of angular momentum via a spin polarized current (the mechanism of spin-transfer torque - STT) or through a direct transfer of angular momentum from the crystal lattice through the spin-orbit interaction (the mechanism of spin-orbit torque - SOT). Over the five past years, SOT gained a lot of attention especially for the new possibilities that it offers for data storage application. However, the quantification and the comparison of both mechanisms' efficiencies remains uncertain. In this work, we compare for the first time the STT and SOT efficiencies in individual devices. For this, we created 3-terminal spin-torque oscillators (STO) composed of spin-valves (SV) on top of a Pt wires. The devices can be excited either by STT or by SOT depending on whether the current is applied through the SV or through the Pt wire. By varying the Pt width and the dimensions of the SV, we tune the SOT and STT and compare their efficiencies. We will discuss the complexity of such a structure and the differences in the magnetization dynamics induced by the different excitation mechanisms.

**12:27PM L6.00007 Characterization of perpendicular STT-MRAM by spin torque ferromagnetic resonance<sup>1</sup>**, CHENG CEN SHA, LIU YANG, HAN KYU LEE, IGOR BARSUKOV, JIEYI ZHANG, ILYA KRIVOROTOV, University of California, Irvine — We describe a method for simple quantitative measurement of magnetic anisotropy and Gilbert damping of the MTJ free layer in individual perpendicular STT-MRAM devices by spin torque ferromagnetic resonance (ST-FMR) with magnetic field modulation. We first show the dependence of ST-FMR spectra of an STT-MRAM element on out-of-plane magnetic field. In these spectra, resonances arising from excitation of the quasi-uniform and higher order spin wave eigenmodes of the free layer as well as acoustic mode of the synthetic antiferromagnet (SAF) are clearly seen. The quasi-uniform mode frequency at zero field gives magnetic anisotropy field of the free layer. Then we show dependence of the quasi-uniform mode linewidth on frequency is linear over a range of frequencies but deviates from linearity in the low and high frequency regimes. Comparison to ST-FMR spectra reveals that the high frequency line broadening is linked to the SAF mode softening near the SAF spin flop transition at 5 kG. In the low field regime, the SAF mode frequency approaches that of the quasi-uniform mode, and resonant coupling of the modes leads to the line broadening. A linear fit to the linewidth data outside of the high and low field regimes gives the Gilbert damping parameter of the free layer.

<sup>1</sup>This work was supported by the Samsung Global MRAM Innovation Program.

**12:39PM L6.00008 Spin-torque ferromagnetic resonance (ST-FMR) spectroscopy of localized spin wave modes engineered by applied dipole-field localization**, CHI ZHANG, YONG PU, SERGEI A. MANUILOV, DENIS V. PELEKHOV, P. CHRIS HAMMEL, The Ohio State University — Maintaining efficient spin-Hall anti-damping torque in micron-scale devices is challenging near the critical current for auto-oscillation, likely due to spin wave mode degeneracies and nonlinear magnon scattering between them [1]. Localized spin wave modes confined by the strongly inhomogeneous dipole magnetic field of a nearby micro-spherical magnet [2] provides a potentially powerful tool to study these multi-mode interactions by allowing systematic tunability while avoiding potential spurious effects arising from imperfections in fabricating microscopic structures. We demonstrate electrical ST-FMR detection of well-resolved localized modes in a Py/Pt stripe. We find that magnon spectral engineering by means of a micromagnetic particle enables clear observation of damping control and significant reduction of linewidth by means of the anti-damping torque arising from an imposed DC current. The observed linewidth variation suggests that localized modes can be controlled as effectively as the uniform mode. References: [1] V. E. Demidov et al, Phys. Rev. Lett. 107, 107204 (2011) Z. Duan et al, Nat. Commun. 5, 5616 (2014) [2] I. Lee et al., Nature 466, 845 (2010) H.-J. Chia et al., Phys. Rev. Lett. 108, 087206 (2012)

**12:51PM L6.00009 First-principles theory of current-induced spin torques in noncollinear antiferromagnets**, ALLAN MACDONALD, HUA CHEN, The University of Texas at Austin, YIMING WU, Peking University, YASUFUMI ARAKI, Tohoku University — We propose a new theoretical approach for calculating current induced torques in hybrid systems containing magnetic and heavy metal thin films. The theory is based on ab-initio density functional theory (DFT) and appeals explicitly to the local-spin-density approximation for exchange and correlation. Because the effective magnetic field from exchange and correlation is everywhere parallel to the spin-density in the ferromagnet, it does not contribute to the current-induced torque, which is due entirely to spin-orbit coupling near heterojunctions involving heavy metals. The theoretical picture can be combined with any theory of the electronic steady state produced by electrochemical potential gradients, and involves response of the single-particle density matrix that is partially diagonal and partially off-diagonal in an unperturbed eigenstate representation. The theory is formulated using the basis of Wannier functions and can be readily interfacing with existing DFT codes. This approach predicts strong current-induced torques due to either antiferromagnetic or non-magnetic heavy metal layers. As an illustration, we use it to calculate specifically the spin torque in a ferromagnet induced by an adjacent noncollinear antiferromagnet (Mn3Ir).

**1:03PM L6.00010 Spin Torque Generated by the Spin Hall Effect in Ferromagnets**, JONATHAN GIBBONS, Department of Physics, Cornell University, ROBERT BUHRMAN, School of Applied and Engineering Physics, Cornell University, DANIEL RALPH, Department of Physics, Cornell University — Ferromagnetic materials exhibit the anomalous Hall effect, the generation of a transverse charge current due to spin-orbit coupling. The anomalous Hall effect is closely related to the spin Hall effect, and hence this transverse charge current is expected to be accompanied by a strong transverse spin current, whose direction can be manipulated by rotating the magnetic moment. We measure the torque from this spin current generated by Gd-doped Fe and acting on an in-plane magnetized free layer. We use the harmonic measurement technique, applying a current to an in-plane pinned ferromagnet/spacer/in-plane free ferromagnet stack and measuring the second harmonic Hall voltage. We report the angular dependence of the spin torque for a variety of initial exchange bias directions, and as the spin torque changes with an external magnetic field.

**1:15PM L6.00011 Enhanced spin orbit torques by oxygen incorporation in tungsten films**, TIMOTHY PHUNG, KAI-UWE DEMASIU, WEIFENG ZHANG, BRIAN P. HUGHES, SEE-HUN YANG, ANDREW KELLOCK, WEI HAN, AAKASH PUSH, STUART S. P. PARKIN, IBM Almaden Res Ctr — Spin orbit torques are generated by the conversion of charge to spin currents in non-magnetic materials. The origin of these torques is of considerable debate. One of the most interesting materials is metallic tungsten for which large spin orbit torques have been found in thin films that are stabilized in the A15 ( $\beta$ -phase) structure. Here we report, using spin transfer torque ferromagnetic resonance, large spin Hall angles of up to  $\sim 0.5$  by incorporating oxygen into tungsten films. Whilst the incorporation of oxygen into the tungsten leads to significant changes in its microstructure and electrical resistivity, the large spin Hall angles measured are found to be remarkably insensitive to the oxygen doping level (12-44%). This invariance of the spin Hall angle with the bulk W(O) properties for higher oxygen concentrations suggests that the spin orbit torques in this system may actually be partly interfacial in origin, and induced by scattering of the electrons at the W(O) | CoFeB interface rather than from the interior of the W(O) film. Our results show an intriguing novel path towards enhanced spin orbit torques.

**1:27PM L6.00012 Optically Detected Ferromagnetic Resonance in Metallic Ferromagnets Via Off-Resonant Detection of Nitrogen Vacancy Centers in Diamond**, MICHAEL R. PAGE, VIDYA P. BHALLAMUDI, JOE SCHULZE, CAROLA M. PURSER, SERGEI MANUILOV, CHRISTOPHER WOLFE, JACK T. BRANGHAM, FENGYUAN YANG, P. CHRIS HAMMEL, The Ohio State University Department of Physics — We report optical detection of ferromagnetic resonance in thin film metallic ferromagnets using a recently discovered approach employing nitrogen vacancy centers in nanodiamonds. While conventional optically detected magnetic resonance measures magnetic fields through their impact on the magnetic resonance frequency of the nitrogen vacancy center, we measure a change in the nitrogen vacancy center photoluminescence at the ferromagnets resonance condition without need to work at the NV resonance frequency. This measurement technique allows sensitive, local detection of ferromagnetic resonance and can enable the study of magnetic dynamics at the nanoscale in a wide range of materials. While this measurement protocol was first reported in the study of ferromagnetic resonance in YIG, here we demonstrate the measurement in commonly used metallic ferromagnets to establish the generality of the technique and open the possibility of measuring nanoscale patterned devices and magnetic textures based on metallic ferromagnets of both commercial and scientific interest.

**1:39PM L6.00013 Phase-resolved ferromagnetic resonance detection using heterodyning**, SEUNGHA YOON, ROBERT D. MCMICHAEL, National Institute of Standards and Technology — We have developed a new phase-resolved ferromagnetic (FMR) detection method using a heterodyne method. Phase resolution is important to determine the characteristics of spin transfer torques in magnetization dynamics under microwave excitation [1]. Specifically, field-like torques and damping-like torques result in magnetization precession with different phases. In this method, we drive spin precession in a Permalloy thin film using microwaves. The resulting precession is detected using 1550 nm laser light, that is modulated at a frequency slightly shifted with respect to the driving frequency. In the reflected light, beating of the spin precession and the light modulation produces an oscillating Kerr rotation signal with a phase equal to the precession phase plus a phase due to the path length difference between the excitation microwave and the optical signal. This detection method eliminates the need for field modulation and allows detection at higher frequencies where the  $1/f$  noise floor is reduced. [1] M. Weiler, J. M. Shaw, H. T. Nembach, and T. J. Silva, *Phys. Rev. Lett.* 113, 157204 (2014).

**1:51PM L6.00014 Anomalous Hall Effect in a Kagome Ferromagnet**<sup>1</sup>, LINDA YE, CHRISTINA WICKER, TAKEHITO SUZUKI, JOSEPH CHECKELSKY, Massachusetts Inst of Tech-MIT, JOSEPH CHECKELSKY TEAM — The ferromagnetic kagome lattice is theoretically known to possess topological band structures [1,2]. We have synthesized large single crystals of a kagome ferromagnet  $\text{Fe}_3\text{Sn}_2$  which orders ferromagnetically well above room temperature [3]. We have studied the electrical and magnetic properties of these crystals over a broad temperature and magnetic field range. Both the scaling relation of anomalous Hall effect and anisotropic magnetic susceptibility show that the ferromagnetism of  $\text{Fe}_3\text{Sn}_2$  is unconventional. We discuss these results in the context of magnetism in kagome systems and relevance to the predicted topological properties in this class of compounds. [1] *Phys. Rev. B* 87 144101 (2013) [2] *Phys. Rev. Lett.* 106 236802 (2011) [3] *J. Phys. Cond. Mat.* 21 452202 (2009)

<sup>1</sup>This research is supported by DMR-1231319.

**2:03PM L6.00015 Interaction and multiband effects in the intrinsic spin-Hall effect of an interacting multi-orbital metal**, NAOYA ARAKAWA, RIKEN CEMS — The spin-Hall effect is a spin-current version of the usual-Hall effect, and its potential for application may be great. For the efficient application utilizing the spin-Hall effect, an understanding of interaction effects may be helpful because the interaction effects sometimes become remarkable in transport phenomena (e.g., fractional-quantum-Hall effect). However, a lot of theoretical studies neglected the interaction effects, and the interaction effects in the spin-Hall effect had been little understood. To improve this situation, I developed a general formalism for the intrinsic spin-Hall effect including the interaction effects and multiband effects by using the linear-response theory with approximations appropriate for an interacting multi-orbital metal (see arXiv:1510.03988). In this talk, I explain how the electron-electron interaction modifies the spin-Hall conductivity and show several new and remarkable interaction effects, new mechanisms of the damping dependence and a crossover of the damping dependence in a clean system and a temperature-dependent correction due to the spin-Coulomb drag. I also show guidelines useful for general formulations of other transport phenomena including the interaction effects and multiband effects.

## Wednesday, March 16, 2016 11:15AM - 2:15PM –

### Session L7 DMP FIAP: Dopants and Defects in Semiconductors: Novel experimental techniques

303 - James Speck, University of California, Santa Barbara

**11:15AM L7.00001 Tailoring of materials properties under extreme conditions**<sup>1</sup>, THOMAS SCHENKEL, Lawrence Berkeley Natl Lab — Materials can be driven far from equilibrium e. g. with intense pulses of lasers and ions, in mostly destructive processes. When combined with micro- and nano-structuring, the ability to rapidly excite and then quench local excitations opens up. Now opportunities emerge to form and stabilize novel materials phases and to tailor materials properties for applications. Examples are color centers in diamond and silicon carbide for sensing and qubit applications and proposed ordered dopant structures in cuprate superconductors. Results from studies of materials processing under transient extreme conditions, far from equilibrium will be presented.

<sup>1</sup>This work was supported by the Director, Office of Science, Office of Fusion Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

**11:51AM L7.00002 Polarization spectroscopy of defect-based single photon sources in ZnO**<sup>1</sup>, NICHOLAS JUNGWIRTH, HUNG-SHEN CHANG, MINGDE JIANG, GREGORY FUCHS, Cornell University — Isolated point-defects in wide bandgap semiconductors are promising candidates for future applications requiring quantum light sources. Recently, defect-based single photon sources have been observed in ZnO that are very bright ( $>100$  kCounts/s) and remain photoactive from 4.5 K to room temperature. Despite several investigations, the structure and electronic states of these emitters remain unknown. In this work, we establish a procedure to distinguish a Z dipole from an XY dipole when studying quantum emitters that are randomly oriented. Our cryogenic and room temperature polarization measurements collectively establish that these unidentified ZnO quantum emitters have a Z dipole. We show that the associated absorption and emission dipoles are parallel within experimental uncertainty for all 32 individuals studied. Additionally, we apply group theory and find that, assuming the defect symmetry belongs to a point-group relevant to the ZnO wurtzite lattice, the ground and excited states are orbital singlets. These results are a significant step in identifying the structure and electronic states of defect-based single photon sources in ZnO.

<sup>1</sup>We acknowledge support from the National Science Foundation.

**12:03PM L7.00003 A first principle approach using Maximally Localized Wannier Functions for computing and understanding elasto-optic response**<sup>1</sup>, XIN LIANG, SOHRAB ISMAIL-BEIGI, Yale University — Strain-induced changes of optical properties are of use in the design and functioning of devices that couple photons and phonons. The elasto-optic (or photo-elastic) effect describes a general materials property where strain induces a change in the dielectric tensor. Despite a number of experimental and computational works, it is fair to say that a basic physical understanding of the effect and its materials dependence is lacking: e.g., we know of no materials design rule for enhancing or suppressing elasto-optic response. Based on our previous work, we find that a real space representation, as opposed to a k-space description, is a promising way to understand this effect. We have finished the development of a method of computing the dielectric and elasto-optic tensors using Maximally Localized Wannier Functions (MLWFs). By analyzing responses to uniaxial strain, we find that both tensors respond in a localized manner to the perturbation: the dominant optical transitions are between local electronic states on nearby bonds. We describe the method, the resulting physical picture and computed results for semiconductors.

<sup>1</sup>This work is supported by the National Science Foundation through grant NSF DMR-1104974.

**12:15PM L7.00004 Modification of a scanning electron microscope (SEM) for insitu, nanometer size contact, electrical measurements of III-nitride transistors**, CAMELIA SELCU, Department of Physics, The Ohio State University, ZHICHAO YANG, SRIRAM KRISHNAMOORTHY, SIDDHARTH RAJAN, Department of Electrical and Computer Engineering, The Ohio State University — As the transistors become smaller and smaller, proximity effects become important, therefore there is a need for characterization instruments. We modified a scanning electron microscope (SEM) by adding the capability to make mechanical contacts to devices for electrical measurements with nanometer precision. We will discuss ongoing work involving III-nitride transistors and nanowires.

**12:27PM L7.00005 Second-Harmonic Generation scanning microscopy of strain fields around Through-Silicon-Vias**, YUJIN CHO, FARBOD SHAFIEI, Univ of Texas, Austin, BERNARDO MENDOZA, Centro de Investigaciones en Optica, Leon, Mexico, TENGFEI JIANG, PAUL HO, MICHAEL DOWNER, Univ of Texas, Austin — Through-Silicon-Vias (TSVs) improve electrical performance of integrated circuits and reduce power consumption by interconnecting vertically stacked silicon layers. Cu has been commonly used for TSVs because of its good electrical and mechanical properties. However, mismatch in thermal expansion coefficient of Si and Cu induces strain fields on the surfaces, which can degrade the performance of nearby devices and crack the surfaces. In this work, using non-invasive Second Harmonic Generation (SHG) microscopy, we successfully characterized inhomogeneous distribution of the thermally induced strain fields. High strain gradients strengthen SHG intensity, since it breaks centrosymmetry in Si. In p-polarized incoming beam and s-polarized SHG configuration, we were able to see the strain effect directly, while in p-in/ p-out polarization, strain-induced SHG was coupled with background SHG from Si [1]. We will present SHG micrographs compared with Raman measurement and the theory of strain-induced SHG, as well as wavelength and power dependence of SHG. [1] Mendoza et al. 'Surface second harmonic generation induced by 3D strain fields', Phys. Status Solidi B. 1-8 (2015)

**12:39PM L7.00006 Probing the effect of dopants (donors) within InAs/InGaAs/InAlAs Asymmetric Heterostructure wafer by magneto-THz spectroscopy**, MEHDI PAKMEHR, University at Buffalo (SUNY), Shiraz University, CHRISTIAN HEYN, WOLFGANG HANSEN, University of Hamburg — Probing the effect of impurities within semiconductor structures have been the topic of interest both from applied and scientific point of views. We studied the effect of dopants (donors) within InAs/InGaAs/InAlAs asymmetric heterostructure wafer by means of THz magneto-transmission (TR) spectroscopy, in conjunction with THz magneto-photoresponse (PR) spectroscopy. The sample wafer has been immersed in pumped liquid Helium at 1.6 K, while being exposed to sweeping magnetic field up to 10 Tesla, with THz laser beam (1.4 THz) being focused on sample by off-axis parabolic mirror. The transmitted beam was detected by silicon composite bolometer. Two broad absorption features other than sharp Cyclotron resonance (CR) absorption dip within magneto-TR signal attributed to  $1s \rightarrow 2P$  transition within donors of doped layer (InAlAs) in heterostructure. We plan to discuss the analysis of magneto-TR signal, in conjunction with Magneto-PR signals from Hall bar samples made from same type of wafer at same frequency to clarify how dopants could possibly alter these signals.

**12:51PM L7.00007 Sub-surface single ion detection in diamond: A path for deterministic color center creation**, JOHN ABRAHAM, BRANDON AGUIRRE, JOSE PACHECO, RYAN CAMACHO, EDWARD BIELEJEC, Sandia National Laboratories, SANDIA NATIONAL LABORATORIES TEAM — Deterministic single color center creation remains a critical milestone for the integrated use of diamond color centers. It depends on three components: focused ion beam implantation to control the location, yield improvement to control the activation, and single ion implantation to control the number of implanted ions. A surface electrode detector has been fabricated on diamond where the electron hole pairs generated during ion implantation are used as the detection signal. Results will be presented demonstrating single ion detection. The detection efficiency of the device will be described as a function of implant energy and device geometry. It is anticipated that the controlled introduction of single dopant atoms in diamond will provide a basis for deterministic single localized color centers. This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy Office of Science. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

**1:03PM L7.00008 ABSTRACT WITHDRAWN —**

**1:15PM L7.00009 Uniaxial stress studies of H centers in  $\text{In}_2\text{O}_3$** <sup>1</sup>, PHILIP WEISER, MICHAEL STAVOLA, W. BEALL FOWLER, Lehigh University, LYNN A. BOATNER, Oak Ridge National Laboratory —  $\text{In}_2\text{O}_3$  single crystals have been grown for our experiments that are sufficiently large to make possible IR absorption measurements in conjunction with uniaxial stress. The introduction of H produces an IR line at  $3306\text{ cm}^{-1}$  that has been assigned to the OH stretching mode of an interstitial H shallow donor in  $\text{In}_2\text{O}_3$  [1]. We have performed IR absorption experiments in which the splitting of the  $3306\text{ cm}^{-1}$  line under stresses applied at low temperatures provides information about the symmetry of the OH center. Stress measurements made at elevated temperatures reveal a stress-induced dichroism that provides information about the motion of hydrogen associated with the  $3306\text{ cm}^{-1}$  center. [1] W. Yin et al., Phys. Rev. B **91**, 075208 (2015).

<sup>1</sup>NSF Grant DMR 1160756

**1:27PM L7.00010 Diffusion of H in  $\text{In}_2\text{O}_3$  single crystals**<sup>1</sup>, YING QIN, WEIKAI YIN, MIKE STAVOLA, BEALL FOWLER, Lehigh University, LYNN BOATNER, Oak Ridge National Laboratory — An IR absorption line observed at  $3306\text{ cm}^{-1}$  for  $\text{In}_2\text{O}_3$  single crystals annealed in an  $\text{H}_2$  ambient has been assigned to an interstitial hydrogen center that acts as a shallow donor [1]. Experiments have been performed to determine the indiffusion depth of interstitial H into  $\text{In}_2\text{O}_3$  at temperatures near 400 C. We have also performed annealing experiments in which the outdiffusion of interstitial H is monitored by IR spectroscopy. The goal of these studies is to determine the diffusion constant of interstitial H in  $\text{In}_2\text{O}_3$  over a range of temperatures so that the activation energy for diffusion can be determined. [1] W. Yin et al., Phys. Rev. B **91**, 075208 (2015).

<sup>1</sup>Supported by NSF grant DMR 1160756

**1:39PM L7.00011 Profiling the local carrier concentration and dopant distribution across a semiconductor quantum dot**, J.C. WALRATH, A.S. CHANG, Y.H. LIN, S. HUANG, R.S. GOLDMAN, Univ of Michigan - Ann Arbor — We profile the local carrier concentration,  $n$ , across epitaxial InAs/GaAs quantum dots (QDs) consisting of 3D islands on top of a 2D alloy layer. We use scanning thermoelectric microscopy to profile the temperature gradient-induced voltage, which is converted to a profile of the local Seebeck coefficient,  $S$ . The  $S$  profile is then converted to a conduction band-edge profile and compared with Poisson-Schrodinger band-edge simulations. Our combined computational-experimental approach suggests a reduced carrier concentration in the QD center in comparison to that of the 2D alloy layer. We further use 3D atom probe tomography, which enables 3D imaging with a few Angstrom resolution, to profile the distribution of Si dopants. We discuss the correlation between the Si dopant distribution and the observed carrier concentration profile.

**1:51PM L7.00012 Characterisation of potential barriers in a donor quantum dot defined by hydrogen resist lithography.**<sup>1</sup>, ANDREAS FUHRER, NIKOLA PASCHER, IBM Research - Zurich — We use a four terminal donor quantum dot (QD) to characterize potential barriers between degenerately doped nanoscale contacts. The QD is fabricated by hydrogen resist lithography on Si(001) in combination with n-type doping from the gas-phase. The four contacts have different separations ( $d = 9, 12, 16$  and  $29$  nm) to a central  $6 \text{ nm} \times 6 \text{ nm}$  island, leading to different tunnel- and capacitive coupling. We use cryogenic transport measurements in the Coulomb blockade regime to simultaneously probe current flow in the four terminals for various voltage configurations. The magnitude of the measured tunnelling currents as a function of applied bias and contact separation sets a limit of about  $15 \text{ nm}$  for tunnelling contacts and shows a strong increase of the barrier transmission with applied bias. Using a constant interaction picture we extract the mutual capacitances between the QD and the four contacts which are found to be in excellent agreement with numerically calculated values. Our results contribute to a better understanding of tunnelling barriers and gate electrodes in planar dopant devices and pave the way towards reliable quantum device fabrication at the atomic scale.

<sup>1</sup>Support from EU grants PAMS, SiSpin, SiAM and from Swiss NCCR QSIT is gratefully acknowledged

**2:03PM L7.00013 Nanoscale Imaging of Band Gap and Defects in Polycrystalline CdTe Photovoltaic Devices**, NIKOLAI ZHITENEV, CNST, NIST, YOHAN YOON, JUNGSEOK CHAE, AARON KATZENMEYER, HEAYOUNG YOON, SANGMIN AN, U. Maryland / CNST, JOSHUA SHUMACHER, ANDREA CENTRONE, CNST, NIST — To further increase the power efficiency of polycrystalline thin film photovoltaic (PV) technology, a detailed understanding of microstructural properties of the devices is required. In this work, we investigate the microstructure of CdTe PV devices using two optical spectroscopies. Sub-micron thickness lamella samples were cut out from a PV device, either in cross-section or in-plane, by focused ion beam. The first technique is the photothermal induced resonance (PTIR) used to obtain absorption spectra over a broad range of wavelengths. In PTIR, a wavelength tunable pulsed laser is combined with an atomic force microscope to detect the local thermal expansion of lamella CdTe sample induced by light absorption. The second technique based on a near-field scanning optical microscope maps the local absorption at fixed near-IR wavelengths with energies at or below CdTe band-gap energy. The variation of the band gap throughout the CdTe absorber determined from PTIR spectra is  $\approx 20 \text{ meV}$ . Both techniques detect strong spatial variation of shallow defects over different grains. The spatial distribution of mid-gap defects appears to be more uniform. The resolution, the sensitivity and the applicability of these two approaches are compared.

## Wednesday, March 16, 2016 11:15AM - 2:15PM – Session L8 DMP: Electron Transport in Nanowires 304 - Jonathan Baugh, University of Waterloo

**11:15AM L8.00001 1D Coulomb drag between coupled nanowires formed at oxide interfaces**<sup>1</sup>, YUHE TANG, MICHELLE TOMCZYK, MENGCHEN HUANG, Univ of Pittsburgh, HYUNGWOO LEE, CHANG-BEOM EOM, Univ of Wisconsin at Madison, PATRICK IRVIN, JEREMY LEVY, Univ of Pittsburgh — “Coulomb drag” is a transport phenomenon where Coulomb interaction between two close but electrically isolated conductors induces voltage in one conductor when an electric current is injected in the other conductor. It is a powerful approach to probe electronic correlations. Here we examine 1D electronic correlations in a proximally coupled nanowire system where two parallel nanowires are created with conductive atomic force microscopy at the  $\text{LaAlO}_3/\text{SrTiO}_3$  interface. Coulomb drag measurements are made by injecting current into one wire (drive wire) and measuring the induced voltage in the other wire (drag wire). This geometry offers experimental insights into the interplay of electron pairing and superconductivity in reduced dimensions.

<sup>1</sup>We gratefully acknowledge financial support from DOE DE-SC0014417 (JL).

**11:27AM L8.00002 1D-1D Coulomb drag in a 6 Million Mobility Bi-layer Heterostructure**, SIMON BILODEAU, McGill University, DOMINIQUE LAROCHE, Sandia National Laboratories, JIAN-SHENG XIA, University of Florida, MIKE LILLY, JOHN RENO, Sandia National Laboratories, LOREN PFEIFFER, KEN WEST, Princeton University, GUILLAUME GERVAIS, McGill University — We report Coulomb drag measurements in vertically-coupled quantum wires. The wires are fabricated in  $\text{GaAs}/\text{AlGaAs}$  bilayer heterostructures grown from two different MBE chambers: one at Sandia National Laboratories ( $1.2\text{M}$  mobility), and the other at Princeton University ( $6\text{M}$  mobility). The previously observed positive and negative drag signals are seen in both types of devices, demonstrating the robustness of the result. However, attempts to determine the temperature dependence of the drag signal in the 1D regime proved challenging in the higher mobility heterostructure (Princeton), in part because of difficulties in aligning the wires within the same transverse subband configuration. Nevertheless, this work, performed at the Microkelvin laboratory of the University of Florida, is an important proof-of-concept for future investigations of the temperature dependence of the 1D-1D drag signal down to a few mK. Such an experiment could confirm the Luttinger charge density wave interlocking predicted to occur in the wires. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL8500.

**11:39AM L8.00003 Electronic structure and transport properties of III-V core/shell nanowires**, FLORINDA VIÑAS, MARTIN LEIJNSE, Solid State Physics, Lund University, Sweden — We have modeled electron structure and low-temperature transport in III-V core/shell nanowires to establish a relationship between electron-hole hybridization and signatures in thermoelectrical measurements. Nanowires with a  $\text{GaSb}$  core and an  $\text{InAs}$  shell (and inverted) are interesting for studies of hybridization effects due to the bulk broken band gap alignment at the material interface. By varying the core radius and shell thickness of such wires we can modify the size of the band gap and create wires with band structures that exhibit hole-electron hybridization states. The band structures are obtained using 8-band  $k \cdot p$  theory together with the envelope function approximation. The calculated energy dispersions are used as input to the Boltzmann equation to study thermoelectric transport quantities such as the Seebeck coefficient, in the diffusive limit.

**11:51AM L8.00004 Visualizing One-Dimensional Electronic States and their Scattering in Semi-conducting Nanowires**<sup>1</sup>, HAIM BEIDENKOPF, JONATHAN REINER, ANDREW NORRIS, ABHAY KUMAR NAYAK, NURIT AVRAHAM, HADAS SHTRIKMAN, Department of Condensed Matter Physics, Weizmann Institute of Science — One-dimensional electronic systems constitute a fascinating playground for the emergence of exotic electronic effects and phases, within and beyond the Tomonaga-Luttinger liquid paradigm. More recently topological superconductivity and Majorana modes were added to that long list of phenomena. We report scanning tunneling microscopy and spectroscopy measurements conducted on pristine, epitaxially grown  $\text{InAs}$  nanowires. We resolve the 1D electronic band structure manifested both via Van-Hove singularities in the local density-of-states, as well as by the quasi-particle interference patterns, induced by scattering from surface impurities. By studying the scattering of the one-dimensional electronic states off various scatterers, including crystallographic defects and the nanowire end, we identify new one-dimensional relaxation regimes and yet unexplored effects of interactions. Some of these may bear implications on the topological superconducting state and Majorana modes therein.

<sup>1</sup>The authors acknowledge support from the Israeli Science Foundation (ISF)

**12:03PM L8.00005 Electrical characterization of surface passivation in III-V nanowires**, GREGORY HOLLOWAY, University of Waterloo, RAY LAPIERRE, McMaster University, JONATHAN BAUGH, University of Waterloo — III-V nanowires are promising for implementing many useful technologies including optical sensing and quantum information processing. However, most native nanowires have a significant density of surface states, which cause electron accumulation at the surface and make the optoelectronic characteristics very sensitive to surface conditions and variable from device to device. To achieve optimum device performance it is imperative to decrease the density of these defects, since they are responsible for charge noise (e.g. random telegraph noise) and decreased carrier mobility. Here we report on experimental results from low temperature transport studies of a series of InAs nanowire field effect transistors, each fabricated with a different surface passivation technique. The different surface treatments include combinations of chemical passivation, growth of a thermal oxide, and deposition of a high- $k$  dielectric to determine the optimum process for passivating the surface states. To better quantify the density of surface states, we also study the axial field magnetoconductance of short-channel nanowire transistors, and show how the results can be used to estimate the degree of surface band-bending.

**12:15PM L8.00006 Electron transport in doped GaAs nanowires contacted by evaporated metal films<sup>1</sup>**, ZHUTING SUN, ANDREI KOGAN, Univ of Cincinnati, TIMOTHY BURGESS, CHENNUPATI JAGADISH, Australian National University — We present electron transport measurements in doped GaAs nanowire samples contacted by metal interfaces as function of temperature. We show that the contact resistance is strongly dependent on  $T$  ( $5K < T < 300K$ ), even though the resistance of the moderately doped nanowires ( $N_D \approx 10^{18} \text{ cm}^{-3}$ ), as expected, display little or no variation with  $T$ . We further show that the classical treatment of the Schottky barriers by Padovani and Stratton [1] fails to adequately describe the temperature dependence of the metal-nanowire interface, and present a corrected model that takes into account charge distribution in the contact region and the effect of the surface states on the nanowire. The nanowires, 100 nm in diameter, were grown by MOCVD growth method. The metal contacts, a 20nm Ti/ 300nm Al films were deposited via e-beam and thermal evaporation. We perform a detailed comparison between data on 9 nominally identical samples to the modified theory and find a good agreement. We also show how the measurement can be used to obtain an estimate of the effective doping density and the mobility of the nanowire. [1]: F.A. Padovani, R. Stratton, Field and thermionic-field emission in Schottky barriers, Solid-State Electronics, Volume 9, Issue 7, 1966

<sup>1</sup>The work is supported by NSF grant DMR-1206784 and University of Cincinnati

**12:27PM L8.00007 Electrostatically-tuned dimensional crossover in nanowires<sup>1</sup>**, MICHELLE TOMCZYK, GUANGLEI CHENG, MENGCHEN HUANG, Univ of Pittsburgh, HYUNGWOO LEE, CHANG-BEOM EOM, Univ of Wisconsin-Madison, PATRICK IRVIN, JEREMY LEVY, Univ of Pittsburgh — The electron system at the interface of two complex oxides,  $\text{LaAlO}_3$  and  $\text{SrTiO}_3$ , exhibits a number of interesting strongly-correlated electronic properties, such as superconductivity and spin-orbit coupling. Reduced dimensionality is made accessible through nanowire devices created with conducting AFM lithography. Here, we describe an electrostatically-controlled dimensionality crossover in weak antilocalization behavior of  $\text{LaAlO}_3/\text{SrTiO}_3$  nanowires at low temperature. These measurements give insight to the interplay of spin-orbit coupling and dimensionality. Characterizing the behavior of the strongly-correlated electronic properties in these reduced dimensions is necessary in order to develop this system as a multifunctional nanoelectronics platform.

<sup>1</sup>We gratefully acknowledge financial support from the following agencies and grants: ARO (W911NF-08-1-0317), AFOSR FA9550-10-1-0524 (JL) and FA9550-12-1-0342 (CBE), and NSF (DMR-1104191, DMR-1124131 (JL), ONR N00014-15-1-2847 (JL) and DMR-1234096 (CBE).

**12:39PM L8.00008 Transport studies of quantum dots sensitized single Mn-ZnO nanowire field effect transistors<sup>1</sup>**, KESHAB R SAPKOTA, FRANCIS SCOTT MALONEY, GAURAB RIMAL, UMA POUDYAL, JINKE TANG, WENYONG WANG, Univ of Wyoming — We present opto-electrical transport properties of Mn-CdSe quantum dots (QDs) sensitized single Mn-ZnO nanowire (NW) field effect transistors (FET). The ZnO NWs with 2 atomic % of Mn doping are grown by chemical vapor deposition. The NWs are ferromagnetic at low temperature. The as grown nanowires are transferred to clean  $\text{SiO}_2/\text{Si}$  substrate and single nanowire field effect transistors (FET) are fabricated by standard e-beam lithography. Mobility and carrier concentration of Mn-ZnO NWs are estimated from FET device measurement which shows NWs are n-type semiconductors. Pulse laser deposition of Mn-CdSe QDs on the single NW FET significantly increases carrier concentration of the QD-NW system in dark where the QD monolayer conduction is negligibly small. The photoconductivity study of QD sensitized NW FET enlightens the conduction spectrum of QD-NW system and QD to NW carrier transfer mechanism.

<sup>1</sup>This work has been supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02- 10ER46728.

**12:51PM L8.00009 Thermally Active Screw Dislocations in Si, SiC, PbSe, and SiGe Nanowires.**, JIHONG AL-GHALITH, YUXIANG NI, University of Minnesota, Twin Cities, SHIYUN XIONG, Max Planck Institute for Polymer Research, SEBASTIAN VOLZ, Ecole Centrale Paris, TRAIAN DUMITRICA, University of Minnesota, Twin Cities — We elucidate thermal conductivity along the screw dislocation line, which represents a transport direction inaccessible to classical theories. By using equilibrium and non-equilibrium molecular dynamics simulations, and the atomistic Green function method, we uncover a Burgers vector dependent thermal conductivity reduction in Si, SiC, PbSe, and SiGe nanowires. The effect is uncorrelated with the classical theory of Klemens. The influence of dislocations on thermal transport originates in the highly deformed core region, which represents a significant source of anharmonic phonon-phonon scattering. High strain reduces the phonon relaxation time, especially in the longitudinal acoustic branches, and creates an effective internal thermal resistance around the dislocation axis. The effect can be distinguished from the thermal transport reduction caused by the nanowire surface imperfections and vacancies. Our results have implications for designing materials useful for high-temperature electronics and thermoelectric applications.

**1:03PM L8.00010 A New One-dimensional Quantum Material -  $\text{Ta}_2\text{Pd}_3\text{Se}_8$  Atomic Chain**, XUE LIU, JINYU LIU, JIN HU, CHUNLEI YUE, ZHIQIANG MAO, JIANG WEI, Tulane University, LIUBOV ANTIPINA, PAVEL SOROKIN, Technological Institute for Superhard and Novel Carbon Materials, ANA SANCHEZ, University of Warwick — Since the discovery of carbon nanotube, there has been a persistent effort to search for other one dimensional (1D) quantum systems. However, only a few examples have been found. We report a new 1D example - semiconducting  $\text{Ta}_2\text{Pd}_3\text{Se}_8$ . We demonstrate that the  $\text{Ta}_2\text{Pd}_3\text{Se}_8$  nanowire as thin as 1.3nm can be easily obtained by applying simple mechanical exfoliation from its bulk counterpart. High resolution TEM shows an intrinsic 1D chain-like crystalline morphology on these nano wires, indicating weak bonding between these atomic chains. Theoretical calculation shows a direct bandgap structure, which evolves from 0.53eV in the bulk to 1.04eV in single atomic chain. The field effect transistor based on  $\text{Ta}_2\text{Pd}_3\text{Se}_8$  nanowire achieved a promising performance with  $10^4$  On/Off ratio and  $80 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$  mobility. Low temperature transport study reflects two different mechanisms, variable range hopping and thermal activation, which dominate the transport properties at different temperature regimes.  $\text{Ta}_2\text{Pd}_3\text{Se}_8$  nanowire provides an intrinsic 1D material system for the study low dimensional condensed matter physics.

**1:15PM L8.00011 Gate field induced switching of electronic current in Si-Ge Core-Shell nanowire quantum dots: A first principles study**, KAMAL B DHUNGANA, University of Iowa, MEGHNATH JAISHI, RANJIT PATI, Michigan Technological University — Core-shell nanowires are formed by varying the radial composition of the nanowires. One of the most widely studied core-shell nanowire groups in recent years is the Si-Ge and Ge-Si core-shell nanowires. Compared to their pristine counterparts, they are reported to have superior electronic properties. For example, the scaled ON state current value in a Ge-Si core-shell nanowire field effect transistor (FET) is reported to be three to four times higher than that observed in state-of-the-art-metal oxide semiconductor FET (MOSFET) (*Nature*, 441, 489 (2006)). Here, we study the transport properties of the pristine Si and Si-Ge core-shell nanowire quantum dots of similar dimension to understand the superior performance of Si-Ge core-shell nanowire field effect transistor. Our calculations yield excellent gate field induced switching behavior in current for both pristine Si and Si-Ge core-shell hetero-structure nanowire quantum dots. The threshold gate bias for ON/OFF switching in the Si-Ge core-shell nanowire is found to be much smaller than that found in the pristine Si nanowire. A single particle many-body Green's function approach in conjunction with density functional theory is employed to calculate the electronic current.

**1:27PM L8.00012 Exploring Dynamics and Band Structure in Mid Infrared GaAsSb and GaAsSb/InP Nanowire Heterostructures<sup>1</sup>**, LEIGH SMITH, YUDA WANG, NADEEKA WICKRAMASURIYA, SAMUEL LINSE, HOWARD JACKSON, Department of Physics, University of Cincinnati, XIAOMING YUAN, PHILIPPE CAROFF, HOE TAN, CHENNUPATI JAGADISH, Department of Electronic Materials Engineering, Australian National University — We study the carrier recombination dynamics and band structure of GaAs<sub>1-x</sub>Sb<sub>x</sub> and GaAs<sub>1-x</sub>Sb<sub>x</sub>/InP core/shell nanowires (NWs) grown by MOCVD. Using Transient Rayleigh Scattering (TRS) measurements and Raman scattering measurements in single unstrained bare core and strained core-shell NWs, we measure the strain distributions in the core and shell and its effect on band structures. At 10 K, the band gap of the GaAs<sub>0.7</sub>Sb<sub>0.3</sub> core is seen using TRS to move to lower energy because of the tensile strain from the InP shell. This tensile strain is confirmed by micro-Raman which show the InP phonons shift to higher frequencies while the GaAs<sub>0.7</sub>Sb<sub>0.3</sub> phonons move to lower frequencies. The recombination lifetimes in bare GaAs<sub>0.7</sub>Sb<sub>0.3</sub> NWs are found to be less than the 50 ps at all temperatures, which is limited by our system response. In contrast, the lifetimes measured in the GaAs<sub>0.7</sub>Sb<sub>0.3</sub>/InP core/shell NWs are 820ps at 10K and 130ps at 300K. This significant lifetime enhancement reflects the effectiveness of the InP shell surface passivation. We infer that the surface recombination velocity reduces from ~100,000 cm/s to ~3,000 cm/s in the core-shell NW.

<sup>1</sup>We acknowledge the financial support of NSF DMR 1507844, DMR 151373 and ECCS 1509706 and the Australian Research Council.

**1:39PM L8.00013 ABSTRACT WITHDRAWN —**

**1:51PM L8.00014 WHY A MAGNETIZED QUANTUM WIRE CAN ACT AS AN OPTICAL AMPLIFIER**, MANVIR KUSHWAHA, Rice University — We discuss the fundamental issues associated with the magnetoplasmon excitations in a semiconducting quantum wire characterized by a harmonic confining potential and subjected to an applied (perpendicular) magnetic field. The problem involves two length scales:  $l_0 = \sqrt{\hbar/m^*\omega_0}$  and  $l_c = \sqrt{\hbar/m^*\omega_c}$ , which characterize the strengths of the confinement and the magnetic field ( $B$ ). Essentially, we focus on the device aspects of the intersubband collective (magnetoroton) excitation, which observes a negative group velocity between maxon and roton. Existence of the negative group velocity is a clear manifestation of a medium with population inversion brought about due to a metastable state caused by the magnetic field that satisfies the condition  $B > B_{th}$ ;  $B_{th}$  being the threshold value below which the magnetoroton does not exist. A medium with an inverted population has the remarkable ability of amplifying a small optical signal of definite wavelength. An extensive scrutiny of the gain coefficient suggests an interesting and important application: the electronic device designed on the basis of such magnetoroton modes can act as an optical amplifier<sup>1</sup>. 1. M.S. Kushwaha, J. Appl. Phys. 109, 106102 (2011).

**2:03PM L8.00015 Focused Gold Ion Implantation for Conducting Wires**, TODD BRINTLINGER, Naval Research Lab — With the advent of non-Ga ion sources in commercial focused-ion-beam (FIB) systems, new possibilities have arisen for lithographic devices. We demonstrate that focused gold ions can be directly implanted into silicon nitride to form conducting wires. The focused gold ion beam is formed from a binary alloy AuSi source with a deep eutectic temperature, where the gold ions are sorted from the silicon ions with in an ExB filter. Using a 15 pA beam, single-pass lines (dose 1.0-1.5 nC/cm) are written to create several wires in the gap between existing gold electrodes on a silicon nitride membrane. To allow for overlap between the deposited gold wires and the electrodes, the lines are written on top of the existing gold electrodes, as well as in the gap, giving rise to rapid gold-on-gold sputtering in the electrodes, but leaving behind the aforementioned gold wire in the silicon nitride. Full-width, half-max linewidth of wires is 110-140 nm. Atomic force microscopy reveals significant ion sputtering in existing gold electrodes, as already seen in scanning electron microscope, but shows that implanted gold ion wires exist in subsurface with minimal topographic distortion to silicon nitride membrane. Voltage sweeps reveal linear, length-dependent, currents passing through the gold wires.

**Wednesday, March 16, 2016 11:15AM - 2:15PM —**

**Session L11 DMP: Novel Physics of Fe-Pnictide Superconductors** 307 - Ming Yi, UC Berkeley

**11:15AM L11.00001 Origin of superconductivity in KFe<sub>2</sub>As<sub>2</sub> under positive and negative pressures and relation to other Fe-based families<sup>1</sup>**, ROSER VALENTI, Institute of Theoretical Physics, University of Frankfurt — KFe<sub>2</sub>As<sub>2</sub> shows an intricate behavior as a function of pressure. At ambient pressure the system is superconductor with a low critical temperature  $T_c=3.4$  K and follows a V-shaped pressure dependence of  $T_c$  for moderate pressures with a local minimum at a pressure of 1.5 GPa. Under high pressures  $P_c=15$  GPa, KFe<sub>2</sub>As<sub>2</sub> exhibits a structural phase transition from a tetragonal to a collapsed tetragonal phase accompanied by a boost of the superconducting critical temperature up to 12 K. On the other hand, *negative* pressures realized through substitution of K by Cs or Rb decrease  $T_c$  down to 2.25K. In this talk we will discuss recent progress on the understanding of the microscopic origin of this pressure-dependent behavior by considering a combination of ab initio density functional theory with dynamical mean field theory and spin fluctuation theory calculations [1-3]. We will argue that a Lifshitz transition associated with the structural collapse changes the pairing symmetry from *d*-wave (tetragonal) to  $s_{\pm}$  (collapsed tetragonal) at high pressures while at ambient and negative pressures correlation effects appear to be detrimental for superconductivity. Further, we shall establish cross-links to the chalcogenide family, in particular FeSe under pressure [4]. [1] S. Backes, D. Guterding, H. O. Jeschke, R. Valenti, New J. Phys. 16, 083025 (2014). [2] D. Guterding, S. Backes, H. O. Jeschke, R. Valenti, Phys. Rev. B 91, 140503(R) (2015). [3] S. Backes, H. O. Jeschke, R. Valenti, Phys. Rev. B (in press). [4] J. K. Glasbrenner, I. I. Mazin, H. O. Jeschke, P. J. Hirschfeld, R. Valenti Nature Physics 11, 953 (2015).

<sup>1</sup>The Deutsche Forschungsgemeinschaft (DFG) is gratefully acknowledged for financial support.

**11:51AM L11.00002 ARPES investigation of Fe-based superconductor  $\text{KFe}_2\text{As}_2$  and related compounds**, PIERRE RICHARD, X. SHI, B.-Q. LV, P. ZHANG, T. QIAN, H. DING, Institute of Physics, Chinese Academy of Sciences (CAS), T. K. KIM, M. HOESCH, Diamond Light Source, D.-L. FANG, H.-H. WEN, Nanjing University, X.-H. CHEN, University of Science and Technology of China, A. VAN ROEKEGHEM, P. SETH, S. BIERMANN, Ecole Polytechnique (France) —  $\text{KFe}_2\text{As}_2$  is the end-member of the  $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$  family of Fe-based superconductors. Despite a small  $T_c$  of 3 K, this compound is of particular interest because unlike the other members of this family of superconductors, the Fermi surface of  $\text{KFe}_2\text{As}_2$  is free of electron pocket. Interest for this material was intensified following various reports on possible nodal superconducting order parameters in this system. Due to its momentum-resolved capabilities, angle-resolved photoemission spectroscopy (ARPES) is particularly suitable for investigating the key aspects of the electronic structure of materials. In this work we present recent ARPES data of  $\text{KFe}_2\text{As}_2$  and related materials.

**12:03PM L11.00003 Pauli Limiting and Multi-Band Superconductivity in  $\text{KFe}_2\text{As}_2$  Studied by Small-Angle Neutron Scattering**<sup>1</sup>, M.R. ESKILDSEN, S.J. KUHN, University of Notre Dame, H. KAWANO-FURUKAWA, M. ONO, Ochanomizu University, Japan, E.M. FORGAN, E. JELLYMAN, R. RIYAT, University of Birmingham, United Kingdom, C.H. LEE, K. KIHOU, AIST, Japan, F. HARDY, TH. WOLF, C. MEINGAST, Karlsruhe Institute of Technology, Germany, J.L. GAVILANO, Paul Scherrer Institute, Switzerland — We have studied the intrinsic anisotropy of the superconducting state in  $\text{KFe}_2\text{As}_2$ , using used small-angle neutron scattering to image the vortex lattice (VL) as the applied magnetic field is rotated towards the FeAs planes. The anisotropy is found to be strongly field dependent, indicating multi-band superconductivity. Furthermore, the high field anisotropy significantly exceeds that of the upper critical field, providing further support for Pauli limiting in  $\text{KFe}_2\text{As}_2$  for field applied along the basal plane. Finally, we are able determine the contribution to the field modulation in the mixed state due to Pauli Paramagnetic Effects by measuring both the non-spin flip and spin flip VL scattered intensity. This represents the first instance where all the effects listed above have been obtained simultaneously and in a comprehensive manner by a single experimental technique.

<sup>1</sup>This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences under Award DE-FG02-10ER46783.

**12:15PM L11.00004 Correlation-enhanced odd-parity inter-orbital singlet pairing in the iron-pnictide superconductor  $\text{LiFeAs}$** <sup>1</sup>, REZA NOURAFKAN, Université de Sherbrooke, GABRIEL KOTLIAR, Rutgers University, A.-M. S. TREMBLAY, Université de Sherbrooke — The rich variety of iron-based superconductors and their complex electronic structure lead to a wide range of possibilities for gap symmetry and pairing components. Here we solve in the 2-Fe Brillouin zone the full frequency-dependent linearized Eliashberg equations for  $\text{LiFeAs}$  with spin-fluctuation mediated pairing interactions. The magnetic excitations are calculated with the random phase approximation on a correlated electronic structure obtained with density functional theory and dynamical mean field theory. Correlations induce long-lived local moments with orbital-dependent dynamics. The interaction between electrons through Hund's coupling promotes both the intra-orbital  $d_{xz}(yz)$  and the inter-orbital magnetic susceptibility. As a consequence, the leading pairing channel acquires sizeable inter-orbital  $d_{xy}-d_{xz}(yz)$  singlet pairing with odd parity under glide-plane symmetry. These components reduce the superconducting gap magnitude induced by the intra-orbital components of the gap function at the electron pockets intersection where the Fe-d  $t_{2g}$  orbitals strongly mix. The combination of intra- and inter-orbital components makes the results consistent with available experiments on the angular dependence of the gaps observed on the different Fermi surfaces.

<sup>1</sup>Supported by NSERC, CIFAR and the Tier I Canada Research Chair Program

March 14 (Monday) to March 16 (Wednesday) in the program, since I have to depart Baltimore on March 17 (Thursday).

**12:27PM L11.00005 Superconducting mechanism in Fe-based superconductors**, HIROSHI KONTANI, YOUNG KIM, University of Tokyo — The rich variety of the phase diagrams in Fe-based superconductors, such as the coexistence of superconductivity and magnetic order, has been explained by the mean-field level approximations. Recently, we explained the phase diagrams including the Aslamazov-Larkin vertex correction (AL-VC). The nematoclastic study, we analyze the superconducting states in FeSe and  $\text{LaFeAsO}$ , by a study of the structures are induced by the strong orbital and spin fluctuations driven by orbital fluctuations is strongly enlarged by the AL-VC for the anomalous superconducting mechanism. [1] Y. Yamakawa, S. Onari and H. Kontani, arXiv:1509.01163.

I would appreciate your consideration of my request.

**12:39PM L11.00006 ABSTRACT WITHDRAWN —**

**12:51PM L11.00007 The Magnetic Excitations in Optimal Doped  $\text{BaFe}_2(\text{As}_{0.7}\text{P}_{0.3})_2$** <sup>1</sup>, DING HU, SHILIANG LI, Chinese Academy of Sci (CAS), PENGCHENG DAI, Rice University — High temperature superconductivity in iron based superconductors emerges near the boundary of static antiferromagnetic order which is suppressed by doping or pressure. Although spin fluctuations may be responsible for superconductivity, there is still no consensus on the mechanism. As a unique system in 122-type iron pnictides, the phosphorus doping in the arsenic position in  $\text{BaFe}_2\text{As}_2$  does not induce external carrier and impurity scattering, but the maximum  $T_c = 30\text{K}$ . We have carried out inelastic neutron scattering experiment on Time of Flight Spectrometers, and mapped out the whole spin fluctuation up to 300meV. Our results are consistent with the combined DFT and DMFT calculation results, which confirm that pnictogen height is correlated with the electron-electron correlation strength and consequently the effective bandwidth of magnetic excitations in iron pnictides.

<sup>1</sup>Support from MOST and U.S. NSF

**1:03PM L11.00008 Doping evolution of magnetization hysteresis in (Ba<sub>1-x</sub>K<sub>x</sub>)Fe<sub>2</sub>As<sub>2</sub> single crystals: Crossover from the second magnetization peak to peak effect<sup>1</sup>**, YONG LIU<sup>2</sup>, THOMAS LOGRASSO, Ames Lab — Magnetic hysteresis loops (MHLs) have been systematically measured in a series of (Ba<sub>1-x</sub>K<sub>x</sub>)Fe<sub>2</sub>As<sub>2</sub> single crystals from underdoped  $x=0.177$  to end member  $x=1$  with applied magnetic fields parallel to  $c$  axis ( $H//c$ ). The second magnetization peak (SMP) or fishtail effect was observed within the doping range  $0.177 \leq x \leq 0.650$ . Remarkably, with further increasing doping the SMP becomes narrow and emerges very close to the irreversible field ( $H_{irr}$ ) for the samples  $0.692 \leq x \leq 0.910$ . The similar peak effect (PE) had been widely observed in various conventional or low  $T_c$  superconductors. Meanwhile, the magnetization curves change from symmetrical to asymmetric hysteresis loops, which suggests a dominant surface pinning instead of bulk pinning in the samples. Our findings demonstrate that (Ba<sub>1-x</sub>K<sub>x</sub>)Fe<sub>2</sub>As<sub>2</sub> system is a very unique system that links the SMP and PE by its doping dependence. Our results will lead to a better understanding of the underlying mechanisms for the origin of the SMP and PE.

<sup>1</sup>This work was supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences, Materials Science and Engineering Division.

<sup>2</sup>crystal growth, superconductivity, magnetism

**1:15PM L11.00009 Orbital and Pauli limiting effects in heavily doped Ba<sub>0.05</sub>K<sub>0.95</sub>Fe<sub>2</sub>As<sub>2</sub>.<sup>1</sup>**, S. ZHANG, Y. P. SINGH, X. Y. HUANG, Kent State University, X. J. CHEN, Shanghai Laboratory of High Pressure Science & Technology Advanced Research, M. DZERO, C. C. ALMASAN, Kent State University — We investigated the thermodynamic properties of the Fe-based lightly-disordered superconductor Ba<sub>0.05</sub>K<sub>0.95</sub>Fe<sub>2</sub>As<sub>2</sub> in external magnetic field  $H$  applied along the FeAs layers ( $H||ab$  planes). The superconducting (SC) transition temperature for this doping level is  $T_c = 6.6$  K. Our analysis of the specific heat  $C(T,H)$  measured for  $T < T_c$  implies a sign change of the superconducting order parameter across different Fermi pockets. We provide experimental evidence for the three components superconducting order parameter. We find that all three components have values which are comparable with the previously reported ones for the stoichiometric compound KFe<sub>2</sub>As<sub>2</sub>. Our data for  $C(T,H)$  and resistivity  $\rho(T, H)$  can be interpreted in favor of the dominant orbital contribution to the pair-breaking mechanism at low fields, while Pauli limiting effect dominates at high fields, giving rise to a gapless superconducting state with only the leading non-zero gap.

<sup>1</sup>This work has been supported by the US NSF (Grant Nos. DMR-1506547 and DMR-1505826) at KSU. M.D. also acknowledges financial support from KSU and MPI-PKS.

**1:27PM L11.00010 Can oxygen deficient SmFeAsO<sub>1-x</sub> be synthesized?: Unintentional incorporation of hydride ion at oxygen vacancy site**, YOSHINORI MURABA, Materials Research Center for Element Strategy, SUSHI IIMURA, Materials and Structures Laboratory, Tokyo Institute of Technology, SATORU MATSUSHI, HIDEO HOSONO, Materials Research Center for Element Strategy, Tokyo Institute of Technology — Hydrogen substitution and introduction of oxygen vacancy are effective electron doping methods for the  $LnFeAsO$ . However, their  $T_c$  vs  $e^-/Fe$  diagrams do not entirely overlap each other, while  $T_c$  vs lattice dimension relationships are very similar. These contradictions can be understood by assuming that unintentional hydrogen is incorporated into the oxygen vacancy. To examine the preferred electron-dopant species in  $LnFeAsO$  and the influence of the atmosphere during synthesis on the formation of  $LnFeAsO_{1-x}$ , we try to synthesize the SmFeAsO<sub>1-x</sub> under three well-controlled atmosphere ( $H_2O$ ,  $H_2$  and  $H_2O$ - and  $H_2$ -free). Under  $H_2O$  and  $H_2$  atmosphere, hydrogen were incorporated at oxygen sites as the hydride ion and SmFeAsO<sub>1-x</sub>H<sub>x</sub> was formed. On the other hand, when  $H_2O$  and  $H_2$  were removed from synthetic process, nearly stoichiometric SmFeAsO was formed. Furthermore, DFT calculations showed that H-substituted samples are more stable than oxygen deficient samples. These results strongly imply that the reported  $LnFeAsO_{1-x}$  was contaminated with unintentional hydrogen and  $LnFeAsO_{1-x}H_x$  was misidentified as  $LnFeAsO_{1-x}$ .

**1:39PM L11.00011 Neutron diffraction study of 154SmFeAsO<sub>1-x</sub>D<sub>x</sub>**, SUSHI IIMURA, HIROSHI OKANISHI, Materials and Structures Laboratory, Tokyo Tech., SATORU MATSUSHI, Materials Research Center for Element Strategy, Tokyo Tech., HARUHIRO HIRAKA, KAZUTAKA IKEDA, Institute of Materials Structure Science, KEK, THOMAS HANSEN, Institut Laue-Langevin, TOSHIYA OTOMO, Institute of Materials Structure Science, KEK, HIDEO HOSONO, Materials and Structures Laboratory, Tokyo Tech. — Hot issue in unconventional superconductors (SC) is why the 2nd highest- $T_c$  of 56 K after cuprates is accomplished in the 1111-type iron-oxyarsenides  $LnFeAsO_{1-x}Fx$  ( $Ln =$  lanthanide). Recently, utilizing a hydride-substitution-method ( $O^{2-} = H^- + e^-$ ) in the  $LnFeAsO_{1-x}H_x$  [1], we found a second SC phase in  $0.18 \leq x \leq 0.45$  at  $Ln = La$  in addition to the first one adjacent to the antiferromagnetic (AFM) order [2], and another AFM order accompanying a unique structural transition in over-doped region  $x > 0.4$  [3]. However, since the  $T_c$  of La-system is lower than the other systems, i.e.,  $Ln = Ce, Sm$  and so on, it is still unclear whether the second AFM phase is essential for their high- $T_c$  or not. Thus, we synthesized the isotope-substituted 154SmFeAsO<sub>1-x</sub>D<sub>x</sub> and performed neutron powder diffraction (NPD) to examine the structural and magnetic properties of the high- $T_c$  1111 system. In this talk, we show the results of NPD data and discuss the relation between the superconducting, magnetic, and structural properties of the 154SmFeAsO<sub>1-x</sub>D<sub>x</sub> and electron-doping-effect on it. [1] T. Hanna, et al. PRB 85, 024521 (2011). [2] S. Iimura, et al. Nat. Commun. 3, 943 (2012). [3] M. Hiraishi et al. Nat. Phys. 10, 300 (2014).

**1:51PM L11.00012 Role of Hydrogen in the Electronic Properties of H-rich Pnictide Superconductors**, YINA HUANG, University of California Davis, XIANGLONG YU, DAYONG LIU, Institute of Solid State Physics, Chinese Academy of Sciences, LIANGJIAN ZOU, University of Science and Technology of China — The electronic and magnetic properties of the parent material CaFeAsH and its La/Co-doped compounds are investigated using first-principles calculations based on the generalized gradient approximation (GGA). We predict that the ground state of CaFeAsH is a spin-density-wave (SDW)-type striped antiferromagnet driven by Fermi surface nesting. We find a sandglass-type hole pocket near the  $\Gamma$  point in CaFeAsH that is not present in CaFeAsF. In comparison with CaFeAsF, the sandglass-shaped pocket, mainly contributed from Fe  $d_{xz} + d_{yz}$  orbitals, arises from the weak oxidation of CaH layers and the hybridization enhancement between FeAs layers. In contrast, the electronic properties of electron doped Ca<sub>0.75</sub>La<sub>0.25</sub>FeAsH and CaFe<sub>0.75</sub>Co<sub>0.25</sub>AsH indicate that La or Co doping almost does not affect the sandglass-type Fermi surface, while the suppression of Fermi surface nesting in Ca<sub>0.75</sub>La<sub>0.25</sub>FeAsH is weaker than that in CaFe<sub>0.75</sub>Co<sub>0.25</sub>AsH. This features may contribute to the higher  $T_c$  in La-substituted CaFeAsH.

**2:03PM L11.00013 Nanofabrication of Point Contact Junctions for Spectroscopic Studies of High-Temperature Superconductors<sup>1</sup>** , HAN ZHAO, OMAR MEHIO, WAN KYU PARK, JAMES ECKSTEIN, University of Illinois Urbana-Champaign, LAURA GREENE, National High Magnetic Field Laboratory, Florida State University — Point contact spectroscopy (PCS) probes the superconducting order parameter from Andreev reflection conductance spectrum. A new method to achieve robust junctions with a precise control of the geometry of the point contact by focused ion beam (FIB) nanofabrication techniques is currently under development. Preliminary application on niobium thin films shows consistent data that is insensitive to thermal cycling. This opens the possibility to perform PCS on a series of materials as a function of external variables, including temperature, magnetic field as a function of angle, and stress. Our preliminary data as a function of junction size show the expected resistance dependence, which will help us to determine more precisely when junctions are in the ballistic, or spectroscopic regime. Our plan is to apply this newly-developed method to probe the electronic nematic state in iron-based superconductors under applied magnetic field and uniaxial stress, to further understand the origin of the nematicity.

<sup>1</sup>This work is carried out in part in the Materials Research Lab, University of Illinois and is supported by the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the US DOE, Office of Science, Award No. DE-AC0298CH1088.

**Wednesday, March 16, 2016 11:15AM - 2:15PM –**  
**Session L12 DPOLY FIAP: From Nano to Meso: Assembly Structure and Dynamics of Polymers and Polymer Nanocomposite Thin Films II - Industry Day** 308 - Neal Brant, Miliken, Inc.

**11:15AM L12.00001 Nanoparticles in Polymers: Assembly, Rheology and Properties** , YUANQIAO RAO<sup>1</sup>, The Dow Chemical Company — Inorganic nanoparticles have the potential of providing functionalities that are difficult to realize using organic materials; and nanocomposites is an effective mean to impart processibility and construct bulk materials with breakthrough properties. The dispersion and assembly of nanoparticles are critical to both processibility and properties of the resulting product. In this talk, we will discuss several methods to control the hierarchical structure of nanoparticles in polymers and resulting rheological, mechanical and optical properties. In one example, polymer-particle interaction and secondary microstructure were designed to provide a low viscosity composition comprising exfoliated high aspect ratio clay nanoparticles; in another example, the microstructure control through templates was shown to enable unique thermal mechanical and optical properties.

<sup>1</sup>Jeff Munro, Stephanie Potisek, Phillip Hustad; all of the Dow Chemical Company are co-authors

**11:51AM L12.00002 Pressure-Directed Assembly: Nanostructures Made Easy** , HONGYOU FAN, Sandia National Laboratories — Precise control of structural parameters through nanoscale engineering to improve optical and electronic properties of functional nanomaterials continuously remains an outstanding challenge. Previous work has been conducted largely at ambient pressure and relies on specific chemical or physical interactions such as van der Waals interactions, dipole-dipole interactions, chemical reactions, ligand-receptor interactions, etc. In this presentation, I will introduce a new pressure-directed assembly method that uses mechanical compressive force applied to nanoparticle arrays to induce structural phase transition and to consolidate new nanomaterials with precisely controlled structures and tunable properties. By manipulating nanoparticle coupling through external pressure, instead of through chemistry, a reversible change in their assemblies and properties can be achieved and demonstrated. In addition, over a certain threshold, the external pressure will force these nanoparticles into contact, thereby allowing the formation and consolidation of one- to three-dimensional nanostructures. Through pressure induced nanoparticle assembly, materials engineering and synthesis become remarkably flexible without relying on traditional crystallization process where atoms/ions are locked in a specific crystal structure. Therefore, morphology or architecture can be readily tuned to produce desirable properties for practical applications. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

**12:27PM L12.00003 X-ray Studies of Nano Composites<sup>1</sup>** , ALEXANDER HEXEMER, LBNL — Nano composite materials are an exciting and fast expanding field. X-ray scattering has been used in order to study the structure properties relation. During the last few years the field has expanded more towards the field of thin films where there's been a dramatic increase in the use of grazing incidence small angle X-ray scattering (GISAXS). The main issue of GISAXS has been the complex analysis framework necessary for simulating and fitting. In addition, existing software has restricted the scientist in systems that can be simulated and the speed to analyze large amounts of data. Over the last few years we have worked closely with our computational research and supercomputer division to enable the use of supercomputers to simulate at scattering data. We have developed a comprehensive analysis framework to simulate and fit a wide variety of materials and morphologies. The framework is designed to supply scientists with close to real-time feedback during beam times. Therefore, HipGISAXS (High Performance GISAXS) has been developed to run simulations on massively parallel platforms such as the Oak Ridge Supercomputer Titan (OLCF). Further, with inverse modeling algorithms for fitting available in HipGISAXS, such as particle swarm optimization, it can handle a large number of parameters during the structure fitting process. In September of 2014, HipGISAXS was used in a real time demonstration that married the SAXS/WAXS beamline at the ALS with the data handling and processing capabilities at NERSC, and simulation capabilities of running at-scale simulations on Titan at OLCF.

<sup>1</sup>DOE Early Career Award, SPOT and CAMERA

**1:03PM L12.00004 Swelling and viscoelasticity in photoresist thin films** , PRAVEEN AGARWAL, The Dow Chemical Company — For a wide range of electronic applications, polymers are processed in the thin film state with the film thickness lower than 100 nm. Understanding the polymer structure property relationship at those characteristic length scales is important to enable the material design for various applications. Extreme ultraviolet lithography (EUVL) is the next generation lithographic technique using low wavelength (13.5 nm) ultraviolet radiation. Quality of the final pattern in the lithographic process depends on the performance of the photoresist polymer during multiple processing steps. Photoresist material development for the EUV lithography presents several challenges for controlling the thin film swelling, density and outgassing. In particular, it has been proposed in the literature that pattern collapse, a lithographic defect where the desired features become deformed, can be caused by the swelling of the photoresist material. In this presentation, the effect of photoresist formulation and architecture on the thin film swelling and viscoelasticity will be discussed. We find that the quencher base could have a significant effect on the swelling characteristics of the photoresist. Additionally, swelling characteristics of the photoresists with covalently bound vs. blended photoacid generator (PAG) were found to be significantly different.

**1:39PM L12.00005 Patterning Multicomponent Polymer Thin Films via Dynamic Thermal Processing** , GURPREET SINGH, Intel Corporation — Bottom-up patterning is gaining increased importance owing to the physical limitations and rising costs of top-down patterning. One example of bottom-up patterning is self-assembling polymer thin films. Although there are several pathways to facilitate polymer thin film self-assembly, this presentation will focus on dynamic thermal field based processes for patterning multicomponent polymer thin films. Dynamic thermal field processing is an attractive rolltoroll (R2R) amenable directed selfassembly (DSA) method for molecular level organization of multicomponent polymer systems such as block copolymer thin films over large areas without requiring guiding templates. The talk will first outline how parameters such as magnitude of the temperature gradient, velocity of annealing, thermal expansion, and molecular weight of the polymer can be optimized to finely tune the morphology of the block copolymer thin films and also elucidate their associated physical mechanisms. The second part of the talk will outline application of dynamic thermal field processes for fabricating functional nanomaterials and discuss the recent advancements achieved using these processes.

## Wednesday, March 16, 2016 11:15AM - 2:15PM –

Session L13 DAMOP: New Phenomena in 2D Fermi Gases 309 - Cheng Chin, University of Chicago

### 11:15AM L13.00001 A strongly interacting two-dimensional Fermi gas , SELIM JOCHIM, Heidelberg University

— We will present our progress realizing two-dimensional superfluids with ultracold fermionic lithium atoms confined in a quasi two-dimensional potential. In this setting, a generic two-dimensional Fermi gas is realized with interactions tunable to any value within the short-range limit. We measured the phase diagram for this system and found the coherence properties to be decaying algebraically, a signature of the Beresinskii-Kosterlitz-Thouless phase which is expected for a homogeneous two-dimensional superfluid. We furthermore extracted from our data the equation of state, which will be an important benchmark for many body theories. We are currently working to transfer our fermionic atoms into an optical lattice potential. Our vision to realize exotic superfluidity in this system will be discussed.

### 11:51AM L13.00002 Experimental studies of spin-imbalanced Fermi gases in 2D geometries<sup>1</sup> , JOHN THOMAS, North Carolina State University

— We study the thermodynamics of a quasi-two-dimensional Fermi gas, which is not quite two-dimensional (2D), but far from three dimensional (3D). This system offers opportunities to test predictions that cross interdisciplinary boundaries, such as enhanced superfluid transition temperatures in spin-imbalanced quasi-2D superconductors, and provides important benchmarks for calculations of the phase diagrams. In the experiments, an ultra-cold Fermi gas is confined in an infrared CO<sub>2</sub> laser standing-wave, which produces periodic pancake-shaped potential wells, separated by 5.3  $\mu\text{m}$ . To study the thermodynamics, we load an ultra-cold mixture of  $N_1 = 800$  spin-up and  $N_2 < N_1$  spin-down <sup>6</sup>Li atoms into each well and image the individual cloud profiles as a function of interaction strength and spin imbalance  $N_2/N_1$ . The measured properties are in disagreement with 2D-BCS theory, but can be fit by a 2D-polaron gas model, where each atom is surrounded by a cloud of particle-hole pairs of the opposite spin. However, this model fails to predict a transition to a spin-balanced central region as  $N_2/N_1$  is increased.

<sup>1</sup>Supported by the physics divisions of ARO, AFOSR, and NSF and by the Division of Materials Science and Engineering, the Office of Basic Energy Sciences, DOE.

### 12:27PM L13.00003 Fermi-to-Bose crossover in a trapped quasi-2D gas of fermionic atoms , ANDREY TURLAPOV, Institute of Applied Physics, Russian Academy of Sciences

— Neither long-range order nor Bose condensation may appear in uniform 2D systems at finite temperature. Despite that, 2D superconductors, such as cuprates, are among the systems with highest critical temperatures. 2D quantum systems remain intriguing, and their understanding is incomplete despite huge progress seen in the recent decades. Ultracold atoms are a platform for studying 2D physics. Using tunability of atomic gases, we have realized a crossover between a 2D gas of Fermi atoms and a 2D gas of weakly-bound diatomic Bose molecules by varying s-wave interactions in the gas. Between these two asymptotic states, there is a regime of strong interactions, whose quantitative description is challenging, e. g., a mean field of Cooper pairs fails to describe the crossover even qualitatively, unlike in 3D gases. At the lowest achievable temperatures,  $\sim 10\%$  of the Fermi energy, the pressure is measured in the whole Fermi-to-Bose crossover and compared with the available theoretical models, including those which appeared over the last year. In the Fermi regime of weak interactions, the pressure is systematically above a Fermi-liquid-theory prediction, which maybe due to mesoscopic effects. Alternatively, this upshift is partially reproduced within a recent mean-field theory supplemented with fluctuations. On the Bose side of the crossover, the molecules easily condense, which is found in interferometric measurements. On one hand, such condensation is expected because the gas is held in a nearly harmonic trap, which favors condensation unlike the uniform space. On the other hand, each molecule is locally in a flat potential, which is the sum of the trap and the strong repulsive mean field, and this should inhibit the condensation.

### 1:03PM L13.00004 Quasi-condensation in trapped two-dimensional Fermi gases<sup>1</sup> , BRANDON ANDERSON, James Franck Institute

— It is well known that the Mermin-Wagner theorem prohibits true long range order 2D systems. Nevertheless, recent experiments [1,2] provide strong evidence that 2D Fermi gases undergo a form of pair condensation, along with aspects of BKT physics. In this talk we apply a BCS-BEC theory (which is compatible with the Mermin-Wagner theorem) to characterize the nature of pair (quasi-) condensation in 2D Fermi gases. Here we follow the same analysis and protocols of these recent experiments. We find a strong zero momentum peak in the pair momentum distribution which importantly occurs at a reasonably well defined onset temperature. We demonstrate that the resulting phase diagram, pair momentum distribution, and algebraic power law decay are compatible with these experiments throughout the continuum from BEC to BCS. Finally, we present sharp qualitative experimental signatures to test this physical picture. [1] Phys. Rev. Lett. 114, 230401 (2015) [2] Phys. Rev. Lett. 115, 010401 (2015) [3] Phys. Rev. Lett. (To be published.)

<sup>1</sup>This work was supported by NSF-DMR-MRSEC 1420709.

### 1:39PM L13.00005 BKT physics in trapped 2D Bose and Fermi gases , MARKUS HOLZMANN, LPMCM, CNRS and UJF, Grenoble

— I will discuss superfluid and spatial coherence properties of two-dimensional trapped Fermi gases in the BEC-BCS crossover regime [1]. On the bosonic side, experimental data are in quantitative agreement with path-integral quantum Monte Carlo calculations of point like molecules up to large values of the interaction. Algebraic correlations in the first-order correlation function characterize the phase below the Kosterlitz-Thouless transition temperature. Whereas the inhomogeneous trapping potential introduces important quantitative modifications, the effective exponent of the power-law decay at the superfluid transition remains approximately constant for all interaction strengths in the BEC-BCS crossover regime.

P.A. Murthy, I. Boettcher, L. Bayha, M. Holzmann, D. Kedar, M. Neidig, M.G. Ries, A.N. Wenz, G. Zuern, and S. Jochim, Phys. Rev. Lett. 115, 010401 (2015).

## Wednesday, March 16, 2016 11:15AM - 2:15PM –

Session L14 FEd: Impacts and Experiences with Hybrid and Online Courses 310 - Michael Schatz,

Georgia Institute of Technology

### 11:15AM L14.00001 Fully On-line Introductory Physics with a Lab , MICHAEL SCHATZ, School of Physics, Georgia Institute of Technology, Atlanta, GA, USA

— We describe the development and implementation of a college-level introductory physics (mechanics) course and laboratory that is suited for both on-campus and on-line environments. The course emphasizes a Your World is Your Lab approach whereby students first examine and capture on video (using cellphones) motion in their immediate surroundings, and then use free, open-source software both to extract data from the video and to apply physics principles to build models that describe, predict, and visualize the observations. Each student reports findings by creating a video lab report and posting it online; these video lab reports are then distributed to the rest of the class for peer review. In this talk, we will discuss the student and instructor experiences in courses offered to three distinct audiences in different venues: (1) a Massively Open On-line Course (MOOC) for off-campus participants, (2) a flipped/blended course for on-campus students, and, most recently, (3) a fully-online course for off-campus students.

**11:51AM L14.00002 A Flipped Pedagogy for Expert Problem Solving**, DAVID PRITCHARD, MIT — The internet provides free learning opportunities for declarative (Wikipedia, YouTube) and procedural (Kahn Academy, MOOCs) knowledge, challenging colleges to provide learning at a higher cognitive level. Our “Modeling Applied to Problem Solving”<sup>1 2</sup> pedagogy for Newtonian Mechanics imparts *strategic knowledge* - how to systematically determine which concepts to apply and why. Declarative and procedural knowledge is learned online before class via an e-text, checkpoint questions, and homework on edX.org (see <http://relate.mit.edu/physicscourse>); it is organized into five Core Models. Instructors then coach students on simple “touchstone problems”, novel exercises, and multi-concept problems - meanwhile exercising three of the four C's: communication, collaboration, critical thinking and problem solving. Students showed 1.2 standard deviations improvement on the MIT final exam after three weeks instruction, a significant positive shift in 7 of the 9 categories in the CLASS, and their grades improved by 0.5 standard deviation in their following physics course (Electricity and Magnetism).

<sup>1</sup>Modeling Applied to Problem Solving, Pawl, A., et. al., *AIP Conference Proceedings* 1179 2009 Physics Education Research Conference, pp. 51-54, (2009)

<sup>2</sup>Improved Student Performance In Electricity And Magnetism Following Prior MAPS Instruction In Mechanics, Rayyan, S et. al. Physics Education Research Conference 2010 AIP Conf. Proc. 1289, 273(2010).

**12:27PM L14.00003 Online activities to optimize in person learning.**, TIM STELZER, Univ of Illinois - Urbana — Students' unprecedented access to content on the web is providing a unique opportunity to transform the role lectures in education, moving the focus from content delivery to helping students synthesize the content into knowledge. We have introduced a variety of activities to facilitate this transformation at the University of Illinois, including web-based preflight assessments of student understanding before lecture, peer instruction (clickers) to assess and facilitate student understanding during lecture, and web-based multimedia pre-lectures designed to provide students with content before lecture. In this talk I will discuss the pedagogical motivation for introducing these activities, and the impact they have had at the University of Illinois.

**1:03PM L14.00004 Lessons from two decades of hybrid and online physics courses at Michigan State University**, GERD KORTEMEYER, Michigan State University — In Fall 1992, at Michigan State University we first offered online homework to one section of an introductory physics course; students received randomized assignments as printouts and entered answers through Telnet sessions, frequently using text terminals. Now, over two decades later, all of our introductory physics courses have significant online components, and students can choose between different formats, including hybrid courses with free online textbook materials, as well as courses that are completely online. What have we learned over the years about which formats are most effective for which students? What are the respective learning outcomes? Which logistical models work best for homework, exams, videos, and textbook materials? What about academic integrity? In our talk we will reflect on how our courses have been developing over the years, report educational research results, relate anecdotes and experiences, and point out pitfalls that we have encountered.

**1:39PM L14.00005 Apples vs. Oranges: Comparison of Student Performance in a MOOC vs. a Brick-and-Mortar Class**, MICHAEL DUBSON, University of Colorado at Boulder — In the fall of 2013, my colleagues and I taught the calculus-based introductory physics course to 800 tuition-paying students at the University of Colorado at Boulder. At the same time we taught a free massive open online version of the same course (MOOC), through Coursera.com. The initial enrollment in the MOOC was 10,000 students, of whom 255 completed the course. Students in both courses received identical lectures with identical embedded clicker questions, identical homework assignments, and identical timed exams. We present data on participation rates and exam performance for the two groups. We find that the MOOC is like a drug targeted at a very specific population. When it works, it works well, but it works for very few students. This MOOC worked well for older, well-educated students, who already had a good understanding of Newtonian mechanics.

## Wednesday, March 16, 2016 11:03AM - 2:27PM –

Session L15 DCMP DMP: Phenomena in Dirac Systems 314 - Adam Friedman, Naval Research Laboratory

**11:03AM L15.00001 Dirac Materials**, ALEXANDER BALATSKY, Los Alamos Natl Lab — Discoveries of superfluid phases in <sup>3</sup>He, high T<sub>c</sub> superconductors, graphene and topological insulators have brought into focus materials where quasiparticles are described by same Dirac and Weyl equation that governs behavior of relativistic particles. This class of materials, called Dirac materials [1], exhibits unusual universal features: Klein tunneling, chirality and impurity resonances. I will explore these similarities and discuss the unique role of symmetries that protect the Dirac spectrum. As an example of universal behavior of Dirac-Weyl materials I will consider impurity resonances, filling of the gap and gapless spectra in the magnetically doped topological insulators [2]. I will also discuss Dirac materials quantum imaging and how the ripples in the Dirac sea produced by defects can induce fascinating features in local magnetism and Kondo effect. At the end I will outline future opportunities to design Dirac materials that host bosonic Dirac excitations, something that would not be possible in particle physics [3]. Work supported by US DOE E304. [1] T.O. Wehling, A.M. Black-Schaffer, A.V. Balatsky (2014) Dirac materials, *Advances in Physics*, 63:1, 1-76. [2] A. M. Black-Schaffer, A. V. Balatsky, and J. Fransson, *Phys. Rev. B* 91, 201411(R) (2015). [3] S. Banerjee, A. M. Black-Schaffer, J. Fransson, H. Agren, A.V. Balatsky, Bosonic Dirac Materials in 2 Dimensions, preprint [2015], J. Fransson et.al, Dirac Magnons, preprint [2015].

**11:39AM L15.00002 Artificial Graphene in Nano-patterned GaAs Quantum Wells**<sup>1</sup>, SHENG WANG, DIEGO SCARABELLI, Department of Applied Physics, Columbia University, YULIYA Y. KUZNETSOVA, Department of Physics, Columbia University, LOREN N. PFEIFFER, KEN WEST, Department of Electrical Engineering, Princeton University, GEOFF C. GARDNER, MICHAEL J. MANFRA, Department of Physics and Astronomy, and School of Materials Engineering, and School of Electrical and Computer Engineering, Purdue University, VITTORIO PELLEGRINI, Istituto Italiano di Tecnologia, Graphene Labs, Genova, Italy and NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, Pisa, Italy, SHALOM J. WIND, Department of Applied Physics, Columbia University, ARON PINCZUK, Department of Physics and Department of Applied Physics, Columbia University — We report the realization of artificial graphene (AG) in a 2D electron gas in a highly tunable semiconductor quantum well system. Very short period (as small as 40 nm) honeycomb lattices were formed in a GaAs heterostructure by electron beam lithography followed by dry etching. Characterization of the AG samples by photoluminescence at low temperature (about 4K) indicates modulation of 2D electron states. Low-lying electron excitations observed by resonant inelastic light scattering and interpreted with a calculated AG band structure confirm the formation of AG bands with a well-defined Dirac cone, evidence for the presence of massless Dirac fermions. These results suggest that engineered semiconductor nano-scale structures can serve as advanced quantum simulators for probing novel electron behavior in low dimensional systems.

<sup>1</sup>Supported by DOE-BES Award DE-SC0010695

**11:51AM L15.00003 Fabrication of artificial graphene in a GaAs heterostructure<sup>1</sup>**, DIEGO SCARBELLI, SHENG WANG, YULIYA KUZNETSOVA, Columbia University, LOREN PFEIFFER, KEN WEST, Princeton University, GEOFF GARDNER, MICHAEL MANFRA, Purdue University, VITTORIO PELLEGRINI, Italian Institute of Technology, ARON PINCZUK, SHALOM WIND, Columbia University — Engineered honeycomb lattices, known as artificial graphene, constitute a platform for the exploration of graphene-like phenomena in a highly controllable and tunable manner, offering insight into a broader parameter range inaccessible to natural graphene. The electronic states of a 2D electron gas whose density is modulated by a potential with honeycomb topology have been predicted to generate massless Dirac fermions (MDFs) with tunable Fermi velocity. In this work we present the fabrication of artificial graphene in an ultrahigh quality GaAs/AlGaAs quantum well, with lattice period as small as 40nm, the smallest reported so far for this type of system. The combination of high precision electron-beam lithography, used to define an etch mask with honeycomb geometry on the surface of the sample, and precise anisotropic reactive ion etching allows to create artificial graphene with excellent uniformity and long range order. Different methodologies for preparation of the mask are compared and their limits are discussed. Thanks to the achievement of such high-resolution artificial graphene we expected to be able to observe, for the first time, MDFs in an engineered semiconductor and the possibility of access to novel topological phases.

<sup>1</sup>Supported by DOE-BES Award DE-SC0010695

**12:03PM L15.00004 Berry's Phase and Giant Non-Reciprocity in Dirac Quantum Dots**, JOAQUIN RODRIGUEZ-NIEVA, MILDRED DRESSSELHAUS, LEONID LEVITOV, MIT — Recently, nanoscale pn-junction rings have been introduced as a vehicle for coherent control of electronic states in Dirac materials [1]. Confined states in such ring-shaped electron resonators arise due to constructive interference of electronic waves incident at the pn junction at oblique angles and inward-reflected from the ring. Contrary to confined electronic states in conventional quantum dots, Dirac electrons are characterized by a non-trivial Berry's phase. Here we show [2] that the Dirac quantum dot energy levels are sensitive to the Berry's phase. In particular, we predict that the Berry's phase can induce a giant spectral non-reciprocity arising in weak magnetic fields. The effect is maximal for massless Dirac electrons, e.g. graphene, and is manifested in anomalously large splittings of the resonances which are degenerate at B=0 due to time reversal symmetry. This non-reciprocity effect overwhelms the conventional orbital and spin-induced non-reciprocity. The predicted giant non-reciprocity is readily accessible by Faraday and Kerr optical rotation measurements as well as by scanning tunneling spectroscopy. [1] Zhao, et al., Science 348, 672 (2015). [2] JRN, et al., arXiv:1508.06609.

**12:15PM L15.00005 a universal regulation for the angle resolved transport properties of Dirac cones and beyond**, ZHENZHU LI, ZHIRONG LIU, Peking Univ — A universal regulation for the angle resolved transport properties of two-dimensional (2D) Dirac cones, such as graphene, graphynes or even beyond, was established for the first time. The anisotropy and isotropy properties of 2D Dirac cones were investigated theoretically combining with first-principles calculation. It was found the moving direction of Dirac cones ( $\theta_{\text{move}}$ ) varies with the strain orientation ( $\theta_q$ ) can be approximately described by a linear law. Moreover,  $\theta_{\text{move}}$  is related the hopping ( $S_{12}$ ) between two bases with respect to the strain. The coefficients,  $a_x$ ,  $a_y$ ,  $a_z$ , in the Taylor expansion formula of  $S_{12}$  and strain were determined with DFT calculations. Graphene and graphynes were calculated to check the universality of the theory, which turns out to be working well. This new regulation could also be recommended into semiconductive systems to predict their transport behaviors, such as phosphorene or MoS<sub>2</sub>, whose angle resolved transport properties have been widely investigated experimentally for comparison.

**12:27PM L15.00006 Graphene quantum dots for high-performance THz hot electron bolometers<sup>1</sup>**, A EL FATIMY, P HAN, Department of Physics, Georgetown University, Washington DC, 20057, R.L MYERS-WARD, A.K BOYD, K.M DANIELS, U.S. Naval Research Laboratory, Washington, DC 20375, A.B SUSHKOV, D DREW, Department of Physics, University of Maryland, Maryland, 20742, USA, D.K GASKILL, U.S. Naval Research Laboratory, Washington, DC 20375, P BARBARA, Department of Physics, Georgetown University, Washington DC, 20057 — We study graphene quantum dots patterned from epitaxial graphene on SiC with a resistance strongly dependent on temperature. The combination of weak electron-phonon coupling and small electronic heat capacity in graphene makes these quantum dots ideal hot-electron bolometers. We characterize their response to THz radiation as a function of dot size, with sizes ranging from 30 to 700 nm and temperature, from 2.4K to 80K. We show that quantum dots exhibit a variation of resistance with temperature higher than 430 M $\Omega$ /K below 6K, leading to electrical responsivities for an absorbed THz power above 110<sup>10</sup> V/W. The high responsivity, the potential for operation above 80 K and the process scalability show great promise towards practical applications of graphene quantum dot THz detectors. <sup>1</sup>A. El Fatimy, R.L.Myers-Ward, A.K. Boyd, K.M. Daniels, D. K. Gaskill, and P. Barbara, Nature Nanotechnology, Accepted (2015).

<sup>1</sup>This work was sponsored by the U.S. Office of Naval Research (award number N000141310865)

**12:39PM L15.00007 Ballistic Transport in Graphene Antidot Lattices**, RYUTA YAGI, RYOJI SAKAKIBARA, RYOYA EBISUOKA, JUMPEI ONISHI, Hiroshima University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Material Sciences (NIMS), YASUHIRO IYE, Institute for Solid State Physics, the University of Tokyo — We observed commensurability magnetoresistance arising from ballistic electron transport in the triangular antidot lattice of high-mobility graphene. For both the monolayer and bilayer, magnetoresistance peaks were observed at the commensurability magnetic elds of the cyclotron orbit with antidot lattice. This condition was approximately unchanged for massless and massive Dirac fermions. The peaks appeared when the carrier mean free path was roughly larger than the lattice constant of the antidot, which indicates that the effect stems from the short-range characteristics of the carrier's scattering with antidots. We also found that the magnitude of commensurability peak diminished with changing the gate voltages to the charge neutrality point. This arose from the screening of charged impurity in graphene, which is dependent on carrier density.

**12:51PM L15.00008 Magneto Transport of Graphene Monolayer with Antidot Arrays**, LEI WANG, University of South Carolina, MING YIN, Benedict College, TIMIR DATTA, University of South Carolina, GODWIN MBAMALU, Benedict College, DHEYAA ALAMERI, University of South Carolina — Graphene has a significant potential for electronics application as well as in high precision resistive metrological standard. Here we report magneto transport studies of monolayer graphene with antidot in hexagonal arrays on SiO<sub>2</sub>/Si substrate. The choice of antidot array was motivated by the potential to enhance quantum interference effect amongst charge carriers. The graphene-antidot arrays were fabricated by electron beam lithography followed by reactive ion etching. In our samples the dc magnetic field (B) was applied continuously up to 18 Tesla while the measurement temperature (T) was held steady at desired set points, ranging from 200 mK to 20 K. The effect of nanoarrays on the temperature and field dependence of the electrical properties (MR) and quantum hall effect with particular attention to Aharonov-Bohm oscillations will be reported.

**1:03PM L15.00009 An Einzel lens apparatus for deposition of levitated graphene on a substrate in UHV**, JOYCE COPPOCK, PAVEL NAGORNYKH, IAN MCADAMS, University of Maryland, College Park, BRUCE KANE, Laboratory for Physical Sciences, College Park, MD and Joint Quantum Institute, University of Maryland, College Park — The goal of our research is to levitate a charged micron-scale graphene flake in an electrical AC quadrupole trap in ultra-high vacuum (UHV) in order to study its properties and dynamics while decoupled from any substrate [1,2]. As a complement to the optical measurements that can be performed on the levitated flake, we are developing a method of depositing the same flake on a substrate, which can be removed from the system for further study using such probes as atomic force microscopy (AFM) and scanning tunneling microscopy (STM). As the flake is released from the trap and propelled toward the substrate, its trajectory will be controlled by an Einzel (electrostatic) lens to achieve accurate positioning on the substrate. This talk will discuss the design of the lens as well as particle tracing simulations to determine the proper lens voltage to focus the particle's trajectory. In the future, deposited graphene may be used to passivate H-terminated silicon. The method is expected to be generalizable to achieve deposition of 2D materials on surfaces in a clean UHV environment. [1] Kane, B.E. *Phys. Rev. B.*, **82**, 115441 (2010). [2] Nagornyykh, P., et. al. *Appl. Phys. Lett.* **106**, 244102 (2015).

**1:15PM L15.00010 Rotational dynamics of levitated graphite flakes**, PAVEL NAGORNYKH, JOYCE COPPOCK, BRUCE KANE, University of Maryland, College Park — Trapping of charged graphene multilayer flakes in a quadrupole ion trap provides a unique method of characterization of 2D materials via complete separation of the flake and the environment. As the ability to cool the center-of-mass temperature of the flakes levitated in high vacuum was shown in the previous work [1], in this talk we concentrate on probing the internal dynamics of the spinning flake. A 671 nm circularly polarized laser was used to provide a spinning torque to the levitated micron-sized flakes, while a linear 532 nm laser, oriented orthogonal to the first one, acted as a light source. We have studied the effects of 671 nm laser power on measured frequency spectra at pressures of  $10^{-7} - 10^{-9}$  Torr, where spinning frequencies of greater than 6 MHz have been achieved. Frequency decay data was collected by turning the laser on and off, which allowed us to estimate damping ratios from the flake deceleration. The spectra measured during the spinning acceleration showed multiple harmonics and other non-commensurate frequencies. We compare the observed frequencies to the behavior expected from a rigid body and from a membrane under the centrifugal tension. [1] P. Nagornyykh, J. E. Coppock, B. E. Kane, *Appl. Phys. Lett.* **106**, 244102 (2015)

**1:27PM L15.00011 Bosonic Dirac Materials in 2 dimensions<sup>1</sup>**, SAIKAT BANERJEE, Los Alamos Natl Lab, Nordita, A.M. BLACK-SCHAEFFER, J. FRANSSON, Uppsala University, H. AGREN, KTH, Royal Institute of Technology, A.V. BALATSKY, Los Alamos Natl Lab — We examine the low energy effective theory of phase oscillations in a two dimensional granular superconducting sheet where the grains are arranged in honeycomb lattice structure. Two different types of collective phase oscillations are obtained, which are analogous to the massive Leggett and massless Bogoliubov-Anderson-Gorkov modes for two-band superconductor. It is explicitly shown that the spectra of these collective Bosonic modes cross each other at  $\$K\$$  and  $\$K'\$$  points in the Brillouin zone and form a Dirac node. This Dirac node behavior in Bosonic excitations represent the case of Bosonic Dirac Materials (BDM). Dirac node is preserved in presence of an inter-grain interaction despite induced changes of the qualitative features of the two collective modes. Finally, breaking the sub lattice symmetry by choosing different on-site potentials for the two sub lattices leads to a gap opening near the Dirac node, in analogy with Fermionic Dirac material.

<sup>1</sup>Supported by US DOE E304, ERC DM 321031, KAW, VR2012-3447

**1:39PM L15.00012 Double Dirac cones in two-dimensional phononic crystals.<sup>1</sup>**, JUN MEI, South China University of Technology — By utilizing the accidental degeneracy of two double-degenerate Bloch eigenstates, a double Dirac cone is realized at the center of the Brillouin zone of a two-dimensional phononic crystal. Using a perturbation method, we demonstrate that the double Dirac cone is composed of two identical and overlapping Dirac cones whose linear slopes can be accurately predicted by the method from first-principles. A slab of the PC can be mapped onto a slab of zero refractive index material by using a standard retrieval method. Total transmission without phase change and energy tunneling at the double Dirac point frequency are unambiguously demonstrated.

<sup>1</sup>Supported by NSFC (Grant No. 11274120)

**1:51PM L15.00013 Mechanical Flip-Chip for Ultra-High Electron Mobility Devices**, KEYAN BENNACEUR, SIMON BILODEAU, BENJAMIN SCHMIDT, SAMUEL GAUCHER, McGill University, DOMINIQUE LAROCHE, MIKE LILLY, JOHN RENO, Sandia National Laboratories, KEN WEST, LOREN PFEIFFER, Princeton University, GUILLAUME GERVAIS, McGill University — We present a novel “flip-chip” microfabrication method that was used to make a quantum point contact (QPC) on a two-dimensional electron gas (2DEG) without any fabrication process on the 2DEG. Electrostatic gates are of paramount importance for the physics of devices based on 2DEG since they allow depletion of electrons in selected areas. This field-effect gating enables the fabrication of a wide range of devices such as, electron interferometers and quantum dots. To fabricate these gates, processing is usually performed on the 2DEG, which is in many cases detrimental to its electron mobility. Our approach does not require any processing of the 2DEG material leaving it pristine and reusable. It relies on processing a separate wafer that is then mechanically mounted on the 2DEG material in a flip-chip fashion. This technique proved successful to fabricate QPC on GaAs/AlGaAs materials with high electron mobility ranging from  $1e6$  to  $1e7$   $cm^2V/s$ . (Bennaceur, K. et al. Scientific Reports 5, 13494 (2015)). Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

**2:03PM L15.00014 Topological States in Multi-Orbital Honeycomb Lattices of HgTe Quantum Dots**, CHRISTOPHE DELERUE, IEMN, Lille, France, WOUTER BEUGELING, TU Dortmund, Germany, EFTERPI KALES AKI, University of Luxembourg, YANN-MICHEL NIQUET, Grenoble Alpes University and CEA, Grenoble, France, DANIEL VANMAEKELBERGH, CRISTIANE MORAIS SMITH, University of Utrecht, The Netherlands — Recent works demonstrate that 2D single-crystalline sheets of semiconductors forming a honeycomb lattice can be synthesized by oriented attachment of semiconductor nanocrystals. Inspired by these results, we have performed atomistic tight-binding calculations of the band structure of CdSe [1] and HgTe [2] sheets with honeycomb nano-geometry. In the case of CdSe [1], we predict that their conduction band exhibits Dirac cones at two distinct energies. The lowest one has s-orbital character. The bands higher in energy present a Dirac cone and nontrivial flat bands because of their p-orbital character. We show that lattices of HgTe [2] combine the effects of the honeycomb geometry and strong spin-orbit coupling. The conduction bands can be described by a tight-binding lattice model as in graphene, but including multi-orbital degrees of freedom and spin-orbit coupling. This results in very large topological gaps and a flattened band detached from the others. Honeycomb structures of HgTe constitute a promising platform for the observation of a fractional Chern insulator or a fractional quantum spin Hall phase. [1] E. Kalesaki et al., *Phys. Rev. X* **4**, 011010 (2014). [2] W. Beugeling et al., *Nat. Commun.* doi: 10.1038/ncomms7316 (2015).

## 2:15PM L15.00015 Interaction of water molecules with hexagonal 2D systems. A DFT study<sup>1</sup>

, NGELA ROJAS, RAFAEL REY, Universidad Nacional de Colombia — Over the years water sources have been contaminated with many chemical agents, becoming issues that affect health of the world population. The advances of the nanoscience and nanotechnology in the development new materials constitute an alternative for design molecular filters with great efficiencies and low cost for water treatment and purification. In the nanoscale, the process of filtration or separation of inorganic and organic pollutants from water requires to study interactions of these atoms or molecules with different nano-materials. Specifically, it is necessary to understand the role of these interactions in physical and chemical properties of the nano-materials. In this work, the main interest is to do a theoretical study of interaction between water molecules and 2D graphene-like systems, such as silicene (h-Si) or germanene (h-Ge). Using Density Functional Theory we calculate total energy curves as function of separation between of water molecules and 2D systems. Different spatial configurations of water molecules relative to 2D systems are considered. Structural relaxation effects and changes of electronic charge density also are reported.

<sup>1</sup>Universidad Nacional de Colombia

## Wednesday, March 16, 2016 11:15AM - 2:15PM –

Session L16 DMP: Black Phosphorus Device Physics 315 - Yuanbo Zhang, Fudan University, China

## 11:15AM L16.00001 Black Phosphorus Optoelectronics and Electronics<sup>1</sup>, FENGNIAN XIA, Yale University

— Black phosphorus recently emerged as a promising new 2D material due to its widely tunable and direct bandgap, high carrier mobility and remarkable in-plane anisotropic electrical, optical and phonon properties. It serendipitously bridges the zero-gap graphene and the relatively large-bandgap transition metal dichalcogenides such as molybdenum disulfide (MoS<sub>2</sub>). In this talk, I will first cover the basic properties of few-layer and thin-film black phosphorus, followed by a discussion of recent observation of highly anisotropic robust excitons in monolayer black phosphorus. Finally I will present a few potential applications of black phosphorus such as radio-frequency transistors and wideband photodetectors.

<sup>1</sup>We acknowledge support from the Office of Naval Research, the Air Force Office of Scientific Research, the National Science Foundation and Yale University.

## 11:51AM L16.00002 Anisotropic Raman Spectroscopy of Few-Layer Phosphorene<sup>1</sup>, YUCHEN DU, WANGRAN WU, JESSE MAASSEN, ZHE LUO, MARK LUNDSTROM, XIANFAN XU, PEIDE YE, Purdue Univ

— Much recent research of black phosphorus (BP) and phosphorene has been focused on their unique anisotropy of this novel 2D material in terms of electrical, optical and thermal properties. Here we report the emerging Raman spectroscopy measurements of BP with respect to its isolation from bulk BP down to single layer phosphorene. The found frequency shift of BP in Raman spectra is to be correlated with atomic motion of modes, which can be explained by applying classical model of coupled harmonic oscillators. Raman intensity of different modes has also been included in our studies, which is confirmed as a solid strategy to quickly determine BP layer thickness. In addition, more information of their mechanical properties can also be obtained from Raman spectroscopy.

<sup>1</sup>The work was supported in part by NSF ECCS-1449270, NSF/AFOSR EFRI 2DARE Program, and ARO W911NF-15-1-0574.

## 12:03PM L16.00003 Interlayer Interaction that is Decisive in the Energy Gap of a Few Layer Phosphorene, YUKI SUGIHARA, ATSUSHI OSHIYAMA, Dept. of App. Phys., Univ. of Tokyo

— We report on our first-principles calculations that clarify the microscopic origin of the band-gap variation in a few-layer phosphorene (i.e. layered phosphorous) and also rectify a prevailed picture of the electronic structure of this new layered material [1]. Calculations have been done either using GGA with inclusion of van der Waals correction in the density-functional theory or GW approximation in the self-energy. We unequivocally reveal that the interlayer interaction causes the bonding-antibonding splitting of the highest valence band state, thus reducing the fundamental energy gap. This is due to the highest state consists mainly of *p* orbitals along the direction perpendicular to the layers. It was predicted that phosphorene has four polytypes named  $\alpha$  (black),  $\beta$  (blue),  $\gamma$  and  $\delta$  and all these polytypes exhibit common feature of the band-gap variation [2]. Especially,  $\gamma$  phosphorene is proposed to show the metal-insulator transition from the semiconductor mono-layer to the metal bi-layer. We reveal that this transition takes place in thicker region. [1] L. Li, Y. Yu, G. J. Ye, Q. Ge, X. ou, H. Wu, D. Feng, X. H. Chen, and Y. Zhang, Nat. Nanotechnol. 9, 372 (2014), [2] J. Guan, Z. Zhu, and D. Tomanek, PRL, 113, 046804 (2014)

## 12:15PM L16.00004 Quantum Hall Effect in Black Phosphorus Two-dimensional Electron System, LIKAI LI, FANGYUAN YANG, Fudan University, GUO JUN YE, University of Science and Technology of China, ZUOCHENG ZHANG, Tsinghua University, ZENGWEI ZHU, Huazhong University of Science and Technology, WENKAI LOU, XIAOYING ZHOU, Chinese Academy of Sciences, LIANG LI, Huazhong University of Science and Technology, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, KAI CHANG, Chinese Academy of Sciences, YAYU WANG, Tsinghua University, XIAN HUI CHEN, University of Science and Technology of China, YUANBO ZHANG, Fudan University

— The recent advent of black phosphorus has greatly enriched the material base of two-dimensional electron systems (2DES). In this work, we reached a milestone in black phosphorus research: the observation of integer quantum Hall (QH) effect in high quality black phosphorus 2DES. We achieved high carrier mobility by embedding the black phosphorus 2DES in a van der Waals heterostructure close to a graphite back gate; the graphite gate screens the impurity potential in the 2DES, and brings the Hall mobility up to 6000 cm<sup>2</sup>/V.s. The exceptional mobility enabled us, for the first time, to observe QH effect, and to gain important information on the energetics of the spin-split Landau levels in black phosphorus. Our results set the stage for further study on quantum transport and device application in the ultrahigh mobility regime.

## 12:27PM L16.00005 Nanoscopy Reveals Surface-Metallic Black Phosphorus. , YOHANNES ABATE, Georgia State University

— Nanolayer and two-dimensional (2D) materials.....<sup>1</sup> such as graphene...<sup>2,3</sup>, boron nitride...<sup>1,4</sup>, transition metal dichalcogenides...<sup>1,5-8</sup> (TMDCs), and black phosphorus (BP)...<sup>1,9-13</sup> have intriguing fundamental physical properties and bear promise of important applications in electronics and optics...<sup>9,14,15</sup>. Of them, BP...<sup>11,12,16</sup> is a novel layered material that has been theoretically predicted...<sup>10</sup> to acquire plasmonic behavior for frequencies below ~0.4 eV when highly doped. The electronic properties of BP are unique due to its anisotropic structure. Advantages of BP as a material for nanoelectronics and nanooptics are due to the fact that, in contrast to metals, the free carrier density in it can be dynamically controlled by chemical or electrostatic gating, which has been demonstrated by its use in field-effect transistors....<sup>9,14,15</sup> Despite all the interest that BP attracts, near-field and plasmonic properties of BP have not yet been investigated experimentally. Here we report the first observation of nanoscopic near-field properties of BP. We have discovered near-field patterns of outside bright fringes and high surface polarizability of nanofilm BP consistent with its surface-metallic, plasmonic behavior at mid-infrared (mid-IR) frequencies below critical frequency  $\omega_m \approx 1176 \text{ cm}^{-1}$ . This has allowed us to estimate plasma frequency  $\omega_p \approx 0.4 \text{ eV}$ , carrier density  $n \approx 1.1 \times 10^{11} \text{ cm}^{-2}$  and the thickness of the surface metallic layer of ~1nm. We have also observed similar behavior in other nanolayer semiconductors such as TMDC MoS<sub>2</sub> and topological insulator Bi<sub>2</sub>Te<sub>3</sub> but not in insulators such as boron nitride. This new phenomenon is attributed to surface band-bending and charging of the semiconductor nanofilms. The surface plasmonic behavior has been found for 10-40 nm BP thickness but absent for 4 nm BP thickness. This discovery opens up a new field of research and potential applications in nanoelectronics, plasmonics, and optoelectronics.

**12:39PM L16.00006 Near-field optical microscopy and spectroscopy of few-layer black phosphorus** , A. J. FRENZEL, Department of Physics, University of California, San Diego, S. TRAN, Department of Physics & Astronomy, University of California, Riverside, J. P. HINTON, A. J. STERNBACH, Department of Physics, University of California, San Diego, J. YANG, N. GILLGREN, C. N. LAU, Department of Physics & Astronomy, University of California, Riverside, D. N. BASOV, Department of Physics, University of California, San Diego — Few-layer black phosphorous is a recent addition to the family of two-dimensional (2D) materials which exhibits strongly anisotropic transport and optical properties due to its puckered honeycomb structure. It was recently predicted that this intrinsic anisotropy should manifest in the plasmon dispersion. Additionally, tuning layer number and carrier density can control the dispersion of these collective modes. Scanning near-field optical microscopy (SNOM) has been demonstrated as a powerful method to probe electronic properties, including propagating collective modes, in layered 2D materials. We used SNOM to investigate anisotropic carrier response in few-layer black phosphorous encapsulated by hexagonal boron nitride. In addition to exploring gate-voltage tunability of the electronic response, we demonstrate effective modulation of the near-field signal by ultrafast photoexcitation.

**12:51PM L16.00007 Resonant optical third-harmonic generation in few-layer black phosphorus**<sup>1</sup> , CHRISTIANO J. S. DE MATOS, MackGraphe, Mackenzie Presbyterian University, MANUEL J. L. F. RODRIGUES, Centre for Advanced 2D Materials and Graphene Research Centre, National University of Singapore, RAFAEL E. P. DE OLIVEIRA, MackGraphe, Mackenzie Presbyterian University, HÉLDER X. P. PEIXOTO, HSIN-YU WU, HO Y. WEI, ANTONIO H. CASTRO NETO, JOSÉ C. VIANA-GOMES, Centre for Advanced 2D Materials and Graphene Research Centre, National University of Singapore — Black phosphorus (BP), a layered monoatomic anisotropic crystal, has recently re-emerged due to demonstrations of its exfoliation down to few-layer thicknesses. It has been shown that BP remains a direct bandgap semiconductor from the bulk to the monolayer, which has triggered interest in its optoelectronic applications. However, optical characterization has been largely restricted to the linear regime, with nonlinear characterization limited to z-scan and saturable absorption measurements. In this work, we show optical third-harmonic generation measurements in bulk and few-layer BP. Results indicate a resonant increase in the generation efficiency of the latter, with signal intensities reaching values three orders of magnitude higher than those of graphene. The mechanisms leading to the resonant increase will be discussed.

<sup>1</sup>This work is supported by Fapesp (2012/50259-8 and 2015/11779-4), MackPesquisa, NRF-CRP (R-144-000-295-281), and NRF - Medium Sized Centre Programme

**1:03PM L16.00008 Transmission pump-probe spectroscopy on multilayer black phosphorus**<sup>1</sup> , RYAN J. SUESS, MOHAMMAD M. JADIDI, THOMAS E. MURPHY, MARTIN MITTENDORFF, University of Maryland-College Park, Institute for Research in Electronics and Applied Physics — Black phosphorus is a two-dimensional material that has recently attracted interest due to its high mobility and direct bandgap. In this work we examine the pump-induced change in optical transmission of mechanically exfoliated black phosphorus flakes using a two-color optical pump-probe measurement. The time-resolved data reveal a fast pump-induced transparency accompanied by a slower absorption that we attribute to Pauli blocking and free-carrier absorption, respectively. Polarization studies show that these effects are also highly anisotropic - underscoring the importance of crystal orientation in the design of optical devices based on this material. Ongoing work suggests that exploring the carrier density dependence of the pump-probe signals, which can be accessed experimentally via electrostatic gating, may allow for improved understanding of the optical response and carrier dynamics in the material.

<sup>1</sup>Supported by NSF and ONR-MURI

**1:15PM L16.00009 Electronic Structure and Optical Properties of Twisted Bilayer Black Phosphorus**<sup>1</sup> , TING CAO, ZHENGLU LI, DIANA Y. QIU, STEVEN G. LOUIE, Physics Department, UC Berkeley and Lawrence Berkeley National Lab — Using first-principles calculations, we find that the electronic structure and optical properties of bilayer black phosphorus can be modified significantly through changing the interlayer twist angle. We demonstrate the origin of these twist angle dependent effects, and connect our predicted results to experimental measurements.

<sup>1</sup>This work was supported by NSF Grant No. DMR15-1508412, and the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at Lawrence Berkeley National Laboratory's NERSC facility.

**1:27PM L16.00010 Phosphorene Nanoribbons: Electronic Structure and Electric Field Modulation**<sup>1</sup> , SINA SOLEIMANIKAHNOJ, IRENA KNEZEVIC, University of Wisconsin Madison — Phosphorene, a newcomer among the 2D van der Waals materials, has attracted the attention of many scientists due to its promising electronic properties. Monolayer phosphorene has a direct band gap of 2 eV located at the Gamma point of the Brillouin zone. Increasing the number of layers reduces the bandgap due to the van der Waals interaction. The direct nature of the bandgap makes phosphorene particularly favorable for electronic transport and optoelectronic applications. While multilayer phosphorene sheets have been studied, the electronic properties of their 1D counterparts are still unexplored. An accurate tight-binding model was recently proposed for multilayer phosphorene nanoribbons. Employing this model along with the non-equilibrium Greens function method, we calculate the band structure and electronic properties of phosphorene nanoribbons. We show that, depending on the edge termination, phosphorene nanoribbons can be metallic or semiconducting. Our analysis also shows that the electronic properties of phosphorene nanoribbons are highly tunable by in-plane and out-of-plane electric fields. In metallic ribbons, the conductance can be switched off by a threshold electric field, similar to field effect devices.

<sup>1</sup> Support by the NSF through the University of Wisconsin MRSEC Seed (NSF Award DMR-1121288)

**1:39PM L16.00011 Two dimensional disorder in black phosphorus and layered monochalcogenides** , SALVADOR BARRAZA-LOPEZ, MEHRSHAD MEHBOUDI, PRADEEP KUMAR, EDMUND O. HARRISS, HUGH O. H. CHURCHILL, ALEX M. DORIO, University of Arkansas, WENJUAN ZHU, AREND VAN DER ZANDE, University of Illinois, ALEJANDRO A. PACHECO SANJUAN, Universidad del Norte — The degeneracies of the structural ground state of materials with a layered orthorhombic structure such as black phosphorus and layered monochalcogenides GeS, GeSe, SnS, and SnSe, lead to an order/disorder transition in two dimensions at finite temperature. This transition has consequences on applications based on these materials requiring a crystalline two-dimensional structure. Details including a Potts model that explains the two-dimensional transition, among other results, will be given in this talk. References: M. Mehboudi, A.M. Dorio, W. Zhu, A. van der Zande, H.O.H. Churchill, A.A. Pacheco Sanjuan, E.O.H. Harris, P. Kumar, and S. Barraza-Lopez. arXiv:1510.09153.

**1:51PM L16.00012 Two-dimensional massless Dirac fermions, chiral pseudo-spins, and Berry's phase in few-layer black phosphorus<sup>1</sup>**, SEUNG SU BAIK, HYOUNG JOON CHOI, Dept. of Physics, IPAP, and CCSAEMP, Yonsei University, Korea — Black phosphorus (BP) and its two-dimensional (2D) derivative phosphorene are rapidly emerging nanoelectronic materials with potential applicability to field effect transistors and optoelectronic devices. Unlike the gapless semiconductor graphene, multilayer BP has a substantial band gap of 0.2 eV, and this band-gap size is predicted being sensitive to the external perturbations such as pressure, strain, and electric field. Very recently, a semiconductor-semimetal transition in BP was realized by the surface potassium (K) doping, producing a Dirac semimetal state with a linear dispersion in the armchair direction and a quadratic one in the zigzag direction [1,2]. Here, based on first-principles density functional calculations, we present that beyond the critical K density, 2D massless Dirac fermions emerge in K-doped few-layer BP, and the electronic states around Dirac points have chiral pseudo-spins and Berry's phase. These features are robust with respect to the spin-orbit interaction. The switchable massless Dirac fermions discussed here may open a new way for the development of high performance devices in 2D materials beyond graphene. [1] J. Kim, S. S. Baik, S. H. Ryu, Y. Sohn, S. Park, B. Park, J. Denlinger, Y. Yi, H. J. Choi, and K. S. Kim, *Science* **349**, 723-725, (2015). [2] S. S. Baik, K. S. Kim, Y. Yi and H. J. Choi, arXiv:1508.04932.

<sup>1</sup>This work was supported by NRF of Korea (Grant No. 2011-0018306) and KISTI supercomputing center (Project No. KSC-2015-C3-039).

**2:03PM L16.00013 Two-dimensional exciton states in monolayer semiconducting phosphorus allotropes<sup>1</sup>**, ALEXANDRE R ROCHA, CESAR E P VILLEGAS, Instituto de Física Teórica - Unesp, São Paulo, Brazil — During the last decade, novel two-dimensional (2D) semiconducting materials have been synthesized and characterized. As a result, there have been several theoretical and experimental proposals to incorporate 2D materials for designing next generation electronic and optoelectronics devices. In particular, it has been demonstrated that light absorption in phosphorus-based monolayers can span the whole visible spectrum, suggesting they could be used for optoelectronic applications. A key ingredient for optoelectronic applications is the presence of excitons and their subsequent diffusion along a donor material. This is influenced by the character of the different excitations taking place, as well as, the exciton binding energy. Therefore, in this work we use accurate many-body corrected density functional theory by means of GW-BSE methodology to elucidate the most important optical transitions, exciton energy spectrum as well as exciton extension in different types of phosphorene materials. In addition, we solve the Schrödinger equation for different 2D screened potentials and estimate the 2D exciton energy levels and radius extension. Finally, in order to assess further studies based on these systems, we provide a simple analytic expression for estimating 2D exciton energy levels.

<sup>1</sup>Research funded by FAPESP-Brazil

## Wednesday, March 16, 2016 11:15AM - 2:15PM —

Session L17 DMP: 2D Devices: Charge, Spin, and Valley Control 316 - Kin Fai Mak, Penn State University

**11:15AM L17.00001 Properties of Edge States at the Graphene P-N Junction Interface**, SON LE, NIKOLAI KLIMOV, DAVID NEWELL, NIST - Natl Inst of Stds & Tech, JUN YAN, University of Massachusetts, Amherst, JI UNG LEE, SUNY PI, NY, CURT RICHTER, NIST - Natl Inst of Stds & Tech — The Landau level edge states from the p- and the n-section of a graphene P/N junction (*pnJ*) interact with each other differently across the junction depending upon the properties of the junction and the graphene. Full equilibration was reported for a two terminal graphene *pnJ* device in Williams et al. [1]. In our four-terminal device, however, only the lowest Landau level edge state is equilibrated across the *pnJ* [2]. When the two devices are compared, the LL energy spacings, the length of the edge states along the *pnJ* interface, and the carrier mobility are similar. Electrostatic simulations for our device geometry and that of [1] contrast the rate of change of the electrostatic potential across the *pnJs*. Edge states at an electrostatically smooth junction are spatially further apart than those at a relatively abrupt junction, which decreases the probability of edge states mixing. Thus, we attribute the difference in equilibration in our device and that of [1] to the dramatic difference in the shape of the electrostatic junction. [1] J. R. Williams, L. DiCarlo, and C. M. Marcus, *Science* **317**, 638 (2007) [2] Nikolai N. Klimov, Son T. Le, *et al.*, *Phys. Rev. B: Rapid Comm.* (2015)

**11:27AM L17.00002 Quantum oscillations as a probe of massive Dirac fermions**, SCOTT DIETRICH, CARLOS FORSYTHE, JESSE BALGLEY, CORY DEAN, Department of Physics, Columbia University — Significant band structure engineering has been recently accomplished by stacking monolayer and bilayer graphene onto hexagonal Boron Nitride (hBN). The slightly mismatched lattice constants and varying alignment angle of the two materials creates a tunable moiré superlattice potential and breaks the naturally occurring valley symmetry of graphene. These effects open a gap and distort the band dispersion near the charge neutrality point as well as at location of the moiré minibands. In this study, effective band mass as a function of density is extracted from Shubnikov-de Haas oscillations in devices with varying superlattice wavelengths. Our results demonstrate quantitative control of band mass in graphene devices, and could help clarify the possible role of the many-body physics in these systems.

**11:39AM L17.00003 Nanoscale Tunable Strong Carrier Density Modulation of 2D Materials for Metamaterials and Other Tunable Optoelectronics**, CHENG PENG, DMITRI EFETOV, REN-JYE SHIUE, Massachusetts Institute of Technology, SEBASTIEN NANOT, ICFO, the Institute of Photonic Sciences, MAREK HEMPEL, JING KONG, Massachusetts Institute of Technology, FRANK KOPPENS, ICFO, the Institute of Photonic Sciences, DIRK ENGLUND, Massachusetts Institute of Technology — Strong spatial tunability of the charge carrier density at nanoscale is essential to many 2D-material-based electronic and optoelectronic applications. As an example, plasmonic metamaterials with nanoscale dimensions would make graphene plasmonics at visible and near-infrared wavelengths possible. However, existing gating techniques based on conventional dielectric gating geometries limit the spatial resolution and achievable carrier concentration, strongly restricting the available wavelength, geometry, and quality of the devices. Here, we present a novel spatially selective electrolyte gating approach that allows for in-plane spatial Fermi energy modulation of 2D materials of more than 1 eV (carrier density of  $n = 10^{14} \text{ cm}^{-2}$ ) across a length of 2 nm. We present electrostatic simulations as well as electronic transport, photocurrent, cyclic voltammetry and optical spectroscopy measurements to characterize the performance of the gating technique applied to graphene devices. The high spatial resolution, high doping capacity, full tunability and self-aligned device geometry of the presented technique opens a new venue for nanoscale metamaterial engineering of 2D materials for complete optical absorption, nonlinear optics and sensing, among other applications.

**11:51AM L17.00004 Optical study of low-dimensional materials**, FENG WANG, Univ of California - Berkeley — Electrons in monolayer graphene are described by massless Dirac electrons, which exhibit unique quantum phenomena due to the pseudospin and Berry phase of the massless electrons. In this talk, I will discuss our effort in probing massive Dirac electrons in gapped bilayer graphene, which can be described by a quantum valley Hall insulator with non-trivial Chern number for individual valleys. A topologically protected 1D conducting channel was predicted to exist at the layer-stacking domain boundary of AB-BA bilayers. We show that near-field infrared imaging provides a versatile tool to visualize the layer stacking domain walls, and demonstrate conducting channels arising from the quantum valley Hall edge states through electrical transport in gapped bilayer graphene.

**12:27PM L17.00005 Pseudo Magnetic Faraday and Quantum Hall Effect In Oscillating Graphene<sup>1</sup>**, ANITA BHAGAT, KIERAN MULLEN, Homer L. Dodge Department of Physics and Astronomy, Univ. of Oklahoma — When a graphene layer is stressed, the strain changes the phase between sites in a tight binding model of the system. This phase can be viewed as a pseudo-magnetic vector potential. The corresponding pseudo-magnetic field has been experimentally verified in static cases.<sup>2</sup> We examine the case of oscillating graphene ribbons and explore two new effects. The first is to investigate an oscillating pseudo-magnetic field that produces a quantum Hall effect: we calculate the I-V characteristic of an oscillating graphene nanoribbon as a function of frequency, and amplitude in both the oscillations and the applied driving voltage. Second, the time dependent pseudo-magnetic field should produce a pseudo-Faraday effect driving electrons in different valleys in opposite directions. In both cases, we make explicit calculations for experiment.

<sup>1</sup>This project was supported in part by the US National Science Foundation under Grant DMR-1310407.

<sup>2</sup> N. Levy et al. *Science* **329**, 544 (2010)

**12:39PM L17.00006 Twisted bilayer graphene with interlayer potential asymmetry<sup>1</sup>**, PILKYUNG MOON, New York University Shanghai, YOUNG-WOO SON, Korea Institute for Advanced Study, MIKITO KOSHINO, Tohoku University — A twisted stack of two graphene layers (twisted bilayer graphene) exhibits an extremely long potential period arising from the moiré interference between the layers<sup>2-3,4</sup>. We investigate the band structure and optical absorption spectrum of twisted bilayer graphenes with changing interlayer bias and Fermi energy simultaneously<sup>5</sup>. We show that the interlayer bias lifts the degeneracy of the superlattice Dirac point, while the amount of the Dirac point shift is significantly suppressed in small rotation angles, and even becomes opposite to the applied bias, by the interlayer interaction. In addition, we show that the spectroscopic features are highly sensitive to the interlayer bias and the Fermi energy, and widely tunable by the external field effect.

<sup>1</sup>P.M. acknowledges the support of NYU Shanghai and the NYU-ECNU Institute of Physics at NYU Shanghai. Y.-W.S. was supported by the NRF of Korea grant funded by the MSIP. M.K. was funded by JSPS Grant-in-Aid for Scientific Research.

<sup>2</sup>C. Berger et al., *Science* **312**, 1191 (2006).

<sup>3</sup>P. Moon and M. Koshino, *Phys. Rev. B* **85**, 195458 (2012).

<sup>4</sup>P. Moon and M. Koshino, *Phys. Rev. B* **87**, 205404 (2013).

<sup>5</sup>P. Moon, Y.-W. Son, and M. Koshino, *Phys. Rev. B* **90**, 155427 (2014).

**12:51PM L17.00007 Control of commensuration between graphene and boron nitride**, MATTHEW YANKOWITZ, University of Arizona, K. WATANABE, T. TANIGUCHI, National Institute for Materials Science, PABLO SAN-JOSE, Instituto de Ciencia de Materiales de Madrid, BRIAN J. LEROY, University of Arizona — The electronic properties of van der Waals (vdW) heterostructures can be controlled through the choice and ordering of materials, as well as through the relative rotation between the atomic layers. However, little has been done to directly control the interactions between these layers, which may act as another tunable degree of freedom in these systems. Here, we demonstrate the ability to control the interlayer interaction strength between graphene and boron nitride using pressure resulting from the vdW interaction of a nearby STM tip. In particular, controlling the relative layer separation dynamically modifies the adhesion-induced strains in the graphene as it forms a partially commensurate structure with the boron nitride.

**1:03PM L17.00008 Negative Electronic Compressibility and Tuneable Spin Splitting in WSe<sub>2</sub>**, J.M. RILEY, Univ of St Andrews and Diamond Light Source, W. MEEVASANA, Suranaree Univ of Tech, L. BAWDEN, Univ of St Andrews, M. ASAKAWA, Tokyo Inst of Tech, T. TAKAYAMA, Univ of Tokyo, T. EKNAPAKUL, Suranaree Univ of Tech, T.K. KIM, M. HOESCH, Diamond Light Source, S.-K. MO, Advanced Light Source, H. TAKAGI, Univ of Tokyo, T. SASAGAWA, Tokyo Inst of Tech, M.S. BAHARAMY, Univ of Tokyo and RIKEN, P.D.C. KING, Univ of St Andrews — Recently, semiconducting transition metal dichalcogenides have gained attention for their extraordinarily large exciton-binding energies [1,2] and locking of the spin with valley and layer pseudospins [3,4]. Through sub-monolayer deposition of alkali metals onto the surface of WSe<sub>2</sub>, analogous to the gating in a field-effect transistor, we create a 2DEG at the sample surface with tuneable carrier concentration [5]. Counter-intuitively, we find that the addition of carriers induces a reduction of the chemical potential in the near-surface. We attribute this to negative electronic compressibility [6] where strong Coulomb effects lead to the lowering of the chemical potential with band filling, which we find persists to remarkably high electron densities. Simultaneously, we show this is accompanied by a giant tuneable spin-splitting of the valence band states and a reduction of the quasiparticle band gap. [1] Ugeda, et al., *Nature Mat.* **13** (2014) 1091 [2] Ye et al., *Nature* **513** (2014) 214 [3] Xu et al., *Nature Phys.* **10** (2014) 343 [4] Riley et al., *Nature Phys.* **10** (2014) 835 [5] Riley et al. doi:10.1038/nnano.2015.217 [6] Eisenstein et al. *Phys. Rev. Lett.* **68** (1992) 674

**1:15PM L17.00009 Floquet-Engineered Valleytronics in Dirac Systems<sup>1</sup>**, BABAK SERADJEH, ARIJIT KUNDU<sup>2</sup>, HERBERT FERTIG, Indiana University — Valley degrees of freedom offer a potential resource for quantum information processing if they can be effectively controlled. We discuss an optical approach to this problem in which intense light breaks electronic symmetries of a two-dimensional Dirac material. The resulting quasienergy structures may then differ for different valleys, so that the Floquet physics of the system can be exploited to produce highly polarized valley currents. This physics can be utilized to realize a valley valve whose behavior is determined optically. We propose a concrete way to achieve such valleytronics in graphene as well as in a simple model of an inversion-symmetry broken Dirac material, such as monolayer transition-metal dichalcogenides. Simulating the system numerically, we find that the effect is robustness against moderate disorder and small deviations in optical parameters. We also study designs for coherent manipulation of valley degrees of freedom suitable for quantum information processing.

<sup>1</sup>This work was supported in part by the NSF through Grant Nos. DMR-1350663 and DMR-1506460, the US- Israel Binational Science Foundation, and by Indiana University.

<sup>2</sup>Present Address: Israel Institute of Technology

**1:27PM L17.00010 Transition-metal dichalcogenide-based dipolariton optoelectronic devices**, GERMAN KOLMAKOV, NYC College of Technology, CUNY, TIM BYRNES, New York University, ANDY HE, ROMAN YA. KEZERASHVILI, NYC College of Technology, CUNY — Using computational modeling, we simulate the dynamics of dipolaritons in an optical microcavity, which encompasses the transition-metal dichalcogenide double-layer structure. We demonstrate that dipolaritons, a three-way superposition of photons, direct excitons and indirect excitons, are guided by a pattern deposited on the microcavity and can be driven by an external electric field or voltage applied to the structure. Focusing on a normal dipolariton gas in Y- and Psi-shaped patterns, we isolate conditions when the dipolariton flow can be switched between the channel branches of the pattern by the electric field. We also studied the superfluid dynamics of dipolariton Bose-Einstein condensates in patterned substrates at low temperatures, showing that the condensate in the channels can be accelerated and then directed by the electric field. We compare the obtained results with those for GaAs-based microcavities and demonstrate that dipolaritons in transition-metal dichalcogenide-based microcavities can be utilized for the design of optical switches and transistors for optoelectronic integrated circuits.

**1:39PM L17.00011 Electrical and optical properties of SnS<sub>2</sub>/WSe<sub>2</sub> van der Waals Heterojunction FETs**, AHMAD ZUBAIR, AMIRHASAN NOURBAKSH, MILDRED DRESSSELHAUS, TOMAS PALACIOS, Massachusetts Institute of Technology — Two dimensional crystals based on atomically thin films of transition metal dichalcogenides offer an exciting platform for various optoelectronic applications. Their unique crystal properties make them particularly attractive for van der Waals heterostructures which open up an additional degree of freedom to tailor the material properties into new physics and device applications. In this work, we explore, for the first time, the optoelectronic properties of van der Waals SnS<sub>2</sub>/WSe<sub>2</sub> heterojunction. WSe<sub>2</sub> is an ambipolar semiconductor while SnS<sub>2</sub> is an *n*-type wide bandgap semiconductor. We use the pickup and dry transfer methods to fabricate SnS<sub>2</sub>/WSe<sub>2</sub> heterojunction transistors (hetero-FETs). We observe negative differential transconductance in the SnS<sub>2</sub>/WSe<sub>2</sub> hetero-FET. Also, the heterostructure couples strongly to incident light and shows high photovoltaic responsivity which can find applications in nano-devices such as photo-detectors and solar cells.

**1:51PM L17.00012 Mapping of the photo-induced metastable and hidden phases in 2D electronic materials**, FARAN ZHOU, TIANYIN SUN, TZONG-RU HAN, Michigan State University, CHRISTOS MALLIAKAS, Northwestern University, PHILLIP DUXBURY, SUBHENDRA MAHANTI, Michigan State University, MERCOURI KANATZIDIS, Northwestern University, CHONG-YU RUAN, Michigan State University, MSU TEAM, NU TEAM — Using the ultrafast electron imaging techniques, we studied the light-induced phase transitions in transition-metal dichalcogenide materials. A succession of different phases was introduced transiently using femtosecond mid-infrared pulses and the local atomic scale charge-density-wave dynamics and morphological evolution of the long-range textured domains were *in situ* characterized using the ultrashort coherent electron pulses. The various metastable and hidden states emerging under the controlled nonthermal, nonadiabatic driving highlight the interaction-driven nature of these transitions with limited involvement of lattice entropy. The methodology introduced here can be generally applied to survey the complex energy landscape in strongly correlated electron systems, avoiding the difficulty of electrostatic gating or confounding effects due to defects and/or disorder. In particular, the observation of robust non-thermal switching at meso-scales and at ultrafast timescales, provides a platform for designing high-speed low-energy consumption nano-photonics and electronics devices.

**2:03PM L17.00013 Transport properties of heterostructures composed of Mo(S,Se)<sub>2</sub> on *h*-BN**, QIONG ZHOU, NIHAR PRADHAN, SHAHRIAR MERAMAN, DANIEL RHODES, LUIS BALICAS, National High Magnetic Field Laboratory and Florida State University — The thickness-dependent tunable band gap of transition metal dichalcogenides in the visible region has generated a lot of interest on their optoelectronic properties. Our single crystals of molybdenum disulphide (MoS<sub>2</sub>) and molybdenum diselenide (MoSe<sub>2</sub>) were grown through a chemical vapor transport technique. Few-layered flakes of MoS<sub>2</sub> and MoSe<sub>2</sub> were mechanically exfoliated and transferred onto *h*-BN flakes, with this stack subsequently transferred onto pre-evaporated molybdenum bottom gate(s). Here, we report the fabrication and temperature-dependent electrical transport properties of few-layered MoS<sub>2</sub> and MoSe<sub>2</sub> field-effect transistors on *h*-BN.

## Wednesday, March 16, 2016 11:15AM - 2:15PM –

Session L18 GMAG DMP FIAP: Ultrafast Magnetization Dynamics 317 - Emrah Turgut, Cornell University

**11:15AM L18.00001 Tabletop soft x-ray magnetic circular dichroism measurements using circularly polarized high harmonic sources**, T FAN, R KNUT, C HERNANDEZ GARCA, D HICKSTEIN, D ZUSIN, C GENTRY, F DOLLAR, C MANCUSO, C HOGLE, J ELLIS, K DORNEY, JILA - University of Colorado, D LEGUT, Charles University, K CARVA, P OPPENEER, Department of Physics - Uppsalla University, O SHPYRKO, E FULLERTON, University of California at San Diego, O KFIR, O COHEN, Physics Department - Technion, D MILOSEVIC, University of Sarajevo, A BECKER, A JARON BECKER, T POPMINTCHEV, M MURNANE, H KAPTEYN, P GRYCHTOL, JILA - University of Colorado — X-ray magnetic circular dichroism (XMCD) allows for the extraction of the orbital and spin contributions to the magnetization and its interaction with phononic and electronic degrees of freedom on fs time and nm length scales, with element-specificity. However, to date, circular soft x-ray beams were restricted to large-scale x-ray facilities. These facilities have great advantages of high peak and average powers, but have limited access and temporal resolution. In this work, we present the first direct tabletop approach for generating bright circularly polarized light exceeding 160 eV. This makes it possible to implement XMCD on the tabletop for the first time, allowing to probe not only the 3d ferromagnets, but also the 4f rare earth materials with element-specificity. We demonstrate the stability, circularity and brightness of our high harmonic source by extracting the magneto-optical coefficients near the *N* edge of Gd (145 eV), as well as at the *M* edges of Fe (52eV), for an out-of-plane magnetized Gd/Fe multilayer sample thus enabling ultrafast studies of magnetization dynamics.

**11:27AM L18.00002 Localization of Fe d-states in Ni-Fe-Cu alloys and implications for ultrafast demagnetization**, TOM SILVA, NIST, Boulder, CO, USA, RONNY KNUT, JILA, Boulder, CO, USA, ERNA DELCZEG-CZIRJAK, Uppsalla University, Uppsalla, Sweden, JUSTIN SHAW, HANS NEMBACH, NIST, Boulder, CO, USA, PATRIK GRYCHTOL, DMITRIY ZUSIN, CHRISTIAN GENTRY, EMRAH TURGUT, HENRY KAPTEYN, MARGARET MURNANE, JILA, Boulder, CO, USA, DARIO ARENA, University of South Florida, Tampa, FL, USA, OLLE ERIKSSON, OLOF KARIS, Uppsalla University, Uppsalla, Sweden — Ni<sub>0.8</sub>Fe<sub>0.2</sub> (Py) and Py-Cu exhibit intriguing ultrafast demagnetization behavior, where the Ni magnetic moment shows a delayed response relative to the Fe. To unravel the mechanism responsible for this behavior, we have studied Py-Cu alloys for a wide range of Cu concentrations using X-ray magnetic circular dichroism (XMCD). The magnetic moments of Fe and Ni are found to respond very differently to Cu alloying: Fe becomes a strong ferromagnet in Py, with the magnetic moment largely unaffected by Cu alloying. In contrast, the Ni magnetic moment decreases continuously with increasing Cu concentration. Ab-initio calculations corroborate these results and we discuss the electronic structure in the framework of virtual bound states (VBSs). Fe exhibits VBSs in the minority band that lie approximately 1 eV above the Fermi level in pure Py, and which move closer to the Fermi level upon Cu alloying. A strong interaction between the VBSs and electrons above the Fermi level enhances the formation of magnons at Fe sites. This mechanism is consistent with a demagnetization delay between Fe and Ni, as found experimentally.

**11:39AM L18.00003 Time Resolved X-ray Magnetic Circular Dichroism at the Linac Coherent Light Source**<sup>1</sup>, W. SCHLOTTER, D. HIGLEY, E. JAL, G. DAKOVSKI, E. YUAN, J. MACARTHUR, A. LUTMAN, K. HIRSCH, P. GRANITZKA, Z. CHEN, G. COSLOVICH, M. HOFFMAN, A. MITRA, A. REID, P. HART, H.-D. NUHN, H. DUERR, SLAC - Natl Accelerator Lab, E. ARENHOLZ, P. SHAFER, P. DENNES, J. JOSEPH, Lawrence Berkeley Natl Lab, L. GUYADER, Helmholtz-Zentrum Berlin, Germany, A. TSUKAMOTO, Nihon University, Chiba, Japan — We demonstrate ultrafast time resolved X-ray Magnetic Circular Dichroism on optically switchable GdFeCo thin film samples. This method extends the element specificity of time resolved x-ray absorption spectroscopy to characterize the evolution of electron spin and orbital angular momenta. These measurements were enabled by a recent upgrade at the Linac Coherent Light Source (LCLS) to generate circularly polarized x-rays. Additionally these measurements were enhanced by new detection systems that benefit all x-ray absorption spectroscopy experiments performed in transmission. Consequently static XMCD data are in excellent agreement with similar measurements at synchrotron light sources. The LCLS is an x-ray free electron laser user facility accessible via a peer-reviewed proposal process.

<sup>1</sup> Acknowledgement: The Linac Coherent Light Source (LCLS), SLAC National Accelerator Laboratory, is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-76SF00515.

### 11:51AM L18.00004 Spin pumping in electrodynamically coupled magnon-photon systems<sup>1</sup>

LIHUI BAI, Department of Physics and Astronomy, University of Manitoba, Winnipeg, Canada R3T 2N2 — The electronics industry is quickly approaching the limitation of Moore's Law due to Joule heating in high density-integrated devices. To achieve new higher-speed devices and reduce energy consumption, researchers are turning to spintronics where the intrinsic spin, rather than the charge of electrons, is used to carry information in devices. Advances in spintronics have led to the discovery of giant magnetoresistance (GMR), spin transfer torque etc. Another subject, cavity electrodynamics, promises a completely new quantum algorithm by studying the properties of a single electron interacting with photons inside of a cavity. By merging both spintronics and cavity electrodynamics, a new cutting edge field called Cavity Spintronics is forming, which draws on the advantages of both subjects to develop new spintronics devices utilizing light-matter interaction. In this work, we use electrical detection, in combination with microwave transmission, to investigate both resonant and nonresonant magnon-photon coupling in a microwave cavity at room temperature. Spin pumping in a dynamically coupled magnon-photon system is found to be distinctly different from previous experiments. Characteristic coupling features such as modes anticrossing, linewidth evolution, peculiar line shape, and resonance broadening are systematically measured and consistently analyzed by a theoretical model set on the foundation of classical electrodynamic coupling. Our experimental and theoretical approach paves the way for pursuing microwave coherent manipulation of pure spin current via the combination of spin pumping and magnon-photon coupling.

<sup>1</sup>Co-authored with M. Harder, C.-M. Hu from University of Manitoba, Y. P. Chen, J. Q. Xiao from University of Delaware, and X. Fan from University of Denver

### 12:27PM L18.00005 Ultrafast magnetization dynamics in heterogeneous granular FePt media

PATRICK GRANITZKA, ALEXANDER REID, EMMANUELLE JAL, TIANMIN LIU, SLAC - National Accelerator Laboratory, WILLIAM SCHLOTTER, SLAC - Linac Coherent Light Source, PADRAIC SHAFER, LBNL, VIRAT METHA, OLAV HELLWIG, HGST, YUKIKO TAHAKASHI, National Institute for Materials Science, Japan, ERIC FULLERTON, UCSD, Center for Magnetic Recording Research, JOACHIM STOHR, HERMANN DURR, SLAC - National Accelerator Laboratory — Granular FePt in the L<sub>10</sub> phase is a key material for future magnetic data storage devices, supporting stable magnetic domains less than 10 nm in diameter. To switch the magnetization of magnetically hard materials like FePt, new writing techniques are needed such as Heat Assisted Magnetic Recording (HAMR). However, it is not known how HAMR works on the fundamental length and time scales of magnetization in FePt. Here we investigate the nanoscale aspects of magnetization dynamics in FePt HAMR with fs X-ray pulses from the Linac Coherent Light Source at Stanford using resonant X-ray diffraction. We show that while many spins display switching in a magnetic field following a fs duration optical excitation. The remaining spins do not switch. Surprisingly the ratio of spins that switch to spins that do not, stays constant over a large fluence range. Furthermore we observe that the spin reservoir which displays heat assisted magnetic recording is quenched homogeneously over the size distribution of grains, while the spins that do not follow the field display a length-scale dependent quenching.

### 12:39PM L18.00006 A simple and effective theory for all-optical helicity-dependent spin switching<sup>1</sup>

GUOPING ZHANG, Department of Physics, Indiana State University, Terre Haute, IN 47809, USA, YIHUA BAI, Office of Information Technology, Indiana State University, USA, THOMAS F GEORGE, University of Missouri-St. Louis — All-optical helicity-dependent spin switching (AOS) represents a new frontier in magnetic recording technology, where a single ultrafast laser pulse, without any assistance from an external magnetic field, can permanently switch spin within a few hundred femtoseconds. By contrast, the existing theory does rely on an artificial magnetic field to switch spins. Here we develop a microscopic spin switch theory, free of any artificial field, and demonstrate unambiguously that both circularly and linearly polarized lights can switch spins faithfully. Our theory is based on the Hookean theory, but includes two new elements: spin-orbit coupling and exchange interaction. We predict that left (right) circularly polarized light only flips (flops) spin, a symmetry constraint that strongly favors ferrimagnetic orderings over ferromagnetic ones, with the allowable exchange interaction within 10 meV, consistent with all prior theories. The effect of the laser amplitude is highly nonlinear: If it is too weak, AOS does not occur, but if too strong, the spin cants; a compromise between them produces a narrow spin reversal window as observed experimentally. We envision that our model can be easily extended to describe spin frustrated systems and multiferroics, where the light-spin interaction

<sup>1</sup>Supported by the U.S. Department of Energy under Contract No. DE-FG02-06ER46304 and the National Energy Research Scientific Computing Center

### 12:51PM L18.00007 A fast time-dependent density functional theory method for the simulation of ultrafast demagnetization induced by laser

ZHANGHUI CHEN, LIN-WANG WANG, Lawrence Berkeley Natl Lab, MAGNETIC PROJECT TEAM — We present a fast real-time time-dependent density functional theory method to investigate the ultrafast spin dynamics induced by laser. The Hamiltonian considers non-collinear magnetic moment, spin-orbital coupling and electron-laser interaction. An accelerated method with leapfrog prediction of charge matrix is used to solve the time-evolving equation. The investigation of Ni bulk found that the spin demagnetization consists of one time-lag stage and one fast demagnetization stage followed by one slow demagnetization stage. The time-lag and fast stages are mainly affected by the spin-electron interaction and their interactions with photons while the slow stage is affected by phonon-related interaction. Demagnetization appears only when spin-orbital coupling effect is considered. We further demonstrated how to manipulate the spin dynamics by changing laser fluence, duration and wavelength.

### 1:03PM L18.00008 A comparative study of laser-induced demagnetization dynamics in Fe, Co, and Ni

MAITHREYI GOPALAKRISHNAN, CHRISTIAN GENTRY, DMITRIY ZUSIN, PATRIK GRYCHTOL, RONNY KNUT, JILA, University of Colorado Boulder, JUSTIN SHAW, HANS NEMBACH, Electromagnetics Division, NIST, Boulder, STEFAN MATHIAS, Department of Physics, Georg-August-Universität Göttingen, MARTIN AESCHLIMANN, Department of Physics, University of Kaiserslautern, PETER OPPENEER, Department of Physics and Astronomy, Uppsala University, CLAUDIUS SCHNEIDER, Peter Grünberg Institut, Forschungszentrum Jülich, HENRY KAPTEYN, MARGARET MURNANE, JILA, University of Colorado Boulder — Even twenty years after the discovery of ultrafast demagnetization of ferromagnetic materials induced by a femtosecond laser pulse there is still an ongoing debate about the mechanisms that drive the process. Surprisingly, a comprehensive study that compares demagnetization dynamics in different materials on equal footing is lacking. Yet, the scientific community would greatly benefit from such study. We fill this gap by performing a systematic comparison of ultrafast demagnetization behavior in Iron, Cobalt and Nickel, the simplest itinerant ferromagnets, under a wide range of pump fluences. In this experiment, we utilize a tabletop broadband extreme ultraviolet source to probe magnetization dynamics at the M<sub>2,3</sub> absorption edges of these three elements using the transverse magneto-optical Kerr effect. The obtained data can be used to inform theory and, thereby, assist in resolving the remaining questions about the micro- and macroscopic mechanisms behind ultrafast laser-induced magnetization dynamics in materials.

**1:15PM L18.00009 Ultrafast demagnetization, spin-dependent Seebeck effect, and thermal spin transfer torque in Pt/TbFe/Cu and Pt/TbFe/Cu/Fe thin films<sup>1</sup>**, JOHANNES KIMLING, University of Illinois, BIRGIT HEBLER, University of Augsburg, JUDITH KIMLING, University of Illinois, MANFRED ALBRECHT, University of Augsburg, DAVID G. CAHILL, University of Illinois — We investigate diffusive spin currents in Pt(20nm)/TbFe(10nm)/Cu(100nm) and Pt(20 nm)/TbFe(10nm)/Cu(100nm)/Fe(3nm) stacks using time-resolved magneto-optic Kerr effect (TRMOKE) and time-domain thermoreflectance measurements. Our experiments are based on two hypothesis: (1) fast changes of magnetization due to laser excitation are transferred into spin accumulation, e.g., via electron-magnon scattering; the generated spin accumulation drives a diffusive spin current into adjacent normal metal layers; (2) electronic thermal transport through the ferromagnetic layer injects a spin current into adjacent normal metal layers, based on the spin-dependent Seebeck effect. [1] We excite the Pt layer with ps-laser pulses. Resulting diffusive spin currents generate nonequilibrium magnetization in the Cu layer (sample I) and induce a precession of the magnetization of the Fe layer via spin transfer torque (sample II). Both responses are probed using TRMOKE. Prior experiments used [Co(0.2nm)/Pt(0.4nm)]<sub>x5</sub>/Co(0.2nm) instead of TbFe. [1] The ferrimagnetic TbFe layer with introduces two major modifications: (1) slow demagnetization behavior, and (2) large thermal resistance. Hence, thermal spin transfer torques can be observed on significantly longer time scales. [1] G.-M. Choi, C.-H. Moon, B.-C. Min, K.-J. Lee, and D. G. Cahill, Nature Physics 11, 576 (2015).

<sup>1</sup> Financial support by the German Research Foundation under DFG-Grant No. KI 1893/1-1 and DFG-Grant No. AL 618/21-1 are kindly acknowledged.

CNRS-SOLEIL Synchrotron

L'Orme des Merisiers , Saint Aubin

91192 Gif sur Yvette

**1:27PM L18.00010 Electronic properties of solids excited with intermediate laser power densities.**, FAUSTO SIROTTI, None, TEMPO BEAMLINE TEAM — Intermediate laser power density up to about 100 GW/cm<sup>2</sup> is below the surface damage threshold is currently used to induce modification in the physical properties on short time scales. The absorption of a short laser pulse induces non-equilibrium electronic distributions followed by lattice-mediated equilibrium taking place only in the picosecond range. The role of the hot electrons is particularly important in several domains as for example fast magnetization and demagnetization processes [1], laser induced phase transitions, charge density waves. Angular resolved photoelectron spectroscopy measuring directly energy and momentum of electrons is the most adapted tool to study the electronic excitations at short time scales during and after fast laser excitations. The main technical problem is the space charge created by the pumping laser pulse. I will present angular resolved multiphoton photoemission results obtained with 800 nm laser pulses [2] showing how space charge electrons emitted during fast demagnetization processes can be measured.

[1] N. Beaulieu et al., Journal of Electron Spectroscopy and Related Phenomena, 2013, 189 Supp: 40–45

[2] F. Sirotti et al., Physical Review B, 2014, 90(3): art.n035401

France

**1:39PM L18.00011 Ultrafast Study of Dynamic interfacial Exchange Coupling in Ferromagnet/Oxide/Semiconductor Heterostructures<sup>1</sup>**, YU-SHENG OU, YI-HSIN CHIU, The Ohio State University, NICHOLAS HARMON, The University of Iowa, PATRICK ODENTHAL, University of California, Riverside, MATTHEW SHEFFIELD, MICHAEL CHILCOTE, ROLAND KAWAKAMI, The Ohio State University, MICHAEL FLATT, The University of Iowa, EZEKIEL JOHNSTON-HALPERIN, The Ohio State University — Time-resolved Kerr/Faraday rotation (TRKR/TRFR) is employed to study GaAs spin dynamics in the regime of strong and dynamic exchange coupling to an adjacent MgO/Fe layer. This study reveals a dramatic, resonant suppression in the inhomogeneous spin lifetime (T<sub>2</sub><sup>\*</sup>) in the GaAs layer. Further investigation of the magnetization dynamics of the neighboring Fe layer, also using TRKR/TRFR, reveals not only the expected Kittel-dispersion but also additional lower frequency modes with very short lifetime (65 ps) that are not easily observed with conventional ferromagnetic resonance (FMR) techniques. These results suggest the intriguing possibility of resonant dynamic spin transfer between the GaAs and Fe spin systems. We discuss the potential for this work to establish GaAs spin dynamics as an efficient detector of spin dissipation and transport in the regime of dynamically-driven spin injection in ferromagnet/semiconductor heterostructures.

<sup>1</sup> Center for Emergent Materials; U.S. Department of Energy

**1:51PM L18.00012 Heisenberg vs. Stoner: Ultrafast magnon generation and exchange renormalization in the course of laser-induced demagnetization**, DMITRIY ZUSIN, EMRAH TURGUT, PATRIK GRZYCHOL, RONNY KNUT, JILA, University of Colorado - Boulder, DOMINIK LEGUT, Department of Condensed Matter Physics, Charles University, Prague, JUSTIN SHAW, HANS NEMBACH, THOMAS SILVA, Electromagnetics Division, NIST, Boulder, STEFAN MATHIAS, MARTIN AESCHLIMANN, Department of Physics, University of Kaiserslautern and Research Center OPTIMAS, CLAUS SCHNEIDER, Peter-Grunberg-Institut, Forschungszentrum Julich, KAREL CARVA, PETER OPPENEER, Department of Physics and Astronomy, Uppsala University, HENRY KAPTEYN, MARGARET MURNANE, JILA, University of Colorado - Boulder — In this work, we access the microscopic mechanisms responsible for the ultrafast magnetization dynamics of ferromagnets following a femtosecond laser excitation. Using a tabletop high-harmonic source of extreme ultraviolet light, we perform magneto-optical pump-probe spectroscopic studies across the M<sub>2,3</sub> absorption edge of Cobalt with time, energy and angle resolution. This novel approach allows us to extract the time-dependent resonant magneto-optical properties of the Cobalt sample. In combination with ab-initio calculations of the density of states and the magneto-optical response, this gives us indirect access to ultrafast dynamics of the band structure. A comparison of our theoretical simulations with the experimental measurements suggests a variety of demagnetization mechanisms, which include ultrafast magnon excitations, enhanced electron temperature and transient renormalization of exchange splitting.

**2:03PM L18.00013 Studies of Ultrafast Demagnetization in Ferromagnetic Metal Alloys using TDDFT**, PETER ELLIOTT, KEVIN KRIEGER, JOHN KAY DEWHURST, SANGEETA SHARMA, E.K.U. GROSS, Max Planck Institute of Microstructure Physics — Time dependent density functional theory (TDDFT) has recently [1,2] been applied to study magnetization dynamics in periodic systems. In particular it was found for short intense pulses, a significant source of demagnetization is spin-flips mediated by the spin-orbit interaction. In this work, we perform TDDFT simulations for the case of bulk Heusler compounds under the same conditions, and find a similar loss of the global magnetic moment can occur. Furthermore, we also see local loss of moment due to transfer of moment from one sublattice to another during the optical excitation process. This is then followed by the spin-orbit mediated demagnetization in certain cases. Additionally we will analyze the spin-current densities to better understand the various processes at work. [1] Laser induced ultrafast demagnetization: an ab-initio perspective, K. Krieger, J.K. Dewhurst, P. Elliott, S. Sharma, E.K.U. Gross, J. Chem. Theory and Comput. 11, 4870 (2015). [2] Demonstration of Optimal Control of Laser Induced Spin-Orbit Mediated Ultrafast Demagnetization, P. Elliott, K. Krieger, J. K. Dewhurst, S. Sharma, E. K. U. Gross, submitted (2015).

**Wednesday, March 16, 2016 11:15AM - 2:15PM –**

**Session L19 GMAG DMP: Emergent Magnetic and Electronic States in Oxide Heterostructures**

318 - Gervasi Herranz, ICMAB-CSIC

**11:15AM L19.00001 Engineering a spin-orbital magnetic insulator by tailoring iridate-based superlattices**, JOBU MATSUNO, RIKEN Center for Emergent Matter Science — In 5d Ir oxides with an interplay of spin-orbit coupling and electron correlations, we have tailored a spin-orbital magnetic insulator out of a semimetal SrIrO<sub>3</sub> by tuning the structure through superlattices [(SrIrO<sub>3</sub>)<sub>m</sub>, SrTiO<sub>3</sub>] ( $m = 1, 2, 3, 4$ , and  $\infty$ ) grown on SrTiO<sub>3</sub>(001) substrates. We observed the systematic decrease of the magnetic ordering temperature and the resistivity as a function of  $m$ . The transition from the semimetal to the insulator is found to be closely linked to the appearance of magnetism at  $m \simeq 3$ . Long range magnetic ordering was realized even in the  $m = 1$  single layer superlattice, implying that the design and realization of novel electronic phases is feasible at the level of a single atomic layer in complex Ir oxides. We also report the fabrication of (111)-oriented superlattice structures with alternating  $2m$ -layers ( $m = 1, 2$ , and  $3$ ) of Ca<sub>0.5</sub>Sr<sub>0.5</sub>IrO<sub>3</sub> perovskite and two layers of SrTiO<sub>3</sub> perovskite on SrTiO<sub>3</sub>(111) substrates. In the case of  $m = 1$  bilayer films, the Ir sublattice is a buckled honeycomb, where a topological state may be anticipated. The ground states of the superlattice films were found to be magnetic insulators, which may suggest the importance of electron correlations in Ir perovskites in addition to the much discussed topological effects.

**11:51AM L19.00002 Novel magnetic and electronic states in manganite-iridate heterostructures**<sup>1</sup>, JOHN NICHOLS, SHINBUHM LEE, JON PETRIE, TRICIA MEYER, XIANG GAO, ERJIA GUO, Oak Ridge National Laboratory, JOHN FREELAND, Argonne National Laboratory, DI YI, JIAN LIU, University of Tennessee, DANIEL HASKEL, Argonne National Laboratory, THOMAS ZAC WARD, GYULA ERES, VALERIA LAUTER, MICHAEL R. FITZSIMMONS, HO NYUNG LEE, Oak Ridge National Laboratory — Strong correlation between spin, charge, lattice, and orbital order parameters has proven to give rise to exotic physical phenomena, while epitaxial design of materials with strong interfacial coupling is an efficient technique to tune such parameters. Although there have been numerous studies of interfaces between 3d-3d and 4d-3d compounds, only few studies reported work on 3d and 5d materials and there has been no report on strong interfacial coupling in such systems. We have synthesized high quality [(AMnO<sub>3</sub>)<sub>m</sub>/(SrIrO<sub>3</sub>)<sub>n</sub>]<sub>z</sub> ( $A = \text{Sr, La}$ ) heterostructures by pulsed laser epitaxy on SrTiO<sub>3</sub> (001) substrates and have observed interesting novel magnetic and electronic ground states, which are highly sensitive to the degree of dimensional confinement in the heterostructures. Based on studies with x-ray diffraction, SQUID,  $dc$ -transport, x-ray circular dichroism, and polarized neutron reflectometry measurements, we will report intriguing magnetic and transport properties that provide the first evidence of strong interfacial coupling between 5d and 3d materials.

<sup>1</sup>This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

**12:03PM L19.00003 Strain control of magnetic structure in Sr<sub>3</sub>Ir<sub>2</sub>O<sub>7</sub>**, CHOONG H. KIM, IBS-CCES & Seoul Nat'l Univ. — We have studied from first principles the structural, electronic, and magnetic properties of the layered-perovskite iridates Sr<sub>3</sub>Ir<sub>2</sub>O<sub>7</sub> as a function of epitaxial strain. In Sr<sub>3</sub>Ir<sub>2</sub>O<sub>7</sub>, bilayer iridates, an easy  $c$ -axis collinear antiferromagnetic structure have been reported, a significant contrast to single layer Sr<sub>2</sub>IrO<sub>4</sub> with in-plane canted moments. This behavior is understood by competition among intra- and interlayer bond-directional pseudodipolar interactions. From our first-principles calculations, we show that these two energy scales are controllable via strain to drive spin-flop transition.

**12:15PM L19.00004 Realization of a Ferroelectric-Domain-Wall Tunnel Junction**, JACOBO SANTA-MARIA, G. SANCHEZ-SANTOLINO, J. TORNOS, D. HERNANDEZ-MARTIN, J. I. BELTRAN, M. CABERO, A. PEREZ-MUOZ, Z. SEFRIQUI, C. LEON, M. VARELA, GFMC. Univ Complutense. 28040 Madrid, C. MUNUERA, F. MOMPEAN, M. GARCIA-HERNANDEZ, M. C. MUOZ, Instituto de Ciencia de Materiales de Madrid ICM-ICMM-CSIC 28049 Madrid, S. J. PENNYCOOK, Department of Materials Science & Engineering, National University of Singapore, Singapore 117575. — Incorporating ferroelectric domain walls as an active part of electronic devices holds the promise of interesting new functionalities. Here we form a ferroelectric BaTiO<sub>3</sub> tunnel barrier just 4.4-nanometer thick, with ferromagnetic La<sub>0.7</sub>Sr<sub>0.3</sub>MnO<sub>3</sub> electrodes, containing a head-to-head domain wall within its thickness. A confined electron gas is formed at the domain wall, stabilized by oxygen vacancies, which controls the tunneling transport of the magnetic tunnel junction. Resonant tunneling assisted by the discrete levels of the ferroelectric quantum well gives rise to strong quantum oscillations of the tunneling conductance. Our engineered, highly constrained, domain wall provides a major step forward towards the new concept "The Wall is the Device", exploiting the electronic properties of domain walls for ferroelectric tunnel barriers with new functionalities. Work at UCM supported by MINECO MAT2014-52405-C02-01 and ERC Starting Investigator Grant #239739 STEMOX. MCM acknowledges financial support from MICINN through grant MAT2012-38045-C04-04.

**12:27PM L19.00005 Tailoring magneto-electro-resistance in La<sub>0.7</sub>Sr<sub>0.3</sub>MnO<sub>3</sub>/BaTiO<sub>3</sub>multiferroic tunnel junctions**, MARIONA CABERO, A.M. PEREZ-MUOZ, D. HERNANDEZ-MARTIN, Z. SEFRIQUI, M. VARELA, C. LEON, J. SANTA-MARIA, GFMC Univ Complutense. 28040 Madrid, S. VALENCIA, Helmholtz-Zentrum Berlin fr Materialien & Energie, Albert-Einstein-Strasse 15, 12489 Berlin, Germany, R. ABRUDAN<sup>1</sup>, Helmholtz-Zentrum Berlin fr Materialien & Energie, Albert-Einstein-Strasse 15, 12489 Berlin, S. J. PENNYCOOK, Department of Materials Science & Engineering, National University of Singapore, Singapore 117575. — Controlling and manipulating the electronic states of oxide interfaces using external stimuli has become a major direction towards oxide-based electronics. Here, we present a study of the transport properties of multiferroic La<sub>0.7</sub>Sr<sub>0.3</sub>MnO<sub>3</sub>/BaTiO<sub>3</sub> (LSMO/BTO) ferromagnetic/ferroelectric heterostructures. Multiferroic tunnel junctions (MTJ's) have been obtained introducing an ultrathin La/Sr cuprate (LSCO) layer between the ferroelectric barrier and the top ferromagnetic electrode. The LSCO introduces an asymmetry in the screening of polarization charges at both interfaces, which yields electroresistance values in excess of 105 % and triggers an inversion of the sign of the tunneling magnetoresistance controlled by ferroelectric switching. We will discuss these results in the light of the generation and transport of oxygen vacancies. Work at UCM supported by MINECO MAT2014-52405-C02-01 and ERC Starting Investigator Grant #239739 STEMOX.

<sup>1</sup>AND Institut fr Experimentalphysik/Festkperphysik, Ruhr-Universitt Bochum, 44780 Bochum, Germany.

**12:39PM L19.00006 DFT+ $U$  study of electronic structure and Curie temperature of  $A_2B\text{ReO}_6$  ( $A=\text{Sr, Ca}$  and  $B=\text{Cr, Fe}$ )**, ALEX LEE, CHRIS MARIANETTI, Applied Physics and Applied Math, Columbia University — Re-based double perovskites (DPs) have attracted much attention due to their high Curie temperature ( $T_C$ ) and colossal magneto resistance with large potential for spintronic applications. Here we investigate the electronic and magnetic properties of the Re-based DPs  $A_2B\text{ReO}_6$  ( $A=\text{Sr, Ca}$  and  $B=\text{Cr, Fe}$ ) using density functional theory +  $U$  (DFT+ $U$ ) calculations. While monoclinic Ca<sub>2</sub>CrReO<sub>6</sub> and Ca<sub>2</sub>FeReO<sub>6</sub> (monoclinic) are insulating within GGA+ $U$ , tetragonal Sr<sub>2</sub>CrReO<sub>6</sub> ( $a^0a^0c^0$ ) and Sr<sub>2</sub>FeReO<sub>6</sub> ( $a^0a^0c^-$ ) remain metallic. We show that both on-site interaction  $U$  and octahedral tilting are critical to obtain the insulating phases. The  $a^0a^0c^-$ -phase of Sr<sub>2</sub>CrReO<sub>6</sub> is most stable and insulating with nonzero  $U$ , suggesting that the high quality Sr<sub>2</sub>CrReO<sub>6</sub> film on STO substrate can be a semiconductor as reported in recent experiments. We explain that the insulator-to-metal transition (MIT) of Ca<sub>2</sub>FeReO<sub>6</sub> at 140K is predominantly due to a structural phase transition which drives the insulating state. Curie temperatures of Re-based DPs are calculated using the classical Monte Carlo simulations based on the Heisenberg model.

**12:51PM L19.00007 Magnetism and Nanoscale Structural and Compositional Irregularities in MBE-grown  $\text{La}_2\text{MnNiO}_6$  on  $\text{SrTiO}_3(001)$** , SCOTT CHAMBERS, YINGGE DU, TIMOTHY DROUBAY, PETER SUSHKO, STEVEN SPURGEON, ARUN DEVARAJ, MARK BOWDEN, V SHUTTHANANDAN, Pacific Northwest Natl Lab, TORGNY GUSTAFSSON, Rutgers University — Double perovskites ( $\text{A}_2\text{BB}'\text{O}_6$ ) are a fascinating class of oxides with considerable potential for applications requiring ferromagnetic and semiconducting properties. We have investigated MBE-grown  $\text{La}_2\text{MnNiO}_6$  and have found that despite the fact that Mn and Ni are present as  $4+$  ( $d^3 : t_{2g}^3 e_g^0$ ) and  $2+$  ( $d^8 : t_{2g}^6 e_g^2$ ) respectively, and exhibit suitable XMCD signatures, the volume-averaged moment per formula unit is considerably less than 5 Bohr magnetons. Our electron energy loss spectroscopy (STEM-EELS) and atom probe tomography (APT) results to date reveal that there is considerable disorder in the B-site sublattice for as-deposited films, despite excellent volume-averaged stoichiometry. While air annealing results in substantial ordering, the moment remains low due to the nucleation of NiO inclusions with needle-like shapes revealed only by APT. First principles modeling suggests that even though the double perovskite is quite stable if nucleated in excess O, the presence of O vacancies facilitates structural disorder. In this talk, we will present our latest results on this fascinating material.

**1:03PM L19.00008 Magnetism, Chemical Ordering, and Defects in Epitaxial Double Perovskite  $\text{La}_2\text{MnNiO}_6$  Thin Films.**, TIM DROUBAY, STEVEN SPURGEON, YINGGE DU, ARUN DEVARAJ, Pacific Northwest National Laboratory, STEVE HEALD, Advanced Photon Source, Argonne National Laboratory, PETER SUSHKO, Pacific Northwest National Laboratory, TORGNY GUSTAFSSON, Rutgers University, DAVID KEAVNEY, Advanced Photon Source, Argonne National Laboratory, SCOTT CHAMBERS, Pacific Northwest National Laboratory — Oxide double perovskites ( $\text{A}_2\text{BB}'\text{O}_6$ ) exhibit an interesting variety of electronic and magnetic properties such as half-metallicity and high temperature ferromagnetism holding promise for potential technological applications. We have investigated  $\text{La}_2\text{MnNiO}_6/\text{SrTiO}_3$  grown using molecular beam epitaxy and have found different proportions of two ferromagnetic phase transitions ( $\sim 130\text{K}$  and  $\sim 290\text{K}$ ) and various saturation magnetization values ( $< 4.6 \mu_B/\text{f.u.}$ ) dependent upon post-growth annealing. Contrary to previous reports, neither the increase in the saturation magnetization nor the Curie temperature(s) after annealing can be attributed to changing Mn and Ni valence. Instead, using aberration-corrected transmission electron microscopy and atom probe tomography, we observe large-scale chemical ordering as a result of annealing. We also find the coexistence of NiO-derived extended defects that appear to prevent the magnetic moment from reaching the maximum possible value ( $5 \mu_B/\text{f.u.}$ ). We will describe these results in light of first principles calculations which suggest that local deviations from the ideal stoichiometry facilitate the formation of the NiO phase and structural disorder in the double perovskite phase.

**1:15PM L19.00009 Half-metallic ferromagnetism on surfaces of insulating and antiferromagnetic  $\text{LaFeO}_3$  thin films**, ROHAN MISHRA, Washington University in St. Louis, YOUNG-MIN KIM, Korea Basic Science Institute, QIAN HE, Oak Ridge National Laboratory, SEONG-KEUN KIM, Korea Institute of Science & Technology, SEOHYOUNG CHANG, ANAND BHATTACHARYA, Argonne National Laboratory, SOKRATES T. PANTELIDES, Vanderbilt University, Oak Ridge National Laboratory, ALBINA BORISEVICH, Oak Ridge National Laboratory — The surfaces of perovskite transition metal oxides having correlated electrons show novel electronic and magnetic phenomena. In this work, we combine scanning transmission electron microscopy imaging and electron energy loss spectroscopy (EELS) with density functional theory (DFT) calculations to study the surface of  $(\text{LaFeO}_3)_m/(\text{SrFeO}_3)_n$  heterostructure thin films. Using EELS, we observe a reduction in the oxidation state of Fe on moving from the bulk to the surface over a length of  $\sim 5$  unit cells. Simultaneously acquired STEM images allow us to map the associated changes in their structure, such as cation displacements and changes in oxygen polyhedral tilts. DFT calculations coupled with the STEM results show that by reducing the surface layer of a  $\text{LaFeO}_3$  film such that the surface is terminated with  $\text{FeO}_4$  tetrahedra instead of the  $\text{FeO}_6$  octahedra as present in the bulk, it is possible to stabilize an exotic phase where the surface layer displays a half-metallic ferromagnetic behavior, while the bulk remains antiferromagnetic and insulating, similar to the class of topological insulators. The calculations also predict that the magnetism and conductivity at the surface can be controlled by the partial pressure of oxygen.

**1:27PM L19.00010 X-ray Magnetic circular dichroism study of hexagonal  $\text{YbFeO}_3$  thin films**, XIAO WANG, Bryn Mawr College, KISHAN SINHA, XIAOSHAN XU, University of NebraskaLincoln, YAOHUA LIU, Oak Ridge National Laboratory, DAVID KEAVNEY, Argonne National Laboratory, X.M. CHENG, Bryn Mawr College — Multiferroic materials exhibit multiple ferroic orders simultaneously and thus have potential applications in information technology, sensing, and actuation. Hexagonal  $\text{YbFeO}_3$  is a promising candidate for a multiferroic material with room temperature ferromagnetism because of the expected enhanced Fe moment and higher transition temperature due to the exchange interaction between magnetic Yb and Fe ions. Here we report an x-ray magnetic circular dichroism (XMCD) study of (0001) Hexagonal  $\text{YbFeO}_3$  thin films deposited on (111) yttria-stabilized zirconia substrates via pulsed laser deposition. XMCD spectra for the Fe  $L_{2,3}$  edges and Yb  $M_5$  edge were measured with the magnetic field applied parallel to the x-ray propagation direction and 20 degree away from the film normal at beamline 4ID-C of the APS at ANL. Field dependence of the XMCD spectra show that Fe and Yb each has a ferromagnetic ordering at around 6.7 K but with opposite orientations in between. The saturation magnetic moment for Fe is determined by the sum rules to be  $0.07 \mu_B / \text{Fe cation}$  at around 6.7 K, about 4 times larger than that in Hexagonal  $\text{LuFeO}_3$ .

**1:39PM L19.00011 MAGNETO-OPTIC ENHANCEMENT IN NANO-SCALE IRON GARNET FILMS**, ASHIM CHAKRAVARTY, MIGUEL LEVY, Physics Department, Michigan Technological University, 49931, USA — This work addresses dimensionality-induced magneto-optic effects in liquid-phase-epitaxy magnetic garnet thin films. It is found that the Faraday rotation (FR) per unit length evinces a marked and steady enhancement as the film thickness is reduced approximately below 100 nm in  $\text{Bi}_{0.8}\text{Gd}_{0.2}\text{Lu}_2\text{Fe}_5\text{O}_{12}$ , although it remains constant in the micron- and most of the sub-micron-regime. The reported specific FR change in such reduced dimensions is due to size-dependent modifications in diamagnetic transition processes in the garnet film. These processes correspond to the electronic transitions from the singlet  $^6\text{S}$  ground state to spin-orbit split excited states of the  $\text{Fe}^{3+}$  ions in the garnet. A measurable reduction in the corresponding ferrimagnetic resonance linewidths is found, thus pointing to an increase in electronic relaxation times and longer lived excitations at reduced thicknesses than in the bulk. These changes together with a shift in vibrational frequency of the Bi-O bonds in the garnet at reduced thicknesses result in magneto-optical enhancement in ultra-thin garnet films.

**1:51PM L19.00012 Enhancement of Magnetization in  $\text{Y}_3\text{Fe}_5\text{O}_{12}$  Epitaxial Thin Films.**, JACK T. BRANGHAM, JAMES C. GALLAGHER, ANGELA S. YANG, SHANE P. WHITE, ROHAN ADUR, WILLAM T. RUANE, BRYAN D. ESSER, MICHAEL R. PAGE, P. CHRIS HAMMEL, Ohio State Univ - Columbus, DAVID W. MCCOMB, Center for Electron Microscopy and Analysis, Dept of Materials Science and Engineering, The Ohio State University, Columbus, OH 43212, FENGYUAN YANG, Ohio State Univ - Columbus — The ability to generate pure spin currents has applications in telecommunications, radar, and spin-based logic.  $\text{Y}_3\text{Fe}_5\text{O}_{12}$  (YIG) is one of the best materials for dynamic generation of spin currents due to its low damping, narrow ferromagnetic resonance (FMR) linewidth, and insulating behavior. We grow stoichiometric, high quality, epitaxial YIG thin films with thicknesses ranging from 4 to 250 nm on  $\text{Gd}_3\text{Ga}_5\text{O}_{12}$  by off-axis magnetron sputtering and characterize the YIG films by various techniques. The temperature dependence of the saturation magnetization was independently measured by in-plane vibrating sample magnetometry, out-of-plane magnetic shape anisotropy, and angular-dependent FMR absorption from 10 K to the Curie temperature of 530 K. The room temperature saturation magnetization was also measured with frequency dependent FMR. All measurements show a magnetization enhancement of 15% or greater when compared to reported magnetization values of bulk YIG crystals. We speculate this is due to suppression of the long wavelength magnons due to the finite size of the films.

**2:03PM L19.00013 Strain induced structural, electronic, and magnetic properties of SrFeO<sub>2</sub> and BaFeO<sub>2</sub>**, WEIDONG LUO, XIAOLE ZHANG, Shanghai Jiao Tong University, China — The structural, electronic and magnetic properties of SrFeO<sub>2</sub> and BaFeO<sub>2</sub> under tensile strains are studied using first-principles density-functional theory calculations. Strain-induced Jahn-Teller-like behaviors involving the cooperative displacements of oxygen atoms are predicted in both compounds. Lattice dynamical properties are also investigated and the strain-induced imaginary phonon modes are consistent with the Jahn-Teller-like distortion. The usual Jahn-Teller instability of degenerate energy levels does not contribute to the interesting phenomena. Besides the structural and electronic properties, a transition of magnetic orderings from G-type anti-ferromagnetic phase to C-type anti-ferromagnetic phase is predicted in both compounds, which originates from the combined effects of the lattice-orbital coupling and the spin-orbital coupling due to exchange interaction between orthogonal Fe 3d orbitals.  
We acknowledge funding support from the National Natural Science Foundation of China.

**Wednesday, March 16, 2016 11:15AM - 2:15PM –**  
**Session L20 DCOMP: Quantum Many-Body Systems and Methods II** 319 - Eric Andrade, TU Dresden, Germany

**11:15AM L20.00001 Scaling and Locality properties of the Entanglement Hamiltonian in Critical Fermionic systems**, NICOLA LANATA, Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32306, USA, YONG-XIN YAO, Ames Laboratory-U.S. DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa, XIAOYU DENG, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08856-8019, USA, MOHAMMAD POURANVARI, Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32306, USA — We study the entanglement Hamiltonian of several gapless Fermionic systems. In particular, we consider an infinite metallic one dimensional chain of free Fermions, and show that the corresponding entanglement Hamiltonian  $F(L)$  for a subsystem of length  $L$  is local. Furthermore, we show that  $F(L)$  displays a well defined continuum limit, which is related with the so called logarithmically enhanced area law of the entanglement entropy,  $S(L) \sim \log(L)$ . Finally, using the “Gutzwiller renormalization group” [arXiv:1509.05441], we discuss these concepts in relation with the physics of the Anderson impurity model.

**11:27AM L20.00002 Entanglement dynamics in quantum many-body systems<sup>1</sup>**, WEN WEI HO, DMITRY ABANIN, Department of Theoretical Physics, University of Geneva — The dynamics of quantum entanglement  $S(t)$  has proven useful to distinguishing different quantum many-body phases. In particular, the growth of entanglement following a quantum quench can be used to distinguish between many-body localized ( $S(t) \sim \log t$ ) and ergodic ( $S(t) \sim t$ ) phases. Here, we provide a theoretical description of the growth of entanglement in a quantum many-body system, and propose a method to experimentally measure it. We show that entanglement growth is related to the spreading of local operators. In ergodic systems, the linear spreading of operators results in a universal, linear in time growth of entanglement. Furthermore, we show that entanglement growth is directly related to the decay of the Loschmidt echo in a composite system comprised of many copies of the original system, subject to a perturbation that reconnects different parts of the system. Using this picture, we propose an experimental set-up to measure entanglement growth by using a quantum switch (two-level system) which controls connections in the composite system. Our work provides a way to directly probe dynamical properties of many-body systems, in particular, allowing for a direct observation of many-body localization.

<sup>1</sup>This work was partially supported by Sloan Foundation, Ontario Early Researcher Award and NSERC Discovery Grant.

**11:39AM L20.00003 Measuring Entanglement Spectrum via Density Matrix Exponentiation**, GUANYU ZHU, ALIREZA SEIF, Joint Quantum Institute, University of Maryland, College Park, Maryland, USA, HANNES PICHLER, PETER ZOLLER, Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, Innsbruck, Austria, MOHAMMAD HAFEZI, Joint Quantum Institute, University of Maryland, College Park, Maryland, USA — Entanglement spectrum (ES), the eigenvalues of the reduced density matrix of a subsystem, serves as a powerful theoretical tool to study many-body systems. For example, the gap and degeneracies of the entanglement spectrum have been used to identify various topological phases. However, the usefulness of such a concept in real experiments has been debated, since it is believed that obtaining the ES requires full state tomography, at a cost which exponentially grows with the systems size. Inspired by a recent density matrix exponentiation technique, we propose a scheme to measure ES by evolving the system with a Hamiltonian that is the subsystem's own reduced density matrix. Such a time evolution can be induced by an ancilla photon that is coupled to multiple qubits at the same time. The phase associated with the time evolution can be detected and converted into ES through either a digital or an analogue scheme. The digital scheme involves a modified quantum phase estimation algorithm based on random time evolution, while the analogue scheme is in the spirit of Ramsey interferometry. Both schemes are not limited by the size of the system, and are especially sensitive to the gap and degeneracies. We also discuss the implementation in cavity/circuit-QED and ion trap systems.

**11:51AM L20.00004 Flow equation holography**, STEFAN KEHREIN<sup>1</sup>, University Goettingen — The Ryu-Takayanagi conjecture [1] about the holographic derivation of the entanglement entropy provides a remarkable geometric picture by relating minimal surfaces to the entanglement entropy. Underlying this conjecture is the AdS/CFT correspondence, which limits the applicability of this geometric picture in its original formulation to a very specific set of theories. In this talk I will show how the flow equation method [2,3] can be used to construct an emergent geometric picture for generic quantum many-body systems. Results for the emergent Riemannian geometry of certain low-dimensional quantum systems are presented based on analytical and numerical solution of the flow equations. Minimal surfaces on these Riemannian manifolds show behavior in agreement with the entanglement entropy of the corresponding quantum theory, both for gapped and critical systems.

[1] S. Ryu and T. Takayanagi, Phys. Rev. Lett. 96, 181602 (2006)

[2] F. Wegner, Ann. Phys. (Leipzig) 3, 77 (1994)

[3] S. Kehrein, The Flow Equation Approach to Many-Particle Systems (Springer, 2006)

<sup>1</sup>See list of reciprocal member societies: I am a member of the Deutsche Physikalische Gesellschaft (DPG), member ID 871489

**12:03PM L20.00005 Irreversibility in Quantum Many-Body Systems**, MARKUS SCHMITT, STEFAN KEHREIN, Univ Goettingen — The question of thermalization in closed quantum many-body systems has received a lot of attention in the past few years. An intimately related question is whether a closed quantum system shows irreversible dynamics. However, irreversibility and what we actually mean by this in a quantum many-body system with unitary dynamics has been explored very little. In our work we investigate the irreversibility of dynamics in quantum many-body systems by studying echo dynamics. In order to quantify the (ir)reversibility we study the time evolution involving an imperfect effective time reversal. Our measure for the recovery of the initial state are the echo peaks occurring in the time evolution of observables. Specifically, we investigate non-interacting and interacting one-dimensional spin chains. We study the characteristics of the echo peak decay and especially focus on whether this depends on the (non-)integrability of the model.

**12:15PM L20.00006 Quantum Quench Dynamics in the Transverse Field Ising Model at Non-zero Temperatures<sup>1</sup>** , NILS ABELING, STEFAN KEHREIN, Univ Goettingen — The recently discovered *Dynamical Phase Transition* denotes non-analytic behavior in the real time evolution of quantum systems in the thermodynamic limit and has been shown to occur in different systems at zero temperature [Heyl *et al.*, Phys. Rev. Lett. **110**, 135704 (2013)]. In this talk we present the extension of the analysis to non-zero temperature by studying a generalized form of the Loschmidt echo, the work distribution function, of a quantum quench in the transverse field Ising model. Although the quantitative behavior at non-zero temperatures still displays features derived from the zero temperature non-analyticities, it is shown that in this model dynamical phase transitions do not exist if  $T > 0$ . This is a consequence of the system being initialized in a thermal state. Moreover, we elucidate how the Tasaki-Crooks-Jarzynski relation can be exploited as a symmetry relation for a global quench or to obtain the change of the equilibrium free energy density.

<sup>1</sup>This work was supported through CRC SFB 1073 (Project B03) of the Deutsche Forschungsgemeinschaft (DFG).

**12:27PM L20.00007 Nonequilibrium electron dynamics: Formation of the quasiparticle peak** , SHARAREH SAYYAD, MARTIN ECKSTEIN, Max Planck Inst Structure and Dynamics of Matter — We characterize how the narrow quasiparticle band of the one-band Hubbard model forms out of a bad metallic state in a time-dependent metal-insulator transition, using nonequilibrium slave-rotor dynamical mean field theory. Our results exhibit a nontrivial electronic timescale which is much longer than the width of the quasiparticle peak itself. To study this timescale, we perform a fast ramp from the insulating phase into the metallic region of the phase diagram, resulting in a highly excited state, and study the equilibration of the system with a weakly coupled phononic bath. The slow relaxation behavior is explained by surveilling the interplay between spinon and rotor degrees of freedom. Since the system is initially prepared in an insulating phase, the quasi-particle peak emerges when spinons catch up the metal-insulator crossover region, which is reached earlier by the rotor. At this point, spinon and rotor become weakly coupled, and the resulting very slow equilibration of the spinon is a bottleneck for the dynamics. After the birth of the quasiparticle peak, its height enhances by the construction of the low-energy spectrum of the rotor, which then lags behind the relaxation of the spinon.

**12:39PM L20.00008 Nonequilibrium Kondo physics in the Anderson impurity model: Auxiliary master equation approach<sup>1</sup>** , ANTONIUS DORDA, Graz University of Technology, MARTIN GANAHL, Perimeter Institute for Theoretical Physics, HANS GERD EVERTZ, WOLFGANG VON DER LINDEN, ENRICO ARRIGONI, Graz University of Technology — An accurate investigation of the evolution of the Kondo peak as a function of bias voltage is presented for the single impurity Anderson model (SIAM). We greatly enhance the capability of the recently introduced auxiliary master equation approach (AMEA) [1,2] by making use of matrix product states [3]. This allows us to obtain highly accurate spectral functions and observables for the SIAM at large values of the interaction and low temperatures  $T$ , well below the Kondo scale  $T_K$ . For  $T \approx T_K/4$  and  $T \approx T_K/10$  we find a clear splitting of the Kondo resonance into a two-peak structure at bias voltages just above  $T_K$ . A benchmark in the equilibrium case for  $T \approx T_K/4$  reveals a remarkably close agreement to the numerical renormalization group. This, together with the high flexibility and the applicability to various problems such as dynamical mean field theory [1,4,5], demonstrates the great potential of AMEA for correlated systems, both in nonequilibrium as well as in equilibrium situations.

[1] E. Arrigoni *et al.*, PRL **110**, 086403 (2013)

[2] A. Dorda *et al.*, PRB **89**, 165105 (2014)

[3] A. Dorda *et al.*, PRB **92**, 125145 (2015)

[4] I. Titvinidze *et al.*, arXiv:1508.02953

[5] A. Dorda *et al.*, arXiv:1509.09255

<sup>1</sup>This work was supported by the Austrian Science Fund (FWF): P24081 and P26508, as well as SFB-ViCoM projects F04103 and F04104.

**12:51PM L20.00009 Fixed Order Real-Time Simulation of Nonequilibrium Transport** , JONG HAN, University at Buffalo, SUNY — Finding a reliable formalism for an impurity model out of equilibrium, despite intense effort in recent years, is still one of the major obstacles in nonequilibrium quantum many-body theory. We note that the Keldysh formalism with the close-time contour has the statistical weight given by the non-interacting limit, which enables direct evaluation of perturbation series at a fixed order. The Green function expansions are carried out up to the sixth order of the Coulomb parameter in the Anderson impurity model out of equilibrium, and demonstrate how the self-energy evolves as the voltage bias increases. We discuss the remarkable cancellation between self-energy diagrams in equilibrium which justifies the low-order approximations, and further investigate the deviation of this behavior in nonequilibrium.

**1:03PM L20.00010 State of the Polaron: Criticality in the Spin Boson Model** , ZACH BLUNDEN-CODD, Imperial College London, AHSAN NAZIR, University of Manchester, ALEX CHIN, University of Cambridge — In strongly coupled open quantum systems it can become necessary to take into account the behaviour of environmental degrees of freedom more rigorously than is usual with standard weak coupling techniques. We investigate the use of a variational ansatz, making use of a multitude of coherent states, to obtain more precise information about the interaction between an open system and its environment. We provide a thorough study of the ground state of the ubiquitous spin boson model; presenting analytic and numerical results concerning the nature of its much debated quantum phase transition.

**1:15PM L20.00011 Quantum Phase Transitions detected by a local probe using Time Correlations and Violations of Leggett-Garg Inequalities** , FERNANDO GOMEZ, Universidad de los Andes, JUAN MENDOZA, University of Oxford, FERNEY RODRIGUEZ, Universidad de los Andes, CARLOS TEJEDOR, Universidad Autónoma de Madrid, LUIS QUIROGA, Universidad de los Andes — We introduce a new way of identifying quantum phase transitions of many-body systems by means of local time correlations and Leggett-Garg inequalities. This procedure allows to experimentally determine the quantum critical points not only of finite-order transitions but also those of infinite-size as the Kosterlitz-Thouless transition that is not always easy to detect with current methods. By means of an analytical calculation on a general spin-1/2 Hamiltonian, and matrix product simulations of one-dimensional  $XXZ$  and anisotropic  $XY$  models, we argue that finite-order quantum phase transitions can be determined by singularities of the time correlations or their derivatives at criticality. The same features are exhibited by corresponding Leggett-Garg functions, which remarkably indicate violation of the Leggett-Garg inequalities for early times and all the Hamiltonian parameters considered. In addition, we find that the infinite-order transition of the  $XXZ$  model at the isotropic point can be revealed by the maximal violation of the Leggett-Garg inequalities.

**1:27PM L20.00012 Scaling behaviors at discontinuous quantum transitions** , JACOPO NESPOLO, MASSIMO CAMPOSTRINI, Dipartimento di Fisica dell'Università di Pisa and INFN, Sez. di Pisa, ANDREA PELISSETTO, Dipartimento di Fisica di 'Sapienza' Università di Roma and INFN, Sez. di Roma I, ETTORE VICARI, Dipartimento di Fisica dell'Università di Pisa and INFN, Sez. di Pisa — First-order (or discontinuous) quantum phase transitions (FOQTs) are characterized by a vanishing energy gap and jumps in the values of some observables across the critical point in the thermodynamic limit. Unlike what happens at continuous transitions, the correlation lengths remain finite at FOQTs. Nevertheless, finite systems at FOQTs exhibit finite-size effects, in the form of a rounding and smoothing of the discontinuities. We show that a scaling theory, similar to the usual finite-size scaling, can be formulated at FOQTs, and that the relevant scaling variable is extremely sensitive to the choice of boundary conditions. We further consider the scaling effects due to the presence of spatial inhomogeneities, in analogy with trap-size scaling at continuous transitions. Our results are supported by numerical simulations on the ferromagnetic quantum Ising chain and on the  $q$ -state quantum Potts chain with  $q > 4$ . We provide FSS predictions for the energy gap and the magnetization of finite quantum chains, which can be relevant for quantum computation applications.

**1:39PM L20.00013 Order  $O(1)$  algorithm for first-principles transient current through open quantum systems**, KING TAI CHEUNG, ZHIZHOU YU, BIN FU, JIAN WANG, The University of Hong Kong — First principles transient current through molecular devices is known to be extremely time consuming with typical computational complexity  $T^3N^3$  where  $N$  and  $T$  are the dimension of the scattering system and the number of time steps respectively. Various algorithms have been developed which eventually brings the complexity down to  $cTN^3$ , a linear scaling in  $T$ , where  $c$  is a large coefficient comparable to  $N$ . Here we provide an order  $O(1)$  algorithm that reduces it further to  $c_1N^3 + c_2TN^2$  where  $c_1$  and  $c_2$  are  $\sim 50$  and  $0.1$  respectively. Hence for  $T < N$ , the transient calculation is independent of  $T$ , thus order  $O(1)$  is achieved. To make this happening four important ingredients are essential: (1). availability of exact solution based on non-equilibrium Green's function (NEGF) that goes beyond wideband limit; (2). the use of complex absorbing potential (CAP) so that all the pole of Green's function can be found; (3). the exact solution is separable between real space and time domain; (4). the exploit of Vandermonde matrix further reduces the scaling of  $TN^2$  to  $T\ln TN$  for  $T > N$ . Benchmark calculation has been done on graphene nanoribbons using Tight-binding (TB) Hamiltonian with a huge speed up factor of  $100T$ , confirmed the  $O(1)$  scaling.

**1:51PM L20.00014 Generalized non-equilibrium vertex correction method in coherent medium theory for quantum transport simulation of disordered nanoelectronics<sup>1</sup>**, JIAWEI YAN, YOUQI KE, School of Physical Science and Technology, ShanghaiTech University — In realistic nanoelectronics, disordered impurities/defects are inevitable and play important roles in electron transport. However, due to the lack of effective quantum transport method, the important effects of disorders remain poorly understood. Here, we report a generalized non-equilibrium vertex correction (NVC) method with coherent potential approximation to treat the disorder effects in quantum transport simulation. With this generalized NVC method, any averaged product of two single-particle Greens functions can be obtained by solving a set of simple linear equations. As a result, the averaged non-equilibrium density matrix and various important transport properties, including averaged current, disordered induced current fluctuation and the averaged shot noise, can all be efficiently computed in a unified scheme. Moreover, a generalized form of conditionally averaged non-equilibrium Green's function is derived to incorporate with density functional theory to enable first-principles simulation. We prove the non-equilibrium coherent potential equals the non-equilibrium vertex correction. Our approach provides a unified, efficient and self-consistent method for simulating non-equilibrium quantum transport through disorder nanoelectronics.

<sup>1</sup>ShanghaiTech start-up fund

**2:03PM L20.00015 Efficient heat-bath sampling in Fock space<sup>1</sup>**, ADAM HOLMES, Laboratory of Atomic and Solid State Physics, Cornell University, HITESH CHANGLANI, University of Illinois at Urbana-Champaign, CYRUS UMRIGAR, Laboratory of Atomic and Solid State Physics, Cornell University — We introduce an algorithm for sampling many-body quantum states in Fock space. The algorithm efficiently samples states with probability approximately proportional to an arbitrary function of the second-quantized Hamiltonian matrix elements connected to the current state. We apply the new sampling algorithm to the recently-developed Semistochastic Full Configuration Interaction Quantum Monte Carlo method (S-FCIQMC), a semistochastic implementation of the power method for projecting out the ground state energy in a basis of Slater determinants. The heat-bath sampling requires modest additional computational time and memory compared to uniform sampling but results in newly-spawned weights that are approximately of the same magnitude, thereby greatly improving the efficiency of projection. A comparison in efficiency between uniform and approximate heat-bath sampling is performed on the all-electron nitrogen dimer at equilibrium in Dunning's cc-pVXZ basis sets with  $X \in \{D, T, Q, 5\}$ , demonstrating a large gain in efficiency that increases with basis set size.

<sup>1</sup>This work was supported in part by grants NSF CHE-1112097, DOE DE-SC0006650, and NSF ACI-1534965.

**Wednesday, March 16, 2016 11:15AM - 2:15PM –**  
**Session L21 GSCCM DCOMP DMP: Materials in Extremes: Energetic Materials** 320 - Tariq Aslam, Los Alamos National Laboratory

**11:15AM L21.00001 Modeling the anisotropic shock response of single-crystal RDX**, DARBY LUSCHER, Los Alamos National Laboratory — Explosives initiate under impacts whose energy, if distributed homogeneously throughout the material, translates to temperature increases that are insufficient to drive the rapid chemistry observed. Heterogeneous thermomechanical interactions at the meso-scale (i.e. between single-crystal and macroscale) leads to the formation of localized hot spots. Direct numerical simulations of mesoscale response can contribute to our understanding of hot spots if they include the relevant deformation mechanisms that are essential to the nonlinear thermomechanical response of explosive molecular crystals. We have developed a single-crystal model for the finite deformation thermomechanical response of cyclotrimethylene trinitramine (RDX). Because of the low symmetry of RDX, a complete description of nonlinear thermoelasticity requires a careful decomposition of free energy into components that represent the pressure-volume-temperature (PVT) response and the coupling between isochoric deformation and both deviatoric and hydrostatic stresses. An equation-of-state (EOS) based on Debye theory that defines the PVT response was constructed using experimental data and density functional theory calculations. This EOS replicates the equilibrium states of phase transformation from alpha to gamma polymorphs observed in static high-pressure experiments. Lattice thermoelastic parameters defining the coupled isochoric free energy were obtained from molecular dynamics calculations and previous experimental data. Anisotropic crystal plasticity is modeled using Rowan's expression relating slip rate to dislocation density and velocity. Details of the theory will be presented followed by discussion of simulations of flyer plate impact experiments, including recent experiments diagnosed with in situ X-ray diffraction at the Advanced Photon Source. Impact conditions explored within the experimental effort have spanned shock pressures ranging from 1-10 GPa for several crystallographic orientations. Simulation results will be used to motivate conclusions about the nature of dislocation-mediated plasticity in RDX, as well as, future directions to improve these models and quantitatively compare them to the average lattice response recorded with in situ X-ray diffraction.

**11:51AM L21.00002 Role of microstructure and thermal transport in determining the rate of hot spot growth in aluminized PBX**, KAUSHIK JOSHI, SANTANU CHAUDHURI, Univ of Illinois - Urbana — The mechanisms of initiation and propagation of a hot spot in non-ideal explosives with aluminum additives are poorly understood due to greater complexity introduced by the different thermal and mechanical behavior of the components. In aluminized composites such as PBXN-109, the binder, RDX and Aluminum phases have been studied separately. However, not much is known about deflection of hot spots in the microstructured composite. Especially, the role of adhesion, debonding and thermal conductivity of binder phase is critical in moderating the sensitivity of such interfaces. Using reactive molecular dynamics simulations, the primary binder interfaces in PBXN-109 was investigated. Depending on the temperature of the growing hot spot reaching an RDX or Al/Al<sub>2</sub>O<sub>3</sub> grain, the thermal conductivity and viscoplastic behavior of the binder interface determine the attenuation of reaction front and thermal shock leading the hot spot. Different mechanisms like melt-dispersion and failure of oxide layer for the release of Al in the hot spot regions remain underexplored to connect the chemistry to the microstructure. Although Al/Al<sub>2</sub>O<sub>3</sub>/RDX and Al/Al<sub>2</sub>O<sub>3</sub>/HTPB interfaces are chemically stable, the hot spot melts the Al<sub>x</sub>O<sub>y</sub> layers and create shear bands in aluminum domain due to thermomechanical strain created due to different thermal environment. In a shock-compressed microstructure without voids, the cohesive interaction and chemical composition of such interfaces for different phases of RDX will be presented.

**12:03PM L21.00003 An extreme pressure attenuation in metals from a miniaturized pyrotechnic train configuration<sup>1</sup>**, JACK YOH, BOHOON KIM, HYEONJU YU, Seoul National University, SEOUL NATIONAL UNIVERSITY TEAM — A pyrotechnic device that consists of donor/acceptor pair separated by a bulkhead relies on shock attenuation in metal and shock sensitivity of the energetic materials. Despite of its common use, full-scale numerical simulation of such explosive train configuration is seldom reported because the proper modeling of the entire process requires precise capturing of extreme pressure waves from the donor charge during its attenuation in the metal before triggering of an acceptor charge and the accurate material modeling of high strain rate dynamics of both reactive and inert solids. The considered train consists of HMX as donor, STS 304 as the bulkhead, and RDX as acceptor. The simulation of such multi-material configuration reveals the critical bulkhead thickness for successful initiation of a pyrotechnic device. Furthermore, the miniaturization of such system is considered by obtaining the distance to shock front sharpening for building an analytical theory of pressure attenuation in STS sample of microscale thickness, and a new shock Hugoniot data is provided from the laser-based shock experiment using such samples.

<sup>1</sup>Hanwha Research Grant 2015

**12:15PM L21.00004 Mechanisms of laser-induced photocatalytic decomposition of high explosives**, ANATOLY MITROFANOV, ANTON ZVEREV, Kemerovo State University, Russia, SERGEY RASHKEEV, ROMAN TSYSHEVSKY, University of Maryland, MAIJA KUKLJA, National Science Foundation — Using laser irradiation for triggering explosive decomposition of high density energy materials opens up new opportunities in design of safe optical detonators by removing primary explosive from the devices. Precise tuning of sensitivity to initiation of detonation via photo-excitation appears challenging because all secondary explosives are insulators with the band gap of 4-8 eV. We will discuss our combined experimental and theoretical studies that suggest feasible mechanisms of photocatalytic decomposition of explosives triggered by the laser excitation with the energy of 1.17 - 2.3 eV and the wavelength of 1064-532 nm. The first approach considers tuning the optical absorption via the controlled modification of the electronic structure of the explosive-metal oxide interfaces. The second approach involves incorporating photoactive organic molecules in the crystalline matrix of the explosive material.

**12:27PM L21.00005 Emergent molecular theory of initiation of detonation: the effect of molecular and crystal structure on thermal stability of high density energy materials**, MAIJA KUKLA, National Science Foundation, ROMAN TSYSHEVSKY, ONISE SHARIA, University of Maryland — The sensitivity to detonation initiation of high density energy materials along with their performance are two most important criteria for choosing the best material for explosive formulations, booster engines, detonators, etc. After numerous experimental and theoretical attempts to develop a single parameter describing sensitivity of different classes of energetic materials, one concludes that the complexity of physical and chemical explosive properties cannot be trivialized. We report here the results of our theoretical and computational studies of thermal decomposition mechanisms and kinetics of five classes of EM: pentaerythritol tetranitrate (PETN), nitramine cyclotetramethylene-tetranitramine (HMX), diamino-dinitroethene (DADNE), bis-(nitrofurazano)-furoxane (BNFF) and benchmark triamino-trinitrobenzene (TATB). Our modeling reveals how the thermal stability depends on the molecular structure of the material and how the crystal structure may additionally hinder or catalyze decomposition reactions. We will also discuss an effect of crystalline defects on sensitivity and performance of materials.

**12:39PM L21.00006 Ignition Prediction of Pressed HMX based on Hotspot Analysis Under Shock Pulse Loading**, SEOKPUM KIM, CHRISTOPHER MILLER, Georgia Institute of Technology, YASUYUKI HORIE, (ret.) Air Force Research Lab, CHRISTOPHER MOLEK, ERIC WELLE, Air Force Research Lab, MIN ZHOU, Georgia Institute of Technology — The ignition behavior of pressed HMX under shock pulse loading with a flyer is analyzed using a cohesive finite element method (CFEM) which accounts for large deformation, microcracking, frictional heating, and thermal conduction. The simulations account for the controlled loading of thin-flyer shock experiments with flyer velocities between 1.7 and 4.0 km/s. The study focuses on the computational prediction of ignition threshold using James criterion which involves loading intensity and energy imparted to the material. The predicted thresholds are in good agreement with measurements from shock experiments. In particular, it is found that grain size significantly affects the ignition sensitivity of the materials, with smaller sizes leading to lower energy thresholds required for ignition. In addition, significant stress attenuation is observed in high intensity pulse loading as compared to low intensity pulse loading, which affects density of hotspot distribution. The microstructure-performance relations obtained can be used to design explosives with tailored attributes and safety envelopes.

**12:51PM L21.00007 The Dynamic Behaviors of Single Crystal RDX Under Ramp Wave Loading to 15GPa**, GUIJI WANG, JINTAO CAI, JIANHENG ZHAO, FENG ZHAO, GANG WU, FULI TAN, CHENGWEI SUN, institute of fluid physics — Based on high pulsed power generator CQ-4, the single crystal RDX explosive was researched along different crystal orientations under ramp wave loadings up to 15 GPa. The typical three-wave structures were obtained by means of laser interferometry PDV, which show the elastic-plastic transition and  $\alpha$  to  $\gamma$  phase transition. The ramp elastic limit (REL) and yield strength of RDX along 210 and 100 crystal orientations were respectively calculated and the results show obvious effects of crystal orientations for RDX. The ramp elastic limit  $\sigma_{IEL}$  of RDX along 210 orientation is 0.688-0.758GPa, and the  $\sigma_{IEL}$  of RDX along 100 is 1.039 -1.110 GPa. The  $\alpha$  to  $\gamma$  phase transformation characteristics were also analyzed based on the experimental data. The initial phase transition pressure for the two crystal orientation of RDX are about 3.5 to 4 GPa, which agree well with the data of about 4-5GPa given by MD simulation. The data directly validate the results given by Raman Spectrum under shock compression and static high pressure, which couldn't be observed by wave profiles. The experimental data can be used to verify and validate the new models of RDX under dynamic loading. Supported by NSFC of China under contract No.11327803 and 11176002

**1:03PM L21.00008 Experimental and numerical study of deformation modes of a pressed HMX-based explosive composition**, DIDIER PICART, JEROME VIAL, CEA DAM Le Ripault, PATRICE BAILLY, INSA Centre Val de Loire — Safety of industrial or military explosives is still studied to prevent inadvertent ignition of pressed HMX-based explosive compositions submitted to a low-velocity impact. Our aim is to determine the dissipative mechanisms leading to the local heating of the material. To observe the dissipative mechanisms, a reversed edge-on impact test has been developed. This test enables real-time observations of the microstructural scale. No friction is observed between the biggest HMX grains and the matrix (the smallest grains, the binder and the porosity). Plasticity of HMX grains is obtained as well as damage by micro-cracking. Meanwhile, a biphasic numerical representation (HMX grains and matrix) is used to mimic our material. A comparison between experimental observations and simulations is used to determine the yield stress of HMX. The behavior of the matrix has been determined to account for the effect of strain rate and damage. Lastly, a comparison between tests and simulations has highlighted (1) that heating should rather be located in the matrix than in the biggest HMX grains and (2) that the most likely heating mechanism is the friction of micro(or meso)-cracks lips.

**1:15PM L21.00009 Decomposition products of TATB under high static pressure.**, JONATHAN CROWHURST, ELISSAIOS STAVROU, JOSEPH ZAUG, Lawrence Livermore Natl Lab — We have investigated the decomposition products of 2,4,6-triamino-1,3,5-trinitrobenzene (TATB) at static pressures up to 50 GPa using Raman and IR absorption spectroscopy. Decomposition was driven by various continuous wave and pulsed laser drives. We compare decomposition behavior and products obtained at the different pressures. Preliminary results at lower pressures indicate the formation of carbon dioxide, nitrogen, amorphous carbon and possibly hydrogen. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract No. DE-AC52-07NA27344

**1:27PM L21.00010 Modified Gap Experiment and Simulation** , GERRIT SUTHERLAND, RICHARD BENJAMIN, U.S. Army Research Laboratory — Modified Gap Experiment hydrocode simulations and data are presented. The modified gap experiment is a variation of the large scale gap test (LSGT) experiment. A 50.8-mm diameter  $\times$  12.7-mm long disk of sample explosive replaces the confined sample and witness plate in the LSGT. Either a framing camera or a photonic Doppler velocimeter measures the free surface velocity. The free surface velocity is measured for varying levels of input pressure. The Plexiglas gap thickness controls the input pressure. Features of the free surface velocity versus input pressure curve show the pressure at which detonation and ignition thresholds occur. The amount of reaction in various regions of the sample is predicted by the simulations and compared to experiment. Additionally, the simulations will predict how the release waves traveling backward into the sample affect the amount of reaction in the sample. Further, simulations of a non-ideal explosive will predict the response of an explosive whose reaction zone length is on the order of the 12.7-mm sample length.

**1:39PM L21.00011 ABSTRACT WITHDRAWN —**

**1:51PM L21.00012 Secondary decomposition reactions in nitramines<sup>1</sup>** , IGOR SCHWEIGERT, U.S. Naval Research Laboratory — Thermal decomposition of nitramines is known to proceed via multiple, competing reaction branches [1], some of which are triggered by secondary reactions between initial decomposition products and unreacted nitramine molecules. Better mechanistic understanding of these secondary reactions is needed to enable extrapolations of measured rates to higher temperatures and pressures relevant to shock ignition. I will present density functional theory (DFT) based simulations of nitramines that aim to re-evaluate known elementary mechanisms [2,3] and seek alternative pathways in the gas and condensed phases. [1] S. Maharrey and R. Behrens, J. Phys. Chem. A, 109, 11236 (2005) [2] C. F. Melius and M. C. Piqueras, P. Combust. Inst., 29, 2863 (2002) [3] K. Irikura, J. Phys. Chem. A, 117, 2233 (2013)

<sup>1</sup>This work was supported by the Office of Naval Research, both directly and through the Naval Research Laboratory.

**2:03PM L21.00013 Shock-induced decomposition of high energy materials: A ReaxFF molecular dynamics study<sup>1</sup>** , SUBODH TIWARI, ANKIT MISHRA, KEN-ICHI NOMURA, RAJIV KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, University of Southern California — Atomistic simulations of shock-induced detonation provide critical information about high-energy (HE) materials such as sensitivity, crystallographic anisotropy, detonation velocity, and reaction pathways. However, first principles methods are unable to handle systems large enough to describe shock appropriately. We report reactive-force-field ReaxFF simulations of shock-induced decomposition of 1, 3, 5-triamino-2, 3, 6-trinitrobenzene (TATB) and 1,1-diamino 2-2-dinitroethane (FOX-7) crystal. A flyer acts as mechanical stimuli to introduce a shock, which in turn initiated chemical reactions. Our simulation showed a shock speed of 9.8 km/s and 8.23 km/s for TATB and FOX-7, respectively. Reactivity analysis proves that FOX-7 is more reactive than TATB. Chemical reaction pathways analysis revealed similar pathways for the formation of N<sub>2</sub> and H<sub>2</sub>O in both TATB and FOX-7. However, abundance of NH<sub>3</sub> formation is specific to FOX-7. Large clusters formed during the reactions also shows different compositions between TATB and FOX-7. Carbon soot formation is much more pronounced in TATB. Overall, this study provides a detailed comparison between shock induced reaction pathway between FOX-7 and TATB.

<sup>1</sup>This work was supported by the Office of Naval Research Grant No. N000014-12-1-0555.

**Wednesday, March 16, 2016 11:15AM - 2:15PM —**

**Session L22 DCOMP: Theory and Simulations of Strongly Correlated Systems with Disorder**

321 - Richard Scalettar, University of California, Davis

**11:15AM L22.00001 Magnetic moments and non-Fermi-liquid behavior in quasicrystals<sup>1</sup>** , ERIC ANDRADE, Instituto de Física Terica/UNESP — Motivated by the intrinsic non-Fermi-liquid behavior observed in the heavy-fermion quasicrystal Au<sub>51</sub>Al<sub>34</sub>Yb<sub>15</sub>, we study the low-temperature behavior of dilute magnetic impurities placed in metallic quasicrystals. We find that a large fraction of the magnetic moments are not quenched down to very low temperatures, leading to a power-law distribution of Kondo temperatures, accompanied by a non-Fermi-liquid behavior, in a remarkable similarity to the Kondo-disorder scenario found in disordered heavy-fermion metals.

<sup>1</sup>This work was supported by FAPESP (Brazil) Grant No. 2013/00681-8.

**11:51AM L22.00002 The Knight shift anomaly in the disordered periodic Anderson model** , RAIMUNDO DOS SANTOS, NATANAEL COSTA, THEREZA PAIVA, Universidade Federal do Rio de Janeiro, NICHOLAS CURRO, RICHARD SCALETTAR, UC Davis — In some materials, the coherence temperature  $T^*$  signals the regime in which one has a heavy-electron fluid and 'dissolved' local moments. An experimental signature of  $T^*$  is provided by the Knight shift anomaly in NMR measurements. Further, the contribution of the heavy-electron fluid to the Knight shift,  $K_{\text{HF}}$ , displays universal character over a wide range of temperatures. An important probe of the physical mechanisms at play is the random substitution of say, La for Ce in CeRhIn<sub>5</sub>: this amounts to removing local moments at random sites, and one may wonder whether these universal features are sensitive to the presence of disorder. The Periodic Anderson Model (PAM) captures many aspects of heavy-fermion materials, so here we consider the two-dimensional PAM with a fraction  $x$  of the  $f$ -sites removed at random. Through Determinant Quantum Monte Carlo simulations we find that universality of  $K_{\text{HF}}$  persists even in the presence of disorder, which, in turn, allows us to establish that  $T^*$  decreases monotonically with  $x$ , in agreement with available experimental data. Our simulations also shed light into the low temperature behavior of the disordered PAM at low temperatures: the spin liquid phase of the local moments is suppressed upon dilution.

**12:03PM L22.00003 Strong correlations generically protect d-wave superconductivity against disorder** , SHAO TANG, V. DOBROSAVLJEVIĆ, Department of Physics and National High Magnetic Field Laboratory, Florida State University, E. MIRANDA, Campinas State University, Brazil — We address the question of why strongly correlated d-wave superconductors, such as the cuprates, prove to be surprisingly robust against the introduction of non-magnetic impurities. We show that, very generally, both the pair-breaking and the normal state transport scattering rates are significantly suppressed by strong correlations effects arising in the proximity to a Mott insulating state. We also show that the correlation-renormalized scattering amplitude is generically enhanced in the forward direction, an effect which was previously often ascribed to the specific scattering by charged impurities outside the copper-oxide planes.

**12:15PM L22.00004 Study of the Anderson localization in real materials using typical medium dynamical cluster approximation**, YI ZHANG, RYKY NELSON, Louisiana State Univ - Baton Rouge, HANNA TERLETSKA, University of Michigan, CONRAD MOORE, Louisiana State Univ - Baton Rouge, CHINEDU EKUMA, United States Naval Research Laboratory, KA-MING TAM, Louisiana State Univ - Baton Rouge, TOM BERLIJN, Oak Ridge National Laboratory, WEI KU, Brookhaven National Laboratory, JUANA MORENO, MARK JARRELL, Louisiana State Univ - Baton Rouge — We generalize the typical medium dynamical cluster approximation to multi-orbital disordered systems. Combining it with the first principals downfolding and unfolding methods to derive an effective low energy model, we apply our extended formalism to real materials where strong disorder exists. These include, e.g., the iron selenide superconductors  $K_xFe_{2-y}Se_2$  with Fe vacancies,  $Ga_{1-x}Mn_xN$  and S doped Si. By looking at the typical density of states, we study the mobility edge and the localization effects in these materials, which is useful to understand the mechanism of their insulating behavior. We find for example, that even the disorder associated with 12% vacancies in  $K_xFe_{2-y}Se_2$  together with the anisotropy is not sufficient to cause localization.

**12:27PM L22.00005 Rounding of the first-order phase transition in the four-color Ashkin-Teller model**, AHMED IBRAHIM, THOMAS VOJTA, Missouri Univ of Sci & Tech — The two-dimensional four-color Ashkin-Teller model is investigated by Monte Carlo simulations to analyze the effects of quenched disorder on the first-order phase transition. We show that the quenched disorder destroys the first-order phase transition and turns into a continuous one. We study the emerging critical behavior of the disordered Ashkin-Teller model by using a finite-size-scaling analysis and confirm it to be in the clean two-dimensional Ising universality class with universal logarithmic corrections. This concurs with perturbative renormalization-group predictions by Cardy. We discuss the universality of the arising critical behavior and we compare with earlier results in the literature.

**12:39PM L22.00006 Charge density waves in disordered media circumventing the Imry-Ma argument**, NORM TUBMAN, University of California, Berkeley, HITESH CHANGLANI, TAYLOR HUGHES, University of Illinois — Two powerful theoretical predictions, Anderson localization and the Imry-Ma argument, impose significant restrictions on which phases of matter can exist in the presence of even the smallest amount of disorder in one-dimensional systems. These predictions forbid conducting states and ordered states respectively. It was thus of great interest to find out that Anderson localization can indeed be circumvented in one dimensional systems in the presence of correlated disorder. In a similar manner, but for a different physical phenomenon, we show that the Imry-Ma argument can be circumvented resulting in the formation of stable ordered states in disordered one dimensional systems. We explicitly simulate a family of Hamiltonians of spinless fermions with correlated disorder, where we find that a charge density wave is stable up to a finite critical disorder strength. Having circumvented the Imry-Ma mechanism, we then investigate other mechanisms in which disordered systems can destroy an ordered state.

**12:51PM L22.00007 Entanglement Holographic Mapping of Many-Body Localized System by Spectrum Bifurcation Renormalization Group**, YI-ZHUANG YOU, University of Californian, Santa Barbara, XIAO-LIANG QI, Stanford University, CENKE XU, University of Californian, Santa Barbara — We introduce the spectrum bifurcation renormalization group (SBRG) as a generalization of the real-space renormalization group for the many-body localized (MBL) system without truncating the Hilbert space. Starting from a disordered many-body Hamiltonian in the full MBL phase, the SBRG flows to the MBL fixed-point Hamiltonian, and generates the local conserved quantities and the matrix product state representations for all eigenstates. The method is applicable to both spin and fermion models with arbitrary interaction strength on any lattice in all dimensions, as long as the models are in the MBL phase. In particular, we focus on the  $1d$  interacting Majorana chain with strong disorder, and map out its phase diagram using the entanglement entropy. The SBRG flow also generates an entanglement holographic mapping, which duals the MBL state to a fragmented holographic space decorated with small blackholes.

**1:03PM L22.00008 Disordered XYZ Spin Chain Simulations using the Spectrum Bifurcation Renormalization Group**, KEVIN SLAGLE, YI-ZHUANG YOU, CENKE XU, Univ of California - Santa Barbara — We study the disordered XYZ spin chain using the recently developed Spectrum Bifurcation Renormalization Group (SBRG) numerical method. With large disorder, the phase diagram of the eigenstates consists of three many body localized (MBL) spin glass phases separated by marginal MBL critical phases. We examine the critical phases of this model by probing the entanglement entropy and Edwards-Anderson spin glass order parameter. We also show how long-range mutual information can be used to distinguish these phases (Jian, Kim, Qi 2015).

**1:15PM L22.00009 Many-body Localization Transition in Rokhsar-Kivelson-type wave functions<sup>1</sup>**, XIAO CHEN, XIONGJIE YU, University of Illinois at Urbana-Champaign, GIL YOUNG CHO, Korea Advanced Institute of Science and Technology, BRYAN CLARK, EDUARDO FRADKIN, University of Illinois at Urbana-Champaign — We construct a family of many-body wave functions to study the many-body localization phase transition. The wave functions have a Rokhsar-Kivelson form, in which the weight for the configurations are chosen from the Gibbs weights of a classical spin glass model, known as the Random Energy Model, multiplied by a random sign structure to represent a highly excited state. These wave functions show a phase transition into an MBL phase. In addition, we see three regimes of entanglement scaling with subsystem size: scaling with entanglement corresponding to an infinite temperature thermal phase, constant scaling, and a sub-extensive scaling between these limits. Near the phase transition point, the fluctuations of the Renyi entropies are non-Gaussian. We find that Renyi entropies with different Renyi index transition into the MBL phase at different points and have different scaling behavior, suggesting a multifractal behavior.

<sup>1</sup>This work was supported in part by DMR-1064319 and DMR-1408713 (XC,GYC,EF) at the University of Illinois, PHY11-25915 at KITP (EF), DOE, SciDAC FG02-12ER46875 (BKC and XY), and the Brain Korea 21 PLUS Project of Korea Government (GYC).

**1:27PM L22.00010 Computational Analysis of many-body localized phases beyond 1D**, BENJAMIN VILLALONGA CORREA, Department of Physics, University of Illinois at Urbana-Champaign, DAVID PEKKER, Department of Physics and Astronomy, University of Pittsburgh, BRYAN CLARK, Department of Physics, University of Illinois at Urbana-Champaign — Anderson localization can persist in the presence of finite interactions, giving rise to what is known as a many-body localized (MBL) phase. The need to access interior eigenstates makes their computational analysis hard for large system sizes. Recently, an MPS ansatz has been successfully applied to the study of long 1D chains in the MBL phase; however, higher dimensional systems remain largely inaccessible to computational methods. We explore a variational approach to overcome this limitation and report on two-dimensional MBL phases.

**1:39PM L22.00011 A tensor network approach to many-body localization<sup>1</sup>**, XIONGJIE YU, University of Illinois at Urbana-Champaign, DAVID PEKKER, University of Pittsburgh, BRYAN CLARK, University of Illinois at Urbana-Champaign — Understanding the many-body localized phase requires access to eigenstates in the middle of the many-body spectrum. While exact-diagonalization is able to access these eigenstates, it is restricted to systems sizes of about 22 spins. To overcome this limitation, we develop tensor network algorithms which increase the accessible system size by an order of magnitude. We describe both our new algorithms as well as the additional physics about MBL we can extract from them. For example, we demonstrate the power of these methods by verifying the breakdown of the Eigenstate Thermalization Hypothesis (ETH) in the many-body localized phase of the random field Heisenberg model, and show the saturation of entanglement in the MBL phase and generate eigenstates that differ by local excitations.

<sup>1</sup>Work was supported by AFOSR FA9550-10-1-0524 and FA9550-12-1-0057, the Kaufmann foundation, and SciDAC FG02-12ER46875.

**1:51PM L22.00012 Absence of diffusion in disordered spin-chains**, SNIR GAZIT, Physics Department, University of California at Berkeley, ILIA KHAIT, Physics Department, Technion, NORMAN YAO, Physics Department, University of California at Berkeley, ASSA AUERBACH, Physics Department, Technion — We study the dynamical properties of the one dimensional XXZ model at infinite temperature in the presence of quench disorder. This model is expected to exhibit a many body localization (MBL) transition at finite disorder. We compute the local dynamical spin correlation function using a non-perturbative continued fraction expansion. The expansion up to 15th order is sufficient to achieve convergence of our extrapolation scheme. We compare the continued fraction result to the exact diagonalization (ED) on 22 sites. The phase diagram is determined in the disorder-anisotropy plane. Our main finding is the emergence of sub-diffusive transport and absence of a diffusive behavior ( $\omega^{-1/2}$  at low frequencies) in the weak disorder regime. The lack of a true diffusive phase contrasts with previous results and expectations obtained from smaller system sizes. In addition, the MBL transition is determined to occur at lower values than those deduced by ED on finite systems. Lastly, the finite frequency-momentum dynamical structure factor is computed and we explore its space-time scaling behavior.

**2:03PM L22.00013 Pseudospin representation of the two-site Anderson-Hubbard model<sup>1</sup>**, RACHEL WORTIS, Trent University, MALCOLM KENNETT, Simon Fraser University — The state of an Anderson localized system can be described in terms of the occupation of a set of single-particle wave functions which are localized in space. When interactions are added, single-particle wave functions are no longer well defined, so what is a useful description of the state of a many-body localized system and what about it is localized? Given that any system with Hilbert-space dimension  $2^N$  may be described by an Ising-type Hamiltonian, it has been proposed that in a fully many-body localized system the Ising pseudospins in this representation may be chosen to be local. Actually constructing these spins is non-trivial. While a number of approaches have been proposed, few explicit examples exist and almost all work has been on spin systems. Here we present the Hamiltonian of a two-site Hubbard model with disorder and nearest-neighbor interactions written in terms of pseudospins, and we explore the form of these pseudospins and their evolution as a function of hopping amplitude.

<sup>1</sup>Supported by NSERC of Canada

**Wednesday, March 16, 2016 11:15AM - 2:15PM –**  
**Session L23 DMP DCOMP: Computational Materials Discovery and Design - Graphene and 2D Materials** 322 - Mahesh Neupane, Army Research Lab

**11:15AM L23.00001 Computational design and optimization of energy materials**, MARIA CHAN, Argonne National Laboratory — The use of density functional theory (DFT) to understand and improve energy materials for diverse applications – including energy storage, thermal management, catalysis, and photovoltaics – is widespread. The further step of using high throughput DFT calculations to design materials and has led to an acceleration in materials discovery and development. Due to various limitations in DFT, including accuracy and computational cost, however, it is important to leverage effective models and, in some cases, experimental information to aid the design process. In this talk, I will discuss efforts in design and optimization of energy materials using a combination of effective models, DFT, machine learning, and experimental information.

**11:51AM L23.00002 High-throughput prediction of novel two-dimensional materials**, NICOLAS MOUNET, PHILIPPE SCHWALLER, ANDREA CEPPELLOTTI, Ecole Polytechnique Federale de Lausanne, Switzerland, ANDRIUS MERKYS, Vilnius University, Lithuania, IVANO ELIGIO CASTELLI, MARCO GIBERTINI, GIOVANNI PIZZI, NICOLA MARZARI, Ecole Polytechnique Federale de Lausanne, Switzerland — As a crucial step towards the identification of novel and promising 2D materials, we provide here a large scale first-principles exploration and characterization of such compounds. More than 300,000 three-dimensional structures from several crystallographic databases are screened systematically by checking the absence of chemical bonds between adjacent layers, identifying close to 5,000 layered systems. Then DFT calculations of the van der Waals interlayer bonding are performed with automatic workflows, while systematically assessing the metallic, insulating or magnetic character of the materials obtained. Following full atomic and cell relaxations, phonon dispersions are computed as a first step towards the assessment of thermodynamic properties. Thanks to the AiiDA materials' informatics platform [1], and in particular its automatic workflow engine, database structure, sharing capabilities, and pipelines to/from crystallographic repositories, the systematic and reproducible calculation of these properties becomes straightforward, together with seamless accessibility and sharing. [1] G. Pizzi, A. Cepellotti, R. Sabatini, N. Marzari and B. Kozinsky, Comp. Mat. Sci. 111, 218 (2016).

**12:03PM L23.00003 New Monolayered Materials Exhibiting Unusual Electronic Properties<sup>1</sup>**, ALEJANDRO LOPEZ-BEZANILLA, IVAR MARTIN, Argonne Natl Lab, PETER B. LITTLEWOOD, Argonne Natl Lab & James Franck Institute, University of Chicago — Computationally based approaches are allowing to progress in the discovery and design of nano-scaled materials. Here we propose a series of new mono-layered compounds with exotic properties. By means of density functional theory calculations we demonstrate that the pentagonal arrangement of SiC<sub>2</sub> yields an inverted distribution of the p-bands which leads to an unusual electronic behaviour of the material under strain [J. Phys. Chem. C, 2015, 119 (33), pp 19469]. A different pentagonal arrangement of C atoms enables the formation of Dirac cones which, unlike graphene, exhibit a strain-mediated tunable band gap.

<sup>1</sup>This work is supported by DOE-BES under Contract No. DE-AC02-06CH11357

**12:15PM L23.00004 First-principles Study of Size and Edge Dependent Properties of MXene Nanoribbons<sup>1</sup>**, LIANG HONG, ROBERT KLIE, SERDAR OGUT, Univ of Illinois - Chicago — One-dimensional nanoribbons can be created with considerably different physical properties from their two-dimensional (2D) counterparts due to quantum confinement and surface effects. MXenes are a new class of 2D materials with many potential applications and have drawn significant attention. We perform first-principles calculations to explore the size and edge dependent properties of a wide range of MXene nanoribbons cut from 2D semiconducting MXenes. Our results suggest that semiconducting versus metallic nature as well as the size of the band gap for semiconducting MXene nanoribbons can be tuned as a function of size, chemical composition, and functional groups, which can be useful for future designs of MXene nanostructures with interesting electronic and optical properties.

<sup>1</sup>This work was supported by the National Science Foundation (Grant No. DMR-1408427) and used resources of the National Energy Research Scientific Computing Center supported by the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

**12:27PM L23.00005 First-principles study of 2D electride : Gadolinium carbide**, CHANDANI NADADASA, SEONG-GON KIM, SUNGHO KIM, Mississippi State University, Starkville, MS39762, SUNG WNG KIM, sungkyunkwan university, Suwon, Korea — Electrides are an exclusive class of ionic compounds in which some electrons are occupying crystal voids instead of attaching to specific atoms or bonds. Using first-principles density functional theory calculations, we study structural, electronic and magnetic properties of Gd<sub>2</sub>C. The theoretically predicted structure of Gd<sub>2</sub>C is in good agreement with the available experimental data. Energy band diagram of Gd<sub>2</sub>C shows that they are crossing the Fermi level. Projected electronic density of states plots indicate that the interstitial sites are the main contributor to the density of states at the Fermi level. Charge of individual atoms including interstitial site are obtained using Bader analysis. Magnetic properties of Gd<sub>2</sub>C is determined from magnetization density plots. Work functions of Gd<sub>2</sub>C are determined for (001) and (100) surfaces with the technique of macroscopic average of electrostatic potential with the Fermi energy of bulk.

**12:39PM L23.00006 Phase Transition between Black and Blue Phosphorenes: A Quantum Monte Carlo Study**, LESHENG LI, YI YAO, KYLE REEVES, YOSUKE KANAI, Univ of NC - Chapel Hill — Phase transition of the more common black phosphorene to blue phosphorene is of great interest because they are predicted to exhibit unique electronic and optical properties[1]. However, these two phases are predicted to be separated by a rather large energy barrier. In this work, we study the transition pathway between black and blue phosphorenes by using the variable cell nudge elastic band method combined with density functional theory calculation. We show how diffusion quantum Monte Carlo method can be used for determining the energetics of the phase transition and demonstrate the use of two approaches for removing finite-size errors. Finally, we predict how applied stress can be used to control the energetic balance between these two different phases of phosphorene. [1] Zhu, Zhen, and David Tománek. "Semiconducting layered blue phosphorus: A computational study." *Physical review letters* 112.17 (2014): 176802.

**12:51PM L23.00007 Induced Magnetization and Band Gap in Graphene-Like Materials: Towards Spintronics**, XUAN LUO, National Graphene Research and Development Center, JESSE CAI, Thomas Jefferson High School for Science and Technology, NGRD-TJHSST TEAM — We use first principles calculations incorporated within the ABINIT package to analyze the potential of two dimensional graphene-like materials in spintronics. Spintronics has potential to vastly improve upon and decrease the size of existing silicon based technology. We use four transition metals, Mn, Fe, Co, and Ni, to dope six graphene-like materials: graphene, boron nitride, silicene, molybdenum disulfide, molybdenum diselenide and black phosphorene. With the addition of a transition metal dopant, boron nitride, silicene, molybdenum disulfide, molybdenum diselenide and black phosphorene all displayed magnetization and a band gap in at least one configuration. Doped graphene, however, showed magnetization but no band gap. By using a hybrid graphene/boron nitride surface, or by placing graphene on top of boron nitride, magnetization and a band gap was observed. By altering the surface and the metal dopant, we have the ability to tune the band gap and magnetization. In conclusion, we find that all six graphene-like materials show promise in developing spintronics.

**1:03PM L23.00008 Anisotropic Dirac Fermions in Novel 2D Carbon and Silicon Allotropes**, ZHENHAI WANG, Stony Brook University, MINGWEN ZHAO, Shandong University, XIANG-FENG ZHOU, QIANG ZHU, Stony Brook University, XIAOMING ZHANG, Shandong University, HUAFENG DONG, ARTEM R. OGANOV, Stony Brook University, SHUMIN HE, PETER GRÜNBERG, Nanjing University of Posts and Telecommunications — Graphene, due to its unique Dirac cones with linear dispersion, exhibits a number of novel physics, such as high carrier mobility and quantum hall effect. Successful preparation of graphene in 2004 has inspired further searches for other 2D Dirac materials. Using systematic evolutionary structure searching, here we proposed one interesting type of 2D Dirac allotropes, which were named as 'phagraphene' [Nano. Lett. 15, 6182 (2015)] and 'siliceneet' respectively. Compared with the isotropic energy dispersion in graphene, the Dirac cones in these samples are direction-dependent. Further investigations proved that such anisotropic behaviors and the distorted Dirac cones are robust against external strain with tunable Fermi velocities. These predictions pave a new way to construct novel functional Dirac materials that might have potential applications in future.

**1:15PM L23.00009 Carbon Phosphide Monolayers: Novel 2D Materials**, GAOXUE WANG, RAVINDRA PANDEY, Michigan Technological Univ, SHASHI P. KARNA, US Army Research Laboratory — Monolayers of carbon phosphide are investigated using the particle swarm optimization and first-principles methods. The calculated results for  $\alpha$ -,  $\beta$ -, and  $\gamma$ - phases of carbon phosphide show novel properties including the presence of Dirac cones in the band structure. These configurations are composed of  $sp^2$  hybridized C atoms and  $sp^3$  hybridized P atoms in a hexagonal network with three-fold coordinated atoms.  $\alpha$ - and  $\beta$ - phases are semiconducting with highly anisotropic electronic and mechanical properties whereas  $\gamma$ -CP is semi-metallic with a high electron mobility. Our results suggest that the group IV-V binary monolayers can be considered as a new family of 2D materials for electronics and optoelectronics applications at nanoscale.

**1:27PM L23.00010 Influence of Metal Substrates on the Nucleation of Chemical Vapor Deposition Growth of Graphene<sup>1</sup>**, JIA LI, LIXIANG ZHONG, Graduate School at Shenzhen, Tsinghua University, Shenzhen 518055, People's Republic of China, YUANCHANG LI, National Center for Nanoscience and Technology, Beijing 100190, People's Republic of China — Using *ab initio* calculations, we systematically investigate the graphene nucleation on ten kinds of metal substrates that have been reported for the chemical vapor deposition growth of graphene. Noble metals (Cu, Ag and Au) and Co have a kinetic smallest graphene precursor, corresponding to the structural transition from linear chain to  $sp^2$  compact cluster. Ru, Rh, Ir and Pt have a energetic smallest graphene precursor, which is much larger than that in terms of kinetics. While for Ni and Pd, the carbon atoms trend to immerse inside the metals, resulting in the distinctively different growth mechanism from other metals. The different influence of metals is associated with their characterized carbon-metal and carbon-carbon coupling competition. The incorporation of five-membered rings into the  $sp^2$  compact cluster is the result of the competition between the curvature energy and the edge formation energy of graphene islands, and is suitable for the enlargement of graphene domain. And the effect of experimental conditions such as temperature, step or defects on the nucleation of graphene at different metal substrates is also discussed.

<sup>1</sup>This work was supported by the MOST, NSFC and Shenzhen Projects for Basic Research of China.

**1:39PM L23.00011 Stability and Superconductivity of N-(B-) Doped Graphene**, JIAN ZHOU, Virginia Commonwealth Univ, QIANG SUN, QIAN WANG, Peking University, PURU JENA, Virginia Commonwealth Univ — Superconductivity of two-dimensional honeycomb lattice has been predicted to possess a wealth of fascinating properties. For example, if graphene is heavily electron/hole doped, it exhibits high-temperature topological superconductivity. However, to achieve this, the carrier concentration will be too high, and graphene will be dynamically unstable. One possible route will be atomic substitution by B or N atoms, which, unfortunately, again is dynamic instability in nature. Using density functional theory combined with a global structural search and phonon dispersion calculations, we show that an ordered 50% N- (B-) doped graphene can be made energetically and dynamically stable by simultaneous doping carriers and applying biaxial tensile strain. By using a simple model, we show that tensile strain reduces the electrostatic interaction and moves imaginary phonon dispersion to be positive. Electron-phonon coupling calculations show that the N- (B-) doped graphene is superconducting with critical temperature reaching 66 K in the case of 50% N-doped graphene.

**1:51PM L23.00012 Next Generation Monolayer Structures of Group V Elements: Nitrogene and Antimonene**, ONGUN OZCELIK, Princeton University, OLCAY AKTURK, ENGIN DURGUN, SALIM CIRACI, Bilkent University — Based on first-principles density functional theory, we predict that nitrogen and antimony atoms can form single-layer, buckled honeycomb structures called nitrogene[1] and antimonene[2], which are rigid and stable even above room temperature. The 2D crystalline phase of nitrogen, which corresponds to a local minimum in the Born-Oppenheimer surface, is a nonmagnetic insulator with saturated pi bonds. When grown on a substrate like Al(111) surface or graphene, nitrogene binds weakly to substrates and hence preserves its free-standing properties, but it can easily be peeled off. Zigzag and armchair nanoribbons have fundamental band gaps derived from reconstructed edge states. These band gaps are tunable with size and suitable for the emerging field of 2D electronics. Nitrogene and antimonene form not only bilayer, but also 3D graphitic multilayer structures. Single-layer nitrogene can nucleate and grow on the armchair edges of hexagonal boron nitride. Starting from the pseudo-layered character of 3D bulk crystals of antimony, we also demonstrate the formation of monolayer antimonene structure which is similar to nitrogene. [1] Phys. Rev. B 92, 125420, 2015. [2] Phys. Rev. B 91, 235446, 2015.

**2:03PM L23.00013 Design of low work function materials using alkali metal-doped transition metal dichalcogenides**, SOL KIM, Pohang Univ of Sci & Tech, MAN YOUNG LEE, SEONG LEE, 4th RD Institute-4, Agency for Defense Development., SEUNG-HOON JHI, Pohang Univ of Sci & Tech — Engineering the work function is a key issue in surface science. Particularly, discovering the materials that have work functions less than 1eV is essential for efficient thermionic energy conversion. The lowest work function of materials, reported so far, is in a range of about 1eV. To design low work function materials, we chose  $\text{MX}_2$  ( $\text{M}=\text{Mo}$  and  $\text{W}$ ;  $\text{X}=\text{S}$ ,  $\text{Se}$  and  $\text{Te}$ ) as substrates and alkali metals ( $\text{Li}$ ,  $\text{Na}$ ,  $\text{K}$ ,  $\text{Rb}$  and  $\text{Cs}$ ) as dopants, and studied their electronic structures, charge transfer, induced surface dipole moment, and work function using first-principles calculations. We found that the charge transfer from alkali metals to  $\text{MX}_2$  substrates decreases as the atomic radius of alkali metals increases. Regardless of the amount of the charge transfer,  $\text{K}$  on  $\text{WTe}_2$  exhibits the biggest surface dipole moment, which consequently makes the surface work function the lowest. Also, we found a correlation between the binding distance and the work function.

**Wednesday, March 16, 2016 11:15AM - 2:15PM –**

**Session L24 DMP: Mesoscopic Materials and Devices I** 323 - Nitin Samarth, Pennsylvania State University

**11:15AM L24.00001 Manipulating edge transport in quantum anomalous Hall insulators<sup>1</sup>**, ABHINAV KANDALA, IBM T J Watson Research Center/Pennsylvania State University — The quantum anomalous Hall (QAH) effect provides a path to obtain dissipation-less, one-dimensional (1D) edge states at zero magnetic field. Its recent experimental realization in magnetic topological insulator thin films lies at the overlap of several areas of condensed matter physics: dilute magnetic semiconductors, low dimensional electron transport and topologically non-trivial material systems. In this talk, we demonstrate how careful compositional and electrical tuning of epitaxial films of Cr-doped  $(\text{Bi,Sb})_2\text{Te}_3$  enables access to a robust zero-field quantized Hall effect, despite sample roughness [1] and low carrier mobility. In samples that show near-dissipation-less transport, we manipulate the intermixing between edge states and dissipative channels via a tilted-field crossover from ballistic 1D edge transport to diffusive transport [2]. This crossover manifests in a gate-tunable giant anisotropic magneto-resistance effect that we use as a quantitative probe of dissipation in our systems. Finally, we discuss experiments with mesoscopic channels of QAH insulator thin films, and discuss the effect of their modified magnetic anisotropy on edge transport. This work was carried out in collaboration with A. Richardella, C-X Liu, M. Liu, W. Wang, N. P. Ong, and N. Samarth. [1] A. Richardella, A. Kandala et. al APL Materials 3 (8), 083303 (2015) [2] A. Kandala, A. Richardella et. al. Nature Commun. 6:7434 (2015)

<sup>1</sup>Funded by ARO/MURI, DARPA and ONR

**11:51AM L24.00002 Spin-orbit Josephson  $\phi_0$ -junction in nanowire quantum dots**, DANIEL SZOMBATI, STEVAN NADJ-PERGE, TU Delft, DIANA CAR, ERIK BAKKERS, TU Eindhoven, LEO KOUWENHOVEN, TU Delft — The Josephson effect describes supercurrent flowing through a junction connecting two superconducting leads by a thin barrier[1]. This current is driven by a superconducting phase difference  $\phi$  between the leads and it is strictly zero when  $\phi$  vanishes, due to the chiral and time reversal symmetry of the Cooper pair tunneling process[2]. Only if these underlying symmetries are broken the supercurrent for  $\phi = 0$  may be finite[3]. This corresponds to a ground state of the junction being offset by a phase  $\phi_0$ . Here, for the first time, we report such Josephson  $\phi_0$ -junction. Our realization is based on a nanowire quantum dot. We use a quantum interferometer device in order to investigate phase offsets and demonstrate that  $\phi_0$  can be controlled by electrostatic gating. Our results have possible far reaching implications for superconducting flux and phase defined quantum bits as well as for exploring topological superconductivity in quantum dot systems. 1. Josephson, *Phys. Lett.* 1, 251–253 (1962). 2. Yip, S.-K., De Alcantara Bonfim, O. F. & Kumar, P., *Phys. Rev. B* 41, 11214–11228 (1990). 3. Zazunov, A., Egger, R., Jonckheere, T. & Martin, T., *Phys. Rev. Lett.* 103, 147004 (2009).

**12:03PM L24.00003 Controlling the magnetic state of a carbon nanotube Josephson junction with the superconducting phase.**, RAPHAELLE DELAGRANGE, R. WEIL, A. KASUMOV, H. BOUCHIAT, R. DEBLOCK, LPS, CNRS, Univ. Paris-Sud, Orsay, France., D. J. LUITZ, LPT-IRSAMC, Universite de Toulouse and CNRS, Toulouse, France., V. MEDEN, Institut für Theorie der Statistischen Physik, RWTH Aachen University and JARA, Aachen, Germany — The Kondo effect is a many-body phenomenon that screens the magnetic moment of an impurity in a metal. The associated singlet state can be probed in a single impurity by electronic transport in a quantum dot (QD), here made of a carbon nanotube (CNT), which provides a localized electron between the two contacts. Using superconducting leads, one can investigate the competition between the Kondo effect and the superconductivity induced in the CNT. The superconductivity can destroy the Kondo singlet in favor of a magnetic doublet, leading to a sign reversal of the supercurrent in the S-CNT-S junction. This singlet-doublet transition depends on the Kondo temperature and the superconducting gap, as well as the position of the impurity level. We demonstrate experimentally that the superconducting phase difference across the QD can also control this magnetic transition. We use the measurement of the relation between the supercurrent and this superconducting phase as a tool to probe the transition. We show that it has a distinctly anharmonic behavior, that reveals the phase-mediated singlet to doublet transition, in good agreement with finite temperature quantum Monte Carlo calculations. We extract as well a phase diagram of the phase-controlled quantum transition at zero temperature.

**12:15PM L24.00004 Majorana fermions in topological Yu-Shiba-Rusinov chains and lattices with or without spin-orbit interaction.**, PANAGIOTIS KOTETES, Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen, Denmark — Recent spin polarized scanning tunneling microscopy (SPSTM) experiments in magnetic chains (S. Nadj-Perge et al., *Science* 2014) opened new routes for detecting the elusive Majorana fermions (MFs). Within the deep Yu-Shiba-Rusinov (YSR) limit we calculate [1] the spatially resolved tunneling conductance of topological ferromagnetic chains [2] measured by means of SPSTM. Our analysis reveals novel signatures of MFs arising from the interplay of their strongly anisotropic spin-polarization and the magnetization content of the tip. We investigate the occurrence and evolution of zero/finite bias peaks for a single or two coupled chains forming a Josephson junction, when a preexisting chiral symmetry controlling the number of MFs per chain edge is preserved or weakly broken. We also reveal alternative pathways for engineering MFs without spin-orbit interaction (SOI). On one hand, we highlight that antiferromagnetic YSR chains become topological by inducing an artificial SOI using external fields [3], while on the other, we pursue mechanisms for stabilizing magnetic textures and topological YSR lattices [4] following the self-organization principle for topological spiral chains [5]. [1] P. Kotetes et al., *Physica E* 74, 614 (2015), [2] A. Heimes, D. Mandler, and P. Kotetes, *New J. Phys.* 17 023051 (2015), [3] A. Heimes, P. Kotetes, and G. Schön, *PRB* 90, 060507(R) (2014), [4] M. Schechter, P. Kotetes, K. Flensberg, and J. Paaske, [5] M. Schechter et al., arXiv:1509.07399.

**12:27PM L24.00005 Suppressed Conductance From Spin Selection Rules in F-CNT-F Quantum Dots<sup>1</sup>**, NIKOLAUS HARTMAN<sup>2</sup>, TYLER MORGAN-WALL, NINA MARKOVIC<sup>3</sup>, Johns Hopkins University — Conductance through a quantum dot can be suppressed due to spin selection rules governing the hopping of an additional electron onto an already-occupied quantum dot. Measurements of this effect in a carbon nanotube quantum dot with ferromagnetic contacts will be presented. Suppressed conductance peaks are observed in the Coulomb diamond plots at zero field and explained using spin selection rules. The pattern of suppressed peaks is observed to change with applied magnetic field as the spin ground state of the occupied quantum dot changes.

<sup>1</sup>This work was supported by NSF DMR-1106167.

<sup>2</sup>Current address: The University of British Columbia

<sup>3</sup>Current address: Goucher College

**12:39PM L24.00006 Hybrid Quantum Point Contact-Superconductor Devices Using InSb Nanowires**, STEPHEN GILL, JOHN JEFFREY DAMASCO, University of Illinois at Urbana-Champaign, DIANA CAR, ERIK BAKKERS, Eindhoven University of Technology, NADYA MASON, University of Illinois at Urbana-Champaign — Recent experiments using hybrid nanowire (NW)-superconductor (SC) devices have provided evidence for Majorana quasiparticles in tunneling experiments [1,2]. However, these tunneling experiments are marked by a soft superconducting gap, which likely originates from disorder at the NW-SC interface [3]. Hence, clean NW-SC interfaces are important for future Majorana studies. By carefully processing the NW-SC interface, we have realized quantized conductance steps in quantum point contacts fabricated from InSb NWs and superconducting contacts. We study the length dependence of ballistic behavior and the induced superconductivity in InSb NWs by quantum point contact spectroscopy. Additionally, we discuss how the transport in InSb NW-SC quantum point contacts evolves in magnetic field.  
References: 1. V. Mourik et al, Science 336, 1003 (2012). 2. A. Das et al, Nature Phys. 8, 887 (2012). 3. S. Takei et al, Phys. Rev. Lett. 110, 186803 (2013).

**12:51PM L24.00007 Flat band of midgap rotating surface states in 3D Dirac and Weyl semimetals under circularly polarized radiation**, JOSE GONZALEZ, RAFAEL A. MOLINA, Instituto de Estructura de la Materia (CSIC), Madrid, Spain — We report the investigation of novel surface states which develop when 3D Dirac or Weyl semimetals are placed under circularly polarized electromagnetic radiation. We find that a gap opens up from the hybridization between Floquet side bands, which leads to the appearance of midgap surface states in the form of evanescent waves decaying from the surface exposed to the radiation. We observe a phenomenon reminiscent of Landau quantization by which the midgap surface states get a large degeneracy proportional to the radiation flux traversing the surface of the semimetal. We show that all these surface states carry angular current, leading to a modulation of their charge that rotates with the same frequency of the radiation, which should manifest in the observation of a macroscopic chiral current in the irradiated surface.

**1:03PM L24.00008 Quantum coherence of mesoscopic stadia and wires coupled to the environment**<sup>1</sup>, YUANTAO XIE, J. J. HEREMANS, Virginia Tech, Physics Department, C. LE PRIOL, Ecole Polytechnique (France), Physics Department, S. VIJAYARAGUNATHAN, T. D. MISHIMA, M. B. SANTOS, The University of Oklahoma, Homer L. Dodge Dept. of Physics and Astronomy — Quantum phase coherence was measured in quasi-1D wires and in mesoscopic stadia connected to wide sample regions by wire-like necks, to investigate the effects of environmental and interdevice coupling on decoherence as contrasted to intrinsic materials properties. Measurements of quantum phase coherence lengths used weak-antiloocalization on nanolithographic InGaAs/InAlAs structures at 390 mK. For quantum wires, experiments show that longer wire lengths result in longer phase coherence lengths. The result is understood from the observation that longer wires average out decoherence introduced at the end sections by environmental coupling. For stadia with quantum-wire-like necks, stadium-wire coupling dominates decoherence in the stadia, rather than environmental coupling. Stadia with wider and shorter necks show longer phase coherence lengths. The result is understood from the observation that wider and shorter wires are geometrically similar to stadia, implying a stronger wave function hybridization between stadia and connecting necks and thus weaker decoherence from stadium-wire coupling. The work shows that geometry has to be taken into account in measured mesoscopic coherence.

<sup>1</sup>Supported by DOE DE-FG02-08ER46532 and NSF DMR-1207537.

**1:15PM L24.00009 Spin-polarized conductance anomalies in one-dimensional channels**, ALFREDO SANCHEZ, JEAN-PIERRE LEBURTON, Univ of Illinois - Urbana — We explain the emergence of conductance anomalies ( $\sim 0.3G_0$  and  $\sim 0.7G_0$ ,  $G_0 = 2e^2/h$ ) in one-dimensional channels by using an unrestricted Hartree-Fock approach with a three-dimensional Coulomb interaction. The latter predicts the onset of a pair of degenerate spin-polarized configurations (or channels), with specific conductance above a concentration-dependent threshold. The  $0.3G_0$  anomaly is a consequence of the 1D nature of the carrier density of states at the conductance onset, which weakens with temperature. Meanwhile, the second anomaly manifests itself as shoulders in the quantum conductance at the onset of concentration-dependent spin polarization, and becomes more pronounced as the temperature increases above 0 K, in agreement with experimental results. Our model also explains the dependence of the anomalies on drain and gate biases, longitudinal magnetic field, and channel length.

**1:27PM L24.00010 An interacting adiabatic quantum motor**, SILVIA VIOLA KUSMINSKIY, University Erlangen-Nürnberg, ANTON BRUCH, FELIX VON OPPEN, Freie Universität Berlin — We consider the effect of electron-electron interactions on the performance of an adiabatic quantum motor based on a Thouless pump operating in reverse. We model such a device by electrons in a 1d wire coupled to a slowly moving periodic potential associated with the classical mechanical degree of freedom of the motor. This periodic degree of freedom is set into motion by a bias voltage applied to the 1d electron channel. We investigate the Thouless motor with interacting leads modeled as Luttinger liquids. We show that interactions enhance the energy gap opened by the periodic potential and thus the robustness of the Thouless motor against variations in the chemical potential. We show that the motor degree of freedom can be described as a mobile impurity in a Luttinger liquid obeying Langevin dynamics with renormalized coefficients due to interactions, for which we give explicit expressions.

**1:39PM L24.00011 The Quantum Pinch Effect in Semiconducting Quantum Wires**, M.S. KUSHWAHA, Rice University — We investigate a two-component, cylindrical, quasi-one-dimensional quantum plasma subjected to a *radial* confining harmonic potential and an applied magnetic field in the symmetric gauge. It is demonstrated that such a system as can be realized in semiconducting quantum wires offers an excellent medium for observing the quantum pinch effect at low temperatures. An exact analytical solution of the problem allows us to make significant observations: surprisingly, in contrast to the classical pinch effect, the particle density as well as the current density display a *determinable* maximum before attaining a minimum at the surface of the quantum wire. The effect will persist as long as the equilibrium pair density is sustained. Therefore, the technological promise that emerges is the route to the precise electronic devices that will control the particle beams at the nanoscale<sup>1</sup>. 1. M.S. Kushwaha, Appl. Phys. Lett. 103, 173116 (2013).

**1:51PM L24.00012 Control of Nanofilament Structure and Observations of Quantum Point Contact Behavior in Ni/NiO Nanowire Junctions**<sup>1</sup>, SEAN OLIVER, George Mason University, JESSAMYN FAIRFIELD, SUNGHUN LEE, ALLEN BELLEW, Trinity College Dublin, IRIS STONE, George Mason University, LAURA RUPPALT, Naval Research Laboratory, JOHN BOLAND, Trinity College Dublin, PATRICK VORA, George Mason University — Resistive switching is ideal for use in non-volatile memory where information is stored in a metallic or insulating state. Nanowire junctions formed at the intersection of two Ni/NiO core/shell nanowires have emerged as a leading candidate structure where resistive switching occurs due to the formation and destruction of conducting filaments. However, significant knowledge gaps remain regarding the conduction mechanisms as measurements are typically only performed at room temperature. Here, we combine temperature-dependent current-voltage (IV) measurements from 15 - 300 K with magnetoresistance studies and achieve new insight into the nature of the conducting filaments. We identify a novel semiconducting state that behaves as a quantum point contact and find evidence for a possible electric-field driven phase transition. The insulating state exhibits unexpectedly complex IV characteristics that highlight the disordered nature of the ruptured filament while we find clear signs of anisotropic magnetoresistance in the metallic state. Our results expose previously unobserved behaviors in nanowire resistive switching devices and pave the way for future applications where both electrical and magnetic switching can be achieved in a single device.

<sup>1</sup>This work was supported by ONR grant N-00014-15-1-2357.

**2:03PM L24.00013 Puzzling electron behavior analogous to the Braess paradox in a mesoscopic network<sup>1</sup>**, SÉBASTIEN TOUSSAINT, SÉBASTIEN FANIEL, FREDERICO MARTINS, IMCN/NAPS, Université catholique de Louvain, Belgium, MARCO PALA, IMEP-LAHC, Université Grenoble Alpes and CNRS, France, LUDOVIC DESPLANQUE, XAVIER WALLART, IEMN, UMR CNRS and UST, France, SERGE HUANT, HERMANN SELLIER, Institut Néel, Université Grenoble Alpes and CNRS, France, VINCENT BAYOT, BENOIT HACKENS, IMCN/NAPS, Université catholique de Louvain, Belgium — A counterintuitive behavior analogous to the Braess paradox is encountered in a two-terminal mesoscopic network patterned in a two-dimensional electron system (2DES) [1]. Decreasing locally the electron density of one channel in the network paradoxically leads to an increased network conductance. Our scanning gate microscopy experiments reveals this puzzling conductance variation, thanks to tip-induced localized modifications of electron flow throughout the network's channels at low temperature, in the ballistic and coherent regime of transport. We compare the amplitude of the measured anomalous conductance variation with conductance changes induced by other mechanisms at play in the mesoscopic network, such as interference phenomena between different paths, and Coulomb blockade due to disorder-induced localized states. The robustness of this puzzling behavior is inspected by varying the global 2DES density, magnetic field and temperature. [1] M. G. Pala *et al.*, Phys. Rev. Lett. 108, 076802 (2012).

<sup>1</sup>S.T. acknowledges support from the Belgian FRS-FNRS (FRIA)

## Wednesday, March 16, 2016 11:15AM - 2:15PM —

Session L25 DCMP: Superconductivity: Theory II 324 - Alexander Balatsky, Los Alamos National Laboratory

**11:15AM L25.00001 How the Mott and pseudogap states coalesce beneath the superconductor Dome**, ALEJANDRO CABO MONTES DE OCA<sup>1</sup>, ICIMAF, La Habana, Cuba, ALEJANDRO CABO-BIZET, CEADEN, La Habana, Cuba, VICTOR MARTINEZ, YOANDRI VIELZA, Dept. of Physics, University of Pernambuco, Recife, Brasil, COLLABORATION TEAM TEAM — Former results of a Tight-Binding (TB) model of CuO planes in La<sub>2</sub>CuO<sub>4</sub> are reviewed to underline their wider implications. It is noted that physical systems being appropriately described by the TB model can exhibit the main strongly correlated electron system (SCES) properties, when they are solved in the HF approximation, by also allowing crystal symmetry breaking effects and non-collinear spin orientations of the HF orbitals. In particular, it is argued how a simple 2D square lattice system of Coulomb interacting electrons can exhibit insulator gaps and pseudogap states, and quantum phase transitions as illustrated by the mentioned former works. These results allow to understand the nature of the observed quantum phase transition laying “beneath” the superconducting Dome. It corresponds to coalescence under hole doping increase, of an insulator ground state (with a highly degenerated spin order) with an excited pseudogap state, showing a lattice order symmetry breaking. The evolution of the band structure and Fermi surface with doping are determined.

<sup>1</sup>This abstract is associated to an invited talk of the March Meeting after being accepted. If it is not accepted as talk, we request to be considered as an oral presentation. The argue for it is in the invited talk application (Session Ctrl :97854)

**11:27AM L25.00002 Scattering rates and specific heat jumps in high- $T_c$  cuprates<sup>1</sup>**, JAMES STOREY, Victoria University of Wellington — Inspired by recent ARPES and tunneling studies on high- $T_c$  cuprates, we examine the effect of a pair-breaking term in the self-energy on the shape of the electronic specific heat jump. It is found that the observed specific heat jump can be described in terms of a superconducting gap, that persists above the observed  $T_c$ , in the presence of a strongly temperature dependent pair-breaking scattering rate. An increase in the scattering rate is found to explain the non-BCS-like suppression of the specific heat jump with magnetic field. A discussion of these results in the context of other properties such as the superfluid density and Raman spectra will also be presented.

<sup>1</sup>Supported by the Marsden Fund Council from Government funding, administered by the Royal Society of New Zealand

**11:39AM L25.00003 Skyrmion-induced Bound States in Superconductors<sup>1</sup>**, SHO NAKOSAI, RIKEN, SERGEY PERSHOGUBA, Nordia, ALEXANDER BALATSKY, Nordita, Los Alamos National Laboratory — We consider superconducting systems proximity-coupled to magnetic materials with skyrmion structures. Motivated by the progress in experiments which allows us to control the magnetic textures, we consider the case where a single skyrmion is floating in ferromagnetic background. We predict the skyrmion bound state is formed around the core of it. The results are obtained through the numerical calculation on the spin-polarized local density of states in the vicinity of the skyrmion core, which shows good agreement with T-matrix analysis. The bound states can be recognized as skyrmion-version of well-known Yu-Shiba-Rusinov states.

<sup>1</sup>Supported by Grant-in-Aid for Research Activity Start-up (No. 15H06858) and US DOE BES E304.

**11:51AM L25.00004 Theory of quantum fluctuating superconductivity in incoherent metals**, LUCA DELACRETAZ, Department of Physics, Stanford University, RICHARD DAVISON, Department of Physics, Harvard University, BLAISE GOUTERAUX, SEAN HARTNOLL, Department of Physics, Stanford University — Quantum superconducting fluctuations can be important in two-dimensional, disordered thin films. They lead to the appearance of a metallic state characterized by a non-zero resistivity. We construct an effective description of superfluid hydrodynamics where the phase of the order parameter is relaxed, due to Coulomb interactions or the motion of vortices for instance. We predict there should be a Drude-like or a cyclotron-like pole in the spectrum, and corresponding sharp peaks in the optical conductivity. In some cases the finite electrical conductivity in the phase-fluctuating metallic state is found to be related in a novel way to the thermal conductivity of the normal state.

**12:03PM L25.00005 Charge transfer insulators at half-filling in multiband models of cuprates<sup>1</sup>**, PETER MISTARK, CHRISTOPHER LANE, Northeastern University, HSIN LIN, National University of Singapore, ROBERT MARKIEWICZ, ARUN BANSIL, Northeastern University — Self-consistent mean-field three-band and four-band Hubbard models are used to study the collapse of the Mott gap in doped cuprates. While no set of doping-independent parameters can explain the observed gaps for the entire doping range, the experimental results are consistent with a weakly doping dependent Hubbard U. A key finding is that, when the Cu-O splitting energy  $\Delta$  is large, the cuprates behave as Mott insulators. However, for small  $\Delta$ , the cuprates become charge transfer insulators.

<sup>1</sup>Work supported by the U.S.D.O.E

**12:15PM L25.00006 Polar Kerr effect in high temperature cuprate superconductors<sup>1</sup>**, SUMANTA TEWARI, GIRISH SHARMA, Department of Physics and Astronomy, Clemson University, Clemson, SC, PALLAB GOSWAMI, VICTOR YAKOVENKO, Condensed Matter Theory Center, University of Maryland, College Park, MD, SUDIP CHAKRAVARTY, Department of Physics and Astronomy, University of California Los Angeles, Los Angeles, CA — A mechanism is proposed for the tantalizing evidence of polar Kerr effect in a class of high temperature superconductors the signs of the Kerr angle from two opposite faces of the same sample are identical and magnetic field training is non-existent. The mechanism does not break global time reversal symmetry, as in an antiferromagnet, and results in zero Faraday effect. It is best understood in a phenomenological model of bilayer cuprates, such as YBCO, in which intra-bilayer tunneling nucleates a chiral d-density wave such that the individual layers have opposite chirality. Although the presentation is specific to the chiral d-density wave, the mechanism may be more general to any quasi-two-dimensional orbital antiferromagnet in which time reversal symmetry is broken in each plane, but not when averaged macroscopically.

<sup>1</sup>ST and GS supported by AFOSR (FA9550-13-1-0045), PG supported by JQI-NSF-PFC, SC supported by NSF-DMR-1004520

**12:27PM L25.00007 Dirac lines in the superconducting hyper-honeycomb lattice**, ADRIEN BOUHON, ANNICA BLACK-SCHAFER, Uppsala Univ — Motivated by the recent discovery of the hyper-honeycomb  $\beta$ -Li<sub>2</sub>IrO<sub>3</sub> studied in the context of Kitaev spin liquids, we investigate the possibility to realize superconductivity in the hyper-honeycomb lattice. Based on a t-J model we discuss the effect of the band structure and spin-orbit coupling on the most stable superconducting state. Using group theory we construct all symmetry allowed superconducting states and show that we naturally get Dirac line nodes protected by the non-symmorphic symmetries.

**12:39PM L25.00008 Radiation induced oscillating gap states of nonequilibrium superconductors**, HUIYING LIU, JUNREN SHI, Peking Univ — In recent years, non-equilibrium superconducting phenomena induced by light have drawn great interests. We study effects of a light radiation to a BCS superconductor. The phase transition are obtained from the analysis of self-oscillation conditions of the irradiated dynamical systems. We find an oscillating gap phase solution with a frequency not directly related to the radiation frequency but resulting from the asymmetry of electron density of states of the system. When such a superconductor is in contact with another superconductor, it will give rise to an alternating Josephson current. We further discuss the existence conditions and properties of this alternating gap phase solution and its interesting effects on experiments.

**12:51PM L25.00009 Transient Dynamics of d-wave Superconductors after a Sudden Excitation**, MARCO SCHIRO, CNRS, FRANCESCO PERONACI, MASSIMO CAPONE, SISSA — Motivated by recent ultrafast pump probe experiments on high-temperature superconductors, we discuss the transient dynamics of a d-wave BCS model after a quantum quench of the interaction parameter. We find that the existence of gap nodes, with the associated nodal quasiparticles, introduces a dissipation channel which makes the dynamics much faster than in the conventional s-wave model. For every value of the quench parameters, the superconducting gap rapidly converges to a stationary value smaller than the one at equilibrium. Using a sudden approximation for the gap dynamics, we find an analytical expression for the reduction of spectral weight close to the nodes, which is in qualitative agreement with recent experiments.

**1:03PM L25.00010 Chern mosaic: topology of chiral superconductivity in ferromagnetic adatom lattices<sup>1</sup>**, JOEL RONTYNNEN, TEEMU OJANEN, Low Temperature Laboratory, Aalto University — Recent experiments have demonstrated signatures of Majorana bound states in ferromagnetic atomic chains. We show that similar systems, extended to two dimensional geometry, may support chiral topological superconductivity with large Chern numbers. Our observation is based on the fact that magnetic adatoms on an s-wave superconductor bind subgap Shiba states, which can hybridize and form subgap energy bands with nontrivial topology. Such a Shiba lattice supports long-range hopping, leading to a complex, mosaic-like phase diagram with large Chern numbers. We analyze the incidence of different Chern numbers phases and the size of their energy gaps for various lattice geometries. Our findings reveal the studied system as one of the richest platforms of topological matter known to date.

<sup>1</sup>The authors acknowledge the Finnish Cultural Foundation and the Academy of Finland for support.

**1:15PM L25.00011 Weak phase stiffness and nature of the quantum critical point in underdoped cuprates<sup>1</sup>**, WEI KU, YUCEL YILDIRIM, Brookhaven National Laboratory — We demonstrate that the zero-temperature superconducting phase diagram of underdoped cuprates can be quantitatively understood in the strong binding limit, using only the experimental spectral function of the “normal” pseudo-gap phase without any free parameter. In the prototypical (La<sub>1-x</sub>Sr<sub>x</sub>)<sub>2</sub>CuO<sub>4</sub>, a kinetics-driven d-wave superconductivity is obtained above the critical doping  $\delta_c \sim 5.2\%$ , below which complete loss of superfluidity results from local quantum fluctuation involving local p-wave pairs. Near the critical doping, a enormous mass enhancement of the local pairs is found responsible for the observed rapid decrease of phase stiffness. Finally, a striking mass divergence is predicted at  $\delta_c$  that dictates the occurrence of the observed quantum critical point and the abrupt suppression of the Nernst effects in the nearby region. \* Phys. Rev. B 92, 180501(R) (2015); Phys. Rev. X 1, 011011 (2011).

<sup>1</sup>Work supported by U.S. Department of Energy, Office of Basic Energy Science, under Contract No. DE-AC02-98CH10886

**1:27PM L25.00012 p-Orbital Density Wave with d Symmetry in High-Tc Cuprate Superconductors**, MASAHISA TSUCHIIZU, YUICHI YAMAKAWA, HIROSHI KONTANI, Nagoya University — Emergence of the nematic density wave is a fundamental unsolved problem in cuprate superconductors. To understand the origin of the nematicity, we employ the recently-developed functional renormalization-group method with high numerical accuracy, and discover the critical development of the p-orbital-density-wave (p-ODW) instability in the strong-spin-fluctuation region [1]. The obtained p-ODW state possesses the key characteristics of the charge ordering pattern in Bi- and Y-based superconductors, such as the wavevector parallel to the nearest Cu-Cu direction, and the d-symmetry form factor with the antiphase correlation between  $p_x$  and  $p_y$  orbitals in the same unit cell. From the beautiful scaling relation between the spin susceptibility and the p-ODW susceptibility, we conclude that the p-ODW is driven by the strong interference between spin and charge fluctuations. It is clarified that the strong charge-spin interference, which is the origin of the nematicity, is the hidden but significant characteristics of the electronic states in cuprate superconductors. [1] M. Tsuchiizu, Y. Yamakawa, and H. Kontani, arXiv:1508.07218.

**1:39PM L25.00013 Spectral properties of the two-dimensional t-J model near the Mott transition**, MASANORI KOHNO, International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Japan — The single-particle spectral function of the two-dimensional t-J model near the Mott transition is studied using cluster perturbation theory to clarify how the spectral-weight distribution transforms to that of the Mott insulator as the doping concentration decreases. Various anomalous features observed in cuprate high-temperature superconductors are collectively explained in the two-dimensional t-J model near the Mott transition [1] as in the two-dimensional Hubbard model [2]. The results imply that the spectral features are primarily related to the proximity of the antiferromagnetic Mott insulator, which has a low-energy spin-wave mode but no low-energy charge excitation, and to the presence of states characterized by different energy scales rather than to the presence of double occupancy, which is completely removed in the t-J model. The results are confirmed to remain almost unchanged as the cluster size is increased from 4×4 to 6×6 sites in cluster perturbation theory by using the non-Abelian dynamical density-matrix renormalization group method [1]. [1] M. Kohno, Phys. Rev. B 92, 085128 (2015). [2] M. Kohno, Phys. Rev. Lett. 108, 076401 (2012).

**1:51PM L25.00014 Monte Carlo Study of Competing Orders in a Nearly Antiferromagnetic Metal**, EREZ BERG, YONI SCHATTNER, Weizmann Institute of Science, MAX GERLACH, SIMON TREBST, University of Cologne — We study a two-dimensional lattice model of a metal on the verge of an antiferromagnetic transition. The model can be simulated using the quantum Monte Carlo technique with no sign problem. We compute the antiferromagnetic, superconducting, charge density wave, and pair density wave susceptibilities, as well as the superfluid density, across the phase diagram. Near the putative antiferromagnetic quantum critical point, we find a dome-shaped d-wave superconducting phase. The electronic density of states displays an opening of a gap at temperatures moderately above the superconducting  $T_c$ . Our results provide insights into the interplay of antiferromagnetism and unconventional superconductivity at intermediate to strong coupling.

**2:03PM L25.00015 TYPICAL MEDIUM DYNAMICAL CLUSTER APPROXIMATION FOR DISORDERED SUPERCONDUCTORS**<sup>1</sup>, ELISHA SIDDIQUI, Louisiana State University, HANNA TERLETSKA, University of Michigan, CHINEDU EKUMA, Naval Research Laboratory, NS VIDHYADHIRAJA, Jawaharlal Nehru Centre for Advanced Scientific Research, JUANA MORENO, MARK JARRELL, Louisiana State University — We study the effect of disorder on a three dimensional attractive Hubbard model using the typical medium dynamical cluster approximation with the Bogoliubov-de Gennes approach as a cluster solver. We explore the effects of disorder for a fixed interaction strength (U) on the diagonal and off-diagonal typical density of states. Using our results we construct a complete phase diagram in the disorder vs interaction (U) parameter space. As the disorder strength is increased, the pairing parameter or the off-diagonal typical density of states decreases and vanishes at a critical disorder strength while the spectral gap remains finite. This indicates the transition from a superconducting to a super-resistive phase. We observe that at small U the superconductor to super-resistive phase line bends down in the disorder vs interaction (U) parameter space. Also, we find that the superconducting order parameter first rises and then falls with increasing disorder in the small U regime. A further increase in the disorder strength causes the diagonal typical density of states to vanish at a critical value, indicating a transition from a super-resistive to the Anderson insulator phase.

<sup>1</sup>This work is supported in part by National Science Foundation (NSF) [Award No. LA-SiGMA EPS-1003897.]

**Wednesday, March 16, 2016 11:15AM - 2:03PM —**  
**Session L26 DCMP DMP: Electronic and Transport Properties of Insulators** 325 - L. Andrew Wray, New York University

**11:15AM L26.00001 First-principles Studies of the Optical Properties of Eu doped Barium Halides: From Storage Phosphor to Bright Scintillator**, ANDREW CANNING, Lawrence Berkeley National Laboratory, UC Davis, BHARAT MEDASANI, MAURO DEL BEN, GREGORY BIZARRI, Lawrence Berkeley National Laboratory — The Eu doped Ba mixed halide family BaBrX (X=F,Cl,Br,I) changes from being a widely used X-ray Storage Phosphor (BaBrF:Eu) to one of the brightest known gamma ray detector scintillators (BaBrI:Eu). To help understand these contrasting optical properties and guide in the design of new and improved scintillator detectors, in collaboration with experimental groups, we have performed first principles theoretical studies of these materials. In particular we have studied their electron and hole trapping mechanisms and how that can explain their very different optical properties.

**11:27AM L26.00002 Direct experimental characterization of photoemission charge-transfer satellites.**, CONAN WEILAND, National Institute of Standards and Technology, ABDUL RUMAIZ, National Synchrotron Light Source II, Brookhaven National Laboratory, JOSEPH WOICK, National Institute of Standards and Technology — Energy-loss satellites in photoelectron spectroscopy often arise due to different charge-transfer states in condensed matter systems. The specific characterization of these satellites, however, has been controversial, and different theoretical approaches may lead to contradictory characterizations. Here we demonstrate the ability of high energy resonant photoelectron spectroscopy to provide direct experimental evidence of the nature of charge transfer satellites. Analysis of the Ti 1s core line in SrTiO<sub>3</sub> reveals two satellites, located approximately 5 eV and 13 eV lower kinetic energy than the main line. High energy resonant photoelectron spectroscopy reveals that these two peaks originate from ligand 2p  $t_{2g}$  to metal 3d  $t_{2g}$  and ligand 2p  $e_g$  to metal 3d  $e_g$  charge-transfer excitations.

**11:39AM L26.00003 High harmonic generation based time resolved ARPES at 30 eV with 50 meV energy resolution**, TIMM ROHWER, EDBERT J. SIE, FAHAD MAHMOOD, NUH GEDIK, MIT — Angle-resolved photoelectron spectroscopy (ARPES) has emerged as a leading technique in identifying equilibrium properties of complex electronic systems as well as their correlated dynamics. By using femtosecond high harmonic generation (HHG) pulses, this technique can be extended to monitor ultrafast changes in the electronic structure in response to an optical excitation [1]. However, the broad bandwidth of the HHG pulses has been a major experimental limitation. In this contribution, we combine the HHG source with an off-axis Czerny-Turner XUV monochromator and a three-dimensional “ARTOF” photoelectron detector to achieve an unrivaled overall energy resolution of 50 meV in multiple harmonic energies. Moreover, the use of a stack of different gratings enables us to fine control both the photon energy and time vs. energy resolution to its particular needs. The performance of our setup is demonstrated by studies on the transition metal dichalcogenide IrTe<sub>2</sub> which undergoes a first-order structural transition and accompanied reconstruction of the band structure upon cooling without the characteristic opening of an energy gap [2]. [1] T. Rohwer et al., Nature 471 (2011) 490, [2] A. F. Fang et al., Scientific Reports 3 (2013) 1153

**11:51AM L26.00004 Resonant inelastic x-ray scattering study at the oxygen K-edge of corner-shared Sr<sub>2</sub>CuO<sub>3</sub> cuprate**, UMESH KUMAR, Department of Physics and Astronomy, University of Tennessee, Knoxville, USA, JUSTINE SCHLAPPA, European X-Ray Free Electron Laser Facility GmbH, Hamburg, Germany, KEJIN ZHOU, Diamond Light Source, Harwell Science and Innovation Campus, Didcot, Oxfordshire, SURJEET SINGH, Indian Institute of Science Education and Research, Pashan, Pune, India, VLADIMIR STROCOV, Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland, ALEXANDRE REVCOLEVSCHI, Universit Paris-Sud, Orsay Cedex, France, HENRIK RNNOW, Ecole Polytechnique Federale de Lausanne (EPFL), Lausanne, Switzerland, STEVEN JOHNSTON, Department of Physics and Astronomy, University of Tennessee, Knoxville, USA, THORSTEN SCHMITT, Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland — We present a resonant inelastic x-ray scattering (RIXS) study at the oxygen K-edge of the spin-chain system Sr<sub>2</sub>CuO<sub>3</sub>. We investigate this system using small cluster exact diagonalization calculations for a microscopic model that considers all the orbitals of Cu and O in CuO<sub>3</sub>-unit cell. Using a canonical parameter set, we compute the XAS and RIXS spectra in comparison to the experiment. This allows us to identify the dd- and charge transfer excitations in the observed spectrum. We also infer the presence of several low energy excitations that may be related to phononic and/or magnetic excitations.

**12:03PM L26.00005 ABSTRACT WITHDRAWN —**

**12:15PM L26.00006 Temperature-Induced Electronic Structure Evolution of ZrTe5 Revealed by High resolution & Laser Angle-Resolved Photoemission Spectroscopy (ARPES)** , YAN ZHANG, CHENLU WANG, GUODONG LIU, GENFU CHEN, LI YU, SHAOLONG HE, LIN ZHAO, Institute of Physics, Chinese Academy of Science, CHUANGTIAN CHEN, ZUYAN XU, Technical Institute of Physics and Chemistry, Chinese Academy of Science, XINGJIANG ZHOU, Institute of Physics, Chinese Academy of Science — The transition metal pentatellurides ZrTe5 have attracted consideration attention since the 70s, due to the unusual transport properties like resistivity peak at ~140K and the sign change of the Hall coefficient and thermopower. The origin of the most peculiar resistivity peak remains controversial. In this talk we will present high resolution angle-resolved photoemission (ARPES) study on the Fermi surface and band structure of ZrTe5, by using our high resolution ARPES system equipped with the VUV laser and the time-of-flight (TOF) electron energy analyzer. Upon cooling down, we found a gradual transition from hole-like band into electron-like band around the Brillouin zone center. Such an electron state transition forms the underlying physics for the abnormal transport properties. We will also comment on the possibility of a Dirac semimetal in ZrTe5.

**12:27PM L26.00007 Material simulation of charge carrier transport properties of polymer dielectrics** , MIKAEL UNGE, ABB Corporate Research SE 72178 Vsters, Sweden, THOMAS CHRISTEN, ABB Corporate Research Baden-Dttwil, Switzerland, CHRISTER TRNKVIST, ABB Corporate Research SE 72178 Vsters, Sweden, ABB CORPORATE RESEARCH TEAM — To understand electron and hole transport in solid material requires to know its electronic properties, i.e. the density of states (DOS) and whether the states are spatially localized or delocalized. The states closest to the band edges may be localized, states further away can be delocalized. This transition from localized to delocalized states determines the mobility edge, above the mobility edge the mobility is expected to be high. A real polymer is never perfect; it contains a number of oxidative states, bonding defects and molecular impurities. These imperfections yield electronic states that can appear in the band gap of the polymer, traps. Traps can be shallow, i.e. close to the band edges, from these states the charge carrier easily can jump to a state in the band edge or another shallow state. Other traps can be deep, in these states it is likely that the charge carrier remains and become immobile. All these properties related to the electronic structure of the polymer, including its defects, affects the conductivity of the polymer. Linear scaling Density Functional Theory has been applied to calculate electronic structure of amorphous polyethylene. In particular DOS, trap levels and mobility edges are studied.

**12:39PM L26.00008 Generality of anomalous broadening in  $\sigma$  peaks of low-Z compounds** , TERENCE JACH, JOHN VINSON, NIST, Gaithersburg, MD, MATTHIAS MUELLER, RAINER UNTERUMSBERGER, BURKHARD BECKHOFF, PTB, Berlin, Germany — X-ray emission spectra originating from N 1s core holes in some nitrates have displayed extreme broadening(> 4 eV) of a feature identified with the NO  $\sigma$  state. Simple band structure calculations of the valence band derived from this bond in a crystal show it to be quite narrow. Calculations of transitions that take into account many-body corrections in the  $GW$  approximation indicate that the final state has a large imaginary self-energy. We have discovered other compounds that demonstrate this effect experimentally, and we are able to show that they display giant lifetime fluctuations of a similar valence state. We have formulated a criterion of compounds for which this effect should be present.

**12:51PM L26.00009 Novel mechanism for displacive distortions in perovskites: On the orbital ordering transition in  $\text{KCuF}_3$**  , HUNTER SIMS, German Research School for Simulation Sciences, EVA PAVARINI, Institute for Advanced Simulation, Forschungszentrum Jülich, ERIK KOCH, German Research School for Simulation Sciences — The Mott insulating perovskite  $\text{KCuF}_3$  is considered the paradigmatic system with long-ranged orbital order and a cooperative Jahn-Teller distortion of the Cu-F octahedra. However, recent experiments have revealed that the JT-like distortions persist and even grow as temperature is increased. We show that neither superexchange nor Jahn-Teller can accurately describe this behavior—even qualitatively. Supported by GGA+U and model calculations, we explain this anomalous result in terms of a volume-driven lattice instability of purely ionic origin. We examine the effect of ionic size on this mechanism through the related systems  $\text{KCu}_{1-x}\text{Mg}_x\text{F}_3$ ,  $\text{KCrF}_3$ , and  $\text{ACuF}_3$ . As a non-electronic effect, this instability should allow for octahedral distortions even in closed-shell systems with cubic ground states, and we propose design guidelines for the realization of this high-temperature broken-symmetry phase experimentally.

**1:03PM L26.00010 Electrical Breakdown in Solids** , HAROLD HJALMARSON, FRED ZUTAVERN, Sandia National Laboratories, KENNETH KAMBOUR, Leidos, CHRIS MOORE, ALAN MAR, Sandia National Laboratories — During electron breakdown of a solid subjected to a large electric field, impact ionization causes growth of an electron-hole plasma. This growth process is opposed by Auger recombination of the electron-hole pairs. In our work, such breakdown is investigated by obtaining steady-state solutions to the Boltzmann equation. In these calculations, the carriers are heated by the electric field and cooled by phonon emission. Our results imply that breakdown may lead to high carrier-density current filaments. Conductive filaments have been observed in optically-triggered, high-power photoconductive semiconductor switch (PCSS) devices being developed at Sandia Labs. The relationship between the steady-state computed solutions to the observed filaments will be discussed in the presentation. This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energys National Nuclear Security Administration under contract DE-AC04-94AL85000.

**1:15PM L26.00011 Hole conduction pathways in transparent amorphous tin oxides** , MATTHEW WAHILA, ZACHARY LEBENS-HIGGINS, NICHOLAS QUACKENBUSH, LOUIS PIPER, Dept. of Physics, Binghamton University, KEITH BUTLER, CHRISTOPHER HENDON, ARON WALSH, Dept. of Chemistry, University of Bath, GRAEME WATSON, School of Chemistry and CRANN, Trinity College Dublin — P-type transparent amorphous oxide semiconductors (TAOS) have yet to be sufficiently demonstrated or commercialized, severely limiting the possible device architecture of transparent and flexible oxide electronics. The lack of p-type amorphous oxide candidates mainly originates from the directional oxygen  $2p$  character of their topmost valence states. Previous attempts to create p-type oxides have involved hybridization of the O  $2p$  with metal orbitals, such as with  $\text{CuAlO}_2$  and its Cu  $3d$  - O  $2p$  hybridization. However, the highly directional nature of the utilized orbitals means that structural disorder inhibits hybridization and severely disrupts hole-conduction pathways. Crystalline stannous oxide ( $\text{SnO}$ ) and other lone-pair active post-transition metal oxides can have reduced localization at the valence band edge due to complex hybridization between the O  $2p$ , metal  $p$ , and spherical metal  $s$ -orbitals. I will discuss our investigation of structural disorder in  $\text{SnO}$ . Using a combination of synchrotron spectroscopy, and atomistic calculations, our investigation elucidates the important interplay between atomistic and electronic structure in establishing continuous hole conduction pathways at the valence band edge of transparent amorphous oxides.

**1:27PM L26.00012 Topological aspects of nonlinear optical responses** , TAKAHIRO MORIMOTO, University of California, Berkeley, NAOTO NAGAOSA, RIKEN CEMS, University of Tokyo — There are a variety of nonlinear optical effects including higher harmonic generations, photovoltaic effects, and nonlinear Kerr rotations. A recent remarkable progress in the photovoltaic effect is the high efficiency solar cell action in perovskite oxides without inversion symmetry. The crystal structure lacking inversion replaces the role of artificial structures such as p-n junctions in conventional solar cells. One of the proposed mechanisms for this phenomenon is the shift-current which is supported by a band structure lacking inversion and is related to the Berry connection of Bloch wavefunctions. Motivated by these, we explore topological aspects of the nonlinear optical responses. To this end, we employ the Keldysh method combined with the Floquet formalism, where effective band structures can be defined under an electric field periodic in time. This enables us to describe the shift-current, nonlinear Kerr rotation, photovoltaic effect, and the photo-induced change in the order parameters in a unified fashion. We connect these nonlinear optical responses to topological quantities involving the Berry connection and Berry curvature. It is found that vector fields defined with the Berry connections in the space of momentum and/or parameters govern the nonlinear responses.

**1:39PM L26.00013 A compact, low-loss, tunable phase shifter on defect mitigated dielectrics up to 40 GHz**, NATHAN ORLOFF, CHRISTIAN LONG, XIFENG LU, NIST, HARI NAIR, NATALIE DAWLEY, DARRELL SCHLOM, Cornell University, JAMES BOOTH, NIST — With the emergence of the internet-of-things and increased connectivity of modern commerce, consumers have driven demand for wireless spectrum beyond current capacity and infrastructure capabilities. One way the telecommunications industry is addressing this problem is by pushing front-end electronics to higher frequencies, introducing carrier aggregation schemes, and developing spectrum-sharing techniques. Some of these solutions require frequency agile components that are vastly different from what is in today's marketplace. Perhaps the most basic and ubiquitous component in front-end electronics is the phase shifter. Phase shifters are particularly important for compact beam-forming antennas that may soon appear in commercial technology. Here, we demonstrate a compact, tunable phase shifter with very low insertion loss up to 40 GHz on a defect mitigated tunable dielectric. We demonstrate performance compared to barium-doped strontium titanate phase shifters. Such phase shifters could potentially meet the stringent size and performance characteristics demanded by telecommunications industry, readily facilitating massive multiple-input multiple-output antennas in the next-generation of mobile handsets.

**1:51PM L26.00014 Electrode effects in dielectric spectroscopy measurements on (Nb+In) co-doped  $\text{TiO}_2$** <sup>1</sup>, DAVID CRANDLES, SUSAN YEE, Brock University, MAXIM SAVINOV, DIMITRI NUZHNYI, JAN PETZELT, STANISLAV KAMBA, Institute of Physics, Czech Academy of Sciences, JAN PROKES, Charles University in Prague — Recently, several papers reported the discovery of giant permittivity and low dielectric loss in (Nb+In) co-doped  $\text{TiO}_2$ . A series of tests was performed which included the measurement of the frequency dependence of the dielectric permittivity and ac conductivity of co-doped (Nb+In) $\text{TiO}_2$  as a function of electrode type, sample thickness and temperature. The data suggest that the measurements are strongly affected by the electrodes. The consistency between four contact van der Pauw dc conductivity measurements and bulk conductivity values extracted from two contact ac conductivity measurements suggest that the values of colossal permittivity are, at least in part, a result of Schottky barrier depletion widths that depend on electrode type and temperature.

<sup>1</sup>NSERC, Czech Science Foundation (Project 15-08389S)

## Wednesday, March 16, 2016 11:15AM - 2:15PM —

Session L27 DCMP: Quantum Criticality: Theory 326 - Lucile Savary, Massachusetts Institute of Technology

**11:15AM L27.00001 Vestigial nematicity from spin and/or charge order in the cuprates**, LAIMEI NIE, AKASH MAHARAJ, Stanford University, EDUARDO FRADKIN, University of Illinois at Urbana-Champaign, STEVEN KIVELSON, Stanford University — Nematic order (C4 rotation symmetry breaking) has manifested itself in a variety of materials in the cuprates family, yet its origin remains debatable, with possible links to lattice, charge, and spin degrees of freedom across different doping regimes. We propose an effective field theory of a layered system with incommensurate, intertwined spin- and charge-density wave (SDW and CDW) orders, each of which consists of two components related by C4 rotations. Using a variational free energy approach, we study the growth of the associated nematicity from partially melting those density waves by either increasing temperature or adding quenched disorder. Under the assumption that the zero-disorder, zero-interaction SDW transition temperature is higher than CDW at small doping (and vice versa for large doping), we find that for the general case with finite disorder and interactions there is a universal nematic transition across the entire doping range, accompanied by SDW and CDW transitions (or strong fluctuations at large enough disorder) at lower temperatures. We also discuss the issues concerning the difference between La-based materials and the other hole-doped cuprates.

**11:27AM L27.00002 Quantum critical dynamics of a magnetic impurity in a semiconducting host**<sup>1</sup>, NAGAMALLESWARARAO DASARI, Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, 560064, India., SWAGATA ACHARYA, Department of Physics, Indian Institute of Technology Kharagpur, Kharagpur 721302, India., A TARAPHDER, Centre for Theoretical Studies, Indian Institute of Technology Kharagpur, Kharagpur 721302, India., JUANA MORENO, MARK JARRELL, Department of Physics & Astronomy, Louisiana State University, Baton Rouge, LA 70803, USA, N. S. VIDHYADHIRAJA, Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, 560064, India., PROF. N. S. VIDHYADHIRAJA COLLABORATION, PROF. MARK JARRELL COLLABORATION, PROF. A. TARAPHDER COLLABORATION — We have investigated the finite temperature dynamics of the singlet to doublet continuous quantum phase transition in the gapped Anderson impurity model using hybridization expansion continuous time quantum Monte Carlo. Using the self-energy and the longitudinal static susceptibility, we obtain a phase diagram in the temperature-gap plane. The separatrix between the low-temperature local moment phase and the high temperature generalized Fermi liquid phase is shown to be the lower bound of the critical scaling region of the zero gap interacting quantum critical point. We have computed the nuclear magnetic spin-lattice relaxation rate, the Knight shift, and the Korringa ratio, which show strong deviations for any non-zero gap from the corresponding quantities in the gapless Kondo screened impurity case.

<sup>1</sup>This work is supported by NSF DMR-1237565 and NSF EPSCoR Cooperative Agreement EPS-1003897 with additional support from the Louisiana Board of Regents, and by CSIR and DST, India.

**11:39AM L27.00003 Corner entanglement as a probe of quantum criticality**<sup>1</sup>, WILLIAM WITCZAK-KREMPA, Harvard Univ, PABLO BUENO, KU Leuven, ROBERT C. MYERS, Perimeter Institute — The entanglement entropy in many gapless quantum systems in 2+1D receives a contribution from corners in the entangling surface. It is characterized by a universal function  $a(\theta)$  that depends non-trivially on the corner opening angle  $\theta$ . Focusing on a large family of quantum critical theories with emergent Lorentz invariance (CFTs), we argue that the smooth limit  $a(\theta \approx \pi)$  is entirely determined by the energy-density or stress tensor 2-point function coefficient. This explains recent results obtained via cutting edge simulations on the quantum critical Ising, XY and Heisenberg models. We also show how to extract the full thermal entropy of the quantum critical system using corner entanglement of the groundstate alone. \*\* Bueno, Myers, WK, Phys. Rev. Lett. (2015)

<sup>1</sup>Work supported by Perimeter Institute and NSERC.

**11:51AM L27.00004 Deconfined quantum criticality beyond designer Hamiltonians**, THOMAS C. LANG, University of Innsbruck, RIBHU K. KAUL, University of Kentucky — The  $\text{SU}(6)$  symmetric generalization of the Hubbard model on the square lattice provides the simplest microscopic realization of the quantum phase transition from a Néel to a valence bond solid (VBS) ordered phase. By constructing dimensionless quantities such as ratios of the magnetic structure factor and valence bond correlations we are able to unambiguously determine the existence of weak, but robust antiferromagnetic order in the weak coupling regime and a plaquette VBS in the strong coupling limit. Furthermore these ratios provide a tool to accurately determine the (critical) point from both sides of the phase transition separating the two limits. Preliminary results suggest a direct continuous transition for which we extract estimates for the critical exponents and compare the scaling function with the  $\text{SU}(6)$  designer spin-models to investigate whether this quantum phase transition is compatible with the scenario of deconfined quantum criticality.

**12:03PM L27.00005 Fermion-induced quantum critical points: beyond Landau criterion**, HONG YAO, ZI-XIANG LI, YI-FAN JIANG, SHAO-KAI JIAN, Institute for Advanced Study, Tsinghua University, Beijing — According to Landau criterion, phase transitions must be first-order when cubic terms of order parameters in the Landau-Ginzburg free energy are allowed by symmetry. Here, from both renormalization group analysis and sign-problem-free quantum Monte Carlo simulations, we show that second-order quantum phase transitions can occur at such putatively-first-order quantum phase transitions in strongly-interacting Dirac semimetals in two spatial dimensions. Such type of Landau-criterion-violating quantum critical points are induced by massless fermionic modes at the quantum phase transitions. We call them “fermion-induced quantum critical points”. From Majorana-quantum-Monte-Carlo simulations and renormalization analysis, we find that the critical exponents at the Kekulé valence-bond-solid transition of the Dirac fermions on the honeycomb lattice are highly-nonclassical. We also discuss experimental signatures of the Kekulé quantum critical point which may be realized in graphene-like systems.

**12:15PM L27.00006 Nonlinear I-V Curve at a Quantum Impurity Quantum Critical Point**, HAROLD BARANGER, Duke Univ, CHUNG-HOU CHUNG, CHAO-YUN LIN, Chiao-Tung Univ and Natl Center for Theoretical Sciences, Taiwan, GU ZHANG, CHUNG-TING KE, GLEB FINKELSTEIN, Duke Univ — The nonlinear I-V curve at an interacting quantum critical point (QCP) is typically out of reach theoretically. Here, however, we provide a striking example of an analytical calculation of the full nonlinear I-V curve at the QCP. The system that we consider is a quantum dot coupled to resistive leads — a spinless resonant level interacting with an ohmic EM environment in which a QCP similar to the two-channel Kondo QCP occurs. Recent experiments studied this criticality via transport measurements: the transmission approaches unity at low temperature and applied bias when tuned exactly to the QCP (on resonance and symmetric tunnel barriers) and approaches zero in all other cases. To obtain the current at finite temperature and arbitrary bias, we write the problem as a one-dimensional field theory and transform from electrons in the left/right leads to right-going and left-going channels between which there is weak two-body backscattering. Drawing on dynamical Coulomb blockade theory, we thus obtain an analytical expression for the full I-V curve. The agreement with the experimental result is remarkable.

**12:27PM L27.00007 Finite-temperature Dynamics and Quantum Criticality in a Model for Insulating Magnets**, JIANDA WU, WANG YANG, CONGJUN WU, UC San Diego, QIMIAO SI, Rice University — Theoretical understanding of the finite-temperature dynamics in quantum critical systems is a challenging problem, due to the mixing of thermal and quantum fluctuations. Recently, neutron scattering experiments in the three-dimensional quantum dimer material  $\text{TiCuCl}_3$  under pressure tuning have mapped out the magnetic dynamics at finite temperatures in the quantum critical regime [1], thereby providing the opportunity for systematic understandings. In this work, we calculate the spin spectral function of an  $O(n)$  symmetric field theory using a field-theory procedure to two loops. We calculate the temperature dependence of the energy and damping rate of the spin excitations in the quantum critical regime, demonstrate a good agreement with the experimental results, and determine the parameter regime of the field theory that is appropriate for  $\text{TiCuCl}_3$ . From our calculations we can also suggest further experimental means to test the applicability of the underlying field theory in this and related systems. [1] P. Merchant, B. Normand, K.W. Krmer, M. Boehm, D. F. McMorrow and Ch. Regg, Nat. Phys. 10, 373 (2014).

**12:39PM L27.00008 Competing phases in the single-band Hubbard model on the 1/5-depleted square lattice**, MICHAEL MULANIX, EHSAN KHATAMI, San Jose State University — Using exact diagonalization of small clusters, we study the Hubbard model on the 1/5-depleted square lattice. This geometry, which arises in ordered-vacancy iron selenide superconductors, consists of 2 by 2 plaquettes connected through inter-plaquette bonds. Previous determinantal quantum Monte Carlo simulations have shown that the model at half filling displays multiple quantum phase transitions by tuning the ratio of hoppings for the two types of bonds, or by varying the interaction strength. We extend those results to the region away from half filling and study the magnetic, charge and pairing correlation functions for a wide range of interaction strengths and the hopping ratios. We find an interesting variation of the magnetic ordering wavevector as the density changes, particularly if the hopping ratio is tuned in favor of the intra-plaquette bond. We also find that, for small interaction strengths and at low densities, unexpected charge or pair density waves dominate.

**12:51PM L27.00009 Metallic quantum critical points with finite BCS couplings**, SHAMIT KACHRU, SRINIVAS RAGHU, Stanford University, GONZALO TORROBA, Centro Atómico Bariloche and CONICET, HUAJIA WANG, University of Illinois, Urbana-Champaign — We study the fate of superconductivity in the vicinity of a class of metallic quantum critical points obtained by coupling a Fermi surface to a critical boson. In such systems there is a competition between the enhanced pairing tendency due to the presence of long-range attractive interactions near criticality, and the suppression of superconductivity due to the destruction of the Landau quasiparticles. We show that there are regimes in which these two effects offset one another, resulting in a novel non-Fermi liquid fixed point with *finite*, scale invariant, BCS coupling. While these interactions lead to substantial superconducting fluctuations, they do not drive the system into a superconducting ground state. The metallic quantum critical fixed points are connected to the superconducting regime by a continuous phase transition. These results are established using a controlled expansion in the deviation from  $d = 3$  spatial dimensions, as well as in a large number  $N$  of internal flavors. We discuss the possible relevance of our findings to the phenomenon of superconducting domes condensing out of a non-Fermi liquid normal state near quantum critical points.

**1:03PM L27.00010 Metallic quantum critical ferromagnets: a quantum Monte Carlo calculation of Non-Fermi liquid exponents**, SAM RIDGWAY, CHRIS HOOLEY, St Andrews — We study a lattice field theory describing the quantum ferromagnetic transition of a metal in two spatial dimensions, using a sign-problem free quantum Monte Carlo algorithm. We provide evidence for the continuous nature of the transition, and calculate universal critical exponents that indicate non-Fermi liquid behaviour at the critical point.

**1:15PM L27.00011 Violation of hyperscaling at the Ising-nematic quantum critical point in a two-dimensional metal**, ANDREAS EBERLEIN, Harvard University, IPSITA MANDAL, Perimeter Institute for Theoretical Physics, SUBIR SACHDEV, Harvard University and Perimeter Institute for Theoretical Physics — Spatially isotropic critical quantum states in  $d$  spatial dimensions which have the hyperscaling property have an optical conductivity that scales as  $\omega^{(d-2)/z}$  for high frequencies  $\omega \gg T$ , where  $T$  is the temperature and  $z$  the dynamic critical exponent. We examine the Ising-nematic quantum critical point in  $d = 2$  using the fixed point theory by Dalidovich and Lee (Phys. Rev. B 88, 245106 (2013)) and compute the optical conductivity in an expansion in  $\epsilon = 5/2 - d$ . We show that hyperscaling is violated at this quantum critical point and discuss the scaling behaviour of the optical conductivity at  $T = 0$ .

**1:27PM L27.00012 Rescuing a Quantum Phase Transition with Quantum Noise**<sup>1</sup>, GU ZHANG, Duke Univ, EDUARDO NOVAIS, UFABC, HAROLD BARANGER, Duke Univ — We show that placing a quantum system in contact with an environment can enhance non-Fermi-liquid correlations, rather than destroying quantum effects as is typical. The system consists of two quantum dots in series with two leads; the highly resistive leads couple charge flow through the dots to the electromagnetic environment (noise). The similarity to the two impurity Kondo model suggests that there will be a quantum phase transition between a Kondo phase and a local singlet phase. However, this transition is destabilized by charge tunneling between the two leads. Our main result is that sufficiently strong quantum noise suppresses this charge transfer and leads to stabilization of the quantum phase transition. We present the phase diagram, the ground state degeneracy at the four fixed points, and the leading temperature dependence of the conductance near these points.

<sup>1</sup>Partially supported by (1) the U.S. DOE, Division of Materials Sciences and Engineering, under Grant No. DE-SC0005237 and (2) FAPESP (BRAZIL) under grant 2014/26356-9.

**1:39PM L27.00013 Anisotropic Non-Fermi Liquids**, SHOUVIK SUR, National High Magnetic Field Laboratory, and Florida State University, SUNG-SIK LEE, McMaster University, and Perimeter Institute for Theoretical Physics — We study non-Fermi liquids that arise at quantum critical points associated with spin (SDW) and charge density wave (CDW) transitions in metals with twofold rotational symmetry. We use the 'codimensional' regularization scheme, where a one-dimensional Fermi surface is embedded in  $3 - \epsilon$  dimensional momentum space. In three dimensions, quasilocal marginal Fermi liquids arise at the SDW and CDW critical points. Below three dimensions, a perturbative anisotropic non-Fermi liquid state is realized at the SDW critical point, where not only time but also different spatial coordinates develop distinct anomalous dimensions. The stable non-Fermi liquid exhibits an emergent algebraic nesting as the patches of the Fermi surface are deformed into a universal power-law shape near the hot spots. Due to the anisotropic scaling, the energy of spin fluctuations disperse with different power laws in different momentum directions. In contrast, at the CDW critical point, the perturbative expansion breaks down immediately below three dimensions as the interaction renormalizes the speed of charge fluctuations to zero within a finite renormalization group scale.

**1:51PM L27.00014 Universal quantum criticality in Hubbard models with massless Dirac dispersion**, YUICHI OTSUKA, SEIJI YUNOKI, RIKEN Advanced Institute for Computational Science, SANDRO SORELLA, SISSA - International School for Advanced Studies — We investigate the metal-insulator transition of two-dimensional interacting electrons with massless Dirac-like dispersion, describe by the Hubbard models on two geometrically different lattices: honeycomb and  $\pi$ -flux square lattices. By performing large-scale quantum Monte Carlo simulations followed by careful finite-size scaling analyses, we find that the transition from semi-metallic to antiferromagnetic insulating phases is continuous and evaluate the critical exponents with a high degree of accuracy for the corresponding universality class, which is described in the continuous limit by the Gross-Neveu model. We furthermore discuss the fate of the quasiparticle weight and the Fermi velocity across this transition.

**2:03PM L27.00015 Mott Quantum Criticality in the Anisotropic 2D Hubbard Model<sup>1</sup>**, BENJAMIN LENZ, SALVATORE R. MANMANA, THOMAS PRÜSCHKE, Institute for Theoretical Physics, University of Göttingen, FAKHER F. ASSAAD, MARCIN RACZKOWSKI, Institute for Theoretical Physics and Astrophysics, University of Würzburg — We present evidence for Mott quantum criticality in an anisotropic two-dimensional system of coupled Hubbard chains at half-filling. In this scenario emerging from variational cluster approximation and cluster dynamical mean-field theory, the interchain hopping  $t_{\perp}$  acts as control parameter driving the second-order critical endpoint  $T_c$  of the metal-insulator transition down to zero at  $t_{\perp}^c/t \simeq 0.2$ . Below  $t_{\perp}^c$  the volume of hole and electron Fermi pockets of a compensated metal vanishes continuously at the Mott transition. Above  $t_{\perp}^c$  the volume reduction of the pockets is cut off by a first-order transition. We discuss the relevance of our findings to a putative quantum critical point in layered organic conductors whose location remains elusive so far.

<sup>1</sup>We acknowledge support by DFG research units FOR1807 and FOR1346, ERC Starting Grant No. 306897 and NSF Grant No. PHY11-25915, and computer support by the GWDG and Jülich Supercomputing Centre.

## Wednesday, March 16, 2016 11:15AM - 2:15PM – Session L28 DMP: Topological Crystalline Insulators 327 - Liang Fu, Massachusetts Institute of Technology

**11:15AM L28.00001 Searching for ideal topological crystalline insulators and topological superconductors in the Pb-Sn-In-Te system<sup>1</sup>**, GENDA GU, Brookhaven national laboratory — The discovery of 3D topological insulator materials and topological superconductor open up a new research field in the condensed matter physics. In order to search for the ideal topological insulator, topological crystalline insulator and topological superconductor, we have grown a large number of the single crystals of Pb-system (Pb-Sn-In-Te) topological crystalline insulator and their topological superconductor. We have measured the physical properties on these single crystals by various techniques. We have studied the effect of crystal growth condition, impurity and composition on the bulk electrical conductivity of these single crystals. We try to find out which composition and crystal growth condition is the best for the ideal topological insulator, topological crystalline insulator and topological superconductor. We have got the bulk topological superconductor with  $T_c = 5K$ .

<sup>1</sup>Work was supported by the Office of Basic Energy Sciences (BES), Division of Materials Sciences and Engineering, U.S. Department of Energy (DOE), through Contract No. DE-SC00112704.

**11:51AM L28.00002 Interplay of Dirac Fermions and Structural Deformations in Topological Crystalline Insulators**, ILIJA ZELJKOVIC, Boston College — Topological crystalline insulators (TCIs) are a new class of topological materials which harbor massless Dirac surface states (SS). Theory postulates that these SS are protected by crystalline symmetries, and that SS electrons can acquire a mass if these symmetries are broken. Moreover, this unique crystalline protection has led to a series of intriguing predictions of strain-generated phenomena, such as the appearance of pseudo-magnetic fields and topological phase transitions. In this talk, I will present our scanning tunneling microscopy (STM) investigations of two TCI systems: single crystals of  $Pb_{1-x}Sn_xSe$  and strained thin films of SnTe. Simultaneous imaging of the atomic and electronic structures in TCI single crystals reveals that a fraction of the Dirac electrons acquire mass due to a surface distortion that breaks a crystalline mirror symmetry. Furthermore, we discover that even in the absence of any symmetry breaking, local strain in TCI heteroepitaxial thin films can induce spatially dependent changes in the SS dispersion associated with the momentum-space shift of the Dirac nodes. Our experiments provide the first direct visualization of the effects of strain on the SS band structure in topological materials and suggest a novel pathway for manipulation of Dirac electrons via structural deformations.

**12:27PM L28.00003 Modulation of the surface states of SnTe films by doping impurities<sup>1</sup>**, CHI-HSUAN LEE, CHIH-KAI YANG, National Chengchi University — Electronic structures of SnTe films doped by impurities are investigated using density functional calculations. There are surface states crossing the Fermi level in bulk SnTe, which is a topological crystalline insulator. For thin SnTe films, however, an energy gap is opened due to quantum tunneling. The gap can be reduced and even eliminated by doping impurities at the surfaces of the films, all the while keeping the mirror symmetry associated with bulk SnTe intact. Impurities with magnetic moments, on the other hand, can destroy the mirror symmetry.

<sup>1</sup>This work was supported by the Ministry of Science and Technology of the Republic of China under grant number MOST 104-2112-M-004-003

**12:39PM L28.00004 Nanomaterials of the topological crystalline insulators,  $Pb_{1-x}Sn_xTe$  and  $Pb_{1-x}Sn_xSe$ .**, MOHAMMED SAGHIR, ANNA SANCHEZ, STEVE HINDMARSH, STEVE YORK, GEETHA BALAKRISHNAN, University of Warwick — The study of topological insulators and their derivatives, in both 1D and 2D forms, has been the subject of great interest which has grown vastly in recent years. Topological insulators (TIs) and Topological Crystalline insulators (TCIs) exhibit exotic surface properties which are thought to be difficult to detect due to the surface signal being overwhelmed by that arising from the bulk of the material. As a result, by increasing the surface area to volume ratio, the signal from the surface states could be easier to investigate. We present results of the growth and characterisation of nanomaterials for the TCIs,  $Pb_{1-x}Sn_xTe$  and  $Pb_{1-x}Sn_xSe$ . Bulk crystals were used as starting materials for the growth, from which various morphologies of these TCIs were obtained. Nanowires of  $Pb_{1-x}Sn_xTe$  have been produced with a Sn composition of  $\sim x = 0.25$ , at which a transition from trivial to non-trivial insulator has been reported for bulk materials. The results obtained on the growth of nanomaterials of  $Pb_{1-x}Sn_xSe$  are also described, all of which were characterised using various x-ray diffraction and electron microscopy techniques.

**12:51PM L28.00005 Anomalous electronic states in  $\text{Pb}_{1-x}\text{Sn}_x\text{Te}$  induced by hydrostatic pressure<sup>1</sup>**, TIAN LIANG, SATYA KUSHWAHA, QUINN GIBSON, R. J. CAVA, N. P. ONG, Princeton University — Dirac/Weyl semimetals have attracted strong interest. In Dirac semimetals  $\text{Cd}_3\text{As}_2$ ,  $\text{Na}_3\text{Bi}$ , the Dirac nodes split into Weyl states in a magnetic field, which leads to novel phenomena, such as ultrahigh mobility ( $10^7 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ ) in  $\text{Cd}_3\text{As}_2$  [1], and the chiral anomaly in  $\text{Na}_3\text{Bi}$  [2]. The chiral anomaly appears as a negative longitudinal magnetoresistance. A new path to realize Weyl states is via the closing of the bulk gap in a system with broken inversion symmetry. As the gap is tuned, a Weyl semimetallic state is predicted to appear between two insulating phases [3]. We performed the hydrostatic pressure measurement for  $\text{Pb}_{1-x}\text{Sn}_x\text{Te}$  and observed that the gap of the system closes under pressure and the system shows insulator to metal phase transition. Interestingly, in the metallic phase, we observed giant negative magnetoresistance as well as anomalous hall effect which onsets only in the quantum limit. We discuss the implication of these phenomena and their relation with the Berry curvature. [1] Liang, T. et al., *Nature Materials*, **14**, 280 (2015). [2] Xiong, J. et al., *Science*, **350**, 413 (2015). [3] Murakami, S et al., *Phys. Rev. B* **78**, 165313 (2008); *New J. Phys.* **9**, 356 (2007).

<sup>1</sup>Supported by MURI grant (ARO W911NF-12-1-0461), Army Research Office (ARO W911NF-11-1-0379), Gordon and Betty Moore Foundation (EPiQS Initiative GBMF4539)

**1:03PM L28.00006 Topological crystalline semimetals in non-symmorphic lattices without time-reversal symmetry**, YIGE CHEN, HEUNG-SIK KIM, HAE-YOUNG KEE, University of Toronto — Numerous efforts have been devoted to reveal exotic semimetallic phases with topologically non-trivial bulk and surface states in materials with strong spin-orbit coupling. Recent theoretical works on orthorhombic perovskite iridates  $\text{SrIrO}_3$  have indicated that non-symmorphic symmetry is crucial to protect a nodal line Fermi surface (FS) in addition to space-time inversion symmetry [C. Fang *et.al.*, *PRB* **92**, 081201(R) (2015), Y. Chen *et.al.*, *Nat. Commu.* **6**, (2015)]. In this work, we investigate possible topological semimetals in the absence of time-reversal symmetry. In principle, an anti-unitary operator, defined as a product of time-reversal and glide operators, can protect a four-fold or two-fold degenerate nodal FS. Indeed this happens in  $\text{SrIrO}_3$  with the magnetic field along a particular direction. A trivial gapped insulator can also occur due to a lack of such anti-unitary operation. This study shows that non-symmorphic crystals with multiple fractional lattice translations exhibit rich topological properties.

**1:15PM L28.00007  $\text{SU}(3)$  Quantum Hall Ferromagnetism in  $\text{SnTe}$** , CHENG-CHENG LIU, The University of Texas at Dallas, XIAO LI, University of Maryland, FAN ZHANG, The University of Texas at Dallas, A. H. MACDONALD, The University of Texas at Austin — The (111) surface of  $\text{SnTe}$  hosts one isotropic G-centered and three degenerate anisotropic M-centered Dirac surface states. We predict that a nematic phase with spontaneously broken  $C_3$  symmetry will occur in the presence of an external magnetic field when the  $N=0$  M Landau levels are  $1/3$  or  $2/3$  filled. The nematic state phase boundary is controlled by a competition between intravalley Coulomb interactions that favor a valley-polarized state, and weaker intervalley scattering processes that increase in relative strength with magnetic field. An in-plane Zeeman field alters the phase diagram by lifting the three-fold M Landau level degeneracy, yielding a ground state energy with  $2\pi/3$  periodicity as a function of Zeeman-field orientation angle.

**1:27PM L28.00008 Interplay of imperfections and surface states in topological crystalline insulators**, EVGENY PLEKHANOV, CEDRIC WEBER, Kings College, London — The conducting states, recently discovered at the surface of a special class of insulators topological insulators - are distinguished for their insensitivity to local and non-magnetic surface defects. Their behavior in the presence of magnetic impurities and macroscopic imperfections of the surface is puzzling and hard to analyze quantitatively. Here, we present a systematic study of the imperfections (magnetic impurities and deviations from perfect surface cleavage) in topological crystalline insulators of the tin telluride family by using realistic first-principles-derived tight-binding models. The theoretical framework proposed is quite general and easily permits the extensions to other TI families and impurity types. The influence of the strong local correlations of the impurity atoms on the topological states stability is also discussed within the frame of the Dynamical Mean Field Theory.

**1:39PM L28.00009 Space group constraints on weak indices in topological crystalline insulators**, DANIEL VARJAS, FERNANDO DE JUAN, Univ of California - Berkeley, YUAN-MING LU, The Ohio State University — In this work we derive constraints on weak indices of topological insulators and superconductors coming from space group symmetry. Weak indices are topological invariants of lower dimensional slices of the Brillouin zone, notable examples are the Chern numbers in class A and weak  $Z_2$  indices in class AII in 3D. The components of the weak indices form a momentum space vector that transforms in a simple fashion under space group symmetries, using results of momentum space crystallography we find the allowed values for each Bravais lattice. Nonsymmorphic symmetries, such as screw axes and glide planes pose additional constraints. Accounting for both of these we find that most space groups experience some restriction, to the extent that some cannot support nontrivial weak topological insulators and superconductors at all. This result puts a strong constraint on candidates in the experimental and numerical search for topological materials based on the lattice structure alone.

**1:51PM L28.00010 Quantized electric quadrupole moment in Topological Crystalline Insulators**, WLADIMIR A. BENALCAZAR, Department of Physics, Univ of Illinois - Urbana, B. ANDREI BERNEVIG, Department of Physics, Princeton University, TAYLOR HUGHES, Department of Physics, Univ of Illinois - Urbana — We define the quadrupole moment as a bulk topological quantity in 2-dimensional insulators. When protected by spatial symmetries, a non-trivial quadrupole with full open boundaries exhibits robust, quantized and corner-localized half-charges. Alternatively, the non-trivial quadrupole state manifests as an edge-localized non-trivial polarization (i.e. edge-localized 1-dimensional topological insulators) in systems with open boundaries along one direction but closed along the other. We characterize this phase and explore new phenomena, as well as generalizations of this moment to higher dimensions.

**2:03PM L28.00011 Temperature dependence of angle-resolved photoemission of the crystalline topological insulator  $\text{Pb}_{1-x}\text{Sn}_x\text{Se}(111)$** , OLIVER RADER, PARTHA S. MANDAL, Helmholtz-Zentrum Berlin, GUNTHER SPRINGHOLZ, GUNTHER BAUER, VALENTYN VOLOBUIEV, Johannes-Kepler-Universitt Linz, ANDREI VARYKHALOV, EVANGELOS GOLIAS, JAIME SNCHEZ-BARRIGA, Helmholtz-Zentrum Berlin — The system  $\text{Pb}_{1-x}\text{Sn}_x\text{Se}$  is a topological insulator protected by mirror symmetry. Angle-resolved photoemission investigations have so far been concentrating on (100) surfaces of bulk single crystals. Here, we systematically study (111) epitaxial films under variation of the Sn concentration (10

**Wednesday, March 16, 2016 11:15AM - 2:15PM —**  
Session L29 DCMP DMP: Two-Dimensional Topological Insulators: Heterostructures and Beyond 328 - Fan Zhang, University of Texas, Dallas

**11:15AM L29.00001 Topological Phases in Perovskite Oxide Heterostructures**, ROKYEON KIM, CCES, IBS & Seoul National University, JAEJUN YU, Seoul National University, HOSUB JIN, Ulsan National Institute of Science and Technology — Quantum spin Hall (QSH) insulator is a new state of matter characterized by gapless edge states and insulating bulk states. Because the edge states are topologically protected and therefore robust against non-magnetic perturbations, it has a potential to be utilized in spintronics devices. Quantum valley Hall (QVH) phase, on the other hand, is another class of topological state exhibiting valley-contrasting Berry curvature and spin splitting, which could yield novel transport properties, such as valley Hall effect and valley spin Hall effect. We propose a new kind of perovskite (111) heterostructures which can host both QSH and QVH phases with appropriate choices of composing elements. By carrying out first-principles calculations, we demonstrate that a Dirac cone emerges in a particular choice of heterostructure, and a sizable spin-orbit coupling turns the system into the QSH phase. In addition, the QVH phase with different Berry phases and spin textures in each valley is shown to be realized in the heterostructure with broken inversion symmetry. We propose that these perovskite heterostructures can provide a feasible platform for spintronics, valleytronics, and topological engineering of the two-dimensional electron system.

**11:27AM L29.00002 Structure of the Surface States at Topological Insulator-Semiconductor Interfaces<sup>1</sup>**, MAHMOUD M. ASMAR, DANIEL SHEEHY, ILYA VEKHTER, Louisiana State University — Topologically-protected surface states of three-dimensional topological insulators (TIs) are characterized by spin and momentum locking. In the simplest picture the emergent two dimensional semimetal displays opposite helicities around the point of degeneracy. Possible applications of TIs rely on forming interfaces with other materials, such as semiconductors or superconductors. In such heterostructures, the dispersion and quantum numbers of the surface states become not only dependent on bulk properties but also on the specifics of the boundaries between the TI and the material in contact. Making use of the three dimensional  $k \cdot p$  Hamiltonian describing TIs, and taking in to account surface potentials compatible with the symmetries of the TI and the semiconducting material, we find the effects of the latter on the energy-momentum dispersion and spin structure of the surface state and explore the consequences this may have on physical observables.

<sup>1</sup>Supported by: NSF grant No. DMR-1105339, NSF grant No. DMR-1410741 and NSF grant No. DMR-1151717.

**11:39AM L29.00003 Interplay of Dirac surface states and magnetic fluctuations in topological insulator heterostructures**, HILARY M. HURST, DMITRY K. EFIMKIN, VICTOR GALITSKI, Joint Quantum Institute and Condensed Matter Theory Center, University of Maryland, College Park — We consider the proximity effect between Dirac states at the surface of a topological insulator and a ferromagnet with easy plane anisotropy, which is described by the XY-model and undergoes a Berezinskii-Kosterlitz-Thouless (BKT) phase transition. Classical magnetic fluctuations interacting with the surface states of a topological insulator can be described by an effective gauge field. This model can be mapped onto the problem of Dirac fermions in a random magnetic field, however this analogy is only partial in the presence of electron-hole asymmetry or warping of the Dirac dispersion which results in screening of magnetic fluctuations. We show that this proximity coupling leads to anomalous transport behavior of the surface states near the BKT transition temperature.

**11:51AM L29.00004 Transforming common III-V/II-VI insulating building blocks into topological heterostructure via the intrinsic electric polarization<sup>1</sup>**, ALEX ZUNGER, XIUWEN ZHANG, LEONARDO ABDALLA, QIHANG LIU, University of Colorado, Boulder — Currently known topological insulators (TIs) are limited to narrow gap compounds incorporating heavy elements, thus severely limiting the material pool available for such applications. We show how a heterovalent superlattice made of common semiconductor building blocks can transform its non-TI components into a topological heterostructure. The heterovalent nature of such interfaces sets up, in the absence of interfacial atomic exchange, a natural internal electric field that along with the quantum confinement leads to band inversion, transforming these semiconductors into a topological phase while also forming a giant Rashba spin splitting. We demonstrate this paradigm of designing TIs from ordinary semiconductors via first-principle calculations on III-V/II-VI superlattice InSb/CdTe. We illustrate the relationship between the interfacial stability and the topological transition, finding a “window of opportunity” where both conditions can be optimized. This work illustrates the general principles of co-evaluation of TI functionality with thermodynamic stability as a route of identifying realistic combination of common insulators that could produce topological heterostructures.

<sup>1</sup>This work was supported by Basic Energy Science, MSE division (Grant DE-FG02-13ER46959)

**12:03PM L29.00005 Emergence of quantum spin Hall and “half-topological” states at Graphene/TMDC heterostructures<sup>1</sup>**, DENIS KOCHAN, MARTIN GMTIRA, PETRA HÖGL, JAROSLAV FABIAN, University of Regensburg — We discuss orbital and spin-orbital proximity effects emerging in graphene deposited on a monolayer transition-metal dichalcogenides (TMDCs: MoS<sub>2</sub>, MoSe<sub>2</sub>, WS<sub>2</sub>, WSe<sub>2</sub>) and analyze the impact on spin transport in such graphene/TMDC heterostructures. First-principles investigations show that graphene on MoS<sub>2</sub>, MoSe<sub>2</sub>, and WS<sub>2</sub> has a topologically trivial band structure, while graphene on WSe<sub>2</sub> exhibits inverted bands. The essential low energy physics can be well described by a symmetry inspired realistic tight-binding Hamiltonian. We predict topologically protected helical edge states for graphene zigzag nanoribbons on WSe<sub>2</sub>, demonstrating the emergence of the quantum spin Hall effect. Our model also features “half-topological states”, which are protected against time-reversal disorder on one edge only. Unlike in pristine graphene, the proximity spin-orbit coupling in graphene on TMDCs is significant (orders of meV), making the predicted effect testable experimentally. References: M. Gmitra, D. Kochan, P. Högl, J. Fabian; Trivial and inverted Dirac bands, and emergence of quantum spin Hall states in graphene on transition-metal dichalcogenides, arXiv:1510.00166

<sup>1</sup>This research was supported by DFG SFB 689, GRK 1570 and by the EU Seventh Framework Programme under Grant Agreement No. 604391 Graphene Flagship.

**12:15PM L29.00006 Tunneling spectroscopy in engineered SrTiO<sub>3</sub> heterostructures**, ADRIAN SWARTZ, HISASHI INOUE, TYLER MERZ, Stanford University, YASUYUKI HIKITA, SLAC National Accelerator Laboratory, HAROLD HWANG, Stanford University and SLAC National Accelerator Laboratory — Despite decades of intense research on the topic, superconductivity in the dilute high- $k$  semiconductor SrTiO<sub>3</sub> (STO) has posed a long-standing problem. In light of the recent reports of unconventional 2D superconductivity in STO-based heterostructures, this problem deserves renewed attention in the bulk limit. Tunneling spectroscopy, which directly measures the electronic density of states, is a powerful tool to investigate the superconducting ground state as well as the relevant electron-phonon couplings. A limiting obstacle for employing this technique is the long depletion lengths formed when semiconducting SrTiO<sub>3</sub> is contacted with a metal in Schottky junctions, which obstructs access to the intrinsic bulk electronic properties. Here, using band alignment engineered planar tunneling junctions to minimize these long depletion lengths, we experimentally re-examine canonical tunneling experiments in Nb-doped STO. We discuss our results on the extraction of the electron-phonon coupling in SrTiO<sub>3</sub> and its relevance to the superconducting condensate.

**12:27PM L29.00007 Origins of conducting channel at  $\text{LaAlO}_3/\text{SrTiO}_3$  heterointerface investigated by *in situ* ARPES**, HYANGKEUN YOO, LUCA MORESCHINI, AARON BOSTWICK, Advanced Light Source, LBNL, ANDREW WALTER, Brookhaven National Laboratory, NSLS II, TAE WON NOH, Seoul National University, YOUNG JUN CHANG, University of Seoul, ELI ROTENBERG, Advanced Light Source, LBNL — The high-mobility conducting interface (CI) between  $\text{LaAlO}_3$  (LAO) and  $\text{SrTiO}_3$  (STO) has revealed many fascinating phenomena. But the formation mechanism of the CI has not been conclusively explained. Here, we investigated the CI formation between LAO and STO by *in situ* angle-resolved photoemission spectroscopy. By directly imaging the LAO polarity-induced built-in potential ( $V_i$ ) at each step of the LAO growth, we demonstrated that the  $V_i$  is proportional to the LAO thickness and the conducting interface is appeared above 3 unit cells of LAO. However, we found that the  $V_i$  and the critical thickness are strongly dependent on the amount of the surface oxygen vacancies controlled by the synchrotron ultraviolet-irradiation and the oxygen gas exposure. This indicates that the only polar catastrophe, theorized to explain the CI formation above a critical thickness, is not adequate. Instead, our results point to a decisive role played by the oxygen vacancy, and explain why the  $V_i$  and the critical thickness as reported in several works show some variation, rather than being a universal quantity.

**12:39PM L29.00008 Electronic structure study of UV photodoping evolution on the  $\text{TiO}_2$  terminated  $\text{SrTiO}_3$** , CHAOFAN ZHANG, SIMES, Stanford University, ZHONGKAI LIU, ZHUOYU CHEN, Department of Applied Physics, Stanford University, CHUNJING JIA, YAO WANG, SIMES, Stanford University, YANWU XIE, Department of Applied Physics, Stanford University, WEI LI, SIMES, Stanford University, JAMES. -J LEE, TAO JIA, SLAVKO REBEC, ERIC YUE MA, Department of Applied Physics, Stanford University, SUNGKWAN MO, ALS, Lawrence Berkeley National Laboratory, BRIAN MORITZ, ROBERT MOORER, SIMES, Stanford University, RUIHUA HE, Department of Physics, Boston College, T.-P. DEVEREAUX, SIMES, Stanford University, WORAWAT MEEVASANA, School of Physics, Suranaree University of Technology, Thailand, ZHIXUN SHEN, SIMES, Stanford University — The metallic two dimensional electron gas (2DEG) has been observed on the UV light irradiated bare  $\text{SrTiO}_3$  surface of various terminations ((001),(110),(111)) using angular resolved photoemission spectroscopy (ARPES). The study of electronic structure of 2DEG opens a window to study the complex physical properties on the bare  $\text{SrTiO}_3$  surface, such as the superconductivity, the high mobility and ferromagnetism. In this talk, we will show the clear polaron band that due to the electron phonon coupling formed at low carrier density gradually screening out and vanishing as the photodoping increases, instead of that, the quantum well states start appearing at higher doping level. Besides that, the upshifting of both the incoherent in-gap and deep valence states towards the Fermi level suggests a huge gap shrinking, which we believe to be the negative electronic compressibility on the 2DEG surface on  $\text{SrTiO}_3$ . All the properties mentioned above were observed at all the three terminations. We also would like to compare their behavior at similar carrier density range.

**12:51PM L29.00009 Quasi 2D electronic states with high spin-polarization in centrosymmetric  $\text{MoS}_2$  bulk crystals**, L. PLUCINSKI, M. GEHLMANN, PGI-6, FZ Juelich, G. BIHLMAYER, I. AGUILERA, PGI-1, FZ Juelich, E. MLYNCZAK, M. ESCHBACH, S. DÖRING, P. GOSPODARIC, PGI-6, FZ Juelich, B. KARDYNAL, PGI-9, FZ Juelich, S. BLÜGEL, PGI-1, FZ Juelich, C. M. SCHNEIDER, PGI-6, FZ Juelich — Time reversal dictates that nonmagnetic, centrosymmetric crystals cannot be spin-polarized. However, it has been recently shown that the electronic structure in these crystals can in fact show a high spin-polarization, as long as it is probed locally in real and in reciprocal space [1]. We present the first observation of this type of compensated polarization in  $\text{MoS}_2$  bulk crystals. Using spin- and angle-resolved photoemission spectroscopy we directly observed a spin-polarization of more than 65% for distinct valleys in the electronic band structure. By additionally evaluating the probing depth of our method we find that these valence band states at the K point in the Brillouin zone are close to fully polarized for the individual atomic trilayers of  $\text{MoS}_2$ , which is confirmed by our density functional theory calculations. Furthermore, we show that these states are almost completely confined within two dimensions. Our findings prove that these highly desired properties of  $\text{MoS}_2$  can be accessed without thinning it down to the monolayer limit. Our results are accessible at the pre-print server: M. Gehlmann et al., arXiv:1510.04101 (2015). [1] X. Zhang, Q. Liu, J.-W. Luo, A. J. Freeman, and A. Zunger, Nat. Phys. 10, 381 (2014).

**1:03PM L29.00010 Dirac State in Giant Magnetoresistive Materials<sup>1</sup>**, Y. WU, N.H. JO, Ames Laboratory & Iowa State University, M. OCHI, RIKEN Center for Emergent Matter Science & Tohoku University, L. HUANG, D. MOU, T. KONG, E. MUN, L. WANG, Y. LEE, S. L. BUD'KO, P. C. CANFIELD, Ames Laboratory & Iowa State University, N. TRIVEDI, Ohio State University, R. ARITO, RIKEN Center for Emergent Matter Science & Tohoku University, A. KAMINSKI, Ames Laboratory & Iowa State University — We use ultrahigh resolution, tunable, vacuum ultraviolet laser-based angle-resolved photoemission spectroscopy (ARPES) to study the electronic properties of materials that recently were discovered to display titanic magnetoresistance. We find that that several of these materials have Dirac-like features in their band structure. In some materials those features are “ordinary” Dirac cones, while in others the linear Dirac dispersion of two crossing bands forms a linear object in 3D momentum space. Our observation poses an important question about the role of Dirac dispersion in the unusually high, non-saturating magnetoresistance of these materials.

<sup>1</sup>Research was supported by the US DOE, Office of Basic Energy Sciences under Contract No. DE-AC02-07CH11358; Gordon and Betty Moore Foundation EPIQS Initiative (Grant No. GBMF4411); CEM, a NSF MRSEC, under Grant No. DMR-1420451.

**1:15PM L29.00011 ABSTRACT WITHDRAWN —**

**1:27PM L29.00012 Topological protection from random Rashba spin-orbit backscattering: Ballistic transport in a helical Luttinger liquid<sup>1</sup>**, HONG-YI XIE, Rice Univ, HEQIU LI, Zhejiang University, YANG-ZHI CHOU, MATTHEW FOSTER, Rice Univ — Rashba spin-orbit coupling enables irrelevant backscattering in a time-reversal symmetric helical Luttinger liquid (HLL). We study the Landauer conductance  $G$  of a HLL in the presence of random Rashba coupling as well as the density-density (Luttinger) interaction. We prove that the transport is purely ballistic ( $G = e^2/h$ ) at any temperature due to the topology. The solution involves a unitary transformation that corresponds to a spin-1/2 in a random, two-component time-dependent magnetic field that preserves the projection of the spin along one fluctuating component (integrable dynamics). Our result is exact for a fixed realization of disorder, and avoids difficulties that arise in disorder-averaged perturbative calculations such as bosonization. We compare the HLL with random Rashba coupling to the Dyson model describing an ordinary spinless quantum wire with particle-hole symmetry, which exhibits non-ballistic transport even at zero temperature.

<sup>1</sup>This research was supported by the Welch Foundation under Grant No. C-1809 and by an Alfred P. Sloan Research Fellowship No. BR2014-035

**1:39PM L29.00013 Detection of topological states in two-dimensional Dirac systems by the dynamic spin susceptibility**, MASAAKI NAKAMURA, Department of Physics, Ehime University, AKIYUKI TOKUNO, Centre de Physique Theorique, Ecole Polytechnique/College de France — We discuss dynamic spin susceptibility (DSS) in two-dimensional (2D) Dirac electrons with spin-orbit interactions to characterize topological insulators. The imaginary part of the DSS appears as an absorption rate in response to a transverse AC magnetic field, just like an electron spin resonance experiment for localized spin systems. We found that when the system is in a static magnetic field, the topological state can be identified by an anomalous resonant peak of the imaginary part of the DSS as a function of the frequency of the transverse magnetic field  $\omega$ . This anomalous peak is related to a transition between two Landau levels close to the Fermi level, which is not allowed in the trivial state. In the absence of the static magnetic field, the imaginary part of the DSS becomes a continuous function of  $\omega$  with a threshold frequency  $\omega_c$ . In this case, the topological and the trivial phases can also be distinguished by the values of  $\omega_c$  and by the line shapes. Thus the DSS is an essential and an experimentally observable physical quantity to characterize the topological insulators.

**1:51PM L29.00014 Magnetic moment coupled to a helical edge can make weak correlations seem strong**, JUKKA VAYRYNEN, Yale University, FLORIAN GEISSLER, University of Würzburg, LEONID GLAZMAN, Yale University — We study the effect of a localized magnetic moment on the helical edge electron transport. The spin flips caused by the moment can be effective in the electron backscattering. We evaluate the resulting differential conductance as a function of temperature  $T$  and applied bias  $V$  for any value of  $V/T$ . At temperatures  $T$  above the Kondo temperature, the deviation of the conductance from its quantized value displays a power-law temperature dependence,  $\delta G \propto T^{-\alpha}$ . We show that the Luttinger liquid effects with  $3/4 < K < 1$  may lead to a small exponent  $\alpha < 1/2$ . Values of  $K$  close to 1 correspond to weakly-correlated electrons. Our results provide an alternative interpretation of the recent experiment by Li et al. [1] where a power-law behavior of the conductance was attributed to strong correlation effects with the value of  $K$  fine-tuned close to  $1/4$ .

#### References

Li et al. Phys. Rev. Lett. **115**, 136804 (2015)

**2:03PM L29.00015 Chiral exciton in the topological insulator  $\text{Bi}_2\text{Se}_3$** <sup>1</sup>, HSIANG-HSI KUNG, MARYAM SALEHI, XUEYUN WANG, NIKESH KOIRALA, MATTHEW BRAHLEK, ALEXANDER LEE, SANG-WOOK CHEONG, SEONGSHIK OH, GIRSH BLUMBERG, Department of Physics & Astronomy, Rutgers University — Materials with novel band structures can host “chiral excitons”, where the exciton emission preserves the helicity of the excitation photon, as recently demonstrated in transition metal dichalcogenide monolayers<sup>2,3</sup>. Here, we report the observation of a highly polarized photoluminescence peak, which is due to chiral exciton emission in the topological insulator  $\text{Bi}_2\text{Se}_3$ . Surprisingly, the energy of the emission is centered at 2.26 eV, much higher than the 0.3 eV bulk band gap of  $\text{Bi}_2\text{Se}_3$ . The excitation profile shows maximum polarization around 2.60 eV excitation, suggesting the chiral exciton is due to interband transition between the topological surface states and a bulk band. We demonstrate that the polarization of the exciton emission is insensitive to temperature and  $\text{Bi}_2\text{Se}_3$  film thickness, providing a convenient and robust platform for optoelectronic applications.

<sup>1</sup>GB, HHK and AL acknowledge support from NSF Award DMR-1104884. MS, NK, MB and SO are funded by Gordon and Betty Moore Foundation’s EPiQS initiative (GBMF4418) and NSF(DMR-1308142). XYW and SWC acknowledge support from NSF Award DMREF-1233349.

<sup>2</sup>H. Zeng, J. Dai, W. Yao, D. Xiao and X. Cui *Nature Nanotech.* **7** 490

<sup>3</sup>K.F. Mak, K. He, J. Shan and T.F. Heinz *Nature Nanotech.* **7** 494

## Wednesday, March 16, 2016 11:15AM - 2:15PM –

Session L30 DMP: Functional Defects in Oxide Heterostructures 329 - Hanghui Chen, Columbia University

**11:15AM L30.00001 Structural and electronic response via oxygen vacancy control in  $\text{SrFeO}_3$  heterostructures**, ALEX KRICK, EUN JU MOON, AMANDA HUON, STEVEN MAY, Drexel University — The electronic and structural properties of complex perovskite oxide thin films are often directly influenced by their oxygen vacancy concentration. Here, we investigate epitaxial films of  $\text{SrFeO}_3$ , which exhibits a variety of structural and electronic phases as a function of oxygen content. The ability to control these functional properties via temperature or external fields is not present in conventional semiconductors and is attractive from an application perspective. As-grown films are oxidized using a post-growth anneal in dilute ozone, yielding metallic behavior consistent with bulk  $\text{SrFeO}_3$ . X-ray diffraction and temperature dependent resistivity collected at different stages of oxidation and reduction reveal minute structural transformations that yield large changes in electronic behavior due to oxygen loss.

**11:27AM L30.00002 A new kind of line defect in  $\text{NdTiO}_3$  perovskite**<sup>1</sup>, MEHMET TOPSAKAL, JONG SEOK JEONG, PENG XU, BHARAT JALAN, RENATA WENTZCOVITCH, ANDRE MKHOYAN, University of Minnesota — We report an observation of a new line defect in strained  $\text{NdTiO}_3$  perovskite. Aberration-corrected analytical scanning transmission electron microscopy and first-principles calculations are used to characterize its atomic structure and electronic properties. The defect represents a shift and rotation of the core Ti-O-Nd unit accommodating the deficiency of Ti-O units in neighboring columns and strain. The core of the defect has considerably different electronic properties resulting from Ti being in different oxidation states. This observation closes the dimensionality gap between previously observed point and planar defects in complex oxides needed to accommodate the alterations of stoichiometry and strain. This new line defect should also exist in other multi-valent perovskites, and could open a new avenue for tailoring unexpected and highly-desirable electronic properties.

<sup>1</sup>NSF DMR- 0819885, DMR-1420013, NSF DMR-1410888, NSF EAR-134866 and EAR- 1319361

**11:39AM L30.00003 Interplay of oxygen vacancies and electronic correlations in  $\text{SrVO}_3$** <sup>1</sup>, STEFFEN BACKES, AARAM J. KIM, Institut für Theoretische Physik, Universität Frankfurt, FRANK LECHERMANN, Institut für Theoretische Physik, Universität Hamburg, HARALD O. JESCHKE, Institut für Theoretische Physik, Universität Frankfurt, MARCELO J. ROZENBERG, Laboratoire de Physique des Solides, Université Paris-Sud, ANDRES F. SANTANDER SYRO, CSNSM, Université Paris-Sud and CNRS/IN2P3, ROSER VALENTI, Institut für Theoretische Physik, Universität Frankfurt — We investigate the role of oxygen vacancies in  $\text{SrVO}_3$  within LDA+DMFT (density functional theory combined with dynamical mean-field theory). We show that, in addition to the usual  $t_{2g}$  lower Hubbard band, oxygen vacancies are responsible for an additional peak around  $-1$  eV of V  $3d_{z^2}$  orbital character, which is not present in the bulk system without vacancies. We discuss our results in the light of recent angle-resolved photoemission (ARPES) experiments.

<sup>1</sup>Financial support by DFG SPP 1458 and FOR 1346.

**11:51AM L30.00004 Strain induced defects and charge state transitions in oxides**, ULRICH ASCHAUER, University of Bern — It recently became apparent that bi-axial strain in coherent epitaxial perovskite oxide thin films or heterostructures can not only be accommodated by changes in structural parameters such as bond lengths or octahedral-rotation angles, but also by the formation of point defects. The redox reactions accompanying the formation of anion and cation vacancy defects lead to local volume changes, which facilitate the formation of either defect species under bi-axial strain. In this talk we will, after a general introduction to the phenomenon, use density functional theory (DFT) calculations to explore the generality of this concept for perovskite oxides and binary rock-salt oxides and put an emphasis on defects in different charge states. Moreover we will discuss the interaction of defects with ferroelectric domain walls, leading to novel functionalities in strained thin films.

**12:27PM L30.00005 Antisite defects at oxide interfaces**<sup>1</sup>, HANGHUI CHEN, ANDREW MILLIS, Columbia Univ — We use ab initio calculations to estimate formation energies of cation (transition metal) antisite defects at oxide interfaces and to understand the basic physical effects that drive or suppress the formation of these defects. We find [1] that antisite defects are favored in systems with substantial charge transfer across the interface, while Jahn-Teller distortions and itinerant ferromagnetism can prevent antisite defects and help stabilize atomically sharp interfaces. Our results enable identification of classes of systems that are more and less susceptible to the formation of antisite defects and motivate a range of experimental studies and further theoretical calculations to further explicate the oxide interface systems. [1] H. Chen and A. J. Millis, arXiv:1509.06643, (2015).

<sup>1</sup>This research was supported by National Science Foundation under Grant No. DMR-1120296 (H. Chen) and DOE-ER-046169 (A. J. Millis).

**12:39PM L30.00006 Metal-Insulator Transition and Weak Localization in Oxygen Vacancy Doped  $\text{BaSnO}_{3-\delta}$  Thin Films<sup>1</sup>**, KOUSTAV GANGULY, ABHINAV PRAKASH, JONG SEOK JEONG, K. ANDRE MKHOYAN, BHARAT JALAN, CHRIS LEIGHTON, University of Minnesota — We present detailed temperature-dependent electronic transport in oxygen vacancy doped  $\text{BaSnO}_3$  films grown on  $\text{MgO}(001)$ ,  $\text{LaAlO}_3(001)$ , and  $\text{GdScO}_3(110)$  using high pressure oxygen sputter deposition. Various modes of high-resolution X-ray diffraction and scanning transmission electron microscopy confirm phase-pure, close to stoichiometric, smooth, epitaxial  $\text{BaSnO}_3(001)$ . [1] As-grown films are insulating, but can be made conductive with *n*-type carriers via vacuum annealing, resulting in 300 K Hall mobilities up to  $35 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$  at  $510^{19}$  carriers per  $\text{cm}^3$ . [1] Film thickness, reduction temperature, and substrate (*i.e.* lattice mismatch) have been systematically varied, enabling study of the insulator-metal transition, and, in particular, 2D weak localization at low temperatures. The results provide significant insight into the active transport mechanisms in  $\text{BaSnO}_3$  films. [1] Ganguly *et al.* APL Materials 3, 062509 (2015).

<sup>1</sup>Work supported by NSF through the UMN MRSEC.

**12:51PM L30.00007 Tuning optical absorption and photoexcited recombination dynamics in  $\text{La}_{1-x}\text{Sr}_x\text{FeO}_{3-\delta}$  through A-site substitution and oxygen vacancies<sup>1</sup>**, SERGEY SMOLIN, MARK SCAFETTA, AMBER CHOQUETTE, Drexel Univ, MATTHEW SFEIR, Brookhaven National Lab, JASON BAXTER, STEVEN MAY, Drexel Univ — We study optical absorption and recombination dynamics in  $\text{La}_{1-x}\text{Sr}_x\text{FeO}_{3-\delta}$  thin films, uncovering the effects of tuning nominal Fe valence via A-site substitution and oxygen stoichiometry. Variable angle spectroscopic ellipsometry was used to measure static optical properties, revealing a linear increase in absorption coefficient at 1.25 eV and a red-shifting of the optical absorption edge with increasing Sr fraction. The absorption spectra can be similarly tuned through the introduction of oxygen vacancies, indicating the critical role that nominal Fe valence plays in optical absorption. Dynamic optoelectronic properties were studied with ultrafast transient reflectance spectroscopy, revealing similar nanosecond photoexcited carrier lifetimes for oxygen deficient and stoichiometric films with the same nominal Fe valence. These results demonstrate that while the static optical absorption is strongly dependent on Fe valence tuned through cation or anion stoichiometry, oxygen vacancies do not appear to play a significantly detrimental role in the recombination kinetics.

<sup>1</sup>NSF: ECCS-1201957, MRI DMR-0922929, MRI DMR-1040166. This research used resources of the Center for Functional Nanomaterials, which is a U.S. DOE Office of Science Facility, at Brookhaven National Laboratory under Contract No. DE-SC0012704.

**1:03PM L30.00008 Low Dimensional Oxygen Vacancy Ordering and Diffusion in  $\text{SrCrO}_{3-\delta}$** , PHUONG VU ONG, PETER V. SUSHKO, Physical & Computational Sciences Directorate, Pacific Northwest National Laboratory, Richland, WA 99352, U.S.A., PHYSICAL & COMPUTATIONAL SCIENCES DIRECTORATE, PACIFIC NORTHWEST NATIONAL LABORATORY, RICHLAND, WA 9 TEAM — Oxygen vacancies ( $V_O$ ) are known to strongly affect the structure and electronic properties of complex oxides. An ability to control local concentration and spatial distribution of the vacancies, as well as stability and dimensionality of their aggregates, would enable generating novel materials functionalities, such as fast directional charge and mass transport. We use first-principles simulations to study mechanisms of formation, aggregation and diffusion of oxygen vacancies in  $\text{SrCrO}_{3-\delta}$ . We found that at low concentrations oxygen vacancies have a tendency to aggregate into one-dimensional (1D) structures oriented along a [110] direction. These  $V_O$  clusters induce rearrangements of oxide ions and conversion of Cr-centered perovskite lattice octahedra into tetrahedra. In turn, aggregation of these 1D  $V_O$  clusters enables formation of 2D vacancy aggregates parallel to the (111) plane of the cubic perovskite lattice. We provide a simple physical picture for the formation and growth of such low-dimensional  $V_O$ -structures. Moreover, we found mechanisms of  $V_O$  migration which enable a diffusion and expansion of the  $V_O$ -structures with low activation energies. Our results elucidate the atomic-scale mechanisms of efficient and reversible reduction and oxidation process observed in this material. These mechanisms could be extended to other complex oxides and used in design of high performance electrolytes and cathodes.

**1:15PM L30.00009 Structure and Electronic Transport of Oxygen-Deficient  $\text{SrTiO}_3$  Thin Films Buffered with  $\text{DyScO}_3$** , PURNIMA BALAKRISHNAN, URUSA ALAAN, MATTHEW GRAY, YURI SUZUKI, Stanford Univ — Oxygen deficiency in  $\text{SrTiO}_3$  (STO) induces metallic behavior in bulk and thin film form. Thus far, reports of STO thin film metallicity have been limited to homoepitaxial growth on bulk STO substrates. Growth on other substrates has suppressed metallicity, suggesting the important role of lattice distortions. In this presentation, we report on the metallicity and corresponding structure of oxygen-deficient STO films deposited on  $\text{DyScO}_3$  (DSO) buffered STO substrates and compare to STO films deposited directly on STO substrates. These films are epitaxial, atomically flat, expanded out-of-plane by  $\sim 0.6\%$ , and coherently strained to the STO substrate. Oxygen-deficient STO thin films grown on STO and DSO-buffered STO substrates are metallic, while films deposited on  $\text{LaAlO}_3$ ,  $(\text{LaAlO}_3)(\text{SrTaO}_3)$ , and DSO substrates are insulating. The resistivities of metallic films follow a  $T^3$  dependence near room temperature, transitioning to a  $T^2$  dependence below  $\sim 100$  K, and are increased by the addition of a DSO buffer. Comparison of sheet resistance across films of various thicknesses indicates the presence of an insulating layer around 7 unit cells thick. These properties indicate the importance of both oxygen deficiency and lattice structure in obtaining metallicity.

**1:27PM L30.00010 Non-Fermi liquids in two and three-dimensional doped  $\text{SrTiO}_3$** , EVGENY MIKHEEV, SANTOSH RAGHAVAN, JACK ZHANG, PATRICK MARSHALL, ADAM KAJDOS, Materials Department, University of California, Santa Barbara, CA 93106-5050, USA, LEON BALENTS, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, California 93106-4030, USA, SUSANNE STEMMER, Materials Department, University of California, Santa Barbara, CA 93106-5050, USA — A remarkable feature of transport in doped  $\text{SrTiO}_3$  is the temperature dependence of the electrical resistivity that is proportional to  $T^n$  with  $n \leq 2$ . This power law suggests electron-electron scattering is the dominant scattering mechanism. It extends to room temperature and above in both three-dimensional, uniformly doped  $\text{SrTiO}_3$  and in two-dimensional electron liquids (2DELs) at oxide interfaces. In case of  $n = 2$ , the behavior is traditionally identified as that of a Landau Fermi liquid. Here we argue that Landau Fermi liquid theory does not apply to the electron liquid in  $\text{SrTiO}_3$ , even when  $n = 2$ . Using electrostatic gating and chemical doping, we demonstrate that this regime is associated with a scattering rate and an energy scale that are independent of carrier density. This is in fundamental conflict with the premise of the Fermi liquid theory, where this energy scale is the Fermi energy. This work raises important questions in terms of microscopic scattering mechanism. It appears to be relevant for understanding of transport in many other strongly correlated systems, which also show very robust  $T^n$  regimes with carrier density independent scattering rates.

**1:39PM L30.00011 Understanding the Origin of Surface Depletion in  $\delta$ -doped  $\text{SrTiO}_3$  Structures**, HYEOK YOON, HISASHI INOUE, ADRIAN G. SWARTZ, Stanford Univ, YASUYUKI HIKITA, SLAC National Accelerator Laboratory, HAROLD Y. HWANG, Stanford Univ, SLAC National Accelerator Laboratory — Unlike most of the conventional semiconductors, the large dielectric constant of  $\text{SrTiO}_3$  results in a pronounced surface depletion width [1]. In thin films, the effect of surface depletion is even more dramatic: reduction of mobility and two-dimensional carrier density. To avoid this effect, capping and buffering a narrow channel of *n*-type doped  $\text{SrTiO}_3$ , so called  $\delta$ -doping, is designed to make the channel free from surface scattering, resulting in highly mobile carriers [2-4] We have investigated systematic changes in electronic transport by tuning the thicknesses of the undoped surface buffering cap and the  $\delta$ -doped layer. This has allowed us to map the phase diagram consisting of a three-dimensional metal, two-dimensional metallic behavior, and an insulating phase. We also show the surface depletion width as a function of doping density in order to study the origin of surface depletion of  $\text{SrTiO}_3$  [1] A. Ohtomo and H. Y. Hwang, *Appl. Phys. Lett.* **84**, 1716 (2004). [2] Y. Kozuka *et al.*, *Appl. Phys. Lett.* **97**, 222115 (2010). [3] Y. Kozuka, M. Kim *et al.*, *Nature* **462**, 487 (2009). [4] M. Kim *et al.*, *Phys. Rev. Lett.* **107**, 106801 (2011).

**1:51PM L30.00012 High-mobility SrTiO<sub>3</sub> delta-doped field-effect transistors**, HISASHI INOUE, ADRIAN SWARTZ, GLAM, Stanford University, YASUYUKI HIKITA, SIMES, SLAC National Accelerator Laboratory, HAROLD HWANG, GLAM, Stanford University, SIMES, SLAC National Accelerator Laboratory — Two-dimensional electron systems in SrTiO<sub>3</sub> show intriguing properties such as high mobility transport, magnetism, and possible unconventional superconductivity. A delta-doped structure, sandwiching a narrow two-dimensional conducting SrTiO<sub>3</sub> channel between two insulating SrTiO<sub>3</sub> layers, provides a clean platform to realize such electronic states, with symmetric confining potential in the absence of interface or surface scattering. Electric field gating of the conducting channel in a field-effect transistor (FET) geometry is a powerful method for tuning low-dimensional systems via carrier density modulation. We have synthesized high quality SrTiO<sub>3</sub> delta-doped structures using pulsed laser deposition, and optimized the device processing steps to achieve ideal FET characteristics at room temperature. This progress enabled examination of high-mobility transport in the carrier density regime as low as  $3 \times 10^{12} \text{ cm}^{-2}$  at low-temperatures, opening promising avenues to investigate quantum transport and realization of exotic quantum phases in SrTiO<sub>3</sub> two-dimensional electron systems.

**2:03PM L30.00013 A model of dopant diffusion through a strongly correlated p-n junction.**, JEDRZEJ WIETESKA, Columbia University, RICHARD BRIERLEY, Yale University, GIAN GUZMAN-VERRI, University of Costa Rica and Argonne National Laboratory, GUNNAR MOLLER, University of Cambridge, PETER LITTLEWOOD, Argonne National Laboratory, University of Chicago, LITTLEWOOD GROUP COLLABORATION — The diffusion of charged ions in a solid depends on an equation of state that balances diffusive and screened electrostatic forces, and is well understood in the case of conventional semiconductors and metals. In the case of a strongly-correlated material, the physics is different, and expected to be relevant, for example, in Li-ion battery cathodes. We propose a model of dopant ion motion through a strongly correlated p-n junction. Our approach is to consider diffusive (Nernst-Planck) dynamics of dopants under screened electrostatic interactions computed [1] within a mean-field (Thomas-Fermi) approximation. Dopant profiles as function of time are calculated for a p-n junction held at constant voltage. In the case where filling levels are near a correlation-induced gap, Mott insulating regions can form at the p-n interface and their dynamics is studied. References: 1. Charlebois et al., Phys. Rev. B, 87 035137 (2013)

## Wednesday, March 16, 2016 11:15AM - 2:15PM –

Session L31 DCP: Advances in Density Functional Theory VI 331 - Marivi Fernandez Serra, SUNY-Stony Brook

**11:15AM L31.00001 Fast RPA and GW calculations: cubic system size scaling**, GEORG KRESSE, Faculty of Physics, Univ. Vienna — The random phase approximation (RPA) to the correlation energy and the related GW approximation are among the most promising methods to obtain accurate correlation energy differences and QP energies from diagrammatic perturbation theory at reasonable computational cost. The calculations are, however, usually one to two orders of magnitude more demanding than conventional density functional theory calculations. Here, we show that a cubic system size scaling can be readily obtained reducing the computation time by one to two orders of magnitude for large systems. Furthermore, the scaling with respect to the number of k points used to sample the Brillouin zone can be reduced to linear order. In combination, this allows accurate and very well-converged single-point RPA and GW calculations, with a time complexity that is roughly on par or better than for self-consistent Hartree-Fock and hybrid-functional calculations [1-2]. Furthermore, the talk discusses the relation between the RPA correlation energy and the GW approximation: the self-energy is the derivative of the RPA correlation energy with respect to the Green's function. The calculated self-energy can be used to compute QP-energies in the GW approximation, any first derivative of the total energy, as well as corrections to the correlation energy from the changes of the charge density when switching from DFT to a many-body description (GW singles energy contribution) [3]. [1] Merzuk Kaltak, Jiří Klimeš, and Georg Kresse, J. Chem. Theory Comput., 10, 2498–2507 (2014). [2] Merzuk Kaltak, Jiří Klimeš, and Georg Kresse, Phys. Rev. B 90, 054115 (2014). [3] Jiří Klimeš, M. Kaltak, E. Maggio, and G. Kresse, J. Chem. Phys. 140, 084502 (2015).

**11:51AM L31.00002 Influence of *xc* functional on thermal-elastic properties of Ceria: A DFT-based Debye-Grüneisen model approach<sup>1</sup>**, JI-HWAN LEE, YOUNGJOO TAK, TAEHUN LEE, ALOYSIUS SOON, Department of Materials Science and Engineering, Yonsei University — Ceria (CeO<sub>2-x</sub>) is widely studied as a choice electrolyte material for intermediate-temperature (~ 800 K) solid oxide fuel cells. At this temperature, maintaining its chemical stability and thermal-mechanical integrity of this oxide are of utmost importance. To understand their thermal-elastic properties, we firstly test the influence of various approximations to the density-functional theory (DFT) *xc* functionals on specific thermal-elastic properties of both CeO<sub>2</sub> and Ce<sub>2</sub>O<sub>3</sub>. Namely, we consider the local-density approximation (LDA), the generalized gradient approximation (GGA-PBE) with and without additional Hubbard *U* as applied to the 4f electron of Ce, as well as the recently popularized hybrid functional due to Heyd-Scuseria-Ernzerhof (HSE06). Next, we then couple this to a volume-dependent Debye-Grüneisen model to determine the thermodynamic quantities of ceria at arbitrary temperatures. We find an explicit description of the strong correlation (e.g. via the DFT+*U* and hybrid functional approach) is necessary to have a good agreement with experimental values, in contrast to the mean-field treatment in standard *xc* approximations (such as LDA or GGA-PBE).

<sup>1</sup>We acknowledge support from Samsung Research Funding Center of Samsung Electronics (SRFC-MA1501-03)

**12:03PM L31.00003 Catalytic Effects of Oxide Surfaces on Diels-Alder Cycloaddition between Furan and Methyl Acrylate: A DFT Study.**, TAHA SALAVATI-FARD, GLEN JENNESS, STAVROS CARATZOULAS, DOUGLAS DOREN, University of Delaware — Using density functional theory with periodic boundary conditions, we study the catalytic effects of oxide surfaces such as ZrO<sub>2</sub> and HfO<sub>2</sub> on Diels-Alder reaction between furan and methyl acrylate. The cycloadduct can be dehydrated later to produce methyl benzoic which is an important step toward benzoic acid production. The gas-phase and on-surface reaction mechanisms are studied in detail. The surface hydration effects on the reaction mechanism and energy profile are studied as well. Our calculations show that the oxide surfaces catalyze the reaction significantly through the interaction of metal sites with methyl acrylate. The calculations are interpreted by making use of electronic density of states and band structure of the catalyst.

**12:15PM L31.00004 Role of Exchange and Correlation in Predicting Structures and Properties of Fluoride Materials**, NENIAN CHARLES, Drexel University, JAMES RONDINELLI, Northwestern University — The study of fluorine-based inorganic compounds has captured the attention of condensed matter physicists as a route to engineer novel states of matter. Here, we present a density functional theory (DFT) study on fluorides with structures ranging from simple to complex, including KF (rock salt), MnF<sub>2</sub> and VF<sub>2</sub> (rutile), KMnF<sub>3</sub> (perovskite), and Na<sub>3</sub>MnF<sub>6</sub> and Na<sub>6</sub>ScF<sub>6</sub> (cryolite). The focus is on understanding the accuracy of various exchange-correlation functionals for the prediction of structural, electronic, and phonon properties at four different levels of theory, i.e., the local density approximation (LDA), generalized gradient approximation (GGA), meta-GGA, and hybrid functional level with exact exchange. Specifically, we draw attention to the meta-GGA functional MS2 [Sun *et al*, Phys. Rev. Lett., **111**, 106401 (2013)], demonstrating that although it shows improvements over the LDA and GGA functionals in predicting structural properties of fluorides, MS2 generally performs poorer for the electronic and phonon properties. Our study provides useful insights for predictive design of functional halide compounds using computational models based on DFT.

## 12:27PM L31.00005 Bond Breaking in Epoxy Systems: A Combined QM/MM Approach

STEPHEN BARR, UTC, Air Force Research Laboratory, GARY KEDZIORA, Engility Corp., Air Force Research Laboratory, ALLISON ECKER, SOCHE, Air Force Research Laboratory, JAMES MOLLER, Miami University, RAJIV BERRY, TIM BREITZMAN, Air Force Research Laboratory — A novel method to combine molecular mechanics and quantum mechanics (QM/MM) is developed with the intent to accurately and efficiently account for covalent bond breaking in polymer systems. Since classical force fields cannot accurately account for bond breaking, and QM is too demanding to simulate large systems, a hybrid approach is required. In the method demonstrated here, strain is applied to the system using a classical force field. When a bond break is likely, a zone surrounding the bond is used in a QM calculation to determine which, if any, bonds break. The QM result is then used to reconstitute the system to continue the classical simulation until another QM calculation is triggered. In this way a QM calculation is only computed when and where it is needed, allowing for an efficient simulation. A key component of this method is a density functional theory (DFT) method which provides accurate forces as bonds are pulled past their breaking points. To find the best method, a number of functionals are compared with high level QM calculations by pulling various small molecules, representative of epoxies, past a bond breaking event. Appropriate values for the QM zone size and the QM trigger criteria are also determined. The overall QM/MM method is then applied to an epoxy system.

## 12:39PM L31.00006 Bayesian Error Estimation Functionals

KARSTEN W. JACOBSEN, CAMD, Dept. of Physics, Technical University of Denmark — The challenge of approximating the exchange-correlation functional in Density Functional Theory (DFT) has led to the development of numerous different approximations of varying accuracy on different calculated properties. There is therefore a need for reliable estimation of prediction errors within the different approximation schemes to DFT. The Bayesian Error Estimation Functionals (BEEF) have been developed with this in mind. The functionals are constructed by fitting to experimental and high-quality computational databases for molecules and solids including chemisorption and van der Waals systems. This leads to reasonably accurate general-purpose functionals with particular focus on surface science. The fitting procedure involves considerations on how to combine different types of data, and applies Tikhonov regularization and bootstrap cross validation. The methodology has been applied to construct GGA and metaGGA functionals with and without inclusion of long-ranged van der Waals contributions. The error estimation is made possible by the generation of not only a single functional but through the construction of a probability distribution of functionals represented by a functional ensemble. The use of the functional ensemble is illustrated on compound heat of formation and by investigations of the reliability of calculated catalytic ammonia synthesis rates.

## 1:15PM L31.00007 Joint Density Functional Theory for the electrode/electrolyte interface: Benchmarking liquid structure with experiment and *ab initio* molecular dynamics

KENDRA LETCHWORTH-WEAVER, Argonne National Laboratory, Cornell University, CHRISTINE UMBRIGHT, Cornell University, MARIA CHAN, PAUL FENTER, Argonne National Laboratory, T. A. ARIAS, Cornell University — Understanding the physics of the interface between a charged electrode surface and a fluid electrolyte would inform design of electrochemical energy storage and conversion devices. However, such studies require a simultaneously accurate yet inherently multi-scale theory. Joint density-functional theory (JDFT) bridges the relevant length-scales by joining a fully *ab initio* description of the electrode with a low computational cost, yet atomically detailed classical DFT description of the liquid electrolyte structure. Leveraging JDFT within our framework to treat charged systems in periodic boundary conditions, we can predict the voltage-dependent structure and energetics of solvated ions at the interface between graphitic and single-crystalline metallic electrodes and technologically relevant liquid electrolytes. First, we elucidate the physical origin of the experimentally measured voltage-dependent differential capacitance of an Ag(111) electrode in aqueous NaF electrolyte, examining the crucial role of ion de-solvation and physisorption onto the electrode surface. We go on to compare the JDFT-predicted interfacial liquid structure next to a graphitic electrode with results obtained from X-ray reflectivity measurements and *ab initio* molecular dynamics simulations.

## 1:27PM L31.00008 Role of Van der Waals interactions in determining the structure of liquid tellurides<sup>1</sup>

MATTHIEU MICOULAUT, HUGO FLORES-RUIZ, Paris Sorbonne Universités, VANESSA COULET, Universités Aix-Marseille, ANDREA PIARRISTEGUY, Université Montpellier II, MARK JOHNSON, GABRIEL CUELLO, Institut Laue Langevin, ANNIE PRADEL, Université Montpellier II — The simulation of tellurides using standard density functional (DFT) theory based molecular dynamics usually leads to an overestimation of the bond distances and a noticeable mismatch between theory and experiments when e.g. structure functions are being directly compared. Here, the structural properties of several compositions of Ge-Te and Ge-Sb-Te liquids are studied from a combination of neutron diffraction and DFT-based molecular dynamics. Importantly, we find an excellent agreement in the reproduction of the structure in real and reciprocal spaces, resulting from the incorporation of dispersion forces in the simulation. We then investigate structural properties including structure factors, pair distribution functions, angular distributions, coordination numbers, neighbor distributions, and compare our results with experimental findings.

### References:

- Physical Review B 92, 134205 (2015)
- Physical Review B 89, 174205 (2014)
- Physical Review B 90, 094207 (2014)

<sup>1</sup>Support from Agence Nationale de la Recherche (ANR) (Grant No. ANR- 11-BS08-0012) is gratefully acknowledged.

## 1:39PM L31.00009 Ti $\alpha - \omega$ phase transformation and metastable structure, solid-state nudged elastic band method<sup>1</sup>

NIKOLAI ZARKEVICH<sup>2</sup>, DUANE D. JOHNSON<sup>2</sup>, Ames Laboratory — The four most utilized structural metals, and, hence, its structural changes and potential metastable phases under stress are of considerable interest. DFT+U combined with the generalized solid-state nudged elastic band (SS-NEB) method, we consider the pressure-driven transformation of Ti from  $\alpha$  to  $\omega$  phases, and find an intermediate metastable body-centered orthorhombic (bco) structure of lower density. We verify its stability by calculating its electronic structure, and compare computational results to experiment. Interestingly, standard density functional theory (DFT) yields a ground state, in contradiction to the observed  $\alpha$  phase at low pressure and temperature. We correct this by proper consideration of  $d$ -electrons, and utilize DFT+U method in the SS-NEB to obtain the relevant transformation pathway and structures.

<sup>1</sup>We use methods developed with support by the U.S. Department of Energy (DE-FG02-03ER46026 and DE-AC02-07CH11358) operated for the DOE by Iowa State University under contract DE-AC02-07CH11358.

<sup>2</sup>Ames Laboratory, U.S. Department of Energy at Iowa State University, Ames, Iowa 50011-3020

**1:51PM L31.00010 The effect of the pair correlation function on dynamic density functional theory<sup>1</sup>**, STEPHEN J. TATE, Department of Chemical Engineering, Imperial College London, BENJAMIN D. GODDARD, School of Mathematics, University of Edinburgh, GRIGORIOS A. PAVLIOTIS, Department of Mathematics, Imperial College London, SERAFIM KALLIADASIS, Department of Chemical Engineering, Imperial College London — In a previous study [1], a general dynamical density functional theory (DDFT) to include hydrodynamic interactions (HI) and inertial effects of colloidal particles was derived and validated with stochastic simulations. But the pair correlation function,  $g$ , was approximated with a simplest possible volume-exclusion function, namely a Heaviside step function. Here we explore what effect more accurate  $g$ 's have on the same DDFT. These include a correction giving the Percus-Yevick solution for hard spheres, which is known analytically. Furthermore, since we typically deal with systems outside of equilibrium, we model non-adiabatic effects to the HI terms in the DDFT, including density and momentum dependence. [1] B.D. Goddard, A. Nold, N. Savva, G.A. Pavliotis and S. Kalliadas, "General dynamical density functional theory for classical fluids," Phys. Rev. Lett. 109 (120603) 2012.

<sup>1</sup>Funded by EPSRC grant no EP/L025159/1

**2:03PM L31.00011 Understanding the spurious DFT fractional charge in the electrochemical double layer**, LEANNE CHEN, MICHAL BAJDICH, ALAN LUNTZ, KAREN CHAN, JENS NORSKOV, SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory and Stanford University — An ongoing challenge in computational electrochemistry is the accurate determination of electrochemical barriers at constant electrode potential. Recently, our group developed an efficient scheme to determine the barriers using a simple extrapolation based on the interfacial charge [1]. However, semilocal DFT calculations have shown that the magnitude of the charge of solvated species ( $\text{H}_3\text{O}^+$ ,  $\text{OH}^-$ ,  $\text{Li}^+$ ,  $\text{Na}^+$ ) in the outer Helmholtz plane is not 1e, but always near 0.6e, which suggests a charge delocalization error in DFT. Furthermore, we frequently observe inaccurate alignment of the metal Fermi and solvent energy levels. Using an increasing amount of exact exchange, we first analyze the charge delocalization error in the dissociation of NaCl molecule, where a large amount of exchange is needed to reproduce the step-like transition of charge from +1 to 0 on the dissociated Na and Cl. Next, we apply the same method to the metal-water interface with solvated ions at varying distances from the surface. The performance of hybrid and other fractional charge-corrected functionals will be discussed together with the possibility of a simple correction scheme. [1] Chan, K.; Nørskov, J. K. Electrochemical Barriers Made Simple. *J. Phys. Chem. Lett.* **2015**, 6 (14), 2663–2668.

**Wednesday, March 16, 2016 11:15AM - 2:15PM –**

**Session L32 DCP: Dynamic Interactions Between Nanostructures** 332 - Todd Krauss, University of Rochester

**11:15AM L32.00001 Efficient Light-driven Long Distance Charge Separation and H<sub>2</sub> Generation in Semiconductor Quantum Rods and Nanoplatelets**, TIANQUAN LIAN, Emory University — Quantum confined semiconductor nanocrystals (0D quantum dots, 1D quantum rods and 2D quantum platelets) have been intensively investigated as light harvesting and charge separation materials for photovoltaic and photocatalytic applications. The efficiency of these semiconductor nanocrystal-based devices depends on many fundamental processes, including light harvesting, carrier relaxation, exciton localization and transport, charge separation and charge recombination. The competition between these processes determines the overall solar energy conversion (solar to electricity or fuel) efficiency. Semiconductor nano-heterostructures, combining two or more material components, offer unique opportunities to control their charge separation properties by tailoring their compositions, dimensions and spatial arrangement. Further integration of catalysts (heterogeneous or homogeneous) to these materials form multifunctional nano-heterostructures. Using 0D, 1D and 2D CdSe/CdS/Pt heterostructures as model systems, we directly probe the above-mentioned fundamental exciton and carrier processes by transient absorption and time-resolved fluorescence spectroscopy. We are examining how to control these fundamental processes through the design of heterostructures to achieve long-lived charge separation and efficient H<sub>2</sub> generation. In this talk, we will discuss a new model for exciton dissociation by charge transfer in quantum dots (i.e. Auger assisted electron transfer), mechanism of 1D and 2D exciton transport and dissociation in nanorods, and key factors limiting H<sub>2</sub> generation efficiency in CdSe/CdS/Pt nanorod heterostructures.

**11:51AM L32.00002 How to harvest solar energy with the photosynthetic reaction center.**, ALEXANDER BALAEFF, JUSTIN REYES, University of Central Florida — Photosynthetic reaction center (PRC) is a protein complex that performs a key step in photosynthesis: the electron-hole separation driven by photon absorption. The PRC has a great promise for applications in solar energy harvesting and photosensing. Such applications, however, are hampered by the difficulty in extracting the photogenerated electric charge from the PRC. To that end, it was proposed to attach the PRC to a molecular wire through which the charge could be collected. In order to find the attachment point for the wire that would maximize the rate of charge outflow from the PRC, we performed a computational study of the PRC from the *R. viridis* bacterium. An ensemble of PRC structures generated by a molecular dynamics simulation was used to calculate the rate of charge transport from the site of initial charge separation to several trial sites on the protein surface. The Pathways model was used to calculate the charge transfer rate in each step of the network of heme co-factors through which the charge transport was presumed to proceed. A simple kinetic model was then used to determine the overall rate of the multistep charge transport. The calculations revealed several candidate sites for the molecular wire attachment, recommended for experimental verification.

**12:03PM L32.00003 Managing photons and carriers for photocatalysis**, ISABELL THOMANN, HOSSEIN ROBATJAZI, SHAH BAHAUDDIN, CHLOE DOIRON, XUEJUN LIU, THEJASWI TUMKUR, WEI-REN WANG, PARKER WRAY, Rice University — While small plasmonic nanoparticles efficiently generate energetic hot carriers, light absorption in a monolayer of such particles is inefficient, and practical utilization of the hot carriers in addition requires efficient charge-separation. Here we describe our approach to address both challenges. By designing an optical cavity structure for the plasmonic photoelectrode [1], light absorption in these particles can be significantly enhanced, resulting in efficient hot electron generation. Rather than utilizing a Schottky barrier to preserve the energy of the carriers, our structure allows for their direct injection into the adjacent electrolyte. On the substrate side, the plasmonic particles are in contact with a wide band gap oxide film that serves as an electron blocking layer but accepts holes and transfers them to the counter electrode. The observed photocurrent spectra follow the plasmon spectrum, and demonstrate that the extracted electrons are energetic enough to drive the hydrogen evolution reaction. A similar structure can be designed to achieve broadband absorption enhancement in monolayer MoS<sub>2</sub> [2]. Time permitting, I will discuss charge carrier dynamics in hybrid nanoparticles composed of plasmonic / two-dimensional materials, and applications of photo-induced force microscopy to study photocatalytic processes. [1] Nano Letters, 2015, 15 (9), p 6155 [2] Photon management strategies for monolayer MoS<sub>2</sub>, submitted

## 12:15PM L32.00004 Charge Transfer Dynamics in Semiconductor Quantum Dots Relevant to Solar Hydrogen Production.

, TODD KRAUSS, University of Rochester — Artificial conversion of sunlight to chemical fuels has attracted attention for several decades as a potential source of clean, renewable energy. For example, in light-driven proton reduction to molecular hydrogen, a light-absorbing molecule (the photosensitizer) rapidly transfers a photoexcited electron to a catalyst for reducing protons. We recently found that CdSe quantum dots (QDs) and simple aqueous  $\text{Ni}^{2+}$  salts in the presence of a sacrificial electron donor form a highly efficient, active, and robust system for photochemical reduction of protons to molecular hydrogen. To understand why this system has such extraordinary catalytic behavior, ultrafast transient absorption (TA) spectroscopy studies of electron transfer (ET) processes from the QDs to the Ni catalysts were performed. CdSe QDs transfer photoexcited electrons to a Ni-dihydrolipoic acid (Ni-DHLA) catalyst complex extremely fast and with high efficiency. Even under high fluence, the relative fraction of TA signal due to ET remains well over 80%, and depopulation from exciton-exciton annihilation is minimal (6%). We also found that increasing QD size and/or shelling the core CdSe QDs with a shell of CdS slowed the ET rate, in agreement with the relative efficiency of photochemical  $\text{H}_2$  generation. The extremely fast ET provides a fundamental explanation for the exceptional photocatalytic  $\text{H}_2$  activity of the CdSe QD/Ni-DHLA system and guides new directions for further improvements.

## 12:51PM L32.00005 Multi-photon Photoemission Dynamics in $\text{TiO}_2$

, ADAM ARGONDISO, University of Pittsburgh, XUEFENG CUI, University of Science and Technology of China, CONG WANG, University of Pittsburgh, HUIJUAN SUN, HONGHUI SHANG, JIN ZHAO, University of Science and Technology of China, HRVOJE PETEK, University of Pittsburgh —  $\text{TiO}_2$  is a material of interest in photocatalytic and photovoltaic applications. Until recently, however, the ability to probe the electron dynamics of this system has been limited to optical experiments. By probing the rutile  $\text{TiO}_2(110)$  surface using two-photon photoemission (2PP) with a tunable ultrashort ( $\sim 20$  fs) laser pulse we investigated the dynamics of electrons excited to its conduction band. Previous 2PP experiments on protic solvent covered  $\text{TiO}_2$  surfaces using 400 nm (3.1 eV) light revealed the presence of an unoccupied surface adsorbate-induced wet electron state. By expanding such measurements at higher photon energy we have found a pair of new nearly degenerate unoccupied states located at 2.7 and 2.8 eV above the Fermi level. Based on the calculated electronic structure and optical transition moments, as well as related spectroscopic evidence, we assign these resonances to transitions between Ti-3d bands of nominally  $t_{2g}$  and  $e_g$  symmetry, which are split by crystal field. A detailed understanding of the  $t_{2g}$ - $e_g$  transitions is essential for the characterization of electron dynamics and adsorbate induced resonances in photocatalytic processes on  $\text{TiO}_2$ .

## 1:03PM L32.00006 ABSTRACT WITHDRAWN —

## 1:15PM L32.00007 Hole transfer dynamics from QDs to tethered ferrocene derivatives

, A. PAUL ALIVISATOS, Department of Chemistry, University of California, Berkeley — Quantum dots (QDs) have shown particular promise in recent years as light absorbers in solar energy conversion schemes. However, in solution junction solar devices such as QD-sensitized solar cells and photocatalytic water splitting systems, efficiencies are often limited by hole transfer from the photoexcited QD. This process is sluggish and can lead to oxidative photocorrosion of the QD material. In order to design highly efficient nanocrystal systems with hole transfer rates that outcompete these undesirable processes, a fundamental understanding of the parameters that control these rates is imperative.

We have developed a model system to study charge transfer from QDs to surface bound acceptors, to fundamentally understand the charge transfer processes for QD systems, namely electronic coupling between the donor and acceptor and the thermodynamic driving force for the hole transfer process. Specifically, we examine hole transfer from the nearly spherical CdSe-core CdS-shell QDs with photoluminescence (PL) quantum yields over 80% to ferrocene derivatives bound to the QD surface via an alkane thiol linker. In this system, we mitigate the ill-defined nonradiative charge dynamic pathways that are intrinsic to native CdSe cores, and then controllably engineer on the surface charge acceptors with well-defined oxidation potentials, spatial distribution, and quantity. By measuring the PL lifetime decay and calibrating the number of hole acceptor ligands per QD via quantitative  $^1\text{H}$  NMR, we extracted the hole transfer rate per acceptor. This rate per acceptor could be varied over four orders of magnitude by changing the coupling between donor and acceptor through modulations in the CdS shell thickness and alkane chain length of the molecule. Furthermore, owing to the large number of acceptors on the surface, we achieve systems in which  $\sim 99\%$  of the photoexcited holes are transferred to these well-defined mediators.

We further mapped the relationship between the thermodynamic driving force and hole transfer rate. We systematically tune the driving force over nearly 1 eV by varying the redox potentials of the ferrocene ligands through functionalization of the cyclopentadiene rings. Our results show a monotonic increase in rate as a function of the increasing driving force with no observed inverted region. This behavior is understood by considering the residual electron in the QD conduction band, which could exhibit intraband excitations coupled to the hole transfer, thus creating a many-state system that would eliminate the inverted region. The resulting relationship between rate and energetic driving force for hole transfer can be used to design QD-molecular systems that maximize interfacial charge transfer rates while minimizing energetic losses associated with the driving force.

## 1:51PM L32.00008 Cooperative Electron-Hole Dynamics at the Organic Donor-Acceptor Interface<sup>1</sup>

, CHEE KONG LEE, SHI LIANG, ADAM WILLARD, Massachusetts Institute of Technology — Charge transfer (CT) excitons are Coulombically bound electron and hole pairs located in spatially separate regions. They play an important role in both light emission of organic light emitting devices and the generation of photocurrent in organic photovoltaic. For some donor/acceptor blends the lowest electronic excitations are triplet CT states, and in these materials the photoluminescence and photocurrent generation exhibit a non-trivial magnetic field dependence due to its effect on singlet-triplet intersystem crossing and reverse intersystem crossing rates. Recent experiments have demonstrated that in these materials bound electron-hole pairs can move geminately over distance of 5-10nm confirming the transport of CT excitons despite strong Coulombic attraction. These experiments can be understood with a numerical model combining kinetic Monte Carlo and the quantum master equation. The model contains a minimal set of physical elements, and yet is able to quantitatively reproduce the experimental results. More importantly, the model provides insights into properties that otherwise cannot be obtained from experiments. Here I present the details of this model along with the physical insights it has provided into this particular class of materials.

<sup>1</sup>Cooperative Electron-Hole Dynamics at the Organic Donor-Acceptor Interface

## 2:03PM L32.00009 Probing of Charge Transfer States at Buried Organic Interfaces with Even-Order Spectroscopy

, RAVINDRA PANDEY, AARON MOON, SEAN ROBERTS, University of Texas at Austin — Organic thin film photovoltaics (OPV) are an emerging economically competitive technology that combines manufacturing adaptability, low-cost processing and a lightweight, flexible device end-product. At junctions formed between organic electron-donating and electron-accepting materials, the abrupt change in the dielectric properties can strongly perturb the density of states of the OPV. This can substantially alter the driving force for charge transfer between these materials. Electronic Sum Frequency Generation (ESFG), owing to its inherent interfacial sensitivity, is ideally suited to probe buried interfaces. Here, we report the ESFG spectra of Copper Phthalocyanine (CuPc) films, deposited on  $\text{SiO}_2$  measured for both reflection and transmission geometries. Three peaks are observed that roughly correlate with resonances that comprise CuPc's Q-band absorption but display slight shifts and amplitude changes with respect to CuPc's bulk absorption spectrum. Experimental results are compared with calculations based on a thin film interference model that accounts for ESFG emitted from both the CuPc:Air and CuPc: $\text{SiO}_2$  interface as well as contributions to the signal from higher order source terms from the bulk. The model reveals a difference in the density of states between the two interfaces and suggests that by combining experimental transmission and reflection data it is possible to separate bulk and interfacial contributions to ESFG spectra.

**Wednesday, March 16, 2016 11:15AM - 2:03PM —**

**Session L33 DMP GMAG: Kitaev Physics in Honeycomb Iridates** 336 - George Jackeli, University of Stuttgart

**11:15AM L33.00001 Evidence for coexisting magnetic order in frustrated three-dimensional honeycomb iridates  $\text{Li}_2\text{IrO}_3$**  , NICHOLAS BREZNAY, ALEJANDRO RUIZ, ALEX FRANO, JAMES ANALYTIS, University of California, Berkeley — The search for unconventional magnetism has found a fertile hunting ground in 5d iridium oxide (iridate) materials. The competition between coulomb, spin-orbit, and crystal field energy scales in honeycomb iridates leads to a quantum magnetic system with localized spin-1/2 moments communicating through spin-anisotropic Kitaev exchange interactions. Although early and ongoing work has focused on layered two-dimensional honeycomb compounds such as  $\text{Na}_2\text{IrO}_3$  and a 4d analog,  $\text{RuCl}_3$ , recently discovered polytypes of  $\text{Li}_2\text{IrO}_3$  take on three-dimensional honeycomb structures. Bulk thermodynamic studies, as well as recent resonant x-ray diffraction and absorption spectroscopy experiments, have uncovered a rich phase diagram for these three-dimensional honeycomb iridates. Low temperature incommensurate and commensurate magnetic orders can be stabilized by tuning the applied magnetic field, displaying a delicate coexistence that signals highly frustrated magnetism.

**11:27AM L33.00002 Vacancies in a 3D-Kitaev model on hyper-honeycomb lattice** , G J SREEJITH, Max Planck Institute for Physics of Complex Systems, Dresden, SUBHRO BHATTACHARJEE, International Centre for Theoretical Sciences, Bangalore, RODERICH MOESSNER, Max Planck Institute for Physics of Complex Systems, Dresden — We study the properties of isolated single and pairs of vacancies in an exactly solvable Kitaev model on a three dimensional hyper-honeycomb lattice. We show that each vacancy in the lattice is associated with a low energy spin like degree of freedom, similar to the case of previously studied honeycomb model. We calculate the contribution from these vacancy spin-moments to the low field magnetization response to a  $z$ -directed field. Isolated vacancies in the gapped phase act as free spins. In the gapless phase, these spins interact with the surrounding spin-liquid suppressing the low-field magnetization to  $\frac{1}{\sqrt{\ln[1/h_z]}}$ . Pair of vacancies have a sublattice-dependent, anisotropic, spin-liquid mediated interaction with each other. In the gapless phase, interaction between vacancies in the same (opposite) sublattice enhances (suppresses) the low-field magnetization, indicating a ferromagnetic (anti-ferromagnetic) nature. We also show that, unlike vacancies in the honeycomb lattice, the vacancies here do not bind a flux at low-energies.

**11:39AM L33.00003 Spin-Peierls instability of three-dimensional Kitaev spin liquids with Majorana Fermi surface** , MARIA HERMANNNS, SIMON TREBST, ACHIM ROSCH, University of Cologne — The Kitaev honeycomb model is one of the paradigmatic examples of a frustrated spin system exhibiting a quantum spin liquid ground state. The emergent low-energy degrees of freedom are Majorana fermions that can form various different (semi-)metallic states. Three-dimensional variants of this model can, in particular, harbor gapless quantum spin liquids with a Majorana Fermi surface. In this talk, we discuss Fermi surface instabilities arising from additional spin exchange terms (such as a Heisenberg coupling), which induce interactions between the emergent Majorana fermion degrees of freedom. We show that independent of the details of the interactions, the Majorana Fermi surface is always unstable. Generically, the system spontaneously dimerizes at exponentially small temperatures and forms a quantum spin liquid with nodal lines. Depending on the microscopic details, further symmetries of the system may be broken at this transition. These spin-Peierls instabilities of a 3D spin liquid are closely related to BCS instabilities of fermions<sup>1</sup>.

<sup>1</sup>M. Hermanns, S. Trebst, A. Rosch, PRL 115, 117205 (2015).

**11:51AM L33.00004 Kitaev physics in three dimensional honeycomb iridates<sup>1</sup>** , YONG-BAEK KIM, Univ of Toronto — It has been realized that Mott insulators with strong spin-orbit coupling may allow strongly bond-dependent exchange interactions between local moments. Such interactions may lead to magnetic frustration and possible quantum spin liquid phases. This is in contrast to usual frustrated magnets, where the magnetic frustration comes from the geometry of the underlying lattice structure. Hence, it offers a new avenue to generate exotic phases of matter. Recently, both two-dimensional ( $\alpha$ - $\text{Li}_2\text{IrO}_3$ ) and three-dimensional honeycomb iridates ( $\beta$ - $\text{Li}_2\text{IrO}_3$  and  $\gamma$ - $\text{Li}_2\text{IrO}_3$ ) have been discovered and it has been suggested that the magnetic exchange interactions contain the so-called Kitaev interaction, which depends on bond directions. In particular, the local moments of Ir ions in  $\beta$ - $\text{Li}_2\text{IrO}_3$  and  $\gamma$ - $\text{Li}_2\text{IrO}_3$  reside on the three-dimensional hyper-honeycomb and stripy-honeycomb lattices. The Kitaev model is exactly solvable on these lattices as well as the two-dimensional honeycomb lattice and the ground state is a quantum spin liquid with gapless excitations. We discuss recent progress in theoretical understanding of magnetic exchange interactions, possible presence of quantum spin liquid phases, and unusual magnetic order in  $\beta$ - $\text{Li}_2\text{IrO}_3$  and  $\gamma$ - $\text{Li}_2\text{IrO}_3$ . These theoretical results are used to make connections to recent experimental data.

<sup>1</sup>This work is supported by the NSERC and CIFAR

**12:27PM L33.00005 Detecting Semimetal Surface Modes in Kitaev Spin Liquids** , BRENT PERREAULT, University of Minnesota, JOHANNES KNOLLE, Cavendish Laboratory, NATALIA B. PERKINS, F. J. BURNELL, University of Minnesota — Raman scattering is a useful probe for Kitaev-type spin liquids because it couples only to the dispersing (and potentially gapless) fermionic degrees of freedom in these systems. I will discuss Raman scattering in Kitaev spin liquids on the 3D hyperhoneycomb (H-0) lattice, where these fermionic degrees of freedom realize topologically non-trivial band structures with protected gapless surface states. I will describe Raman signatures both of bulk 3D samples, and thin-film samples of these materials, where the resonant Raman response can detect the protected surface modes.

**12:39PM L33.00006 Large Band Gap of alpha-RuCl<sub>3</sub> Probed by Photoemission and Inverse Photoemission Spectroscopy** , SOOBIN SINN, CHOONG HYUN KIM, LUKE SANDILANDS, IBS-CCES, Seoul National University, KYUNG-DONG LEE, CHOONGJAE WON, IBS-CCES, Inha University, JI SEOP OH, IBS-CCES, Seoul National University, MOONSUP HAN, YOUNG JUN CHANG, University of Seoul, NAMJUNG HUR, Inha University, HITOSHI SATO, Hiroshima Synchrotron Radiation Center, BYEONG-GYU PARK, Pohang Accelerator Laboratory, CHANGYOUNG KIM, HYEONG-DO KIM, TAE WON NOH, IBS-CCES, Seoul National University — The Kitaev honeycomb lattice model has attracted great attention because of its possibility to stabilize a quantum spin liquid ground state. Recently, it was proposed that alpha-RuCl<sub>3</sub> is its material realization and the first 4d relativistic Mott insulator from an optical spectrum and LDA+ $U$ +SO calculations. Here, we present photoemission and inverse photoemission spectra of alpha-RuCl<sub>3</sub>. The observed band gap is about 1.8 eV, which suggests that the previously assigned optical gap of 0.3 eV is misinterpreted, and that the strong peak at about 1.2 eV in the optical spectrum may be associated with an actual optical gap. Assuming a strong excitonic effect of 0.6 eV in the optical spectrum, all the structures except for the peak at 0.3 eV are consistent with our electronic spectra. When compared with LDA+ $U$ +SO calculations, the value of  $U$  should be considerably larger than the previous one, which implies that the spin-orbit coupling is not a necessary ingredient for the insulating mechanism of alpha-RuCl<sub>3</sub>. We also present angle-resolved photoemission spectra to be compared with LDA+ $U$ +SO and LDA+DMFT calculations.

**12:51PM L33.00007 Ab-initio study on crystal structure of  $\alpha$ -RuCl<sub>3</sub>** , HAE-YOUNG KEE, HEUNG-SIK KIM, Univ of Toronto —  $\alpha$ -RuCl<sub>3</sub> was recently proposed as a candidate system for materialization of Kitaev model, but precise structural information of the compound has remained elusive. For the clarification of the full three-dimensional crystal structure of  $\alpha$ -RuCl<sub>3</sub>, we performed ab-initio electronic structure calculations including effects of spin-orbit coupling (SOC) and electron correlations. We found that SOC prevents dimerization between Ru atoms, and keeps the system close to honeycomb lattice. The ground state crystal structure has monoclinic  $C2/m$ -type layer stacking, but trigonal  $P3_112$ -and orthorhombic  $Cmc2_1$ -type stacking orders are comparable to the  $C2/m$  structure in energy, so that stacking faults can be easily introduced. The electronic structure and the  $j_{\text{eff}}=1/2$  pseudospin exchange interactions and possible magnetic states in  $\alpha$ -RuCl<sub>3</sub> will be presented.

**1:03PM L33.00008 Nanoscale structural and electronic characterization of  $\alpha$ -RuCl<sub>3</sub> layered compound**<sup>1</sup> , MAXIM ZIATDINOV, ARTEM MAKSOV, ARNAB BANERJEE, WU ZHOU, TOM BERLIJN, JIAQIANG YAN, STEPHEN NAGLER, Oak Ridge National Laboratory, DAVID MANDRUS, University of Tennessee, ARTHUR BADDORF, SERGEI KALININ, Oak Ridge National Laboratory — The exceptional interplay of spin-orbit effects, Coulomb interaction, and electron–lattice coupling is expected to produce an elaborate phase space of  $\alpha$ -RuCl<sub>3</sub> layered compound, which to date remains largely unexplored. Here we employ a combination of scanning transmission electron microscopy (STEM) and scanning tunneling microscopy (STM) for detailed evaluation of the system's microscopic structural and electronic orders with a sub-nanometer precision. The STM and STEM measurements are further supported by neutron scattering, X-Ray diffraction, density functional theory (DFT), and multivariate statistical analysis. Our results show a trigonal distortion of Cl octahedral ligand cage along the  $C_3$  symmetry axes in each RuCl<sub>3</sub> layer. The lattice distortion is limited mainly to the Cl subsystem leaving the Ru honeycomb lattice nearly intact. The STM topographic and spectroscopic characterization reveals an intra unit cell electronic symmetry breaking in a spin-orbit coupled Mott insulating phase on the Cl-terminated surface of  $\alpha$ -RuCl<sub>3</sub>. The associated long-range charge order (CO) pattern is linked to a surface component of Cl cage distortion. We finally discuss a fine structure of CO and its potential relation to variations of average unit cell geometries found in multivariate analysis of STEM data.

<sup>1</sup>The research was sponsored by the U.S. Department of Energy

**1:15PM L33.00009 Probing Spin Excitations Using Magneto-Raman Spectroscopy** , K. THIRUNAVUKKUARASU<sup>1</sup>, Z. LU, National High Magnetic Field Laboratory, Tallahassee, FL, J. SIMPSON, Department of Physics, Towson University, MD, A. WALKER, National Institute of Standards and Technology, Gaithersburg MD, J. SEARS, Y.-J. KIM, Department of Physics, University of Toronto, Canada, K. BURCH, Department of Physics, Boston College, MA, D. SMIRNOV, National High Magnetic Field Laboratory, Tallahassee, FL — The presence of a 2D quantum spin liquid state was recently suggested for the spin-orbit coupled Mott insulator  $\alpha$ -RuCl<sub>3</sub> with a honeycomb lattice.[Phys. Rev. 90, 041112 (2014)] Optical spectroscopy, Raman scattering, specific heat as well as magnetic susceptibility measurements on  $\alpha$ -RuCl<sub>3</sub> identified elementary excitations due to electronic correlations and spin-orbit coupling.[arXiv:1503.07593, Phys. Rev. Letters 114, 147201 (2015), and Phys. Rev. 91, 144420 (2015)] These observations appear to be consistent with theoretical expectations for Heisenberg-Kitaev model for QSL.[Phys. Rev. 91, 241110 (2015)] The underlying mechanism for the unconventional magnetism in  $\alpha$ -RuCl<sub>3</sub> was further investigated by probing the effect of external magnetic field on the Raman spectroscopic signatures. Raman scattering experiments were performed at temperatures down to 5 K and magnetic fields up to 10 T. The intensity of strongest  $A_{1g}$  phonon was found to decrease with increasing magnetic field strength suggesting the presence of strong magnetic interactions. The experimental observations and its implications will be presented.

<sup>1</sup>Current Affiliation : Florida A and M University

**1:27PM L33.00010 Phase c comb magnet**<sup>1</sup> , IOANNIS ROUSOCHAKIS, Fachbereich Physik, Freie Universität Berlin, Germany, STEPHAN RACHEL, Institut für Experimentelle Physik, Universität Minn - Minneapolis — We show that the coupling  $K_2$ , which has been recently identified to play a central role in  $\alpha$ -RuCl<sub>3</sub>. This coupling explains natural order-by-disorder mechanisms are qualitatively c

Helmholtz-Zentrum Berlin für Materialien und Energie, 14109 Berlin, Germany

<sup>1</sup>NSF DMR-1511768; Freie Univ. Berlin Exce 1170; DFG-SFB 1143, DFG-SPP 1666, and F

**1:39PM L33.00011 High Pressure Transport and Structural Study on the Honeycomb Lattice Iridates  $A_2\text{IrO}_3$  ( $A = \text{Na, Li}$ )** , YOGESH SINGH, Indian Institute of Science Education and Research (IISER) Mohali, Knowledge City, Sector 81, Mohali 140306, India, SAMAR LAYEK, School of Physics and Astronomy, Tel-Aviv University, 69978, Tel-Aviv, Israel, KAVITA MEHLAWAT, Indian Institute of Science Education and Research (IISER) Mohali, Knowledge City, Sector 81, Mohali 140306, India, ERAN GREENBERG, GREGORY KH. ROZENBERG, MOSHE P. PASTERNAK, School of Physics and Astronomy, Tel-Aviv University, 69978, Tel-Aviv, Israel — The honeycomb lattice iridates  $A_2\text{IrO}_3$  ( $A = \text{Na, Li}$ ) have been predicted and shown to exhibit novel magnetic properties which suggest that these materials could realize bond-directional Kitaev-like magnetic exchange interactions [1 - 5]. We will present high pressure (P) electrical transport ( $P \leq 80$  GPa) and powder X-ray diffraction ( $P \leq 40$  GPa) on these materials. The PXRD data for both materials show a structural transition around  $P \sim 5$  GPa. The transport data show a dramatic reduction of the charge gap for  $\text{Na}_2\text{IrO}_3$ . References: [1] J. Chaloupka, G. Jackeli, and G. Khaliullin, Phys. Rev.Lett. **105**, 027204 (2010). [2] Y. Singh and P. Gegenwart, Phys. Rev. B **82**, 064412 (2010). [3] Y. Singh et al., Phys. Rev. Lett. **108**, 127203 (2012). [3] F. Ye et al., Phys. Rev. B **85**, 180403 (2012) [5] S. H. Chun et al. Nature Phys. **11**, 462 (2015).

**1:51PM L33.00012 Order by disorder in Kitaev-Heisenberg models on the honeycomb lattice<sup>1</sup>**, NATALIA PERKINS, YURIY SIZYUK, SAMUEL DUCATMAN, Univ of Minnesota, Minneapolis, PETER WOELFLE, Institute for Condensed Matter Theory and Institute for Nanotechnology, Karlsruhe Institute of Technology — Recent diffuse magnetic x-ray scattering data in Na<sub>2</sub>IrO<sub>3</sub> [1] clearly determined the spin orientation in this zigzag state and showed that, unexpectedly, it is along the 44.3 degrees direction with respect to a axis, which is approximately half way in between the cubic x and y axes. This experiment provides an important check of the validity of any model proposed to describe the magnetic properties of Na<sub>2</sub>IrO<sub>3</sub> as the model should correctly predict not only the type of the magnetic order but also its orientation in space. We propose that order by disorder mechanism in quantum J1-K1-J2-K2-J3 model [2] gives the experimentally observed direction along cubic face diagonals. Our findings are based on both the calculation of the contribution of thermal fluctuations of quantum spins into free energy obtained by Hubbard-Stratonovich transformation and the zero-point correction to the ground state energy due to quantum spin fluctuations obtained by the spin-wave expansion at zero temperature. [1] S. H. Chun et al, Nature Physics 10, 1038 (2015).? [2] Y. Sizyuk, C. Price, P. Woelfle, and N. B. Perkins, Phys. Rev. B 90, 155126 (2014).

<sup>1</sup>NSF Grant DMR-1511768

## **Wednesday, March 16, 2016 11:15AM - 2:15PM –**

**Session L34 FOEP: Forum on Outreach and Engaging the Public** 337 - Yvan Bruynseraede, University of Leuven

**11:15AM L34.00001 How to interact with Congress about Science**, RAYMOND ORBACH, The University of Texas at Austin — The role of Congress is critical to the success of the scientific enterprise, both in terms of authorization and appropriation. As a consequence, it is very important to make the case for science directly with Congress. Every scientist has a representative in the House of Representatives in whose district he/she lives, and in the Senate. Constituents are especially welcomed in their offices. A personal visit is the most effective means for transmitting the importance of science in general, and physics in particular. The AAAS website lists the "Top Ten Rules for Working With Congress." They are: (1) Know your goal; (2) Understand how Congress works; (3) Conduct detailed background research; (4) Determine the timing of your course of action; (5) Be clear and succinct; (6) Understand Congressional staff and their influence; (7) Provide concrete suggestions; (8) Present support of science as a means to meet national and local goals, not as an entitlement; (9) Be willing to say "I don't know"; and (10) Follow up appropriately. Each of these will be described in more detail during the presentation. The March Meeting is an example of a particularly important time period for meeting with representatives (Rule #4). The President's Budget Request has been submitted to Congress, and the individual appropriation subcommittees are in the process of developing their respective "mark ups." Appointments with members or their staff is now timely, and urgent. Authorization bills are also in play, and can have significant impact on the scientific community. Paying attention to their development in key committees (e.g. the Science, Space, and Technology Committee of the House of Representatives), and providing appropriate and timely input, is the responsibility of every scientist.

**11:51AM L34.00002 How to organize a World Renowned Science Festival**, MARC SCHULMAN, USA Science and Engineering Festival — No abstract available.

**12:27PM L34.00003 How to write a scientist based biography for the public**, JOEL SHURKIN, Editor — No abstract available.

**1:03PM L34.00004 How Physics World reaches out in a digital age**, MATIN DURRANI, Editor, Physics World — Physics World is an award-winning international magazine that exists in print and digital formats. Exploiting the opportunities available with digital publishing and apps, our output has expanded hugely in recent years to include technology-linked focus issues, regional special reports on the likes of China, India, Mexico and Brazil, plus audio, video and interactive material too. This growth in content - and new media for presenting physics - reflects wider changes in communication. People increasingly want to access content in a manner and time of their choosing, seeking out information presented in a way that suits them and their needs. That can be challenging for physics communicators because it means tailoring your message to different audiences and the medium they are using. But it's exciting too as you can reach out to many more people into physics - and in many different ways - than was possible in the past. This talk outlines some principles of good communication, including telling a good story, bearing the reader, viewer or listener in mind, using appropriate media, keeping up with social media, and exploiting the power of video. But with new forms of communication constantly emerging, it's worth remembering there is no one "right answer".

**1:39PM L34.00005 Physics in a Brewery**, JEREMIE PALACCI, UC, San Diego — Looking through the glass, and what Physics found there. A story of beer. Bubbles, heads and temperature make for a great pint, and a vast playground for the physicist. We will discuss a variety of aspects of the science of beer and reflect on the rational of the tricks pulled by professional brewers! – In partnership with Mike Hess Brewery, San Diego.

## **Wednesday, March 16, 2016 11:15AM - 2:15PM –**

**Session L35 DMP: Thermoelectrics Low Dimensional Materials** 338 - Jeff Urban, Lawrence Berkeley National Laboratory

**11:15AM L35.00001 Reversible electron-hole separation in a hot carrier solar cell**, HEINER LINKE, Lund University — Hot-carrier solar cells are envisioned to utilize energy filtering to extract power from photogenerated electron-hole pairs before they thermalize with the lattice, and thus potentially offer higher power conversion efficiency compared to conventional, single absorber solar cells. The efficiency of hot-carrier solar cells can be expected to strongly depend on the details of the energy filtering process, a relationship which to date has not been satisfactorily explored. Here, we establish the conditions under which electron-hole separation in hot-carrier solar cells can occur reversibly, that is, at maximum energy conversion efficiency. We find that, under specific conditions, the energy conversion efficiency of a hot-carrier solar cell can exceed the Carnot limit set by the intra-device temperature gradient alone, due to the additional contribution of the quasi-Fermi level splitting in the absorber. To achieve this, we consider a highly selective energy filter such as a quantum dot embedded into a one-dimensional conductor. We also establish that the open-circuit voltage of a hot-carrier solar cell is not limited by the band gap of the absorber, due to the additional thermoelectric contribution to the voltage. Additionally, we find that a hot-carrier solar cell can be operated in reverse as a thermally driven solid-state light emitter. In addition this theoretical analysis, I will also report on first experimental results in a nanowire-based energy filter device. Ref: S Limpert, S Bremner, and H Linke, New J. Phys 17, 095004 (2015)

**11:51AM L35.00002 Thermionic energy conversion in carbon nanotube networks**, CHEN LI, KEVIN PIPE, University of Michigan - Ann Arbor, KEVIN PIPE'S GROUP TEAM — We investigate whether efficient carrier ballistic transport in CNT networks can overcome the parasitic effects of high CNT thermal conductance to yield thermionic (TI) devices with high energy conversion efficiency and/or high cooling power density. We simulate semiconducting single-walled carbon nanotube (SWCNT) structures in which inter-tube junctions provide the necessary filtering of high-energy electrons. Using energy-dependent transmission functions, we compare the performances of various junction types in selective filtering, and then perform Monte Carlo (MC) simulations to study the subsequent relaxation of hot electrons within the SWCNTs. Finally, we examine the parasitic effects of high thermal conductance, accounting for reductions in phonon mean free path due to scattering at inter-tube junctions. The results of the junction transmission, MC, and phonon transport simulations suggest optimal CNT types, junction types, and inter-junction spacings that maximize energy conversion metrics such as efficiency and cooling power density. While certain aspects of electron transport and phonon transport in CNT networks remain unresolved, our simulations suggest that CNT-based networks show promise for TI energy conversion.

**12:03PM L35.00003 Enhanced Thermoelectric Properties in Tailored Semiconducting SWCNT Networks**, A.D. AVERY, Metropolitan State University of Denver, B.H. ZHOU, National Renewable Energy Laboratory, J. LEE, E. LEE, Korea Advanced Institute of Science and Technology, E.M. MILLER, R. IHL, National Renewable Energy Laboratory, D. WESENBERG, University of Denver, K.S. MISTRY, S.L. GUILLOT, National Renewable Energy Laboratory, B.L. ZINK, University of Denver, Y. KIM, Korea Advanced Institute of Science and Technology, J.L. BLACKBURN, A.J. FERGUSON, National Renewable Energy Laboratory — Single-walled carbon nanotubes (SWCNTs) are a versatile electronic material being explored as cost-effective, high-performance alternative in a variety of renewable energy applications. In this talk, we present a series of experiments designed to probe the thermal and electrical transport through networks of semiconducting SWCNT dispersed in matrices of polyfluorene polymers. We measured electrical transport as a function of hole density to explore the coupling between the electrical conductivity and Seebeck coefficient (thermopower) in the s-SWCNT networks. These networks exhibit large thermopowers  $> 1000 \mu\text{V/K}$  at very low hole densities. Thermopower values remain high at high doping levels, resulting in thermoelectric power factors greater than  $340 \mu\text{W/m K}$ . Finally, we present measurements that demonstrate our doping process significantly reduces the thermal conductivity relative to undoped networks suggesting s-SWCNTs are a viable material for realizing thermally stable room temperature thermoelectric devices fashioned from inexpensive and abundant organic constituents.

**12:15PM L35.00004 Effects of Defects and Strain on Thermoelectric Properties of Single-walled Carbon Nanotubes<sup>1</sup>**, MASATO OHNISHI, TAKUMA SHIGA, JUNICHIRO SHIOMI, Univ of Tokyo — Carbon nanotubes (CNTs) have attracted much attention as a thermoelectric material. Although CNTs have large lattice thermal conductivity, CNT-based composites are promising candidates for thermoelectric material because the phonon transport is suppressed by scattering at contacts between CNTs. Therefore, previous studies have mainly focused on thermoelectric properties at contacts between CNTs. However, understanding the effects of defects and strain on the thermoelectric properties of CNTs themselves are important because they exist inevitably in real systems. In this study, we study the effects of defects, vacancy and Stone-Wales defect, and uniaxial compressive strain on single-walled CNTs (SWNTs) employing nonequilibrium molecular dynamics simulation and Green's function method. We find that the defects and buckling deformation significantly decrease electron conductance, and the effect is much stronger than that on thermal conductivity and Seebeck coefficient, resulting in severe reduction of the figure of merit. In addition, the estimation of thermoelectric performance including a inter-SWNT contact indicates that the effect of defects and strain can deteriorate the figure of merit of the SWNT networks.

<sup>1</sup>This work is partially supported by Thermal Management Materials and Technology Research Association (TherMAT).

**12:27PM L35.00005 Photoinduced thermoelectric transport in solution-processed semiconductors**, NELSON COATES, CSU Maritime, FAN YANG, AYASKANTA SAHU, JEFFREY URBAN, Lawrence Berkeley National Lab — The ability to fabricate semiconductor materials directly from solution offers a number of advantages over traditional semiconductor processing routes. In addition to the generally lower costs of manufacturing and ability to scale device to large areas, solution-based fabrication techniques also easily allow for extensive physical and chemical tuning of the processed materials. Here, we examine ways to tune the photoinduced thermoelectric transport in solution-processed semiconductors, and in particular explore ways to leverage some of the inherent characteristics of solution processed semiconductors (such as electronic inhomogeneity and large trap densities) to improve the photoinduced thermoelectric response in these materials.

**12:39PM L35.00006 Large local temperature gradient induced by surface plasmon heating of periodic metal structure**, RYOKO SHIMADA, HITOMI SAKAI, Japan Women's University — Mixtures of several gas or solution having different concentration can be separated by the gradient of temperature. This is the so-called Soret effect. This phenomenon is quite important for chemical reaction and material condensation/separation. For activating large Soret effect, it would be useful to focus on the surface plasmon heating (SPH) of metal nanostructures that interact with light. In this work, a local temperature gradient was created with the aid of SPH achieved for periodic silver structures in a mesoscopic length scale fabricated by a nanosphere lithography method. Excitation of this periodic structure (by blue laser, for example) could create a localized periodic temperature gradient, as large as  $\sim 1,000 \text{ K}/\mu\text{m}$ , as suggested from preliminary heat-transfer calculation. Experimental and theoretical results will be presented on site

**12:51PM L35.00007 Valley caloritronics and its realization by graphene nanoribbons<sup>1</sup>**, XIAOBIN CHEN, LEI ZHANG, HONG GUO, McGill University — We propose and theoretically investigate a new idea of **valley caloritronics** where quantum transport of the valley degrees of freedom is thermally induced. Valley caloritronics addresses questions such as thermal generation of valley polarized current and more importantly, pure valley current without an accompanying charge current. After establishing a general physical picture, we show that heat-induced pure valley current can be generated by virtue of wedge-shaped graphene nanoribbons in a two-probe device setup. We discover that the quantum transport properties of the valley degree of freedom can be very different when driven by a voltage bias or by a temperature bias. A very surprising result is that an alternating valley current can be *thermally* generated via gate control: namely the heat-induced valley current changes its flow direction in some quasi-periodic manner versus the value of a gate voltage at a fixed polarity. Our results indicate a vast potential for developing valley caloritronic devices.

<sup>1</sup>NSERC, CSC, MESRS, Calcul Québec, and Compute Canada

**1:03PM L35.00008 Theoretical studies on performance evaluation of solar thermoelectronic energy converter with graphene emitter**, OLUKUNLE OLAWOLE<sup>1</sup>, DILIP DE<sup>2</sup>, Department of Physics, Covenant University, Ota, Nigeria — In this paper we consider detailed energy dynamics of solar thermoelectronic energy converter using graphene as the emitter. The emitter is heated by solar energy concentrated by a parabolic mirror concentrator. We study the performance evaluation of the energy conversion using temperature dependent work function of graphene and model the space charge problem by introducing a factor in the emitter and collector current densities. We present computations on power output and efficiency as function of solar insolation, height of emitter from the base of the mirror, reflection coefficient of the mirror, temperature and work function of collector. Effect of molecular doping on the performance of the graphene solar tech is also discussed.

<sup>1</sup>Please schedule our papers so that they are well separated in time for presentations.

<sup>2</sup>Please send notification of acceptance also to the second author

**1:15PM L35.00009 Graphene-based vdW heterostructure Induced High-efficiency Thermoelectric Devices.** , SHIJUN LIANG, LAY KEE ANG, Singapore University of Technology and Design — Thermoelectric material (TE) can convert the heat into electricity to provide green energy source and its performance is characterized by a figure of merit (ZT) parameter. Traditional TE materials only give ZT equal to around 1 at room temperature. But, it is believed that materials with  $ZT > 3$  will find wide applications at this low temperature range. Prior studies have implied that the interrelation between electric conductivity and lattice thermal conductivity renders the goal of engineering ZT of bulk materials to reach  $ZT > 3$ . In this work, we propose a high-efficiency van der Waals (vdW) heterostructure-based thermionic device with graphene electrodes, which is able to harvest wasted heat (around 400K) based on the newly established thermionic emission law of graphene electrodes instead of Seebeck effect, to boost the efficiency of power generation over 10% around room temperature. The efficiency can be above 20% if the Schottky barrier height and cross-plane lattice thermal conductivity of transition metal dichalcogenides (TMD) materials can be fine-engineered. As a refrigerator at 260 K, the efficiency is 50% to 80% of Carnot efficiency. Finally, we identify two TMD materials as the ideal candidates of graphene/TMD/graphene devices based on the state-of-art technology.

**1:27PM L35.00010 Printable Graphene-based Thermoelectric Device with High Temperature Capability** , TIAN LI, YANAN CHEN, DENNIS DREW, LIANGBING HU, University of Maryland, College Park, NANOMATERIALS FOR EMERGING DEVICES COLLABORATION — Thermoelectric devices are of particular interest due to their capability to convert heat into electrical power. We demonstrate the use of a Graphene-based thermoelectric device that can generate output voltages of hundreds of millivolts with an illuminating Graphene strip as the blackbody source. Our proposed device is superior for thermoelectric conversion mainly due to its high temperature capability that yields a maximum Carnot efficiency limit of 90% (referenced to room temperature) and a high Seebeck coefficient. Our device is also macroscopic with good mechanical strength and stabilized performance, making it attractive for large scale and reliable thermoelectric devices.

**1:39PM L35.00011 Thermal conductivity and rectification study of restructured Graphene** , ANUJ ARORA, University of Tokyo — Electronics' miniaturization, has led to search for better thermal management techniques and discovery of important transport phenomenon. Thermal rectification, directionally preferential heat transport analogous to electrical diode, is one such technique, garnering tremendous interest. Its possibility has been explored through structural asymmetry, introducing a differential phonon density of states in hot and cold regions. As of now, mass and shape asymmetries have been studied, both experimentally and theoretically. However, strict requirements of material length being shorter than phonon mean free path and phonon coherence preservation at surface, makes connecting two materials with different temperature-dependent thermal conductivities, a more natural approach. To avoid resultant thermal boundary resistance and integration complexities, we achieve the affect in single material, by restructuring a region of Graphene by introducing defects. The asymmetry impedes ballistic phonon transport, modulating temperature dependence of thermal conductivity in the two regions. We perform deviational Monte Carlo simulations based on Energy-based formulation to microscopically investigate phonon transport, possibility and optimal conditions for thermal rectification. The proposed method uses phonon properties obtained from first principle, treat phonon-boundary scattering explicitly with properties drawn from Bose-Einstein Distribution.

**1:51PM L35.00012 Experimental Studies of Graphene Antidot Lattices for Thermoelectric Applications<sup>1</sup>** , QING HAO, DONGCHAO XU, HONGBO ZHAO, Department of Aerospace and Mechanical Engineering, University of Arizona, XU DU, Department of Physics, Stony Brook University — Pristine graphene has low thermoelectric performance due to its ultra-high thermal conductivity and zero band gap that leads to a low Seebeck coefficient ( $S$ ). Both issues can be addressed by patterning periodic nano- or sub-1-nm pores (antidots) across graphene, called graphene antidot lattices (GALs). In GALs, a geometry-dependent band gap can be opened up to dramatically increase  $S$ , with significantly reduced thermal conductivity ( $k$ ) due to phonon scattering by antidots. Above will lead to a high thermoelectric figure of merit ( $\sim 1.0$  at 300 K by computations [1]) in GALs to be used for device cooling. Despite numerous calculations, experimental studies of GALs are restricted to electrical conductivity ( $\sigma$ ) measurements for GALs with  $\sim 10$  nm patterns. The critical  $k$  measurements are still lacking. In this work, all three thermoelectric properties ( $S$ ,  $k$ , and  $\sigma$ ) are measured on suspended GALs with sub-10 nm pores. In comparison, electrical properties are also characterized for GALs on a substrate. The results presented here provide important guidance on how to tailor transport properties of general two-dimensional materials with ALs. References: [1] Yan et al., Physics Letters A 376, 2425-2429 (2012).

<sup>1</sup>Qing Hao acknowledges the support from the Young Investigator Program of U.S. Air Force Office of Scientific Research (grant FA9550-15-1-0403)

**2:03PM L35.00013 Ab initio design of low work function complex oxides for thermionic energy conversion** , STEPHANIE MACK, UC Berkeley, GUO LI, Molecular Foundry, LBNL; Joint Center for Artificial Photosynthesis, JEFFREY NEATON, UC Berkeley; Molecular Foundry, LBNL; Kavli Energy Nanosciences Institute at Berkeley — Understanding and controlling work functions, or band edge energies, is of interest for a variety of applications in optoelectronics and energy conversion. In particular, while recent advances in device design have improved the feasibility of thermionic generators, new low work function materials are needed to enable their widespread use. Perovskite-based oxides ( $ABO_3$ ) are a diverse class of materials that, depending on the transition metal atoms on the A and B sites, can give rise to myriad emergent and collective phenomena. Here, we use density functional theory calculations to examine how the work function of one such oxide, SrRuO<sub>3</sub> (SRO), can be tuned by monolayers of SrTiO<sub>3</sub> (STO) and other polar or near-polar oxides. We find that SRO work functions can be tuned by over 1 eV with one layer of STO, although the calculated reduction in work function is an order of magnitude less than would be expected from the bulk polarization. We understand the variation in work function via a detailed analysis of Born effective charges at the surface, which are as small as 10% of their bulk values, and charge rearrangement at the STO surface and SRO/STO interface.

**Wednesday, March 16, 2016 11:15AM - 2:15PM –**

**Session L40 GSNP GSOF: Geometry and Dynamics of Slender Structures** 343 - James Hanna, Virginia Tech

**11:15AM L40.00001 Hamiltonian formulations in the computation of extremely deformed nano-scale hyper-elastic rods.** , JOHN H. MADDOCKS, EPFL FSB MATHGEOM LCVMM — There has been a recent resurgence of interest in models exploiting elastic filaments and ribbons, motivated in large part by nano-scale applications, including DNA. Such models are frequently nearly inextensible or nearly unsharable. I will describe how such systems can be modelled as a smooth limit within a hierarchy of perturbed Hamiltonian formulations of the governing equations. Examples include a sequence-dependent double-strand birod model of DNA, where a more familiar rod model can be obtained as a smooth limit in which the intra-strand degrees of freedom are frozen..

**11:51AM L40.00002 A conserved quantity in thin body dynamics** , JAMES HANNA, HODJAT PENDAR, Virginia Tech — We use an example from textile processing to illustrate the utility of a conserved quantity associated with metric symmetry in a thin body. This quantity, when combined with the usual linear and angular momentum currents, allows us to construct a four-parameter family of curves representing the equilibria of a rotating, flowing string. To achieve this, we introduce a non-material action of mixed Lagrangian-Eulerian type, applicable to fixed windows of axially-moving systems. We will point out intriguing similarities with Bernoulli's equation, discuss the effects of axial flow on rotating conservative systems, and make connections with 19th- and 20th-century results on the dynamics of cables.

**12:03PM L40.00003 Tearing of thin spherical shells adhered to equally curved rigid substrates**, CONNOR MCMAHAN, ANNA LEE, JOEL MARTHELOT, PEDRO REIS, Massachusetts Institute of Technology — Lasik (Laser-Assisted in Situ Keratomileusis) eye surgery involves the tearing of the corneal epithelium to remodel the corneal stroma for corrections such as myopia, hyperopia and astigmatism. One issue with this procedure is that during the tearing of the corneal epithelium, if the two propagating cracks coalesce, a flap detaches which could cause significant complications in the recovery of the patient. We seek to gain a predictive physical understanding of this process by performing precision desktop experiments on an analogue model system. First, thin spherical shells of nearly uniform thickness are fabricated by the coating of hemispherical molds with a polymer solution, which upon curing yields an elastic and brittle structure. We then create two notches near the equator of the shell and tear a flap by pulling tangentially to the spherical substrate, towards its pole. The resulting fracture paths are characterized by high-resolution 3D digital scanning. Our primary focus is on establishing how the positive Gaussian curvature of the system affects the path of the crack tip. Our results are directly contrasted against previous studies on systems with zero Gaussian curvature, where films were torn from planar and cylindrical substrates.

**12:15PM L40.00004 Cracks in Sheets Draped on Curved Surfaces**, NOAH P. MITCHELL, James Franck Institute, University of Chicago, VINZENZ KONING, VINCENZO VITELLI, Instituut-Lorentz for Theoretical Physics, Universiteit Leiden, WILLIAM T.M. IRVINE, James Franck Institute, University of Chicago — Conforming materials to surfaces with Gaussian curvature has proven a versatile tool to guide the behavior of mechanical defects such as folds, blisters, scars, and pleats. In this talk, we show how curvature can likewise be used to control material failure. In our experiments, thin elastic sheets are confined on curved geometries that stimulate or suppress the growth of cracks, and steer or arrest their propagation. By redistributing stresses in a sheet, curvature provides a geometric tool for protecting certain regions and guiding crack patterns. A simple model captures crack behavior at the onset of propagation, while a 2D phase-field model successfully captures the crack's full phenomenology.

**12:27PM L40.00005 Pick-up, impact, and peeling.**, HARMEET SINGH, JAMES HANNA, Virginia Tech — We consider a class of problems involving a one-dimensional, inextensible body with a propagating discontinuity (shock) associated with partial contact with a rigid obstacle providing steric, frictional, or adhesive forces. This class includes the pick-up and impact of an axially flowing string or cable, and the peeling of an adhesive tape. The dynamics are derived by applying an action principle to a non-material volume. The resulting boundary conditions provide momentum and energy jump conditions at the shock. These are combined with kinematic conditions on velocities and accelerations to obtain families of steady-state solutions parameterized by the shock velocity and momentum and energy sources. We find relationships between the jump in stress, injection of momentum, and dissipation of energy, which we apply to specific cases, and compare with other results in the literature on chain fountains, falling folded chains, and impulsively loaded cables. Time permitting, we will briefly discuss the possibility of using kinematic conditions and information about accelerating or otherwise unsteady forms of the adjoining bulk solutions to construct an equation of motion of the shock.

**12:39PM L40.00006 Effect of boundary conditions on the buckling instabilities of a ribbon under twist<sup>1</sup>**, CASEY TRIMBLE, ARSHAD KUDROLLI, Department of Physics, Clark University — We investigate the buckling instabilities of a thin flat sheet in the shape of a ribbon which is held at its ends and twisted under tension. Recently it was shown that such a system with clamped boundary conditions exhibited a rich variety of buckled shapes with longitudinal and transverse wrinkles as a function of applied twist and tension for a given ribbon aspect ratio and elastic modulus [1], which could be described by a far from threshold analysis of the covariant form of the Foppl-von Karman equations [2]. Here, we focus on the effect of the boundary conditions on the observed buckling patterns by constraining the ends only at the midpoint towards imposing free boundary conditions normal to the ribbon. In particular, we compare and contrast the observed phase diagram and the shape of the longitudinal and transverse buckled modes as a function of applied constraints. [1] J. Chopin and A. Kudrolli, Phys. Rev. Lett. 111, 174302 (2013). [2] J. Chopin, V. Demery, and B. Davidovitch J. Elast. 119, 137 (2015).

<sup>1</sup>Supported by NSF DMR - 1508186

**12:51PM L40.00007 Multi-stability and bifurcations of a thin band.**, TIAN YU, JAMES HANNA, Department of Biomedical Engineering and Mechanics, Virginia Tech — Thin band- or strip-like structures are common motifs in flexible and deployable systems, serving as integrated connectors, hinges, and umbilicals. The morphing systems impose variable constraints on these components, inducing complex responses. We experimentally investigate a simple configuration representing the above type, a thin elastic band with end constraints on position and orientation. These constraints correspond to a combination of compression and shear with respect to a flat rectangular rest configuration. We vary the aspect ratio of the band, and the position and clamping angle at its ends. The buckled structure remains developable up to limiting deformations that approach one of two states, each dominated by two singularities. At intermediate deformations, the structure may adopt many distinct stable states. Transitions between these states can be smooth or violent, and depend strongly on constraints such as the clamping angle. Time permitting, we will relate our results to the behavior of anisotropic rods, and of strips subjected to twisting and extension.

**1:03PM L40.00008 Finite and infinite wavelength elastocapillary instabilities with cylindrical geometry**, JOHN BIGGINS, CHEN XUAN<sup>1</sup>, Cambridge University — In an elastic cylinder with shear modulus  $\mu$ , radius  $R_0$  and surface tension  $\gamma$  we can define an emergent elastocapillary length  $l = \gamma/\mu$ . When this length becomes comparable to  $R_0$  the cylinder becomes undergoes a Rayleigh-Plateau type instability, but surprisingly, with infinite wavelength  $\lambda$  rather than with wavelength  $\lambda \sim R_0 \sim l$ . Here we take advantage of this infinite wavelength behaviour to construct a simple 1-D model of the elastocapillary instability in a cylindrical gel which permits a high-amplitude fully non-linear treatment. In particular, we show that the instability is sub-critical and entirely dependent on the elastic cylinder being subject to tension. We also discuss elastocapillary instabilities in a range of other cylindrical geometries, such a cylindrical cavities through a bulk elastic solid, or a solid cylinder embedded in a bulk elastic solid, and show that in these cases instability has finite wavelength. Thus infinite wavelength behaviour is a curiosity of elastic cylinders rather than the generic behaviour or elasto-capillarity.

<sup>1</sup>also Fudan University Shanghai

**1:15PM L40.00009 Sequential buckling of an elastic wall<sup>1</sup>**, JOSE BICO, HADRIEN BENSE, LUDOVIC KEISER, BENOIT ROMAN, PMMH, ESPCI, Paris, France, FRANCISCO MELO, Universidad de Santiago de Chile, MANOUK ABKARIAN, Centre de Biochimie Structurale, Montpellier, France — A beam under quasistatic compression classically buckles beyond a critical threshold. In the case of a free beam, the lowest buckling mode is selected. We investigate the case of a long wall grounded of a compliant base and compressed in the axial compression. In the case of a wall of slender rectangular cross section, the selected buckling mode adopts a nearly fixed wavelength proportional to the height of the wall. Higher compressive loads only increase the amplitude of the buckle. However if the cross section has a sharp shape (such as an Eiffel tower profile), we observe successive buckling modes of increasing wavelength. We interpret this unusual evolution in terms of scaling arguments. At small scales, this variable periodicity might be used to develop tunable optical devices.

<sup>1</sup>We thank ECOS C12E07, CNRS-CONICYT, and Fondecyt Grant No. N1130922 for partially funding this work.

**1:27PM L40.00010 Mechanics of a Knitted Fabric<sup>1</sup>** , SAMUEL POINCLOUX, FREDERIC LECHENAULT, MOKHTAR ADDA-BEDIA, Laboratoire de Physique Statistique, Ecole Normale Supérieure, 24 rue Lhomond, 75005 Paris, France — A simple knitted fabric can be seen as a topologically constrained slender rod following a periodic path. The non-linear properties of the fabric, such as large reversible deformation and characteristic shape under stress, arise from topological features known as stitches and are distinct from the constitutive yarn properties. Through experiments we studied a model stockinette fabric made of a single elastic thread, where the mechanical properties and local stitch displacements were measured. Then, we derived a model based on the yarn bending energy at the stitch level resulting in an evaluation of the displacement fields of the repetitive units which describe the fabric shape. The comparison between the predicted and the measured shape gives very good agreement and the right order of magnitude for the mechanical response is captured. This work aims at providing a fundamental framework for the understanding of knitted systems, paving the way to thread based smart materials.

<sup>1</sup>Contract ANR-14-CE07-0031-01 METAMAT

**1:39PM L40.00011 Crumpling of an Elastic Ring in Two Dimensions** , CARTER VANHUSS, SHENGFENG CHENG, Department of Physics & Macromolecules and Interfaces Institute, Virginia Polytechnic Institute and State University — We use molecular dynamics simulations to study the crumpling of an elastic ring (i.e., a circular elastic line) in two dimensions. The crumpling is triggered by reducing the radius of a circular repulsive wall that is used to confine the ring. The ring is modeled as a bead-spring chain. A harmonic potential describing the bonds between neighboring beads is parameterized to reproduce the Young's modulus of the elastic line in the continuum limit. A modified harmonic angle interaction is used to capture the bending of the elastic line including situations where the line is locally stretched or compressed. We have confirmed that the bead-spring model has the correct continuum limit by comparing results on rings made of different numbers of beads but with parameters derived from the same elastic line. With the computational model, we study the morphological transition of the ring and the local distribution of the bond and bending energies as the ring is compressed at various rates, forced to crumple, and finally confined into a dense-packed structure. We find that the crumpling transition signals a sharp energy transfer from the compression to the bending mode. We further explore the possibility of defining an effective temperature for such crumpled systems.

**1:51PM L40.00012 Natural Curvature as Effective Confinement in Elastic Sheets** , OCTAVIO ALBARRAN, Max Planck Institute for Dynamics and Self-Organization, ELENI KATIFORI, University of Pennsylvania, LUCAS GOEHRING, Max Planck Institute for Dynamics and Self-Organization — The wrinkling and folding transitions of thin elastic sheets have been extensively studied in the last decade. The exchange of energy from stretching to bending acts as a paradigm for a wide range of elastic instabilities, including the wrinkling of the gut, and the crinkling of leaves. In two dimensions this type of problem is typically considered by the model of an Euler-*elastica* in compressive confinement. We show that, even without any external forces, an elastic surface supported by a fluid can bend and wrinkle when it acquires a non-zero natural curvature. Locally, we will demonstrate how a preferential curvature can be related to an effective compression, and hence a confining force that can vary spatially. This suggests a simple experimental setup, where we have characterised a variety of wrinkle patterns that can be generated for different mechanical properties and natural curvatures.

**2:03PM L40.00013 Anomalously soft non-Euclidean spring** , IDO LEVIN, ERAN SHARON, Hebrew Univ of Jerusalem — In this work we study the mechanical properties of a frustrated elastic ribbon spring - the non-Euclidean minimal spring. This spring belongs to the family of non-Euclidean plates: it has no spontaneous curvature, but its lateral intrinsic geometry is described by a non-Euclidean reference metric. The reference metric of the minimal spring is hyperbolic, and can be embedded as a minimal surface. We argue that the existence of a continuous set of such isometric minimal surfaces with different extensions leads to a complete degeneracy of the bulk elastic energy of the minimal spring under elongation. This degeneracy is removed only by boundary layer effects. As a result, the mechanical properties of the minimal spring are unusual: the spring is ultra-soft with rigidity that depends on the thickness,  $t$ , as  $t^{7/2}$ , and does not explicitly depend on the ribbon's width. These predictions are confirmed by a numerical study of a constrained spring. This work is the first to address the unusual mechanical properties of constrained non-Euclidean elastic objects. We also present a novel experimental system that is capable of constructing such objects, along with many other non-Euclidean plates.

## Wednesday, March 16, 2016 11:15AM - 2:15PM –

Session L42 FIAP DPOLY: Industry Day Plenary Session 345 - Jeffrey Hunt, Boeing, Inc.

**11:15AM L42.00001 Antithetical Polymers: Performance Through Structured Incompatible Elements** , A.P. NOWAK, HRL Laboratories, 3011 Malibu Canyon Rd, Malibu, CA — Modern coating technology is often limited by a complex trade space that leaves many applications poorly served. Next generation coatings able to successfully meet these application challenges typically require multiple and often contradictory properties not easily met with traditional homogenous compositions. This presentation describes our efforts to combine highly incompatible coating elements capable of organizing into discrete regions at mesoscopic length scales (0.1-10  $\mu\text{m}$ ) in order to express multiple undiluted physical properties of individual components at the macroscopic scale. Such a strategy requires understanding and controlling the interactions between composition and processing that ultimately drive microstructure and performance. Specific examples presented will include anti-fouling coatings where we have combined a low surface energy component with a lubricating region or anti-freeze element to mitigate accumulation of insect debris or delay freezing, respectively. In collaboration with the following: A.F. Gross, A.R. Rodriguez, E. Sherman, C. Ro, S. Yang, M. Behroozi, and B. Fong, HRL Laboratories, 3011 Malibu Canyon Rd, Malibu, CA

**11:51AM L42.00002 Predicting the In-Service Lifetime of Polymers: A multi-scale modeling approach.** , OM PRAKASH, Boeing Research & Technology India Centre, Bangalore 560016, India — Recent advances in theoretical chemistry have enabled a predictive approach to assessing polymer behaviors without lifetime testing. We report on progress in this area. In collaboration with the following: Priya Parandekar and Nishant Sinha, Boeing Research & Technology India Centre, Bangalore 560016, India

**12:27PM L42.00003 Understanding network forming reactions and properties through combining computational and experimental methods** , JEANNETTE M. GARCIA, IBM Almaden, San Jose CA — Poly(hexahydrotriazine)s (PHTs) represent a class of synthetically tunable and dynamic materials that exhibits broad scope in thermal and mechanical properties. Depending on monomer choice, these thermosets can range from elastomeric and self-healing to strong and brittle. Highly crosslinked thermosetting networks such as these have limited solubility in organic solvents; thus, solid-state analysis was coupled with *in silico* methods to characterize structure-property relationships. Density functional theory (DFT) on small-molecule model systems and molecular dynamics (MD) simulations on network-formation provided a rationale for observed properties and guided ensuing experiments. This talk will focus on the combination of experimental efforts with computational analysis to develop and design new polymeric materials with targeted properties.

1:03PM L42.00004 TBD –

1:39PM L42.00005 TBD –

# Wednesday, March 16, 2016 11:15AM - 1:51PM –

Session L43 GSNP: Complex Networks and their Applications II 346 - Mason Porter, Oxford University

**11:15AM L43.00001 Flexible embedding of networks**, JUAN FERNANDEZ-GRACIA, CAROLINE BUCKEE, JUKKA-PEKKA ONNELA, Harvard T.H. Chan School of Public Health — We introduce a model for embedding one network into another, focusing on the case where network A is much bigger than network B. Nodes from network A are assigned to the nodes in network B using an algorithm where we control the extent of localization of node placement in network B using a single parameter. Starting from an unassigned node in network A, called the source node, we first map this node to a randomly chosen node in network B, called the target node. We then assign the neighbors of the source node to the neighborhood of the target node using a random walk based approach. To assign each neighbor of the source node to one of the nodes in network B, we perform a random walk starting from the target node with stopping probability  $\alpha$ . We repeat this process until all nodes in network A have been mapped to the nodes of network B. The simplicity of the model allows us to calculate key quantities of interest in closed form. By varying the parameter  $\alpha$ , we are able to produce embeddings from very local ( $\alpha = 1$ ) to very global ( $\alpha \rightarrow 0$ ). We show how our calculations fit the simulated results, and we apply the model to study how social networks are embedded in geography and how the neurons of C. Elegans are embedded in the surrounding volume.

**11:27AM L43.00002 Exploring many-body physics with deep networks**, GIACOMO TORLAI, University of Waterloo, JUAN CARRASQUILLA, Perimeter Institute, DAVID SCHWAB, Northwestern University, ROGER MELKO, University of Waterloo — The introduction of neural networks with deep architecture has led to a revolution, giving rise to a new wave of technologies empowering our modern society. Although data science has been the main focus, the idea of generic algorithms which automatically extract features and representations from raw data is quite general and applicable in multiple scenarios. Motivated by the effectiveness of deep learning algorithms in revealing complex patterns and structures underlying data, we are interested in exploiting such tool in the context of many-body physics. In this talk we will focus on how to extract information about the physics of a many-body system from the generative training of a deep network, and ultimately consider discriminative tasks, such as phase diagrams estimation and critical points detection. We will discuss results for different classical spin systems, including models with quenched disorder.

**11:39AM L43.00003 Random walks on networks<sup>1</sup>**, ISAAC DONNELLY, Northeastern — Random walks on lattices are a well used model for diffusion on continuum. They have been to model subdiffusive systems, systems with forcing and reactions as well as a combination of the three. We extend the traditional random walk framework to the network to obtain novel results. As an example due to the small graph diameter, the early time behaviour of subdiffusive dynamics dominates the observed system which has implications for models of the brain or airline networks.

<sup>1</sup>I would like to thank the Australian American Fulbright Association

**11:51AM L43.00004 The Impact of Selectivity on Fitness Evolution in the Multi-Generational Matching Problem<sup>1</sup>**, STEPHEN DIPPLE, TAO JIA, GYORGY KORNISS, BOLESŁAW SZYMANSKI, Rensselaer Polytechnic Institute — The stochastic matching hypothesis has been found to produce self-similar pairing without explicitly requiring self-similarity in the rules for matching. Here, we introduce an added complexity of selectivity in which the relative probability of being matched are modified.<sup>2</sup> This allows for probing in areas between the currently established matching hypothesis, random matching, and the extreme case of super selectivity, where only the very best fitness matches for nodes are created. A higher selectivity parameter has been found to indirectly increase the number of matches in the system monotonically. A fairly simple model is then implemented to produce offspring who inherit fitness based on the inherited fitness distribution which is a function of the parents' fitness. While the results show that the specific distribution used may limit the inherited quality factors to a too narrow range to be broadly applicable, the model does expose some interesting patterns in fitness evolution across multiple generations in the context of selectivity and network degree distribution.

<sup>1</sup>Supported in part by ARL NS-CTA and ONR.

<sup>2</sup>T. Jia, R.F. Spivey, B. Szymanski, G. Korniss, PLOS ONE 10(6): e0129804 (2015)

**12:03PM L43.00005 A matrix product algorithm for stochastic dynamics on locally tree-like graphs**, THOMAS BARTHEL, Duke University, Department of Physics, CATERINA DE BACCO, SILVIO FRANZ, Université Paris-Sud, LPTMS — In this talk, I describe a novel algorithm for the efficient simulation of generic stochastic dynamics of classical degrees of freedom defined on the vertices of locally tree-like graphs. Such models correspond for example to spin-glass systems, Boolean networks, neural networks, or other technological, biological, and social networks. Building upon the cavity method and ideas from quantum many-body theory, the algorithm is based on a matrix product approximation of the so-called edge messages – conditional probabilities of vertex variable trajectories. The matrix product edge messages (MPEM) are constructed recursively. Computation costs and accuracy can be tuned by controlling the matrix dimensions of the MPEM in truncations. In contrast to Monte Carlo simulations, the approach has a better error scaling and works for both, single instances as well as the thermodynamic limit. Due to the absence of cancellation effects, observables with small expectation values can be evaluated accurately, allowing for the study of decay processes and temporal correlations with unprecedented accuracy. The method is demonstrated for the prototypical non-equilibrium Glauber dynamics of an Ising spin system. Reference: arXiv:1508.03295.

**12:15PM L43.00006 Percolation transition in dynamical traffic network with evolving critical bottlenecks**, DAQING LI, BeiHang University — A critical phenomenon is an intrinsic feature of traffic dynamics, during which transition between isolated local flows and global flows occurs. However, very little attention has been given to the question of how the local flows in the roads are organized collectively into a global city flow. Here we characterize this organization process of traffic as “traffic percolation,” where the giant cluster of local flows disintegrates when the second largest cluster reaches its maximum. We find in real-time data of city road traffic that global traffic is dynamically composed of clusters of local flows, which are connected by bottleneck links. This organization evolves during a day with different bottleneck links appearing in different hours, but similar in the same hours in different days. A small improvement of critical bottleneck roads is found to benefit significantly the global traffic, providing a method to improve city traffic with low cost. Our results may provide insights on the relation between traffic dynamics and percolation, which can be useful for efficient transportation, epidemic control, and emergency evacuation.

**12:27PM L43.00007 Properties of the networks of same-spin sites in each Ising Model macrostate**, ROBERT HOSKEN, The Aerospace Corporation — An Ising Model macrostate contains all the microstates with the same energy. Each macrostate is labeled in an energy two-space by the two sums in the Hamiltonian, one for the magnetism and the other for the interaction energy. In a single macrostate, a network can be defined for all the up-spin sites and another network for all the down-spin sites. An exact formula has been derived that explicitly provides the total number of connection links (edges) in both of these macrostate networks. This derivation follows from a meticulous analysis of the calculation of the sum of the product of spins in the Hamiltonian. It is applicable to one, two, and three dimension Ising models with periodic boundary conditions. The formula permits calculation of the total number of nearest-neighbor connections for all of the sites, and thus the average number of connections per site. The number of connections can be used to calculate the probability that a nearest neighbor in a particular direction at a spin site has the same spin. This probability can be used to infer the closeness of any macrostate to the ferromagnetic ground states, the paramagnetic region, or the anti-ferromagnetic ground states. Note that these properties of each macrostate do not require knowledge of the number of microstates in the macrostate (the density of states).

**12:39PM L43.00008 Upper Bound for the Ordering Transition on an Ising Model on a Graph**, TIMOTHY DOWNING, LEONID PRYADKO, Univ of California - Riverside — We present an upper bound for the ordering transition of a ferromagnetic Ising model on a graph. Namely, we show that at any given temperature, the magnetic susceptibility per spin cannot exceed that on an infinite tree, the universal cover of the original graph. Exact solution of the Ising model on the tree can be obtained using Bethe-Peierls expansion (also known as Belief Propagation). The corresponding transition point is given by a solution of an eigenvalue problem.

**12:51PM L43.00009 Spectral renormalization group theory on nonspatial networks**, ASLI TUNCER, AYSE ERZAN, Istanbul Tech Univ — We recently proposed a “spectral renormalization group” scheme, for non-spatial networks with no metric defined on them. We implemented the spectral renormalization group on two deterministic non-spatial networks without translational invariance, namely the Cayley tree and diamond lattice. The thermodynamic critical exponents for the Gaussian model are only functions of the spectral dimension,  $\tilde{d}$ . The Gaussian fixed point is stable with respect to a  $\psi^4$  perturbation up to second order on these lattices with  $\tilde{d} = 2$ , the lower critical dimension for the Ising universality class. This is expected for the Cayley tree, but for the diamond lattice it is an indication that the perturbation expansion up to second order breaks down at  $\tilde{d} = 2$ , as it does for the Wilson scheme on the square lattice. On generalized diamond lattices, with  $2 < \tilde{d} < 4$ , we find non-Gaussian fixed points with non-trivial exponents. For  $\tilde{d} > 4$ , the critical behavior is once again mean field.

**1:03PM L43.00010 Real beards and real networks: a spin-glass model for interacting individuals**, DION O'NEALE, University of Auckland — “I want to be different, just like all the other different people” sang the band King Missile. Whether they are the Beatniks of the 1950s, the punks of the 1970s, or the hipsters of today, non-conformists often tend to look the same, seemingly at odds with their goal of non-conformity. The spin-glass model, originally developed to describe the interaction of magnetic spins, and since applied to situations as diverse as the electrical activity of networks of neurons, to trades on a financial market, has recently been used in social science to study populations of interacting individuals comprised of a mix of both conformists and anti-conformists - or hipsters. Including delay effects for the interactions between individuals has been shown to give a system with non-trivial dynamics with a phase transition from stable behaviour to periodic switching between two states (let's call them bushy bearded and clean shaven). Analytic solutions to such a model are possible, but only for particular assumptions about the interaction and delay matrices. In this work we will show what happens when the interactions in the model are based on real-world networks with “small-world” effects and clustering.

**1:15PM L43.00011 Condensation and transport in the totally asymmetric inclusion process (TASIP)**<sup>1</sup>, JOHANNES KNEBEL, MARKUS F WEBER, LMU Munich, TORBEN KRUEGER, IST Austria, ERWIN FREY, LMU Munich — Transport phenomena are often modeled by the hopping of particles on regular lattices or networks. Such models describe, e.g., the exclusive movement of molecular motors along microtubules: no two motors may occupy the same site. In our work, we study inclusion processes that are the bosonic analogues of the fermionic exclusion processes. In inclusion processes, many particles may occupy a single site and hopping rates depend linearly on the occupation of departure and arrival sites. Particles thus attract other particles to their own site. Condensation occurs when particles collectively cluster in one or multiple sites, whereas other sites become depleted. We showed that inclusion processes describe both the selection of strategies in evolutionary zero-sum games and the condensation of non-interacting bosons into multiple quantum states in driven-dissipative systems. The condensation is captured by the antisymmetric Lotka-Volterra equation (ALVE), which constitutes a nonlinearly coupled dynamical system. We derived an algebraic method to analyze the ALVE and to determine the condensates. Our approach allows for the design of networks that result in condensates with oscillating occupations, and yields insight into the interplay between network topology and transport properties.

<sup>1</sup>Deutsche Forschungsgemeinschaft (SFB-TR12), German Excellence Initiative (Nanosystems Initiative Munich), Center for NanoScience Munich

**1:27PM L43.00012 Multi-frequency and edge localized modes in mechanical and electrical lattices**, LARS ENGLISH, Dickinson College, FAUSTINO PALMERO, University of Seville, PANAYOTIS KEVREKIDIS, University of Massachusetts — We present experimental evidence for the existence of a type of dynamical, self-localized mode called a multi-frequency breather in both a mechanical lattice of pendula and an electrical lattice. These modes were excited and stabilized by subharmonic driving. We also experimentally characterize dynamical modes that are localized on the edges of the pendulum chain, as well as in 2D electrical lattices. In the latter system, we briefly discuss the role of lattice topology in the stability of such modes.

**1:39PM L43.00013 Stokes Trap: Multiplexed particle trapping and manipulation using fluidics**, ANISH SHENOY, CHARLES SCHROEDER, University of Illinois at Urbana-Champaign — We report the development of the Stokes Trap, which is a multiplexed microfluidic trap for control over an arbitrary number of small particles in a microfluidic device. Our work involves the design and implementation of “smart” flow-based devices by coupling feedback control with microfluidics, thereby enabling new routes for the fluidic-directed assembly of particles. Here, we discuss the development of a new method to achieve multiplexed microfluidic trapping of an arbitrary number of particles using the sole action of fluid flow. In particular, we use a Hele-Shaw microfluidic cell to generate hydrodynamic forces on particles in a viscous-dominated flow defined by the microdevice geometry and imposed peripheral flow rates. This platform allows for a high degree of flow control over individual particles and can be used for manufacturing novel particles for fundamental studies, using fluidic-directed assembly. From a broader perspective, our work provides a solid framework for guiding the design of next-generation, automated on-chip assays.

**Wednesday, March 16, 2016 11:15AM - 2:15PM –**  
**Session L44 GQI: Quantum Information Theory and Quantum Foundations** 347 - Bei Zeng, University of Guelph

**11:15AM L44.00001 Quantum Speed Limits, coherence and asymmetry**, IMAN MARVIAN, massachusetts institute of technology, ROBERT SPEKKENS, Perimeter Institute for theoretical physics, PAOLO ZANARDI, University of Southern California — The resource theory of asymmetry is a framework for classifying and quantifying the symmetry-breaking properties of both states and operations relative to a given symmetry. In the special case where the symmetry is the set of translations generated by a fixed observable, asymmetry can be interpreted as coherence relative to the observable eigenbasis, and the resource theory of asymmetry provides a framework to study this notion of coherence. We here show that this notion of coherence naturally arises in the context of quantum speed limits. Indeed, the very concept of speed of evolution, i.e., the inverse of the minimum time it takes the system to evolve to another (partially) distinguishable state, is a measure of asymmetry relative to the time translations generated by the system Hamiltonian. Furthermore, the celebrated Mandelstam-Tamm and Margolus-Levitin speed limits can be interpreted as upper bounds on this measure of asymmetry by functions which are themselves measures of asymmetry in the special case of pure states. Using measures of asymmetry that are not restricted to pure states, such as the Wigner-Yanase skew information, we obtain extensions of the Mandelstam-Tamm bound which are significantly tighter in the case of mixed states.

**11:27AM L44.00002 A Strong Loophole-Free Test of Local Realism**, PETER BIERHORST, LYNDEN SHALM, MARTIN STEVENS, THOMAS GERRITS, SCOTT GLANCY, MICHAEL ALLMAN, KEVIN COAKLEY, SHELLEE DYER, CARSON HODGE, ADRIANA LITA, VARUN VERMA, RICHARD MIRIN, EMANUEL KNILL, SAE WOO NAM<sup>1</sup>, National Institute of Standards and Technology, Boulder, CO — We discuss theoretical and statistical aspects of a recent loophole-free violation of local realism using entangled photon pairs. The experiment ensures that all relevant events in the Bell test are spacelike separated by placing the parties far enough apart and using fast random number generators and high-speed polarization measurements. A high-quality polarization-entangled source of photons, combined with high-efficiency, low-noise, single-photon detectors, allows us to make measurements without requiring any fair-sampling assumptions. We collected six data sets, and for each data set we used a hypothesis test to compute the maximum probability (the p-value) that our experiment, if it had been governed by local realism, would produce a violation as large or larger than we observed. The smallest p-value we observed is  $5.9 \times 10^{-9}$ .

<sup>1</sup>See Phys. Rev. Lett. 115, 250402 for a complete list of authors.

**11:39AM L44.00003 Implications of Einstein-Weyl Causality on Quantum Mechanics**, DAVID BENDANIEL, Cornell University — A fundamental physical principle that has consequences for the topology of space-time is the principle of Einstein-Weyl causality. This also has quantum mechanical manifestations. Borchers and Sen have rigorously investigated the mathematical implications of Einstein-Weyl causality and shown the denumerable space-time  $Q^2$  would be implied. They were left with important philosophical paradoxes regarding the nature of the physical real line  $E$ , e.g., whether  $E = R$ , the real line of mathematics. In order to remove these paradoxes an investigation into a constructible foundation is suggested. We have pursued such a program and find it indeed provides a dense, denumerable space-time and, moreover, an interesting connection with quantum mechanics. We first show that this constructible theory contains polynomial functions which are locally homeomorphic with a dense, denumerable metric space  $R^*$  and are inherently quantized. Eigenfunctions governing fields can then be effectively obtained by computational iteration. Postulating a Lagrangian for fields in a compactified space-time, we get a general description of which the Schrodinger equation is a special case. From these results we can then also show that this denumerable space-time is relational (in the sense that space is not infinitesimally small if and only if it contains a quantized field) and, since  $Q^2$  is imbedded in  $R^{*2}$ , it directly fulfills the strict topological requirements for Einstein-Weyl causality. Therefore, the theory predicts that  $E = R^*$ .

**11:51AM L44.00004 Entanglement Entropy and Mutual Information of Circular Entangling Surfaces in 2+1d Quantum Lifshitz Model<sup>1</sup>**, TIANCI ZHOU, XIAO CHEN, EDUARDO FRADKIN, Univ of Illinois - Urbana — We investigate the entanglement entropy (EE) of circular entangling surfaces in the 2+1d quantum Lifshitz model, where the spatially conformal invariant ground state is a Rokhsar-Kivelson state with Gibbs weight of 2d free Boson. We use cut-off independent mutual information regulator [1] to define and calculate the subleading correction in the EE. The subtlety due to the Boson compactification in the replica trick is carefully taken care of. Our results show that for circular entangling surface, the subleading term is a constant on both the sphere of arbitrary radius and infinite plane. For the latter case, it parallels the constancy of disk EE in 2+1d conformal field theory, despite the lack of full space time conformal invariance. In the end, we present the mutual information of two disjoint disks and compare its scaling function in the small parameter regime (radii much smaller than their separation) with Cardy's general CFT results [2]. 1. H. Casini, M. Huerta, R. Myers, A. Yale, arXiv: 1506.06195 (2015). 2. J. Cardy, J. Phys. A: Math. Theor. 46, 285402 (2013)

<sup>1</sup>This work was supported in part by the National Science Foundation grants NSF-DMR-13-06011(TZ) and DMR-1408713 (XC, EF)

**12:03PM L44.00005 Monogamy of quantum steering**, ANTONY MILNE, DAVID JENNINGS, Imperial College London, SANIA JEVTIC, Brunel University, TERRY RUDOLPH, Imperial College London, HOWARD WISEMAN, Griffith University — The quantum steering ellipsoid formalism naturally extends the Bloch vector picture for qubits to provide a visualisation of two-qubit systems. If Alice and Bob share a correlated state then a local measurement by Bob steers Alice's qubit inside the Bloch sphere; given all possible measurements by Bob, the set of states to which Alice can be steered form her steering ellipsoid. We apply the formalism to a three-party scenario and find that steering ellipsoid volumes obey a simple monogamy relation. This gives us a novel derivation of the well-known CKW (Coffman-Kundu-Wootters) inequality for entanglement monogamy. The geometric perspective also identifies a new measure of quantum correlation, 'obesity', and a set of 'maximally obese' states that saturate the steering monogamy bound. These states are found to have extremal quantum correlation properties that are significant in the steering ellipsoid picture and for the study of two-qubit states in general.

**12:15PM L44.00006 Conflict between the Uncertainty Principle and wave mechanics**, ANTONY BOURDILLON, retired — The traveling wave group that is defined on conserved physical values is the vehicle of transmission for a unidirectional photon or free particle having a wide wave front. As a stable wave packet, it expresses internal periodicity combined with group localization. Heisenberg's Uncertainty Principle is precisely derived from it. The wave group demonstrates serious conflict between the Principle and wave mechanics. Also derived is the phase velocity beyond the horizon set by the speed of light. In this space occurs the reduction of the wave packet which occurs in measurement and which is represented by comparing phase velocities in the direction of propagation with the transverse plane. The new description of the wavefunction for the stable free particle or antiparticle contains variables that were previously ignored. Deterministic physics must always appear probabilistic when hidden variables are bypassed. Secondary hidden variables always occur in measurement. The wave group turns out to be probabilistic. It is ubiquitous in physics and has many consequences.

**12:27PM L44.00007 Coherence-path-information duality relation for N paths**, MARK HILLERY, Department of Physics, Hunter College of CUNY, EMILIO BAGAN, Fisica Teorica: Informacio i Fenomens Quantics, Universitat Autònoma de Barcelona, JANOS BERGOU, Department of Physics, Hunter College of CUNY — For an interferometer with two paths, there is a duality relation between the information about which path the particle took and the visibility of the interference pattern at the output. The more path information we have, the smaller the visibility, and vice versa. We generalize this relation to a multi-path interferometer, and we substitute a recently defined measure of quantum coherence for the visibility. The path information is provided by attaching a detector to each path and applying the minimum-error state discrimination procedure to the detector states.

**12:39PM L44.00008 Axioms for quantum mechanics: relativistic causality, retrocausality, and the existence of a classical limit<sup>1</sup>**, DANIEL ROHRLICH<sup>2</sup>, Physics Department, Ben-Gurion University of the Negev, Beersheba 8410501 — Y. Aharonov and A. Shimony both conjectured that two axioms – relativistic causality (“no superluminal signalling”) and nonlocality – so nearly contradict each other that only quantum mechanics reconciles them. Can we indeed derive quantum mechanics, at least in part, from these two axioms? No: “PR-box” correlations show that quantum correlations are not the most nonlocal correlations consistent with relativistic causality. Here we replace “nonlocality” with “retrocausality” and supplement the axioms of relativistic causality and retrocausality with a natural and minimal third axiom: the existence of a classical limit, in which macroscopic observables commute. That is, just as quantum mechanics has a classical limit, so must any generalization of quantum mechanics. In this limit, PR-box correlations *violate* relativistic causality. Generalized to all stronger-than-quantum bipartite correlations, this result is a derivation of Tsirelson's bound (a theorem of quantum mechanics) from the three axioms of relativistic causality, retrocausality and the existence of a classical limit. Although the derivation does not assume quantum mechanics, it points to the Hilbert space structure that underlies quantum correlations.

<sup>1</sup>I thank the John Templeton Foundation (Project ID 43297) and the Israel Science Foundation (grant no. 1190/13) for support.

<sup>2</sup>Keywords: nonlocal correlations, quantum nonlocality, retrocausality, PR boxes, axioms for quantum mechanics, classical limit

**12:51PM L44.00009 J-holomorphic maps and the uncertainty principle in geometric quantum mechanics** , BARBARA SANBORN, Antioch College — The theory of geometric quantum mechanics describes a quantum system as a Hamiltonian dynamical system, with a complex projective Hilbert space as its phase space. The Kähler structure of the projective space provides quantum mechanics with a Riemannian metric in addition to the symplectic structure characteristic of classical mechanics. By including aspects of the symplectic topology of the quantum phase space, the geometric theory is extended and enriched. In particular, the quantum uncertainty principle is naturally expressed as an inequality from J-holomorphic map theory.

**1:03PM L44.00010 A proposed physical analog for a quantum probability amplitude** , JEFFREY BOYD, retired — What is the physical analog of a probability amplitude? All quantum mathematics, including quantum information, is built on amplitudes. Every other science uses probabilities; QM alone uses their square root. Why? This question has been asked for a century, but no one previously has proposed an answer. We will present cylindrical helices moving toward a particle source, which particles follow backwards. Consider Feynman's book QED. He speaks of amplitudes moving through space like the hand of a spinning clock. His hand is a complex vector. It traces a cylindrical helix in Cartesian space. The Theory of Elementary Waves changes direction so Feynman's clock faces move toward the particle source. Particles follow amplitudes (quantum waves) backwards. This contradicts wave particle duality. We will present empirical evidence that wave particle duality is wrong about the direction of particles versus waves. This involves a paradigm shift; which are always controversial. We believe that our model is the ONLY proposal ever made for the physical foundations of probability amplitudes. We will show that our probability amplitudes in physical nature form a Hilbert vector space with adjoints, an inner product and support both linear algebra and Dirac notation.

**1:15PM L44.00011 Quantum enhanced estimation of a multi-dimensional field.**<sup>1</sup> , ANIMESH DATTA, University of Warwick, TILLMANN BAUMGRATZ, University of Oxford — We present a framework for the quantum-enhanced estimation of multiple parameters corresponding to non-commuting unitary generators. We derive the quantum Fisher information matrix to put a lower bound on the total variance of all the parameters involved. We present the conditions for the attainment of the multi-parameter bound, which is not guaranteed unlike the quantum metrology of single parameters. Our study also reveals that too much quantum entanglement may be detrimental to attaining the Heisenberg scaling in the estimation of unitarily generated parameters. One particular case of our framework is the simultaneous estimation of all three components of a magnetic field. We propose a probe state that demonstrates that the simultaneous estimation of the three components is better than the precision of estimating the three components individually. We provide realistic measurements that come close to attaining the quantum limit, exhibiting the advantage of simultaneous quantum estimation even in the case of non-commuting generators. Our work applies to precision estimation any Hamiltonian, and may be employed in efficient process tomography and verification. Our theoretical proposal can be implemented in any finite dimensional quantum system such as trapped ions and nitrogen vacancy centres in diamond.

<sup>1</sup>Acknowledgement : UK EPSRC

**1:27PM L44.00012 Fisher symmetry and the geometry of quantum states** , JONATHAN A. GROSS, HOWARD BARNUM, CARLTON M. CAVES, Univ of New Mexico — The quantum Fisher information (QFI) is a valuable tool on account of the achievable lower bound it provides for single-parameter estimation. Due to the existence of incompatible quantum observables, however, the lower bound provided by the QFI cannot be saturated in the general multi-parameter case. A bound demonstrated by Gill and Massar (GM) captures some of the limitations that incompatibility imposes in the multi-parameter case. We further explore the structure of measurements allowed by quantum mechanics, identifying restrictions beyond those given by the QFI and GM bound. These additional restrictions give insight into the geometry of quantum state space and notions of measurement symmetry related to the QFI.

**1:39PM L44.00013 Information Thermodynamics applied to the MERA quantum circuit.**<sup>1</sup> , VASILIOS PASSIAS, VICTOR CHUA, APOORV TIWARI, SHINSEI RYU, University of Illinois at Urbana-Champaign — We interpret the MERA (Multiscale Entanglement Renormalization Ansatz) tensor network as a unitary quantum circuit to study excited states of quantum spin-chains. Contrary to the common use of MERA as a variational ground state ansatz, the quantum circuit defined by MERA – adapted to a fixed ground state – is employed as a diagnostic tool to study dynamically evolving excited state wavefunctions. Outputs of the quantum computation emanating from the isometry tensors, which are normally approximate tensor product states, now fluctuate strongly. These “bulk” degrees of freedom in the MERA which act as logical qubits are studied using tools from quantum information theory and information thermodynamics. A local temperature scale based on Landauer's information erasure principle is defined to measure their degree of fluctuation. We investigate properties of this temperature against the expectations of Luttinger's theorem which relates weak field gravity to heat flow.

<sup>1</sup>This work was supported by the Gordon and Betty Moore Foundation.

**1:51PM L44.00014 The Dimensions of Emergent Spacetime in the Influence Network** , KEVIN KNUTH, State Univ of NY - Albany — It has been previously demonstrated that the consistent quantification of a causally ordered set of events (influence network) with respect to observers represented by embedded chains results in a unique consistent quantification scheme that reproduces the Minkowski metric in the case of coordinated chains and Lorentz transformations in the case of linearly-related chains (Knuth and Bahreyni 2014). Here we demonstrate that quantification by multiple coordinated chains can only be consistent in the cases of two and four chains resulting in emergent 1+1 and 3+1 dimensional spacetimes, respectively. Odd numbers of chains are specifically ruled out and numbers of chains greater than four lead to a system that is not closed under chain permutation symmetry in a manner consistent with Galois theory. As a result, the spacetime framework that emerges from the consistent quantification of a causally ordered set of events with respect to embedded observers provides a potential foundation for emergent spacetime as well as an explanation as to the significance and nature of 3+1 spacetime dimensions.

**2:03PM L44.00015 Locality and entanglement in bandlimited quantum field theory** , JASON PYE, University of Waterloo, WILLIAM DONNELLY, University of California Santa Barbara, ACHIM KEMPF, University of Waterloo — We consider a model for a Planck scale ultraviolet cutoff which is based on Shannon sampling. Shannon sampling originated in information theory, where it expresses the equivalence of continuous and discrete representations of information. When applied to quantum field theory, Shannon sampling expresses a hard ultraviolet cutoff in the form of a bandlimitation. This introduces nonlocality at the cutoff scale in a way that is more subtle than a simple discretization of space: quantum fields can then be represented as either living on continuous space or, entirely equivalently, as living on any one lattice whose average spacing is sufficiently small. We explicitly calculate vacuum entanglement entropies in 1+1 dimensions and we find a transition between logarithmic and linear scaling of the entropy, which is the expected 1+1 dimensional analog of the transition from an area to a volume law. We also use entanglement entropy and mutual information as measures to probe in detail the localizability of the field degrees of freedom. We find that, even though neither translation nor rotation invariance are broken, each field degree of freedom occupies an incompressible volume of space, indicating a finite information density.

**Wednesday, March 16, 2016 11:15AM - 2:15PM –**

**Session L45 GQI: Semiconductor Qubits: Quantum Dot Entanglement and Control** 348 - Matthew Rakher, HRL Laboratories

**11:15AM L45.00001 One- and two-qubit logic using silicon-MOS quantum dots<sup>1</sup>**, ANDREW DZURAK, UNSW - Australia — Spin qubits in silicon are excellent candidates for scalable quantum information processing [1] due to their long coherence times and the enormous investment in silicon CMOS technology. While our Australian effort in Si QC has largely focused on spin qubits based upon phosphorus dopant atoms implanted in Si [2,3], we are also exploring spin qubits based on single electrons confined in SiMOS quantum dots [4]. Such qubits can have long spin lifetimes  $T_1 = 2$  s, while electric field tuning of the conduction-band valley splitting removes problems due to spin-valley mixing [5]. In isotopically enriched Si-28 these SiMOS qubits have a control fidelity of 99.6% [6], consistent with that required for fault-tolerant QC. By gate-voltage tuning the electron  $g^*$ -factor, the ESR operation frequency can be Stark shifted by  $>10$  MHz [6], allowing individual addressability of many qubits. Most recently we have coupled two SiMOS qubits to realize a CNOT gate [7] using exchange-based controlled phase (CZ) operations. The speed of the two-qubit CZ-operations is controlled electrically via the detuning energy and over 100 two-qubit gates can be performed within a coherence time of  $8 \mu\text{s}$ . [1] D.D. Awschalom et al., “Quantum Spintronics”, Science 339, 1174 (2013). [2] J.J. Pla et al., “A single-atom electron spin qubit in silicon”, Nature 489, 541 (2012). [3] J.T. Muhonen et al., “Storing quantum information for 30 seconds in a nanoelectronic device”, Nature Nanotechnology 9, 986 (2014). [4] S.J. Angus et al., “Gate-defined quantum dots in intrinsic silicon”, Nano Lett. 7, 2051 (2007). [5] C.H. Yang et al., “Spin-valley lifetimes in a silicon quantum dot with tunable valley splitting”, Nature Comm. 4, 2069 (2013). [6] M. Veldhorst et al., “An addressable quantum dot qubit with fault-tolerant control fidelity”, Nature Nanotechnology 9, 981 (2014). [7] M. Veldhorst et al., “A two-qubit logic gate in silicon”, Nature 526, 410 (2015).

<sup>1</sup>We acknowledge support from the Australian Research Council (CE11E0001017), the US Army Research Office (W911NF-13-1-0024) and the Australian National Fabrication Facility.

**11:51AM L45.00002 Silicon quantum processor with robust long-distance qubit coupling**, GUILHERME TOSI, FAHD A. MOHIYADDIN, STEFANIE TENBERG, UNSW Australia, RAJIB RAHMAN, GERHARD KLIMECK, Purdue University, ANDREA MORELLO, UNSW Australia — Recent demonstration of high-fidelity quantum operations using donors in silicon [1] has ignited an urge in scaling up these systems to a multi-qubit device. However, multi-qubit operations and long-distance donor coupling remain a formidable challenge. We will present a novel scalable design for a silicon quantum processor [2] that allows for long-distance fast 2-qubit gates and does not require precise donor placement. Quantum information is encoded into either the nuclear-spin or the flip-flop states of electron and nucleus. It can be manipulated by biasing the electron wavefunction to be shared between donor and interface, in such a way that the hyperfine interaction strongly depends on electric fields. The qubits are spaced by hundreds of nanometers and coupled through direct electric dipole interactions and/or photonic links. All operations are performed at second-order clock transitions, preserving the qubits' outstanding coherence times. A large number of qubits can then be interconnected in a network robust against errors. Prototypical devices are fabricated to demonstrate the processor's basic units. [1] J. T. Muhonen, et.al. Nature Nanotechnol. 9, 986 (2014). [2] G. Tosi, et.al. arXiv:1509.08538 (2015).

**12:03PM L45.00003 Towards optimizing two-qubit operations in three-electron double quantum dots**, ADAM FREES, University of Wisconsin-Madison, Madison, WI 53706, JOHN KING GAMBLE, Center for Computing Research, Sandia National Laboratories, Albuquerque, NM 87123, SEBASTIAN MEHL, JARA-Institute for Quantum Information, RWTH Aachen University, Peter Grünberg Institute (PGI-2), Forschungszentrum Jülich, MARK FRIESEN, S.N. COPPERSMITH, University of Wisconsin-Madison, Madison, WI 53706 — The successful implementation of single-qubit gates in the quantum dot hybrid qubit motivates our interest in developing a high fidelity two-qubit gate protocol. Recently, extensive work has been done to characterize the theoretical limitations and advantages in performing two-qubit operations at an operation point located in the charge transition region. Additionally, there is evidence to support that single-qubit gate fidelities improve while operating in the so-called “far-detuned” region, away from the charge transition. Here we explore the possibility of performing two-qubit gates in this region, considering the challenges and the benefits that may present themselves while implementing such an operational paradigm. This work was supported in part by ARO (W911NF-12-0607) (W911NF-12-R-0012), NSF (PHY-1104660), ONR (N00014-15-1-0029). The authors gratefully acknowledge support from the Sandia National Laboratories Truman Fellowship Program, which is funded by the Laboratory Directed Research and Development (LDRD) Program. Sandia is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the US Department of Energy's National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

**12:15PM L45.00004 High-Fidelity Entangling Gates for Two-Electron Spin Qubits<sup>1</sup>**, PASCAL CERFONTAINE, JARA-Institute for Quantum Information, RWTH Aachen Univ., SEBASTIAN MEHL, DAVID P. DIVINCENZO, Peter Grünberg Institute (PGI-2), Forschungszentrum Jülich, HENDRIK BLUHM, JARA-Institute for Quantum Information, RWTH Aachen Univ. — High fidelity gate operations for manipulating individual and multiple qubits are a prerequisite for fault-tolerant quantum information processing. Recently, we have shown that single-qubit gates for singlet-triplet qubits in GaAs can be pulse-engineered to reduce systematic errors and mitigate magnetic field fluctuations from the abundant nuclear spins, leading to experimentally demonstrated gate fidelities of 98.5% [1]. We expect that a similar approach will be successful for two-qubit gates. We now describe short gating sequences for exchange-based two-qubit gates, showing that gate infidelities below 0.1% can be reached in realistic quantum dot setups [2]. Additionally, we perform numerical pulse optimization to fully take the experimentally important imperfections into account, minimizing systematic errors and noise sensitivity. Since transferring the optimal control pulses to an experimental setting will inevitably incur systematic errors, we discuss how these errors can be calibrated on the experiment. [1] P. Cerfontaine, T. Botzem, D. Schuh, D. Bougeard, H. Bluhm, in preparation. [2] S. Mehl, H. Bluhm, D. P. DiVincenzo, PRB 90 (2014).

<sup>1</sup>Supported by the Alexander von Humboldt Foundation, Alfried Krupp von Bohlen und Halbach Foundation, DFG grant BL 1197/2- 1, and the Deutsche Telekom Foundation

**12:27PM L45.00005 Error-reducing sequence for capacitively coupled singlet-triplet qubits**, FERNANDO CALDERON-VARGAS, JASON KESTNER, Univ of Maryland-Balt County — Two-qubit gates can be implemented by capacitively coupling singlet-triplet qubits, which has been experimentally demonstrated to be capable of generating entangling operations. However, the fidelity of the entangling two-qubit gates is still far from optimum. In this light, we propose a two-qubit entangling echo sequence that reduces drastically the two-qubit decoherence due to the Overhauser field fluctuation and improves the fidelity of two-qubit gates under charge noise.

**12:39PM L45.00006 Decoherence of two electron spin qubit in Si double quantum dot with g-factor modulations**, PEIHAO HUANG, GARNETT BRYANT, Joint Quantum Institute, National Institute of Standards and Technology and University of Maryland — The rapid progress in the manipulation and detection of semiconductor spin qubits enables the experimental demonstration of high fidelity two qubit gates that are necessary for universal quantum computing. Here, we consider the decoherence of two electron spin due to phonon emission in a Si double quantum dot (DQD). In the large detuning regime, where the two qubit gate is operated, we find that the decoherence depends strongly on the g-factor modulation and the asymmetry of the two dots. The estimated two qubit decoherence rate is comparable to the experimental measured results. We discuss the impact of the decoherence on the single/two qubit operations and ways to reduce the gate errors for the addressable semiconductor spin qubit.

**12:51PM L45.00007 Valley dependent g-factor anisotropy in Silicon quantum dots**, RIFAT FERDOUS, Purdue University, ERIKA KAWAKAMI, PASQUALE SCARLINO, MICHAŁ NOWAK, QuTech and Kavli Institute of Nanoscience, GERHARD KLIMECK, Purdue University, MARK FRIESEN, SUSAN N. COPPERSMITH, MARK A. ERIKSSON, University of Wisconsin-Madison, LIEVEN M. K. VANDERSYPEN, QuTech and Kavli Institute of Nanoscience, RAJIB RAHMAN, Purdue University — Silicon (Si) quantum dots (QD) provide a promising platform for a spin based quantum computer, because of the exceptionally long spin coherence times in Si and the existing industrial infrastructure. Due to the presence of an interface and a vertical electric field, the two lowest energy states of a Si QD are primarily composed of two conduction band valleys. Confinement by the interface and the E-field not only affect the charge properties of these states, but also their spin properties through the spin-orbit interaction (SO), which differs significantly from the SO in bulk Si. Recent experiments have found that the g-factors of these states are different and dependent on the direction of the B-field. Using an atomistic tight-binding model, we investigate the electric and magnetic field dependence of the electron g-factor of the valley states in a Si QD. We find that the g-factors are valley dependent and show 180-degree periodicity as a function of an in-plane magnetic field orientation. However, atomic scale roughness can strongly affect the anisotropic g-factors. Our study helps to reconcile disparate experimental observations and to achieve better external control over electron spins in Si QD, by electric and magnetic fields.

**1:03PM L45.00008 Strong spin relaxation anisotropy in a single-electron quantum dot**, LIUQI YU, L. C. CAMENZIND, D. E. F. BIESINGER, University of Basel, J. ZIMMERMAN, A. C. GOSSARD, UCSB, D. M. ZUMBHL, University of Basel — Spin coherence and relaxation is of crucial importance in operating spin based qubits. In a magnetic field, spins relax predominately through spin-phonon coupling mediated by spin-orbit interaction (SOI) [1]. Here we present measurements of the spin relaxation rate anisotropy in a gate defined single-electron GaAs quantum dot. The spin relaxation rate  $W$  is measured at applied magnetic fields of 4 T in the plane of the 2D electron gas.  $W$  exhibits strong anisotropy: a sinusoidal dependence on the B-field angle  $\varphi$  with a period of 180 degrees, as reported recently [2]. The extrema are observed at fields pointing nearly along the [110] and [1-10] crystal axes, modulated by a factor of about 14 from minimum to maximum. The periodicity is attributed to the interplay of Rashba and Dresselhaus SOIs. To decipher the role of SOI, we perform pulsed-gate spectroscopy to extract orbital excited-state energies, and obtain very good agreement with theory also for the angular dependence  $W(\varphi)$ , indicating that  $\alpha$  and  $\beta$ , Rashba and Dresselhaus coefficients respectively, have the same relative sign and are within 20% of each other. With controllable manipulations of the dot orbitals by varying gate voltages, it is possible to precisely extract values of  $\alpha$  and  $\beta$ . Meanwhile, top- and back gates have been implemented on the device structure, which allows full electrical control over the Rashba SOI in the 2D electron gas [3]. [1] V. N. Golovach et al., Phys. Rev. Lett. **93**, 016601 (2004). [2] P. Scarlino et al., Phys. Rev. Lett. **113**, 256802 (2014). [3] F. Dettwiler et al., arXiv:1403.3518 (2014).

**1:15PM L45.00009 Electron Spin Resonance Characterization of Damage and Recovery of Si/SiO<sub>2</sub> Interfaces from Electron Beam Lithography**, JIN-SUNG KIM, ALEXEI TYRYSKIN, STEPHEN LYON, Department of Electrical Engineering, Princeton University — Electron beam lithography (EBL) is an essential tool for the fabrication of few electron silicon quantum devices. However, high-energy electrons and photons from the EBL process create shallow traps and other defects at the Si/SiO<sub>2</sub> interface, inhibiting the control of electron populations through electrostatic gating. To reduce defect densities, high temperature and forming gas anneals are commonly used. We studied the effect of these anneals on the reduction of shallow traps created by EBL by fabricating two sets of large area ( $\sim 1\text{cm}^2$ ) MOSFETs and characterizing them using transport and electron spin resonance (ESR) measurements. One set was exposed to a typical EBL dosage (10kV,  $40\mu\text{C}/\text{cm}^2$ ) and the other remained unexposed. All MOSFETs were fabricated from the same commercially grown gate stack (30nm dry thermal oxide, 200nm amorphous silicon gate layer) and were annealed at 900C in N<sub>2</sub> and at 435C in forming gas. Our transport data indicate that these annealing steps recover the EBL exposed sample's low temperature (4.2K) peak mobility to 85% of the unexposed sample's. Additionally, our ESR data indicate that annealing the EBL exposed sample reduces its density of shallow traps (2-4 meV) to the same density as the unexposed sample.

**1:27PM L45.00010 Assessing MOS Interface Quality for Silicon Quantum Dot Device Fabrication**, RYAN STEIN, Joint Quantum Institute, University of Maryland, JIN-SUNG KIM, STEVE LYON, Department of Electrical Engineering, Princeton University, NEIL M. ZIMMERMAN, M. D. STEWART, JR., National Institute of Standards and Technology — Defects at the Si-SiO<sub>2</sub> interface are capable of trapping electrons and degrading the operation of silicon-based quantum dot devices. To improve device performance, we are working to characterize the interface quality in MOSCAPs and MOSFETs fabricated at NIST by comparing industry standard defect measurements, such as capacitance-voltage (CV), conductance, and mobility, to electron spin resonance (ESR) measurements. This comparison will give insight into the relative role of defects near the band edge and those distributed throughout the gap in degrading device performance. We will discuss our progress toward this goal as well as our latest data and interpretations.

**1:39PM L45.00011 First-principles hyperfine tensors for electrons and holes in silicon and GaAs**, PERICLES PHILIPPOPOULOS, McGill University, STEFANO CHESI, Beijing Computational Science Research Center, WILLIAM COISH, McGill University — Knowing (and controlling) hyperfine interactions in silicon and III-V semiconductor nanostructures is important for quantum information processing with electron and nuclear spin states. We have performed density-functional theory (DFT) calculations that fully account for spin structure of the Bloch states (in contrast with approaches that rely on the density alone). Using this method, we confirm the known value for the contact hyperfine coupling in the conduction band of silicon, but find a significant deviation in the value for the conduction band of GaAs relative to the accepted value, estimated in ref. [1]. Moreover, this method can be used to calculate the full hyperfine tensor for the valence band, where spin-orbit effects may be strong, precluding methods that determine hyperfine couplings from the density alone. This general method can be applied to a broad class of materials with strong combined spin-orbit and hyperfine interactions. [1] D. Paget, G. Lampel, B. Sapoval, and V. I. Safarov Phys. Rev. B **15**, 5780 (1977)

**1:51PM L45.00012 Quantum quench dynamics of a central-spin system**, ALESSANDRO RICOTTONE, WILLIAM COISH, McGill Univ, STEFANO CHESI, YINAN FANG, Beijing Computational Science Research Center — Quantum effects can significantly influence equilibration dynamics. In quantum annealing, a local tunneling mechanism may accelerate the approach to equilibrium. Similarly, long-range quantum coherence can allow for rapid transitions between macroscopically distinct states of a quantum system. An experimentally relevant example of this is given by a 'central' electron spin coupled to an ensemble of nuclear spins in a quantum dot. This system admits a superradiance-like burst of current through ferromagnetic leads due to long-range nuclear spin coherence [1] with a simultaneous inversion of the nuclear-spin polarization. Here, we study this system coupled to normal leads. In particular, we study quench dynamics of the nuclear spin polarization after passing through a quantum phase transition controlled by an applied magnetic field. As a function of dephasing controlled by a magnetic field gradient, we find a crossover from rapid equilibration via collective states to slow dynamics described by classical (product-state) spin configurations. This understanding may allow us to better control dynamic nuclear spin polarization processes in quantum dots and to control more general quantum states of nuclear-spin ensembles. [1] S. Chesi and W. A. Coish PRB **91**, 245306 (2015)

**2:03PM L45.00013 Theory of Corner States in Silicon Nanowire Devices<sup>1</sup>**, ANDRE SARAIVA, BELITA KOILLER, Universidade Federal do Rio de Janeiro, M FERNANDO GONZALEZ-ZALBA, Hitachi Cambridge Lab — Nanowire-based transistors, such as FinFETs and Tri-gate FETs, form one and zero dimensional states at the corners. These corner states may be manipulated for quantum electronic applications, such as tunable quantum dot-based spin qubits. We discuss the electronic structure of the electrons bound at the corner, considering the effects due to the anisotropy of the effective mass, the splitting of valleys due to the confinement and the scattering at the interface, generalizing our results to corners of arbitrary angle. Our results indicate the optimal conditions for lifting the valley degeneracy, known to impact quantum coherence and control. We finally mention the expected impacts of this geometry on the tunnel and exchange coupling between dots at opposite corners of a wire.

<sup>1</sup>AS and BK performed this work as part of the Brazilian National Institute for Science and Technology on Quantum Information and acknowledge support from the Brazilian agencies FAPERJ, CNPq, CAPES. MFG-Z is funded by the FP7/318397-TOLOP project.

## **Wednesday, March 16, 2016 11:15AM - 2:15PM – Session L46 DCMP: Metals II 311 - David Singh, University of Missouri**

**11:15AM L46.00001 Quantum oscillation signatures of Fermi arc surface states in Weyl semimetals**, ANDREW POTTER, Univ of California - Berkeley — Weyl semimetal states and their crystalline symmetry protected Dirac- analogs have recently been discovered in a variety of materials. These new phases of matter offer an interesting example of topology in the absence of a protecting band- or correlation- gap. The bulk topological character of these materials is revealed upon the application of a magnetic field, which produces chiral Landau level modes that propagate along the field and which mediate inter-valley charge pumping associated with chiral anomaly physics. At a surface, the bulk topology manifests itself in unusual surface states whose Fermi surface consists of disjoint arcs. In this talk, I will describe magnetic field induced quantum oscillation signatures of both the surface and bulk topological features of these materials. These oscillations are associated with unusual magnetic orbits that start on the Fermi arc of one surface, propagate through the bulk on the chiral Landau level, and complete the orbit on the opposite surface. I also will describe some recent experimental evidence for these orbits in Dirac semimetal thin films.

**11:51AM L46.00002 Optical properties of the perfectly compensated semimetal WTe<sub>2</sub><sup>1</sup>**, C. C. HOMES, Condensed Matter Physics and Materials Science Dept., Brookhaven National Laboratory, Upton, New York, M. N. ALI, R. J. CAVA, Department of Chemistry, Princeton University, Princeton, New Jersey — The optical properties of layered tungsten ditelluride have been measured over a wide temperature and frequency range for light polarized in the *a-b* planes. A striking low-frequency plasma edge develops in the reflectance at low temperature where this material is a perfectly compensated semimetal. The optical conductivity is described using a two-Drude model which treats the electron and hole pockets as separate electronic subsystems. At low temperature, one scattering rate collapses by over two orders of magnitude, while the other also undergoes a significant, but less dramatic, decrease; both scattering rates appear to display the quadratic temperature dependence expected for a Fermi liquid. First principles electronic structure calculations reveal that the low-lying optical excitations are due to direct transitions between the bands associated with the electron and hole pockets.<sup>2</sup>

<sup>1</sup>Supported by the Department of Energy under Contract No. DE-SC0012704; Army Research Office, Grant No. W911NF-12-1-0461.

<sup>2</sup>C. C. Homes, M. N. Ali, and R. J. Cava, Phys. Rev. B **92**, 161109(R) (2015).

**12:03PM L46.00003 Role of spin-orbit coupling and evolution of the electronic structure of WTe<sub>2</sub> under an external magnetic field<sup>1</sup>**, DANIEL RHODES, SUVADIP DAS, QIU RUN ZHANG, NHMFL, FSU, BIN ZENG, NIHAR PRADHAN, NHMFL, NAOKI KIKUGAWA, NHMFL, NIMS, EFSTRATIOS MANOUSAKIS, NHMFL, FSU, LUIS BALICAS, NHMFL — Here, we present a study on the temperature and angular dependence of the Shubnikov-de Haas (SdH) effect in the semimetal WTe<sub>2</sub>. This compound has been shown to display a large, nonsaturating magnetoresistance which was attributed to nearly perfectly compensated densities of electrons and holes. We observe four fundamental SdH frequencies and attribute them to spin-orbit split, electron-like, and hole-like Fermi-surface (FS) cross-sectional areas. Their angular dependence is consistent with ellipsoidal FSs that suggest a modest excess in the density of electrons with respect to that of the holes. We show that DFT calculations fail to correctly describe the FSs of WTe<sub>2</sub> and find evidence for field-dependent FS cross-sectional areas. We also observe a pronounced field-induced renormalization of the effective masses. Our observations suggest that the electronic structure of WTe<sub>2</sub> evolves with the magnetic field due to the Zeeman splitting. This evolution is likely to contribute to its pronounced magnetoresistivity.

<sup>1</sup>The work was supported by NSF through Grant No. NSFDMR-1157490, the state of Florida, DOE-BES through award No. DE-SC0002613 and by the Army Research Office through MURI Grant No. W911NF- 11-10362.

**12:15PM L46.00004 Magneto-optic measurements of the Weyl semimetal NbAs**, NATHAN ARMSTRONG, McMaster University, YINMING SHAO, Univ of California - San Diego, ZHUJUN YUAN, International Center for Quantum Materials, Peking University, SHUANG JIA, International Center for Quantum Materials, Peking University; Collaborative Innovation Center of Quantum Matter, Beijing, D.N. BASOV, Univ of California - San Diego, THOMAS TIMUSK, McMaster University; Canadian Institute for Advance Research — NbAs is among the newly discovered Weyl semimetals that are of great interest because they have the potential to confirm the chiral anomaly predicted by particle physics. It has been theorized that two separated Weyl nodes of opposite chirality can have a chiral current flow between them with the application electric and magnetic fields parallel to the displacement of the nodes. Indeed, magnetoresistance measurements on TaAs and NbAs found a negative magnetoresistance with these fields. ARPES and band structure calculations show that NbAs has two different groups of Weyl nodes with all the node splittings in  $k_x - k_y$  planes. In addition to the Weyl nodes there are other trivial bands that create Fermi pockets elsewhere in the BZ that are also observed in reflectance measurements. We will present magneto-optics results from far infrared optical data of NbAs in Voigt geometry up to 8 Tesla. In the far infrared at large fields there are two strong features that show an 11% and 3% change of reflectance in field at 60 and 480  $cm^{-1}$ , respectively. We evaluate these data with comparison to the above mentioned band structure of NbAs.

**12:27PM L46.00005 Linear magnetoresistance and zero-field anomalies in HfNiSn single crystals<sup>1</sup>**, LUCIA STEINKE, Texas AM Univ., JEDEDIAH J. KISTNER-MORRIS, HAIMING DENG, GAYLE GESCHWIND, Stony Brook Univ., MEIGAN C. ARONSON, Texas AM Univ. — The Half-Heusler compound HfNiSn is probably best known as a candidate material for thermoelectric applications, and studies of its properties have mainly focused on polycrystalline samples and thin films. However, magnetotransport studies of HfNiSn show unusual transport properties like linear magnetoresistance (LMR) [1], where single-crystalline samples of HfNiSn exhibit unexpected LMR at very low fields. In this work, we optimized the solution growth of HfNiSn to obtain high-quality single crystals, where electrical transport measurements show that it is a compensated semimetal below  $\approx 200$  K, where the Hall voltage is zero. At higher temperatures, we see a finite Hall contribution from activated excess carriers. In the semimetallic regime, we observe transport anomalies like resistive signals that strongly depend on contact configuration, and LMR below 5 K. Both low-field DC and low frequency AC magnetization measurements show pronounced diamagnetic behavior and the onset of paramagnetism below 4 K. High-frequency diamagnetic screening may be attributed to a decreased skin depth with decreased resistance, but this scenario seems unlikely in HfNiSn since the measured resistance increases steeply at the lowest temperatures. [1] K. Ahilan et al., PRB 69, 245116 (2004).

<sup>1</sup>This research was supported by the Army Research Office.

**12:39PM L46.00006 Landau level quantization and almost flat modes in three-dimensional semimetals with nodal ring spectra**, JUN-WON RHIM, Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany, YONG BAEK KIM, Department of Physics, University of Toronto, Toronto, Ontario, Canada M5S 1A7, CANADIAN INSTITUTE FOR ADVANCED RESEARCH COLLABORATION — We investigate Landau level structures of semimetals with nodal ring dispersions. When the magnetic field is applied parallel to the plane in which the ring lies, there exist almost nondispersive Landau levels at the Fermi level ( $E_F = 0$ ) as a function of the momentum along the field direction inside the ring. We show that the Landau levels at each momentum along the field direction can be described by the Hamiltonian for the graphene bilayer with fictitious interlayer couplings under a tilted magnetic field. Near the center of the ring where the interlayer coupling is negligible, we have Dirac Landau levels which explain the appearance of the zero modes. Although the interlayer hopping amplitudes become finite at higher momenta, the splitting of zero modes is exponentially small and they remain almost flat due to the finite artificial in-plane component of the magnetic field. The emergence of the density of states peak at the Fermi level would be a hallmark of the ring dispersion.

**12:51PM L46.00007 Observation of the Thermal Hall Effect Using Capacitive Thermometers in Bismuth**, COLIN TINSMAN, GANG LI, FAN YU, TOMOYA ASABA, BENJAMIN LAWSON, Univ of Michigan - Ann Arbor, CAROLINE SU, Univ of California - Berkeley, LU LI, Univ of Michigan - Ann Arbor — The thermal Hall effect is the thermal analog of the electrical Hall effect. Rarely observed in normal metals, thermal Hall signals were argued to be a key property for a number of strongly correlated materials, such as high temperature superconductors, correlated topological insulators, and quantum magnets. The observation of the thermal Hall effect requires precise measurement of temperature in intense magnetic fields. Particularly at low temperature, resistive thermometers have a strong dependence on field, which makes them unsuitable for this purpose. We have created capacitive thermometers which instead measure the dielectric constant of strontium titanate ( $\text{SrTiO}_3$ ).  $\text{SrTiO}_3$  approaches a ferroelectric transition, causing its dielectric constant to increase by a few orders of magnitude at low temperature. As a result, these thermometers are very sensitive at low temperature while having very little dependence on the applied magnetic field, making them ideal for thermal Hall measurements. We demonstrate this by making measurements of the thermal Hall effect in Bismuth in magnetic fields of up to 10T.

**1:03PM L46.00008 Gyrotropic magnetic effects in chiral metals**, IVO SOUZA, Universidad del Pais Vasco, San Sebastian, SHUDAN ZHONG, University of California, Berkeley, DAVID VANDERBILT, Rutgers University, JOEL MOORE, University of California, Berkeley — We consider two conjugate transport effects occurring in chiral metals as the low-frequency limit of natural optical activity (optical gyrotropy). One occurs in the clean limit where  $\omega$  is small compared to the minimum energy for interband transitions, but large compared to the scattering rate  $1/\tau$ . It consists of a dissipationless current induced by a magnetic field,  $J_i = \alpha'_{ij} B_j$ , and is different from the chiral magnetic effect requiring a static  $\mathbf{B}$  and an electric-field pulse  $\mathbf{E} \parallel \mathbf{B}$ . In the inverse effect a magnetization is generated by a dissipative current,  $M_i = (1/\omega)\alpha''_{ji} E_j$ , with  $\mathbf{E}$  the field driving the current and  $\omega \ll 1/\tau$ , as discussed by Yoda *et al.*, Sci. Rep. 5, 12024 (2015). The low-frequency gyrotropic responses  $\alpha'$  and  $\alpha''$  in the clean and dirty limits can be combined into a complex tensor  $\alpha = \alpha' + i\alpha''$  given by the Fermi-surface integral of the total (orbital plus spin) intrinsic magnetic moment of the Bloch electrons, with a prefactor proportional to  $1 - i\omega\tau$ . Without spin-orbit coupling, only the orbital moment contributes.

**1:15PM L46.00009 Anomalous optical properties of a multiband metal due to thermal redistribution: The case of  $\text{SrMnSb}_2$** , H. J. PARK, LUKE J. SANDILANDS<sup>1</sup>, CCES-IBS & Dep. of Physics and Astronomy, SNU, J. S. YOU, Dep. of Physics, POSTECH, HYO SEOK JI, Dep. of Chemistry, POSTECH, C. H. SOHN, CCES-IBS & Dep. of Physics and Astronomy, SNU, J. W. HAN, Dep. of Physics and Photon Science, School of Physics and Chemistry, GIST, S. J. MOON, Dep. of Physics, Hanyang Univ., K. W. KIM, Dep. of Physics, Chungbuk National Univ., J. H. SHIM, Dep. of Chemistry & Division of Advanced Nuclear Engineering, POSTECH, JUN SUNG KIM, Dep. of Physics, POSTECH, T. W. NOH<sup>2</sup>, CCES-IBS & Dep. of Physics and Astronomy, SNU — We report an optical spectroscopic study of  $\text{SrMnSb}_2$ , a low carrier density metal. As temperature is decreased, our measurements reveal a large increase in the free carrier plasma frequency, which is unusual for a metal. This seemingly anomalous behavior can be accounted for using a 'three band' model of the multiband electronic structure of  $\text{SrMnSb}_2$  that includes two conduction bands and one valence band close to the Fermi level. The temperature dependence of the low-lying interband optical transitions and the Hall number can also be understood using our model. Our results provide a possible explanation for the puzzling optical properties that have been reported in a number of topical low carrier density metals and semimetals.

<sup>1</sup>H. J. park and Luke J. Sandilands contributed equally to this work.

<sup>2</sup>Corresponding author

**1:27PM L46.00010 Optical Spectroscopy of anomalous Fermi Liquids.**, THOMAS TIMUSK, McMaster Univ — It is customary to classify a metallic conductor as a Fermi liquid if, at low temperatures, the electrical resistivity varies as the square of the absolute temperature. Fermi liquid theory shows that if umklapp scattering dominates then, independent of a particular band structure, this T squared dependence is accompanied by a quadratic frequency dependence where  $\rho(T, \omega) = C(\omega^2 + b(\pi T)^2)$  where the scaling constant  $b = 4$  for a Fermi liquid[1,2]. A survey of literature shows that where spectroscopic data exist,  $b = 4$  has not been generally observed[3]. We find that, surveying the recent literature, that in heavy fermion systems the scaling coefficient  $b = 1$ , pointing to a resonant scattering mechanism [2]. In most other systems an unknown mechanism yields a value of  $b$  of around 2. 1. R. N. Gurzhi, Sov. Phys. JETP 14, 886 (1962). 2. D.L. Maslov and A.V. Chubukov, Phys. Rev. B 86, 155137 (2012). 3. U. Nagel *et al.* PNAS 109, 19161 (2012).

**1:39PM L46.00011 Origin of large electron-phonon coupling in the metallic hydride TiH<sub>2</sub>**<sup>1</sup>, SHANAVAS K. VEEDU, DAVID S. PARKER, Oak Ridge National Laboratory — The recent discovery of large superconducting transition temperature of  $T_c = 190$  K in metallic H<sub>2</sub>S under high pressures of 200 GPa, has renewed the interest in the superconducting properties of metal-hydrogen systems. These materials are expected to be electron-phonon superconductors and hydrogen with its low mass can contribute new optic phonons that may couple with the conduction electrons. Often, though not always, a large electron-phonon coupling parameter  $\lambda$  (and consequently high  $T_c$ ) can result from a high electronic density of states at the Fermi level ( $N(E_F)$ ) and the presence of soft phonons. With the help of first-principles calculations within density functional theory, we studied the cubic TiH<sub>2</sub> which has a large  $3d$   $N(E_F) = 2.8$  states/eV/f.u. Our calculated phonon dispersions show that Ti modes active below frequencies of 10 THz whereas much lighter H modes are active between 32 and 40 THz. Electron-phonon coupling calculations reveal a  $\lambda = 0.98$  which corresponds to a  $T_c = 6.1$  K. However, the large  $N(E_F)$  also leads to a tetragonal instability at low temperatures in TiH<sub>2</sub>, which may be overcome by a uniaxial strain, potentially making it a candidate for electron-phonon superconductor.

<sup>1</sup>This research was supported by the US Department of Energy, Basic Energy Sciences, Office of Science, Materials Sciences and Engineering Division

**1:51PM L46.00012 Structure and dynamics of bulk liquid iron at pressures up to 58 GPa. A first-principles study**<sup>1</sup>, DAVID GONZALEZ, MIRIAM MARQUES, LUIS ENRIQUE GONZALEZ, Dpt. Fisica Teorica, Atomica y Optica, Facultad de Ciencias, Universidad de Valladolid, 47011 Valladolid — The static and dynamic properties of bulk liquid Fe at several high pressure states, have been studied by using first-principles molecular dynamics simulations based on the density functional theory and the projector augmented wave technique. Results are reported for four thermodynamic states at pressures of 27, 42, 50 and 58 GPa for which x-ray scattering data are available. The calculated static structure shows very good agreement with the available experimental data, including an asymmetric second peak which becomes more marked with increasing pressure. The dynamical structure reveals the existence of propagating density fluctuations and the associated dispersion relation has also been determined. The relaxation mechanisms for the density fluctuations have been analyzed in terms of a model with two decay channels (fast and slow, respectively). We found that the thermal relaxation proceeds along the slow decaying channel whereas the fast one is that of the viscoelastic relaxation. Finally, results are also reported for some transport coefficients.

<sup>1</sup>We acknowledge financial support from Spanish MCI (FIS2014-59279-P) and JCyL (CIP13/03 and VA104A11-2)

**2:03PM L46.00013 Thermodynamic properties by Equation of state of liquid sodium under pressure.**<sup>1</sup>, HUAMING LI, Georgia Inst of Tech, YONGLI SUN, XIAOXIAO ZHANG, Taiyuan University of Technology, China, MO LI, Georgia Inst of Tech — Isothermal bulk modulus, molar volume and speed of sound of molten sodium are calculated through an equation of state of a power law form within good precision as compared with the experimental data. The calculated internal energy data show the minimum along the isothermal lines as the previous result but with slightly larger values. The calculated values of isobaric heat capacity show the unexpected minimum in the isothermal compression. The temperature and pressure derivative of various thermodynamic quantities in liquid Sodium are derived. It is discussed about the contribution from entropy to the temperature and pressure derivative of isothermal bulk modulus. The expressions for acoustical parameter and nonlinearity parameter are obtained based on thermodynamic relations from the equation of state. Both parameters for liquid Sodium are calculated under high pressure along the isothermal lines by using the available thermodynamic data and numeric derivations. By comparison with the results from experimental measurements and quasi-thermodynamic theory, the calculated values are found to be very close at melting point at ambient condition. Furthermore, several other thermodynamic quantities are also presented.

<sup>1</sup> Scientific Research Starting Foundation from Taiyuan university of Technology, Shanxi Provincial government (100-talents program), China Scholarship Council and National Natural Science Foundation of China (NSFC) under grant No. 11204200.

## Wednesday, March 16, 2016 11:15AM - 2:03PM –

**Session L47 DCP: Chemical Physics of Condensed Phase Dynamics** 312 - David Nesbitt, JILA, University of Colorado

**11:15AM L47.00001 Quantum thermodynamics for systems out of equilibrium strongly interacting with their surroundings.**, MAICOL OCHOA, University of Pennsylvania, MASSIMILIANO ESPOSITO, University of Luxembourg, MICHAEL GALPERIN, University of California - San Diego — The performance of molecular and nanoscopic systems as nanodevices capable of transforming some form of energy into work is greatly determined by their interaction with the surroundings. When the interaction is strong, one may redefine the part of the universe that can be regarded as the system in order to achieve a full dynamic as well as thermodynamic description. In this work we study a single level strongly interacting with a fermionic bath that undergoes slow driving. The dynamics of the system is estimated using Nonequilibrium Green's functions NEGF. We explore different alternatives for the system bath separation under driving, identifying the corresponding terms for heat and energy transferred as well as the dissipation term. We also formulate the problem in terms of the renormalized spectral density. Our investigations indicate that none of the alternatives can fully reproduce the laws of thermodynamics suggesting that the notion of heat, expressed as the expectation value of some part of the Hamiltonian, is responsible for the inconsistency.

**11:27AM L47.00002 A Variational Statistical-Field Theory for Polar Liquid Mixtures**<sup>1</sup>, BILIN ZHUANG, ZHEN-GANG WANG, California Institute of Technology — Using a variational field-theoretic approach, we derive a molecularly-based theory for polar liquid mixtures. The resulting theory consists of simple algebraic expressions for the free energy of mixing and the dielectric constant as functions of mixture composition. Using only the dielectric constants and the molar volumes of the pure liquid constituents, the theory evaluates the mixture dielectric constants in good agreement with the experimental values for a wide range of liquid mixtures, without using adjustable parameters. In addition, the theory predicts that liquids with similar dielectric constants and molar volumes dissolve well in each other, while sufficient disparity in these parameters result in phase separation. The calculated miscibility map on the dielectric constant-molar volume axes agrees well with known experimental observations for a large number of liquid pairs. Thus the theory provides a quantification for the well-known empirical like-dissolves-like rule.

<sup>1</sup>BZ acknowledges the A-STAR fellowship for the financial support.

**11:39AM L47.00003 Role of solvent environments in single molecule conductance used insulator-modified mechanically controlled break junctions.**<sup>1</sup> , NANDINI MUTHUSUBRAMANIAN<sup>2</sup>, CHANDAN MAITY<sup>3</sup>, ELENA GALAN GARCIA<sup>4</sup>, RIENK EELKEMA<sup>5</sup>, FERDINAND GROZEMA<sup>6</sup>, HERRE VAN DER ZANT<sup>7</sup>, Delft University of Technology, KAVLI INSTITUTE OF NANOSCIENCE COLLABORATION, DEPARTMENT OF CHEMICAL ENGINEERING COLLABORATION — We present a method for studying the effects of polar solvents on charge transport through organic/biological single molecules by developing solvent-compatible mechanically controlled break junctions of gold coated with a thin layer of aluminium oxide using plasma enhanced atomic layer deposition (ALD). The optimal oxide thickness was experimentally determined to be 15 nm deposited at ALD operating temperature of 300C which yielded atomically sharp electrodes and reproducible single-barrier tunnelling behaviour across a wide conductance range between  $1 G_0$  and  $10^{-7} G_0$ . The insulator protected MCBJ devices were found to be effective in various solvents such as deionized water, phosphate buffered saline, methanol, acetonitrile and dichlorobenzene. The yield of molecular junctions using such insulated electrodes was tested by developing a chemical protocol for synthesizing an amphipathic form of oligo-phenylene ethynylene (OPE3-PEO) with thioacetate anchoring groups. This work has further applications in studying effects of solvation, dipole orientation and other thermodynamic interactions on charge transport.

<sup>1</sup> EU Marie Curie Initial Training Network (ITN). MOLECULAR-SCALE ELECTRONICS: MOLESCO Project Number 606728

<sup>2</sup> Kavli Institute of Nanoscience

<sup>3</sup> Department of Chemical Engineering

<sup>4</sup> Department of Chemical Engineering

<sup>5</sup> Department of Chemical Engineering

<sup>6</sup> Department of Chemical Engineering

<sup>7</sup> Kavli Institute of Nanoscience

**11:51AM L47.00004 Inferring mixture Gibbs free energies from static light scattering data**<sup>1</sup> , DAVID ROSS, Rochester Institute of Technology, CHRISTOPHER WAHLE, University of Findlay, GEORGE THURSTON, Rochester Institute of Technology — We describe a light scattering partial differential equation for the free energy of mixing that applies to connected, isotropic ternary and quaternary liquid composition domains, including restricted domains which may not touch all binary axes. For restricted domains, contrasting light scattering efficiency patterns obtained at different wavelengths can correspond to the same underlying free energy, and supplement the available information. We discuss well-posed problems for this fully nonlinear, degenerate elliptic partial differential equation. Using Monte Carlo simulations, we provide estimates of the overall system measurement time and sample spacing needed to determine the free energy to a desired degree of accuracy, and indicate how measurement time depends on instrument throughput. These methods provide a way to use static light scattering to measure, directly, mixing free energies of many systems that contain liquid domains.

<sup>1</sup> Supported by NIH EY018249

**12:03PM L47.00005 *In situ/operando* soft x-ray spectroscopy characterization of ion solvation and catalysis.** , YI-SHENG LIU, JINGHUA GUO, Lawrence Berkeley Natl Lab — Many important systems especially in energy-related regime are based on the complexity of material architecture, chemistry and interactions among constituents within. To understand and thus ultimately control the varying applications calls for *in-situ/operando* characterization tools. We will present the recent development of the *in-situ/operando* soft X-ray spectroscopic in the studies of catalytic and alkali ion solvation under bias condition, and reveal how to overcome the challenge that soft X-rays cannot easily peek into the high-pressure catalytic cells or liquid electrochemical cells. Also the different feasible detection approaches can provide surface and bulk sensitivity experimentally from those *in-situ* cells. The unique design of *in-situ/operando* soft X-ray spectroscopy instrumentation and fabrication principle with examples in Ca, Na, Mg based solutions at ambient pressure/temperature and high temperature (~250C) gas catalysis will be shown.

**12:15PM L47.00006 Excited statemolecular dynamics in polarizable environments** , JOSIAH BJORGAARD, KIRILL VELIZHANIN, SERGEI TRETIAK, Los Alamos Natl Lab — Many experimental measurements of molecular systems are performed in solutions, where the solvent forms a polarizable environment around the solute. The effects of this on important molecular processes such as vibrational relaxation or chemical reaction are often significant. In this talk, recent developments in efficiently simulating solvation effects in quantum molecular dynamics for excited electronic states are presented. These methods fall into the category of multiscale quantum mechanics/continuum methods. To adequately describe polarization of the solvent by the electronically excited states of molecules, state-specific methods have been pursued which allow for polarization effects based on the excited state charge density. Variational formulations of solvation models in linear response time-dependent density functional theory are described which allow analytical gradients and efficient molecular dynamics propagation. Further, recently developed simulation methods for nonequilibrium solvation effects are demonstrated.

**12:27PM L47.00007 Evolution of molecular crystal optical phonons near structural phase transitions** , NIGEL MICHKI, KATHERINE NIESSEN, MENG YANG XU, ANDREA MARKELZ, SUNY at Buffalo — Molecular crystals are increasingly important photonic and electronic materials. For example organic semiconductors are lightweight compared to inorganic semiconductors and have inexpensive scale up processing with roll to roll printing[1]. However their implementation is limited by their environmental sensitivity, in part arising from the weak intermolecular interactions of the crystal. These weak interactions result in optical phonons in the terahertz frequency range. We examine the evolution of intermolecular interactions near structural phase transitions by measuring the optical phonons as a function of temperature and crystal orientation using terahertz time-domain spectroscopy. The measured orientation dependence of the resonances provides an additional constraint for comparison of the observed spectra with the density functional calculations [2], enabling us to follow specific phonon modes. We observe crystal reorganization near 350 K for oxalic acid as it transforms from dihydrate to anhydrous form. We also report the first THz spectra for the molecular crystal fructose through its melting point.

1. Krebs, F.C., et al. J. Materials Chem., 2009, 19(30): p. 5442-5451

2. Singh, R., et al. J. Phys. Chem. C, 2012. 116(42): p. 1035910364.

**12:39PM L47.00008 Transient ultrafast coherent spectroscopy of 2-propanol** , SETH MEISELMAN, MATTHEW DECAMP, Univ of Delaware, VIRGINIA LORENZ, Univ of Illinois at Urbana-Champaign — We use transient coherent spontaneous Raman spectroscopy to measure the coherence lifetimes of vibrational states in liquid propanol. By creating single-photon-level collective excitations of the vibrational states in the system we observe coherence oscillations due to simultaneous excitation of the  $2885\text{ cm}^{-1}$ ,  $2938\text{ cm}^{-1}$ , and  $2976\text{ cm}^{-1}$  modes. These lifetimes and oscillation frequencies agree with frequency-domain lineshape measurements.

**12:51PM L47.00009 Molecular Level-Crossing Dynamics in Condensed Phase from an Optical Hanle Effect Perspective** , RACHEL GLENN, MARCOS DANTUS, None — The molecular optical Hanle effect typically involves field-induced level-splitting to measure excited state lifetimes. Here I will discuss how curve-crossing dynamics probed with a single shaped pulse in the weak field regime can be understood from a perspective of the molecular optical Hanle effect. I will discuss how pulse shaping can be utilized to investigate the curve-crossing dynamics occurring in a large organic molecule in solution. Both Experimental and theoretical results will be presented.

**1:03PM L47.00010 Femtosecond Heterodyne Transient Grating Studies of Nonradiative Decay of the  $S_2$  ( $1^1B_u^+$ ) State of Peridinin: Detection and Spectroscopic Assignment of an  $S_x$  Intermediate State<sup>1</sup>**, SOUMEN GHOSH, MICHAEL M. BISHOP, JEROME D. ROSCIOLI, Michigan State University, AMY M. LAFOUNTAIN, HARRY A. FRANK, University of Connecticut, WARREN F. BECK, Michigan State University — Femtosecond heterodyne transient grating spectroscopy was employed to investigate the nonradiative relaxation dynamics of peridinin from the  $S_2$  state to the  $S_1$  ( $2^1A_g^-$ ) state in methanol. A global target analysis indicates that  $S_2$  decays in 12 fs to populate an intermediate state,  $S_x$ . The absorption and dispersion components of the transient grating signal exhibit a response that is very similar to that of  $\beta$ -carotene in benzonitrile solution. Numerical simulation of the experimental data indicates that the excited state absorption transition from  $S_x$  has a larger oscillator strength than that of  $S_1$ , which rules out an assignment of  $S_x$  to a vibrationally excited  $S_1$  state. The lifetime of  $S_x$  is found to be strongly dependent on the polar solvation timescale. This result indicates that nonradiative decay from  $S_x$  to  $S_1$  involves large-amplitude torsional motions and a concomitant formation of intramolecular charge transfer character. The present work provides the first evidence that peridinin has an ultrashort  $S_2$  lifetime owing to the onset of torsional motions and shows that the  $S_x$  acts as an active state for excitation energy transfer to chlorophyll in light-harvesting proteins.

<sup>1</sup>Work supported by the Photosynthetic Systems program of U.S. Department of Energy under Award Number DE-SC0010847.

**1:15PM L47.00011 Isomerization of one molecule observed through tip enhanced Raman spectroscopy<sup>1</sup>**, YANXING ZHANG, Department of Physics and Astronomy, University of California, JOONHEE LEE, VARTKESS A. APKARIAN, Department of Chemistry, University of California, RUQIAN WU, Department of Physics and Astronomy, University of California, RUQIAN WU, YANXING ZHANG TEAM, JOONHEE LEE, VARTKESS A. APKARIAN TEAM — While exploring photoisomerization of azobenzyl thiols (ABT) adsorbed on Au(111), through joint scanning tunneling microscopy (STM) and tip-enhanced Raman scattering (TERS) studies, the reversible photoisomerization of one molecule is captured in TERS trajectories. The apparently heterogeneously photo-catalyzed reaction is assigned to cis-trans isomerization of an outlier, which is chemisorbed on the silver tip of the STM. In order to clarify the role of the silver tip of the STM, we perform systematic density functional theory (DFT) calculations. The results show that compared with the case on the flat Ag(111) surface, the energy difference between trans and cis states of ABT decrease as we add one silver atom or a tetrahedron silver cluster on Ag(111) surface which mimic the geometry of a silver tip. In particular, the trans stretches away from the surface on the tetrahedral silver cluster, and the energy difference between trans and cis decreases to 0.27 eV, from ~1 eV for ABT on the flat Ag(111) surface. This significantly increases the possibility of cis-trans isomerization, as observed in our experiments.

<sup>1</sup>Work was supported by the National Science Foundation Center for Chemical Innovation on Chemistry at the Space-Time Limit (CaSTL) under Grant No. CHE-1414466

**1:27PM L47.00012 Femtosecond Carrier Dynamics in Gold-MoS<sub>2</sub> Hybrid Nanostructures**, CHLOE DOIRON, XUEJUN LIU, HOSSEIN ROBATJAZI, ISABELL THOMANN, Department of Electrical and Computer Engineering, Rice University — Small plasmonic nanoparticles are known to efficiently generate energetic hot carriers [1] that can be harnessed by injecting them across a Schottky barrier. To understand the role of plasmon-induced hot carrier generation across Schottky junctions in photocatalytic processes, we synthesized quasi-2D MoS<sub>2</sub> monolayer flakes decorated with Au nanoparticles in ethanol. Our goal is to study ultrafast plasmon induced electron injection from Au nanospheres into MoS<sub>2</sub> monolayer flakes. We will present femtosecond transient absorption measurements on MoS<sub>2</sub>/Au hybrid nanoparticles in ethanol solvent, and compare them with neat MoS<sub>2</sub> flakes in ethanol.  
[1] Nano Letters, 2015, 15 (9), p 6155

**1:39PM L47.00013 Is DNA a metal, semiconductor or insulator? A theoretical approach<sup>1</sup>**, RAFAEL REY-GONZALEZ, KAREN FONSECA-ROMERO, CARLOS PLAZAS, Universidad Nacional de Colombia, GRUPO DE PTICA E INFORMACIN CUNTICA TEAM — Over the last years, scientific interest for designing and making low dimensional electronic devices with traditional or novel materials has been increased. These experimental and theoretical researches in electronic properties at molecular scale are looking for developing efficient devices able to carry out tasks which are currently done by silicon transistors and devices. Among the new materials DNA strands are highlighted, but the experimental results have been contradictories pointing to behaviors as conductor, semiconductor or insulator. To contribute to the understanding of the origin of the disparity of the measurements, we perform a numerical calculation of the electrical conductance of DNA segments, modeled as 1D disordered finite chains. The system is described into a Tight binding model with nearest neighbor interactions and a s orbital per site. Hydration effects are included as random variations of self-energies. The electronic current as a function of applied bias is calculated using Landauer formalism, where the transmission probability is determined into the transfer matrix formalism. We find a conductor-to-semiconductor-to-insulator transition as a function of the three effects taken into account: chain size, intrinsic disorder, and hydration

<sup>1</sup>We thank Fundación para la Promoción de la Investigación y la Tecnología, Colombia, and Dirección de Investigación de Bogotá, Universidad Nacional de Colombia, for partial financial support

**1:51PM L47.00014 Femtosecond Heterodyne Transient Grating Detection of Conformational Dynamics in the  $S_0$  ( $1^1A_g^-$ ) State of Carotenoids After Nonradiative Decay of the  $S_2$  ( $1^1B_u^+$ ) State<sup>1</sup>**, JEROME D. ROSCIOLI, SOUMEN GHOSH, MICHAEL M. BISHOP, Michigan State University, AMY M. LAFOUNTAIN, HARRY A. FRANK, University of Connecticut, WARREN F. BECK, Michigan State University — Transient grating spectroscopy was used to study the dynamics of nonradiative decay of the  $S_1$  ( $2^1A_g^-$ ) state in  $\beta$ -carotene and peridinin after optical preparation of the  $S_2$  state. The kinetics of the recovery of the absorption and dispersion components of the third-order signal exhibit significantly different time constants. For  $\beta$ -carotene in benzonitrile, the absorption and dispersion recovery time constants are 11.6 and 10.2 ps. For peridinin in methanol, the time constants are 9.9 and 7.4 ps. These results indicate that the initial product of the decay of the  $S_1$  state is a conformationally displaced structure. The decay rate for the  $S_1$  state and the conformational relaxation rate are both slowed in peridinin as the polarity of the solvent decreases; in ethyl acetate, the conformational relaxation time constant is 45 ps, which rules out a dominant contribution from vibrational cooling. These results indicate that the  $S_1$  state develops intramolecular charge transfer character owing to distortions along torsional and out-of-plane coordinates, with a pyramidal structure favored as the most stable conformation. Recovery of the photoselected ground state conformation involves a reverse charge-transfer event followed by relaxation to a planar structure.

<sup>1</sup>Work supported by Photosynthetic Systems Program of the U.S. Department of Energy under grant DE-SC0010847.

**Wednesday, March 16, 2016 11:15AM - 2:15PM —**  
**Session L48 GQI: Decoherence in Superconducting Qubits: Materials and TLSs** 349 - David Pappas, NIST-Boulder

**11:15AM L48.00001 Characterizing and reducing microfabrication-induced loss in superconducting devices, Part I: Resonators<sup>1</sup>**, ANDREW DUNSWORTH, UC Santa Barbara, A. MEGRANT, Google, Santa Barbara, Z. CHEN, C. QUINTANA, UC Santa Barbara, B. BURKETT, J. KELLY, R. BARENDs, A. FOWLER, E. JEFFREY, T. WHITE, D. SANK, J. MUTUS, Google, Santa Barbara, B. CAMPBELL, UC Santa Barbara, Y. CHEN, Google, Santa Barbara, B. CHIARO, C. NEILL, P.J.J. O'MALLEY, UC Santa Barbara, P. ROUSHAN, Google, Santa Barbara, A. VAINSENCER, J. WENNER, UC Santa Barbara, J.M. MARTINIS, University of California and Google, Santa Barbara — Planar and 3D superconducting qubits have previously been shown to be limited by microfabrication induced loss. Using finite element simulations, we have identified a major source of this decoherence in superconducting qubits. Furthermore, we experimentally verified this dominant loss channel using a novel resonator based approach, which we call 'Hydra' resonators. We fully characterized and then substantially reduced this loss channel using these Hydra resonators. I will report on these measurements and their implications on improving the coherence of superconducting qubits.

<sup>1</sup>This work is supported by Google inc.

**11:27AM L48.00002 Characterizing and reducing microfabrication-induced loss in superconducting devices, Part II: Xmon qubits**, ANTHONY MEGRANT, Google, Santa Barbara, A. DUNSWORTH, C. QUINTANA, UC Santa Barbara, J. KELLY, R. BARENDs, Google, Santa Barbara, B. CAMPBELL, UC Santa Barbara, Y. CHEN, Google, Santa Barbara, Z. CHEN, B. CHIARO, UC Santa Barbara, A. FOWLER, E. JEFFREY, J. MUTUS, Google, Santa Barbara, C. NEILL, P.J.J. O'MALLEY, UC Santa Barbara, P. ROUSHAN, D. SANK, Google, Santa Barbara, A. VAINSENCER, J. WENNER, UC Santa Barbara, T. WHITE, Google, Santa Barbara, J.M. MARTINIS, University of California and Google, Santa Barbara — Microfabrication-induced loss has previously been shown to limit the coherence times of both planar and 3-D superconducting qubits. Energy loss in these qubits arises from interactions with two-level state defects which are located in thin lossy surface dielectrics. More recently, we have identified a major source of this loss and then substantially improved this decoherence channel using a novel resonator structure for characterization and improvement. I will report on recent measurements of Xmon qubits with substantially improved coherence times due to our new fabrication process.

**11:39AM L48.00003 Supercritical Fluid Assisted Cleaning of Patterned Aluminum Microstructures for Removal of Post-Processing Residue and Surface Contamination**, MARVIN G. WARNER, CHRISTOPHER A. BARRETT, CYNTHIA L. WARNER, Pacific Northwest National Laboratory, CHRISTOPHER J.K. RICHARDSON, NATHAN SIWAK, Laboratory for Physical Sciences, University of Maryland — We report the development of preliminary methods for the supercritical CO<sub>2</sub> assisted removal of post-processing residue and surface contamination from delicate aluminum structures, such as those found in superconducting quantum circuits based on Josephson Junctions. The supercritical CO<sub>2</sub> serves as an effective solvent system to assist in the delivery of various co-solvents, stripping agents, and surfactants to the surface of the patterned devices without introducing harsh chemical reagents that can lead to degradation and etching of the aluminum structures. This work was conducted to determine the feasibility and benefits of inserting a supercritical CO<sub>2</sub> cleaning step into device patterning and cleaning processes. The results presented here will discuss our efforts to determine the optimal formulation, shortest exposure time, and exposure methods (*e.g.*, pulsed versus static) necessary to completely remove surface contamination while preserving the integrity of the underlying patterned aluminum structures. The methods presented here could make great strides in removing fabrication based residue and surface contamination, which has been shown to lead to decoherence in superconducting quantum circuits.

**11:51AM L48.00004 Low temperature internal friction of amorphous silicon<sup>1</sup>**, XIAO LIU, THOMAS METCALF, GLENN JERNIGAN, Naval Research Lab, BATTOGTOKH JUGDERSUREN, Sotera Defense Solutions Inc., BRIAN KEARNEY, NRC Postdoctoral Associate, JAMES CULBERSTON, Naval Research Lab — The ubiquitous low-energy excitations, known as two-level tunnelling systems (TLS), are one of the universal phenomena of amorphous solids. These excitations dominate the acoustic, dielectric, and thermal properties of structurally disordered solids. Using the double-paddle oscillator internal friction measurement technique, we have shown that TLS can be made to almost completely disappear in e-beam deposited amorphous silicon (a-Si) as the growth temperature increased to 400C. However, there is a mysterious broad maximum in internal friction at 2-3K, which we suspect to come from metallic contamination of our oscillators and is not related to a-Si. Our new result of a-Si, deposited in a different UHV system and on oscillators with a different type of metallic electrodes, confirms our suspicion. This lowers the upper bound of possible TLS content in a-Si, in terms of tunnelling strength, to below 10<sup>-6</sup>. Our results offer an encouraging opportunity to use growth temperature to improve the structure order of amorphous thin films and to develop high quality amorphous dielectrics for applications, such as in modern quantum devices.

<sup>1</sup>Work supported by the Office of Naval Research

**12:03PM L48.00005 Elastic measurements of TLSs in amorphous silicon at mK temperatures**, ANDREW FEFERMAN, Institut Néel, CNRS and Université Grenoble Alpes, XIAO LIU, THOMAS METCALF, GLENN JERNIGAN, Naval Research Laboratory, EDDY COLLIN, Institut Néel, CNRS and Université Grenoble Alpes — The low temperature properties of glass are distinct from those of crystals due to the presence of poorly understood low-energy excitations. These are usually thought to be atoms tunneling between nearby equilibria, forming tunneling two level systems (TLSs). Elastic measurements on amorphous silicon films deposited with e-beam evaporation showed that this material contains a variable density of TLSs that decreases as the growth temperature increases from 45 to 400 deg C [1]. We will present an analysis of the elastic properties of these films down to the low mK range in the framework of the standard tunneling model. [1] X. Liu, D. R. Queen, T. Metcalf, J. Karel and F. Hellman, Phys. Rev. Lett., 113, 025503 (2014)

**12:15PM L48.00006 Device Applications for the Tunneling Atom Maser**, YANIV ROSEN, SAMARESH GUCHHAIT, Laboratory for physical sciences, College Park, MD, ALEX BURIN, Tulane university, New Orleans, LA, KEVIN OSBORN, Laboratory for physical sciences, College Park, MD — Random two-level system defects in dielectrics absorb energy and limit the coherence of superconducting qubits and resonators used in quantum computing applications. So far attempts to reduce this loss have been confined to device design and material optimization. We present the ability to control the loss of a dielectric by directly manipulating the population of its two level system defects (TLSs). The defect populations can be controlled and the resonator can pass continuously through regimes of ordinary defect loss, to negligible material dissipation, and finally to coherent amplification. The theory behind the device is discussed and matched to experimental results. Using similar methods, we propose devices that control loss, exhibit reduced noise, and amplify signals.

**12:27PM L48.00007 A qubit designed with a dynamically controlled bath of two-level system defects**, TIM KOHLER, YANIV ROSEN, SAMARESH GUCHHAIT, Univ of Maryland-College Park, KEVIN OSBORN, Laboratory of Physical Science — Although superconducting qubits have made tremendous gains, they still suffer decoherence from two level system (TLS) defects that are found at dielectric films including the native oxides on superconductors. Qubits often minimize TLS effects by choosing optimal device geometries. We have previously investigated methods to electrically sweep the energy of a bath of TLSs and control their excited-state population. Here we discuss a qubit design that incorporates a similar control over the TLSs, and which may prove to minimize TLS decoherence effects. In this device the qubit energy can remain constant while the TLS bath is dynamically controlled. We will discuss experimental progress towards realizing this qubit.

**12:39PM L48.00008 Surface Participation Effects in Titanium Nitride and Niobium Resonators<sup>1</sup>**, ALLISON DOVE, JOHN MARK KREIKEBAUM, WILLIAM LIVINGSTON, REMY DELVA, YANJIE QIU, REINHARD LOLOWANG, VINAY RAMASESH, KEVIN O'BRIEN, IRFAN SIDDIQI, Quantum Nanoelectronics Laboratory, UC Berkeley — Improving the coherence time of superconducting qubits requires a precise understanding of the location and density of surface defects. Superconducting microwave resonators are commonly used for quantum state readout and are a versatile testbed to systematically characterize materials properties as a function of device geometry and fabrication method. We report on sputter deposited titanium nitride and niobium on silicon coplanar waveguide resonators patterned using reactive ion etches to define the device geometry. We discuss the impact of different growth conditions (temperature and electrical bias) and processing techniques on the internal quality factor ( $Q$ ) of these devices. In particular, to investigate the effect of surface participation, we use a Bosch process to etch many-micron-deep trenches in the silicon substrate and quantify the impact of etch depth and profile on the internal  $Q$ .

<sup>1</sup>This research was supported by the ARO.

**12:51PM L48.00009 Fabrication and characterization of highly disordered TiN thin films by reactive evaporation for circuit-QED.**, YEN-HSIANG LIN, RAYMOND MENCIA, BAOLONG NGUYEN, VLADIMIR MANUCHARYAN, University of Maryland - College Park — Titanium nitride (TiN) has been identified as one of the potentially new materials for circuit-QED. In particular, disordered TiN films close to superconductor-insulator transition can be beneficial to greatly enhance kinetic inductance due to low superfluid density. Here we report TiN thin films prepared by e-beam evaporation within a nitrogen rich environment. By controlling nitrogen gas flow rate, the normal sheet resistance of TiN film can be tuned higher than 1kOhms while superconductivity still remains above 2K. Here, we present our characterization results and microwave measurement of quality factor  $Q$  and kinetic inductance  $L$ .

**1:03PM L48.00010 TiN superconducting coplanar waveguide resonators with single-photon quality factors of 1.5 million**, GREG CALUSINE, DANNA ROSENBERG, DAVID HOVER, RABINDRA DAS, ALEXANDER MELVILLE, KHOVALIN MILOSHI, WAYNE WOODS, JONILYN YODER, MIT Lincoln Laboratory, WILLIAM OLIVER, MIT Lincoln Laboratory; Research Laboratory of Electronics, MIT — The investigation of loss mechanisms in superconducting coplanar waveguide (CPW) resonator provides an efficient means to elucidate relevant loss mechanisms affecting superconducting qubit circuits. As compared to superconducting qubits, the reduced complexity of CPW fabrication coupled with the straightforward characterization of CPW properties facilitates the deconvolution of the impact of individual fabrication steps on the CPW performance. We assess this impact by characterizing the statistically significant differences in internal quality factors ( $Q_i$ ) at the single-photon level resulting from different fabrication processes in aluminum and titanium nitride (TiN) superconducting thin film CPW resonators on silicon. We demonstrate repeatable  $Q_i$ 's at the single-photon level of approximately  $1.5 \times 10^6$  in TiN CPW resonators with 90 percent of devices showing  $Q_i$ 's above  $1 \times 10^6$  and single  $Q_i$ 's as high as  $3.8 \times 10^6$ . This work is sponsored in part by the Laboratory for Physical Science, IARPA, and the Assistant Secretary of Defense for Research and Engineering under Air Force Contract FA8721-05-0002. Opinions, interpretations, conclusions, and recommendations are those of the authors and are not necessarily endorsed by the United States Government.

**1:15PM L48.00011 Anomalous thickness dependence of quality factor in TiN film resonators grown on functionalized Si substrates**, PENG XU, TIM KOHLER, Laboratory for Physical Sciences, EVGENIYA LOCK, Naval Research Laboratory, YANIV ROSEN, ARUNA RAMANAYAKA, SAMARESH GUCHHAIT, KEVIN OSBORN, Laboratory for Physical Sciences — Various properties affect the quality factor of superconducting resonators at millikelvin temperatures including the presence of nanoscale interfacial dielectric films and residual quasiparticles. Superconducting titanium nitride is polycrystalline such that growth phases may also affect the resonator quality. Here, we functionalize Si substrates in different hydrophobic and hydrophilic plasma environments, sputter titanium nitride on top and pattern the latter films into resonators. For each functionalization we study the quality factor dependence on the superconducting film thickness, where the thicknesses are changed only between 25 and 50 nm. As expected, most functionalizations reveal very little quality factor dependence on superconducting film thickness. However, other functionalizations dramatically, and even anomalously, increase or decrease the quality with thickness. For example, oxygen plasma functionalization causes the quality factor to increase by a factor of more than ten at single photon power with increased thickness. We report on the progress towards finding the intrinsic reason for strong quality factor dependences on surface functionalization.

**1:27PM L48.00012 Optimized Shielding and Fabrication Techniques for TiN and Al Microwave Resonators<sup>1</sup>**, JOHN MARK KREIKEBAUM, EUNSEONG KIM, WILLIAM LIVINGSTON, ALLISON DOVE, Univ of California - Berkeley, GREGORY CALUSINE, DAVID HOVER, DANNA ROSENBERG, WILLIAM OLIVER, MIT Lincoln Laboratory, IRFAN SIDDIQI, Univ of California - Berkeley — We present a systematic study of the effects of shielding and packaging on the internal quality factor ( $Q_i$ ) of Al and TiN microwave resonators designed for use in qubit readout. Surprisingly,  $Q_i = 1.3 \times 10^6$  TiN samples investigated at 100 mK exhibited no significant changes in linewidth when operated without magnetic shielding and in an open cryo-package. In contrast, Al resonators showed systematic improvement in  $Q_i$  with each successive shield. Measurements were performed in an adiabatic demagnetization refrigerator, where typical ambient fields of 0.2 mT are present at the sample stage. We discuss the effect of 100 mK and 500 mK Cu radiation shields and cryoperm magnetic shielding on resonator  $Q$  as a function of temperature and input power in samples prepared with a variety of surface treatments, fabrication recipes, and embedding circuits.

<sup>1</sup>This research was supported by the ARO and IARPA.

**1:39PM L48.00013 Characterizing the performance of waveguide technologies for microwave-frequency quantum communication**, PHILIPP KURPIERS, TOBIAS FREY, ANDREAS WALLRAFF, ETH - Zurich — In circuit quantum electrodynamics (QED) systems quantum communication over distances beyond chip-scale requires low-loss waveguides. We measure the loss per unit length and the phase stability of commercially available waveguide technologies down to Millikelvin temperatures and single photon levels. More specifically, we characterize the frequency dependent attenuation and dispersion properties of a range of semi-rigid microwave cables and waveguides. We study the properties of various, commonly used conducting and dielectric materials with high accuracy in resonant structures to extract the internal quality factor which is inversely proportional to the loss per unit length. Furthermore, we compare our data with corresponding loss models. The results of our characterization are relevant to applications in which quantum communication is needed between nodes of a small network, e.g. between quantum circuits realized on different chips within the same or in distinct cryogenic systems.

**1:51PM L48.00014 Spectrum of a Resonator Coupled to a Driven Superconducting Qubit in the Strong Dispersive Regime of Circuit Quantum Electrodynamics**, YONUK CHONG, HYUN-GUE HONG, DONG-GWANG HA, Korea Research Institute of Standards and Science — The resonator spectrum in the strong dispersive coupling regime of circuit-QED has been a useful nondestructive indicator of a stationary qubit state. Here we present experimental observation of the further modification of the resonator spectrum as the qubit undergoes the dynamic transition by a resonant driving field. The quartet resonance associated with the polarized qubit is observed for the resonant driving at one-photon as well as the multi-photon transition in a 3D transmon qubit. The evolution of the resonance as a function of the driving power and the detuning of the driving field is well understood by a simple model which is based on the analytic diagonalization of Hamiltonian and described in terms of dressed states, Lamb shift, and AC Stark shift.

**2:03PM L48.00015 Characterizing Ensembles of Superconducting Qubits**, ADAM SEARS, JEFF BIRENBAUM, DAVID HOVER, DANNA ROSENBERG, STEVEN WEBER, JONILYN L. YODER, JAMIE KERMAN, MIT Lincoln Laboratory, SIMON GUSTAVSSON, ARCHANA KAMAL, FEI YAN, MIT, WILLIAM OLIVER, MIT Lincoln Laboratory — We investigate ensembles of up to 48 superconducting qubits embedded within a superconducting cavity. Such arrays of qubits have been proposed for the experimental study of Ising Hamiltonians, and efficient methods to characterize and calibrate these types of systems are still under development. Here we leverage high qubit coherence ( $> 70 \mu s$ ) to characterize individual devices as well as qubit-qubit interactions, utilizing the common resonator mode for a joint readout. This research was funded by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA) under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of ODNI, IARPA, or the US Government.

**Wednesday, March 16, 2016 11:15AM - 1:51PM –**

**Session L50 DAMOP: Cold Atomic Gases: Precision Measurement and Few-Body Physics** Hilton  
Baltimore Holiday Ballroom 1 - Shina Tan, Georgia Institute of Technology

**11:15AM L50.00001 ABSTRACT WITHDRAWN –**

**11:27AM L50.00002 Atom interferometric measurement of “Big G” on the International Space Station<sup>1</sup>**, ELIZABETH ASHWOOD, DOGA MURAT KURKCUOGLU, MARK EDWARDS, Georgia Southern Univ, CHARLES CLARK, Joint Quantum Institute — Recent measurements of Newton's universal gravitational constant (“Big G”) using atom interferometric methods have increased the uncertainty in the value of this important fundamental constant<sup>2</sup>. We have developed tools for rapid simulation and evaluation of atom interferometer (AI) schemes that can be implemented in the Cold Atom Laboratory to be deployed to the International Space Station (ISS) in 2017. We have approximated the solution of the rotating-frame Gross-Pitaevskii equation in both one and three dimensions by using the Lagrangian Variational Method (LVM). The LVM trial wave function is a sum of  $N_c$  Gaussian clouds and we have derived equations of motion for the centers, widths, and phase parameters of these clouds. These equations of motion can be rapidly solved for many different AI designs enabling the estimation of interferometer sensitivity and the effects of errors. We present two potential schemes for measuring “Big G” on the ISS. These include a Mach-Zehnder-like scheme as well as a design similar to a Foucault Pendulum.

<sup>1</sup>Supported by NSF grants PHY-1413768 and ARO Atomtronics MURI

<sup>2</sup>See, e.g., S. Schlamminger, *Nature* **510**, 478 (2014)

**11:39AM L50.00003 Sensitivity improvements to the YbF electron electric dipole moment experiment**, ISABEL RABEY, JACK DEVLIN, BEN SAUER, JONY HUDSON, MIKE TARBUTT, ED HINDS, Imperial College London — The electron is predicted to have a small electric dipole moment (EDM). The size of this fundamental property is intimately connected to the breaking of time reversal symmetry (T) in nature. The Standard Model, which does include a small amount of T asymmetry, predicts the EDM to be too small to ever detect at  $d_e < 10^{-38}$  e.cm. However, many extensions of the Standard Model that suggest additional T-violation predict the electron's EDM to be within a measurable regime of both current and proposed experiments. This talk describes our YbF electron EDM experiment and introduces some of the technical improvements made to our machine since the last measurement. We have increased the statistical sensitivity of our interferometer by increasing the number of YbF molecules that participate in the experiment and by increasing their detection probability. We demonstrate several hardware developments that combine laser, microwave and rf fields which, when applied to YbF, can pump six times more population into the initial measurement state. In the detection region we have used techniques developed for molecular laser cooling, including resonant polarisation modulation, to dramatically increase the number of scattered photons by a factor of 10. Combining all improvements, the statistical uncertainty of our measurement is expected to be reduced by a factor of ninety, allowing us to search for physics beyond the Standard Model and below the recent upper limit of  $d_e < 8.9 \times 10^{-29}$  e.cm.

**11:51AM L50.00004 Anti-parity-time symmetry via flying atoms**, JIANMING WEN, Yale Univ, LIANG JIANG, Yale University, YANHONG XIAO, PENG PENG, WANXIA CAO, CE SHEN, WEIZHI QU, Fudan University — We report the first experimental demonstration of optical anti-parity-time (anti-PT) symmetry [1], a counterpart of conventional PT symmetry [2], in a warm atomic-vapor cell. By exploiting rapid coherence transport via flying atoms, our scheme illustrates essential features of anti-PT symmetry with an unprecedented precision on phase-transition threshold, and substantially reduces experimental complexity and cost, in contrast to most previous experimental studies relying highly on the advances of nanotechnologies and sophisticated fabrication techniques to synthesize solid-state materials. Of importance, our results represent a significant advance in non-Hermitian physics by bridging a firm connection with the field of atomic, molecular and optical physics, where novel phenomena and applications in quantum and nonlinear optics aided by (anti-)PT symmetry can be anticipated. [1] P. Peng, W. Cao, C. Shen, W. Qu, J. Wen, L. Jiang, and Y. Xiao, arXiv: 1509.07736 (2015). [2] L. Chang, X. Jiang, S. Hua, C. Yang, J. Wen, L. Jiang, G. Li, G. Wang, and M. Xiao, *Nature Photonics* **8**, 524-529 (2014).

**12:03PM L50.00005 Two-dimensional atom localization via phase-sensitive absorption-gain spectra in five-level hyper inverted-Y atomic systems**, ZHONGHU ZHU, WEN-XING YANG<sup>1</sup>, Department of Physics, Southeast University, Nanjing 210096, PR China, AI-XI CHEN, Department of Applied Physics, School of Basic Science, East China Jiaotong University, Nanchang 330013, PR China — High-precision measurement of an atomic position through a standing-wave field has been the subject of active research over the past few decades because of its potential applications in laser cooling and trapping of neutral atoms, such as atom nanolithography, Bose-Einstein condensation, and coherent patterning of matter waves. More recently, two-dimensional atom localization, achieved by applying two orthogonal standing-wave fields, has been studied extensively for its unique properties. For realizing high-precision two-dimensional atom localization, we explore two-dimensional atom localization based on phase-sensitive probe absorption and gain in a microwave-driven five-level hyper inverted-Y atomic system. Because of the spatial position-dependent atom-field interaction, two-dimensional atom localization can be achieved by the measurements of the probe absorption and gain spectra. It was clearly shown that the precision of two-dimensional atom localization is extremely sensitive to the detuning of the weak probe field, the intensities of the two control fields, and the relative phase of the driving fields. The main advantage of our proposed scheme is that the maximum probability of finding the atom at an expected position in one period of the standing-wave fields is 100%.

<sup>1</sup>Corresponding author: wenxingyang2@126.com

**12:15PM L50.00006 Three-bosons in 2D with a magnetic field**, SETH RITTENHOUSE, Department of Physics, The United States Naval Academy, ANDREW WRAY, BRAD JOHNSON, Department of Physics and Astronomy, Western Washington University — Systems of interacting particles in reduced dimensions in the presence of external fields can exhibit a number of surprising behaviors, for instance the emergence of the fractional quantum Hall effect. Examining few-body interactions and effects can lead to significant insights within these systems. In this talk we examine a system of three bosons confined to two dimensions in the presence of a perpendicular magnetic field within the framework of the adiabatic hyperspherical method. For the case of zero-range, regularized pseudo-potential interactions, we find that the system is nearly separable in hyperspherical coordinates and that, away from a set of narrow avoided crossings, the full energy eigenspectrum as a function of the 2D s-wave scattering length is well described by ignoring coupling between adiabatic hyperradial potentials. In the case of weak attractive or repulsive interactions, we find the lowest three-body energy states exhibit even/odd parity oscillations as a function of total internal 2D angular momentum and that for weak repulsive interactions, the universal lowest energy interacting state has an internal angular momentum of  $M = 3$ .

**12:27PM L50.00007 Three-Body Effects in a Zero-Scattering-Length Condensate**, LAWRENCE PHILLIPS, Heriot Watt University — When pairwise interactions between ultracold Bosons are set to zero using Feshbach resonance, the resulting condensate is well described by replacing the standard two-body contact interaction with a three-body pseudopotential and proceeding with Hartree-Fock theory in the usual way. We give a prescription for calculating the coupling constant appearing in the three-body pseudopotential, and use it to investigate the dependence of the zero-scattering-length dynamics upon the original two-body potential.

**12:39PM L50.00008 Nonadiabatic calculations on hydrogen molecule**, JACEK KOMASA, Adam Mickiewicz University, Poznan, KRZYSZTOF PACHUCKI, Warsaw University, Poland — Since its infancy quantum mechanics has treated hydrogen molecule as a test bed. Contemporary spectroscopy is able to supply the dissociation energy ( $D_0$ ) of  $H_2$  with the accuracy of  $3.7 \cdot 10^{-4} \text{ cm}^{-1}$ , while current theoretical predictions are  $10^{-3} \text{ cm}^{-1}$  in error. Both the uncertainties are already smaller than the quantum electrodynamic (QED) effects contributing to  $D_0$ , which poses a particular challenge to theoreticians. Undoubtedly, in order to increase the predictive power of theory one has to not only account for the multitude of the tiny relativistic and QED effects but, especially, significantly increase precision of the largest component of  $D_0$ —the nonrelativistic contribution. We approach the problem of solving the Schroedinger equation, equipped with new methodology, with the target precision of  $D_0$  set at the level of  $10^{-7} \text{ cm}^{-1}$ .

**12:51PM L50.00009 s-wave resonant short-range interactions in a d-dimensional finite volume**, SHANGGUO ZHU, SHINA TAN, Georgia Inst of Tech — It has been known that the energy spectra of few or many particles with short-range interactions in a finite periodic box are shifted according to the size of the box. In particular, the two-body interaction in a three-dimensional box is described by the Lüscher's formulas. Here we study the energy of one particle scattered by a resonant s-wave short-range center in a d-dimensional finite volume. When  $d = 6$ , this one-body problem is mapped to the scattering of three particles in a three-dimensional box with a resonant three-body interaction.

**1:03PM L50.00010 The Bosonic Kane-Mele Hubbard model**, RAJBIR NIRWAN<sup>1</sup>, Institut für Theoretische Physik, Goethe-Universität, 60438 Frankfurt/Main, Germany, IVANA VASIC, Scientific Computing Laboratory, Institute of Physics Belgrade, University of Belgrade, 11080 Belgrade, Serbia, ALEXANDRU PETRESCU, Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544, USA, KARYN LE HUR, Centre de Physique Théorique, Ecole Polytechnique and CNRS, Université Paris-Saclay, France, WALTER HOFSTETTER, Institut für Theoretische Physik, Goethe-Universität, 60438 Frankfurt/Main, Germany — We investigate the bosonic equivalent of the Kane-Mele model on the honeycomb lattice [1] including spin-orbit and interaction effects. This model is a generalization of the interacting bosonic Haldane model introduced in Ref. [2]. We also allow for an on-site conversion (coherent) term between the two species. We analyze the phase diagram using bosonic dynamical mean-field theory and analytical methods. In the Mott phase, a strong-coupling expansion is performed to investigate the magnetism and frustration effects. A connection is drawn with the quantum theory of an antiferromagnet on a triangular lattice in a magnetic field [3]. This model can be realized in ultra-cold atom systems with current technology. [1] C. L. Kane and E. Mele, Phys. Rev. Lett. 95, 226801 (2005). [2] I. Vasic, A. Petrescu, K. Le Hur and W. Hofstetter, Phys. Rev. B 91, 094502 (2015). [3] A. V. Chubukov and D. I. Golosov, J. Phys. Cond. Matt. 3 69 (1991).

<sup>1</sup>replace MAR16-2015-003145

**1:15PM L50.00011 Strong correlation effects in a two-dimensional Bose gas with quartic dispersion**, JURAJ RADIC, STEFAN NATU, VICTOR GALITSKI, University of Maryland, College Park — We consider a two-dimensional Bose gas at zero temperature with an underlying quartic single-particle dispersion in one spatial direction. This type of band structure can be realized using the NIST scheme of spin-orbit coupling, in the regime where the lower band dispersion has the form  $\varepsilon_{\mathbf{k}} \sim k_x^4/4 + k_y^2 + \dots$ . We numerically compare the ground state energies of the mean-field Bose-Einstein condensate (BEC) and various trial wave-functions, where bosons avoid each other at short distances. We discover that, at low densities, several types of strongly correlated states have an energy per particle ( $\epsilon$ ), which scales with density ( $n$ ) as  $\epsilon \sim n^{4/3}$ , in contrast to  $\epsilon \sim n$  for the weakly interacting Bose gas. These competing states include a Wigner crystal, quasi-condensates described in terms of properly symmetrized fermionic states, and variational wave-functions of Jastrow type, where the latter has the lowest energy and describes a strongly-correlated condensate. Our results show that even for weakly-interacting bosons in higher dimensions, one can explore the crossover from a weakly-coupled BEC to a strongly-correlated condensate by simply tuning the single particle dispersion or density.

**1:27PM L50.00012 Wave function anatomy of ultracold fermions in a double well: Attractive-pairing, Wigner-molecules, and entanglement**<sup>1</sup>, BENEDIKT B. BRANDT, CONSANTINE YANNOULEAS, UZI LANDMAN, School of Physics, Georgia Institute of Technology — We report on exact benchmark configuration-interaction computational solutions of the many-body Hamiltonian, uncovering the spectral evolution, wave function anatomy, and entanglement properties of a few interacting ultracold fermions in the entire parameter range, including crossover from an single-well to a double-well confinement and a controllable energy imbalance between the wells. According to recent experiments, the two wells are taken as quasi-one-dimensional and both the linear and parallel configurations of them are considered. We demonstrate attractive pairing and formation of repulsive, highly correlated, ultracold Wigner molecules, associated with the emergence of Heisenberg spin chains.<sup>2</sup> For two fermions, the entanglement measure of the von-Neumann entropy is used as a diagnostic tool for identifying maximally entangled two-qubit Bell states.<sup>3</sup>

<sup>1</sup>Supported by the Air Force Office of Scientific Research

<sup>2</sup>Yuesong Li, C. Yannouleas, and U. Landman, Phys. Rev. B **76**, 245310 (2007); Ying Li, C. Yannouleas, and U. Landman, Phys. Rev. B **80**, 045326 (2009)

<sup>3</sup>B.B. Brandt, C. Yannouleas, and U. Landman, Nano Lett. **15**, 7105 (2015).

**1:39PM L50.00013 Solvable Models for a Few Atoms in a Few One-Dimensional Wells**, NATHAN HARSHMAN, Department of Physics, American University — This project identifies networks of one-dimensional, few-particle, few-well models that can be smoothly connected by tuning trap shape and two-body interaction parameters. Solvable models within these networks are identified and analyzed by exploiting symmetries in few-body configuration space and phase space. In one-dimension, ordering permutation symmetry is particularly effective for generating new models. Ordering permutation symmetry is distinct from particle permutation symmetry and arises when there are similar regions in configuration space that are completely disconnected due to unitary interactions and/or infinite well barriers. Realistic experiments with a few atoms or with ultracold gases trapped in effectively one-dimensional wells are analyzed by comparison with nearby solvable models using approximation schemes like perturbation theory or variational methods. The transition from systems with a few particles in a few wells to systems with many particles in large lattices can be explored using these techniques.

**Wednesday, March 16, 2016 11:15AM - 2:15PM —**

**Session L51 FIAP: Fractional QHE: Bilayer, & Many-Body Effects** Hilton Baltimore Holiday Ballroom 2  
- John Cumings, University of Maryland

**11:15AM L51.00001 Meron deconfinement in the quantum Hall bilayer at intermediate distances**, MILICA MILOVANOVIC, Institute of Physics Belgrade, EDIB DOBARDZIC, Faculty of Physics, University of Belgrade, ZLATKO PAPIC, University of Leeds — Quantum Hall bilayer phase diagram with respect to interlayer distance bears a remarkable similarity with phase diagrams of strongly correlated systems as a function of doping, with magnetic ordering on the one end and Fermi-liquid-like behavior on the other. Moreover, it has been suggested [1] that a BCS correlated state of composite fermions with p-wave pairing may exist in the intermediate region. We discuss features of this state using the composite boson point of view, and exact diagonalization calculations on the torus. Furthermore, we argue that in the same state there is a possibility for meron deconfinement, i.e., the deconfinement of the vortex excitations of the magnetically ordered phase. [1] G. Moller, S. H. Simon, and E. H. Rezayi, Phys. Rev. Lett. 101, 176803 (2008); G. Moller, S. H. Simon, and E. H. Rezayi, Phys. Rev. B 79, 125106 (2009).

**11:27AM L51.00002 Magnetotransport of a Quantum Hall Double Layer at Landau Level Filling  $1/2 + 3/2^1$** , WU XING-JUN, LIU RUIYUAN, MI JIAN, ZHANG CHI, Peking University, PFEIFFER LOREN, WEST KEN, Princeton University, DU RUI-RUI, Rice University — The effect of interlayer-tunneling on electron transport in quantum Hall double layers in the regime of exciton condensation state at Landau level filling factor one ( $1/2+1/2$ ) has been well established, in that the interlayer coherence promotes a huge zero-bias conductance peak due to resonantly-enhanced tunneling (e.g., Phys. Rev. Lett. 84, 5808, 2000). Consequently, an in-plane magnetic field is found to suppress this tunneling. Recent theoretical work, on a similar system consisting of two layers with fillings  $1/2+3/2$ , suggests that here the resonant-enhanced tunneling would be suppressed and an in-plane magnetic field, conversely, would play a promoting role in tunneling. We investigate this regime in high-mobility GaAs/AlGaAs bilayers of suitable parameters and with individually contacted layers. Preliminary results and a brief discussion will be presented.

<sup>1</sup>supported by National Basic Research Program of China (2012CB921301 and 2014CB920901) and by Collaborative Innovation Center of Quantum Matter

**11:39AM L51.00003 Probing a Wigner Crystal via Composite Fermion Commensurability Oscillations in an Adjacent Layer**, HAO DENG, INSUN JO, YANG LIU, MANSOUR SHAYEGAN, LOREN N. PFEIFFER, KEN W. WEST, KIRK W. BALDWIN, Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544 — At high magnetic fields and low temperatures, two-dimensional electrons form a composite fermion (CF) Fermi sea with a well-defined Fermi wave vector when the Landau level fillings factor ( $\nu$ ) is near  $1/2$ . In contrast, when  $\nu \ll 1$ , the Wigner crystal (WC) is the favored ground state. We report measurements of the magneto-resistance in a bilayer electron system with unequal layer densities at high magnetic fields. One layer has a very low density and is in the WC regime ( $\nu \ll 1$ ), while the other (probe) layer is near  $\nu = 1/2$  and hosts a CF sea. As the magnetic field is swept away from  $\nu = 1/2$  of the CF layer, the CFs feel the periodic electric potential of the WC in the other layer and exhibit magneto-resistance maxima whenever their cyclotron orbit encircles certain integer number of the WC lattice points. Via measuring the temperature dependence of strength of these commensurability features, we probe the melting of the WC.

**11:51AM L51.00004 Spin Transition of Composite Fermion Solids in Wide Quantum Wells Observed with Microwave Spectroscopy**, ANTHONY HATKE, LLOYD ENGEL, National High Magnetic Field Laboratory, YANG LIU, MANSOUR SHAYEGAN, LOREN PFEIFFER, KEN WEST, KIRK BALDWIN, Princeton University — Within a narrow range of Landau filling ( $\nu$ ) near 1, a resonance in the microwave spectrum in high mobility two-dimensional electron systems is known to occur [1]. The resonance is understood as due to a pinning mode of a Wigner solid of quasicarriers and is present in the  $\nu$ -region of vanishing diagonal resistance. In microwave spectroscopy an abrupt jump in the resonance frequency,  $f_{pk}$ , upon decreasing  $\nu$  from 1 was observed in wide quantum wells [2]. This jump was interpreted as a transition between two solid states: S1, which occurred closer to  $\nu = 1$ , and S2 (with enhanced- $f_{pk}$ ), which occurred farther from  $\nu = 1$ . In this talk we discuss microwave measurements using variable carrier density and in plane magnetic field. Typical for a spin-related transition, tilting the sample at fixed  $n$  results in effects similar to those found on increasing  $n$  without tilt. Taken together, the dependencies of the resonance on  $n$  and the tilt angle are consistent with a ground state spin transition between different solids. We discuss our results in terms of interacting two-flux composite fermions. [1] Chen et al., Phys. Rev. Lett. 93, 206805 (2004). [2] Hatke et al., Nat. Commun. 5, 4154 (2014).

**12:03PM L51.00005 Transport Signatures of Dirac Composite Fermions in the  $1/2$ -filled Landau level**, MAKSYM SERBYN, ANDREW C. POTTER, ASHVIN VISHWANATH, Univ of California - Berkeley — The half-filled state plays a special role among the variety of different fractional quantum Hall effect states. Halperin, Lee, and Read (HLR) predicted the existence of compressible state, where gapless excitations consists of electrons bound to a pair of vortices with emergent Fermi surface. There exists ample experimental evidence for this emergent Fermi surface, despite the presence of the strong magnetic field. However, the role of particle hole symmetry of the half-filled Landau level has remained a puzzle. Recently, an alternative, explicitly particle-hole symmetric state was proposed, where composite fermions fill a single Dirac-cone, analogous to the surface state of a topological insulator. These composite Dirac fermions have a quantized  $\pi$  Berry phase due to their spin- $1/2$ , their electric dipole moment, locked to their momentum. In this talk I will consider the experimental probes that can distinguish between HLR and composite Dirac fermions. In particular, I will address the signatures of particle-hole symmetry and Berry phase in the thermoelectric response. In addition, I will discuss other transport experiments which can probe the Fermi surface topology.

**12:15PM L51.00006 Dirac Composite Fermi Liquid in the Half-filled Landau level<sup>1</sup>**, SCOTT GER-AEDTS, Princeton University, MICHAEL ZALETEL, Station Q, Microsoft Research, ROGER MONG, University of Pittsburgh, MAX METLITSKI, Perimeter Institute, ASHVIN VISHWANATH, University of California Berkeley, OLEXEI MOTRUNICH, California Institute of Technology — Quantum Hall fluids at filling fraction one-half exhibit a compressible phase known as the ‘composite Fermi liquid’ (CFL) We use infinite-cylinder density matrix renormalization group to numerically determine that this phase is the ground state of a half-filled Landau level with Coulomb interactions. We find evidence for a Fermi surface of composite fermions, while also probing the non-Fermi liquid character of the phase. It has been recently realized that the traditional theory used to describe the CFL breaks particle-hole symmetry, while the lowest-Landau level projected Hamiltonian does not. We find that the composite Fermi liquid has particle-hole symmetry, inconsistent with the traditional theory but consistent with a recent theory proposed by Son [Phys. Rev. X 5, 031027]. Our results show the Dirac nature of the composite fermions. We also observe the suppression of certain kinds of backscattering processes of the composite fermions, similar to the suppression in topological insulator surface states.

<sup>1</sup>SG acknowledges support from DOE-BES Grant DE-SC0002140 and NSF-DMR 1206096.

**12:27PM L51.00007 Spontaneous polarization of composite fermions in the  $n = 1$  Landau level of graphene<sup>1</sup>**, AJIT COIMBATORE BALRAM, Pennsylvania State University, CSABA TÖKE, Budapest University of Technology and Economics, ARKADIUSZ WÓJS, Wrocław University of Technology, JAINENDRA JAIN, Pennsylvania State University — Motivated by experiments that reveal expansive fractional quantum Hall states in the  $n = 1$  graphene Landau level and suggest a nontrivial role of the spin degree of freedom [Amet *et al.*, Nat. Commun. 6, 5838 (2014)], we perform accurate quantitative study of the competition between fractional quantum Hall states with different spin polarizations in the  $n = 1$  graphene Landau level. We find that the fractional quantum Hall effect is well described in terms of composite fermions, but the spin physics is qualitatively different from that in the  $n = 0$  Landau level. In particular, for the states at filling factors  $\nu = s/(2s \pm 1)$ ,  $s$  integer, a combination of exact diagonalization and the composite fermion theory shows that the ground state is fully spin polarized and supports a robust spin wave mode even in the limit of vanishing Zeeman coupling. Thus, even though composite fermions are formed, a mean field description that treats them as weakly interacting particles breaks down, and the exchange interaction between them is strong enough to cause a qualitative change in the behavior by inducing full spin polarization. We also find that the fully spin polarized composite fermion Fermi sea has lower energy than the paired Pfaffian state at the relevant half fillings.

<sup>1</sup>Award No. DE-SC0005042 (ACB, JKJ), Hungarian Scientific Research Funds No. K105149 (CT), the Polish NCN grant 2014/14/A/ST3/00654 and the EU Marie Curie Grant PCIG09-GA-2011-294186 (AW)

**12:39PM L51.00008 Anisotropic Composite Fermions and Fractional Quantum Hall Effect**, M A MUEED, DOBROMIR KAMBUROV, SUKRET HASDEMIR, MANSOUR SHAYEGAN, LOREN PFEIFFER, KEN WEST, KIRK BALDWIN, Princeton University — We study the role of Fermi sea anisotropy on the transport properties of composite Fermions near Landau level filling factor  $\nu = 1/2$  in two-dimensional hole systems confined to GaAs quantum wells. By applying a parallel magnetic field, we tune the Fermi sea anisotropy and monitor the relative change of the transport scattering time along its principal directions. Interpreted in a simple Drude model, our results suggest that the scattering time is longer along the longitudinal direction of the Fermi sea. Furthermore, we find that the measured energy gap for the fractional quantum Hall state at  $\nu = 2/3$  decreases when anisotropy becomes significant.

**12:51PM L51.00009 Spectral properties of center-of-mass conserving two-body Hamiltonians<sup>1</sup>**, AMILA WEERASINGHE, TAHEREH MAZAHARI, ALEXANDER SEIDEL, Washington University in St. Louis — We study the low energy spectral properties of positive center-of-mass conserving two-body Hamiltonians as they arise in models of fractional quantum Hall states. We explore what general constraints can be obtained for such interactions, both in the presence and absence of particle-hole symmetry. We find general bounds that constrain the evolution of the ground state energy with particle number, and in particular constrain the chemical potential at  $T = 0$ . Special attention is given to Hamiltonians with zero modes, in which case similar bounds on the first excited state are also obtained, using a duality property. In this case, in particular an upper bound on the charge gap is also obtained.

<sup>1</sup>This work has been supported by the National Science Foundation under NSF Grant No. DMR-1206781.

**1:03PM L51.00010 Neutral Excitations in the Gaffnian state**, BYUNGMIN KANG, JOEL E. MOORE, UC Berkeley — The Fractional Quantum Hall Effect (FQHE) is one of the most well-studied systems having topological order. Starting with the pioneering work by Laughlin, the model wave function approach has been shown to provide essential information for understanding topological order in gapped incompressible states. We study a model wave function called the Gaffnian state which is believed to represent a gapless, strongly correlated state that is very different from conventional metals. To understand this exotic gapless state better, we provide a representation in which the pairing structure of the Gaffnian state becomes more explicit. We employ the single-mode approximation of the Girvin-MacDonald-Platzman (GMP) mode, which is a neutral collective excitation mode, in order to have a physical picture of the gaplessness of the Gaffnian state. In particular, we discuss how to extract systematically the relevant physics in the long-distance, large electron number limit of the FQH states using a numerical calculation with relatively few electrons.

**1:15PM L51.00011 Beyond the Plasma Analogy: Collective Field Theory for Quantum Hall States**, TANKUT CAN, State Univ of NY- Stony Brook, MICHAEL LASKIN, PAUL WIEGMANN, University of Chicago — We develop a quantum field theory of collective coordinates describing fractional quantum Hall (FQH) states. We show that the familiar properties of Laughlin states are captured by a Gaussian free field theory with a background charge. Gradient corrections to the Gaussian theory arise from ultraviolet regularization, and go beyond the celebrated plasma analogy. They give rise to a gravitational anomaly described by the Liouville theory of 2D quantum gravity. The field theory simplifies the computation of correlation functions in FQH states and makes manifest the effect of quantum anomalies. This talk is based on the preprint arXiv:1412.8716.

**1:27PM L51.00012 Resistively detected high-order magnetoplasmons in a high-quality 2D electron gas**, M.A. ZUDOV, Q. SHI, University of Minnesota, L.N. PFEIFFER, K.W. WEST, Princeton University, J.D. WATSON, M.J. MANFRA, Purdue University — We report on high-order magnetoplasmon resonances detected in photoresistance in high-mobility GaAs quantum wells. These resonances manifest themselves as a series of resistance extrema in the regime of Shubnikov-de Haas oscillations. Extending to orders above 20, the extrema exhibit alternating strength, being less (more) pronounced at even (odd) order magnetoplasmon modes. The lower magnetoplasmon modes reveal the importance of retardation effects.

**1:39PM L51.00013 Zero modes, bosonization, and topological quantum order: The Laughlin state in second quantization**<sup>1</sup>, TAHEREH MAZAHARI, Department of Physics, Washington University, St. Louis, MO 63160, USA, GERARDO ORTIZ, Department of Physics, Indiana University, Bloomington, IN 47405, USA, ZOHAR NUSSINOV, ALEXANDER SEIDEL, Department of Physics, Washington University, St. Louis, MO 63160, USA — We introduce a “second-quantized” representation of the ring of symmetric functions to further develop a purely second-quantized approach to the study of zero modes of frustration-free Haldane-pseudopotential-type Hamiltonians, which in particular stabilize Laughlin ground states. We present three applications of this formalism. We start demonstrating how to systematically construct all zero modes of Laughlin-type parent Hamiltonians in a framework that is free of first-quantized polynomial wave functions, and show that they are in one-to-one correspondence with dominance patterns. Second, as a by-product, we make contact with the bosonization method, and obtain an alternative proof for the equivalence between bosonic and fermionic Fock spaces. Finally, we explicitly derive the second-quantized version of Read’s nonlocal order parameter for the Laughlin state, extending an earlier description by Stone.

<sup>1</sup>his work has been supported by the National Science Foundation under NSF Grant No. DMR-1206781 (AS) and under NSF Grant No. DMR-1106293 (ZN).

**1:51PM L51.00014 Structure of Ground state Wave Functions for the Fractional Quantum Hall Effect: A Variational Approach**<sup>1</sup>, SUTIRTHA MUKHERJEE, SUDHANSU MANDAL, Indian Association for the Cultivation of Science — The internal structure and topology of the ground states for fractional quantum Hall effect (FQHE) are determined by the relative angular momenta between all the possible pairs of electrons. Laughlin wave function is the only known microscopic wave function for which these relative angular momenta are homogeneous (same) for any pair of electrons and depend solely on the filling factor. Without invoking any microscopic theory, considering only the relationship between number of flux quanta and particles in spherical geometry, and allowing the possibility of inhomogeneous (different) relative angular momenta between any two electrons, we develop a general method for determining a closed-form ground state wave function for any incompressible FQHE state. Our procedure provides variationally obtained very accurate wave functions, yet having simpler structure compared to any other known complex microscopic wave functions for the FQHE states. This method, thus, has potential in predicting a very accurate ground state wave function for the puzzling states such as the state at filling fraction 5/2.

<sup>1</sup>We acknowledge support from Department of Science and Technology, India

**2:03PM L51.00015 Insulating Behavior of Strongly Interacting 2D Electrons in Si MOSFETs**<sup>1</sup>, SHIQI LI, M. P. SARACHIK, City College of New York, CUNY, S. V. KRAVCHENKO, Northeastern University, Boston — Experiments on low disorder strongly-interacting 2D electron systems have shown that in the absence of a magnetic field, the temperature dependence of the resistivity changes from metallic-like to insulating behavior as the electron density  $n_s$  is reduced below a critical density  $n_c$  [1]. It has been shown that a metal to insulator transition also occurs in these systems for fixed electron density  $n_s$  at a critical (density-dependent) in-plane magnetic field which results in complete spin polarization of the electrons [2]. Here we report measurements of the temperature dependence of the resistivity in a high mobility Si-MOSFET sample, where in one case the insulating state is reached by reducing the electron density in zero field, and in the other case it is reached by “quenching” the metallic behavior with an in-plane field of 5 T. We find that the resistivity of the insulating state behaves in very similar ways for both cases, exhibiting Efros-Shklovskii variable range hopping regardless of the degree of polarization of the electron spins. [1] S. V. Kravchenko et al., Phys. Rev. B 51, 7038 (1995) [2] D. Simonian et al., Phys. Rev. Lett. 79, 2304 (1997)

<sup>1</sup>Work at CCNY is supported by NSF Grant DMR-1309008 and BSF Grant 2012210; for S. K. by NSF Grant DMR-1309337 and BSF Grant 2012210.

**Wednesday, March 16, 2016 11:15AM - 1:51PM –**  
**Session L52 GERA FIAP: Solar Energy Including Concentrated Solar, and Solar Thermal** Hilton  
Baltimore Holiday Ballroom 3 -

**11:15AM L52.00001 Free-Carrier Absorption in Silicon from First Principles**<sup>1</sup>, GUANGSHA SHI, EMMANOUIL KIOUPAKIS, Univ of Michigan - Ann Arbor — The absorption of light by free carriers in semiconductors such as silicon results in intraband electron or hole excitations, and competes with optical transitions across the band gap. Free-carrier absorption therefore reduces the efficiency of optoelectronic devices such as solar cells because it competes with the generation of electron-hole pairs. In this work, we use first-principles calculations based on density functional theory to investigate direct and phonon-assisted free-carrier absorption in silicon. We determine the free-carrier absorption coefficient as a function of carrier concentration and temperature and compare to experiment. We also identify the dominant phonon modes that contributing to phonon-assisted free-carrier absorption processes, and analyze the results to evaluate the impact of this loss mechanism on the efficiency of silicon solar cells.

<sup>1</sup>This research was supported by the National Science Foundation CAREER award through Grant No. DMR-1254314. Computational resources were provided by the DOE NERSC facility.

**11:27AM L52.00002 Design principles of shift current photovoltaics**<sup>1</sup>, ASHLEY COOK, Department of Physics, University of Toronto, Department of Physics, University of California, Berkeley, BENJAMIN FREGOSO, FERNANDO DE JUAN, Department of Physics, University of California, Berkeley, JOEL MOORE, Department of Physics, University of California, Berkeley, Materials Sciences Division, Lawrence Berkeley National Laboratory — While the basic principles and limitations of conventional solar cells are well understood, relatively little attention has gone toward evaluating and maximizing the potential efficiency of photovoltaic devices based on shift currents. In this work, a sum rule approach is introduced and used to outline design principles for optimizing shift currents for photon energies near the band gap, which depend on wavefunctions via Berry connections as well as standard band structure. Using these we identify two new classes of shift current photovoltaics, ferroelectric polymer films and orthorhombic monochalcogenides, both of which exhibit peak photoresponsivities larger than predictions for previously-known photovoltaics of this type. Using physically-motivated tight-binding models, the full frequency dependent response of these materials is obtained. Exploring the phase space of these models, we find photoresponsivities that can exceed 100 mA/W. These results show that considering the microscopic origin of shift current via effective models allows one to improve the possible efficiency of devices using this mechanism and better grasp their potential to compete with conventional solar cells.

<sup>1</sup>This work was completed with the support of an NSERC Michael Smith Foreign Study Supplement

**11:39AM L52.00003 Complete voltage recovery due to suppression of capture to quantum dots**, ANDREI SERGEYEV, KIMBERLY SABLON, U.S. Army Research Laboratory, Adelphi, MD 20783, USA, ALEX VARGHESE, MICHAEL YAKIMOV, VADIM TOKRANOV, SERGE OKTYABRSKY, SUNY Polytechnic Institute, Albany, NY, 12203, VLADIMIR MITIN, University at Buffalo - SUNY, Buffalo, NY 14260 — Decrease of the open circuit voltage in quantum dot (QD) solar cells with respect to the reference cell is an essential drawback of QD devices. Despite numerous efforts, the complete voltage recovery in QD cells has been demonstrated only at low temperatures. We propose and investigate a new approach that combines nanoscale engineering of band structure and potential profile. In this work we (i) fabricated and investigated GaAs solar cells with various nano-engineered InAs QD media, (ii) identified the key photocarrier processes responsible for the voltage reduction, (iii) optimized QD devices and demonstrated the complete voltage recovery with respect to the reference cell together with some improvements in the short circuit current.

**11:51AM L52.00004 Enhancing photovoltaic efficiency through radiative cooling of solar cells below ambient temperature.**, TAQIYAH SAFI, JEREMY MUNDAY, University of Maryland — Sunlight heats up solar cells and the resulting elevated solar cell temperature adversely effects the photovoltaic efficiency and the reliability of the cell. Currently, a variety of active and passive cooling strategies are used to lower the operating temperature of the solar cell. Passive radiative cooling requires no energy input, and is ideal for solar cells; however, previously demonstrated devices still operate above the ambient, leading to a lower efficiency as compared to the ideal Shockley-Queisser limit, which is defined for a cell in contact with an ideal heat sink at ambient temperature (300 K). In this talk, we will describe the use of radiative cooling techniques to lower the cell temperature below the ambient temperature. We show that by combining specifically designed radiative cooling structures with solar cells, efficiencies higher than the limiting efficiency achievable at 300 K can be obtained for solar cells in both terrestrial and extraterrestrial environments. We show that these structures yield an efficiency 0.87% higher than a typical PV module at operating temperatures in a terrestrial application. We also demonstrate an efficiency advantage of 0.4-2.6% for cells in an extraterrestrial environment in near-earth orbit.

**12:03PM L52.00005 Tin alloyed acanthite  $\text{Cu}_2\text{S}$  using cluster expansion method and their stability analysis using density functional theory<sup>1</sup>**, SAJIB BARMAN, MUHAMMAD HUDA, Univ of Texas, Arlington, DR. HUDA'S GROUP TEAM —  $\text{Cu}_2\text{S}$  is a widely known semiconductor which has the potential to be used as an efficient solar absorber material. However, complex phase structures and phase instabilities due to spontaneous Cu vacancy formation are big issues which need to be addressed. Based on a recent theoretical study which has predicted acathite like  $\text{Cu}_2\text{S}$  to be more favorable than other known crystal structures, we have used cluster expansion method to look for the most favorable tin alloyed acanthite  $\text{Cu}_2\text{S}$ . We have used density functional theory systematically to assess the stabilities of those tin alloyed acanthite  $\text{Cu}_2\text{S}$  structures. In addition, effect of Cu vacancies in Sn alloying has also been investigated.

<sup>1</sup>This research was supported by NREL.

**12:15PM L52.00006 The Upper Bound on Solar Power Conversion Efficiency Through Photonic Engineering<sup>1</sup>**, YUNLU XU, JEREMY MUNDAY, Univ of Maryland-College Park — The power conversion efficiency is a key parameter by which different photovoltaic devices are compared. The maximum value can be calculated under steady-state conditions where the photon flux absorbed by the device equals the outgoing flux of particles (also known as the principle of detailed balance). The photonic engineering of a solar cell offers a new alternative for boosting efficiency. We show that, for an ideally photonic engineered solar cell, its efficiency is subject to an upper bound dictated by a generalized form of detailed balance equation where nano-concentration is taken into account. Results under realistic operating conditions and recent experimental studies will also be discussed.

<sup>1</sup>Authors acknowledge the University of Maryland for startup funds to initiate this project and support by the National Science Foundation under Grant CBET-1335857

**12:27PM L52.00007 Nonlinear Response in Silicon Solar Cells<sup>1</sup>**, BEHRANG HAMADANI, JOHN ROLLER, ANDREW SHORE, HOWARD YOON, National Institute of Standards and Technology, NIST COLLABORATION — A light emitting diode (LED)-based system utilizing a combinatorial flux addition method was used to measure the nonlinear relationship in silicon solar cells between the output current of the cell and the incident irradiance level. The light flux was controlled by the supplied current to two sets of LEDs, of either monochromatic light or a combination of various wavelengths. The (non)linearity of a variety of cells were measured over many orders of magnitude of light intensity and various trends were observed, including a transition from nonlinear to linear behavior for some cells as a function of intensity or a complete nonlinear response throughout the probed range. Furthermore, nonlinearity was found to be spectral dependent. An explanation for the observed behavior based on fundamental physics will be provided.

<sup>1</sup>Nonlinear Response in Silicon Solar Cells

**12:39PM L52.00008 Contactless Spectral-dependent Charge Carrier Lifetime Measurements in Silicon Photovoltaic Materials**, JOHN ROLLER, BEHRANG HAMADANI, NIST - Natl Inst of Stds & Tech, MARIO DAGENAIS, University of Maryland - College Park — Charge carrier lifetime measurements in bulk or unfinished photovoltaic (PV) materials allow for a more accurate estimate of power conversion efficiency in completed solar cells. In this work, carrier lifetimes in PV-grade silicon wafers are obtained by way of quasi-steady state photoconductance measurements. These measurements use a contactless RF system coupled with varying narrow spectrum input LEDs, ranging in wavelength from 460 nm to 1030 nm. Spectral dependent lifetime measurements allow for determination of bulk and surface properties of the material, including the intrinsic bulk lifetime and the surface recombination velocity. The effective lifetimes are fit to an analytical physics-based model to determine the desired parameters. Passivated and non-passivated samples are both studied and are shown to have good agreement with the theoretical model.

**12:51PM L52.00009 Effect of Long-Range Polar Electron-Phonon Interaction on the Hot Carrier Dynamics of GaAs**, CHIN SHEN ONG, University of California, Berkeley, MARCO BERNADI, California Institute of Technology, STEVEN G. LOUIE, University of California, Berkeley — Hot carrier dynamics plays an important role in the functionality of electronic and photovoltaic devices. Recent interest in harvesting the energy of hot electrons before it is lost through thermalization has led to renewed interest in the microscopic details of hot electron energy loss mechanisms. Gallium arsenide (GaAs) is of particular interest because amongst its many advantages, it is a direct-gap semiconductor, has high electron mobility and is a high-performing candidate for electronic and photovoltaic applications. GaAs is a polar material, and long-range polar (Frölich) electron-phonon interaction has non-trivial effects on the carrier dynamics in the material. In this work, we investigate the effect of this interaction on the hot carrier dynamics of GaAs. This work is supported by NSF grant No. DMR15-1508412 and the DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at Lawrence Berkeley National Laboratory's NERSC facility.

**1:03PM L52.00010 Nano-scale Characteristics of Copper poor ordered defect compound at grain boundary of  $\text{CuInGaSe}_2$** , YAPING MA, Chinese Univ of Hong Kong — This work investigates the copper poor ordered defect compound (ODC) layer at grain boundaries (GB) for  $\text{Cu}_x(\text{Ga}_{0.3}\text{In}_{0.7})\text{Se}_2$  with different Cu composition ratio ( $x = 0.9$  and  $0.68$ ). Same chemical composition while widened ODC layer at GBs with lower Cu ratio were first reported determined by the energy dispersive spectroscopy in scanning transmission microscopy mode. Band structure of the ODC layer was directly measured by scanning tunneling spectroscopy showing a downward offset for conduction band and valence band of 200 eV and 350 eV, respectively. This result was further confirmed by photocurrent accumulation and higher Schottky barrier at GBs measured by the conducting probe atomic force microscopy (CP-AFM). Local photovoltaic performance measurements of individual grain boundaries with different ODC width were investigated, using CP-AFM and the disappearance of the differences of open circuit voltage and shunt resistance between grain interior and grain boundary at low illumination provides a direct evidence for the reduced recombination at widened ODC grain boundary which greatly supports the hole barrier theory for the high efficiency of the Copper Indium Ga Selenide solar cells.

**1:15PM L52.00011 Employing Time-Resolved Terahertz Spectroscopy to Analyze Carrier Dynamics in  $\text{Cu}_2\text{ZnSn}(\text{S},\text{Se})_4$  Absorber Layers**<sup>1</sup>, JASON BAXTER, GLENN GUGLIETTA, SIMING LI, Drexel University, KAUSHIK ROY CHOUDHURY, JONATHAN CASPAR, DuPont Central Research and Development, DOUGLAS BISHOP, MICHAEL LLOYD, BRIAN MCCANDLESS, University of Delaware — We report the application of time-resolved terahertz spectroscopy (TRTS) to measure photoexcited carrier lifetimes and mobility, and to determine recombination mechanisms in  $\text{Cu}_2\text{ZnSn}(\text{S},\text{Se})_4$  (CZTSSe) thin films and single crystals. Ultrafast time resolution permits tracking the evolution of carrier density to determine recombination rates and mechanisms. The carrier generation profile was manipulated by varying the photoexcitation wavelength and fluence to distinguish between surface, Shockley-Read-Hall (SRH), radiative, and Auger recombination mechanisms and determine rate constants. Surface and SRH recombination are the dominant mechanisms for the air/CZTSSe/ $\text{SiO}_2$ /Si film stack. Diffusion to, and then recombination at, the air-CZTSSe interface occurred on the order of 100 picoseconds, while SRH recombination lifetimes were 1 - 2 nanoseconds. Analogous measurements on single crystals reveal the effects of eliminating grain boundaries, reducing point defects and secondary phases, and applying surface treatments to reduce surface recombination velocity. TRTS measurements can provide information that is complementary to conventional time-resolved photoluminescence measurements and can direct the design of efficient thin film photovoltaics. Ref: Guglietta et al., APL, 2014.

<sup>1</sup>NSF DMR-1507988

**1:27PM L52.00012 Surfactant Antimony enhanced Indium incorporation on InGaN -C plane**<sup>1</sup>, YIOU ZHANG, JUNYI ZHU, Chinese Univ of Hong Kong — InGaN is an ideal alloy system for optoelectronic devices due to its tunable band gap. Yet high-quality InGaN with high In concentration is still a challenging issue that limits its use in green-light LEDs and other devices. In this presentation, we report the surfactant effect of Sb on the In incorporation on InGaN (000-1) surface via first-principles approaches. We constructed surface phase diagram to determine surface structures under different growth conditions. By analyzing surface stress under different structures, we found that Sb adatom can induce tensile sites in the cation layer, enhancing the In incorporation. These findings may provide fundamental understandings and guidelines for the growth of InGaN with high In concentration.

<sup>1</sup>This work was supported by the start-up funding and direct grant with the Project code of 4053134 at CUHK.

**1:39PM L52.00013 Probing the Surface Defect States of Gallium Nitride Nanowires**, LAUREN SIMONSEN, YUCHEN YANG, Department of Physics and Astronomy, University of Utah, NICHOLAS BORYS, Molecular Foundry, Lawrence Berkeley National Laboratory, ANIL GHIMIRE, Department of Physics and Astronomy, University of Utah, JAMES SCHUCK, SHAUL ALONI, Molecular Foundry, Lawrence Berkeley National Laboratory, JORDAN GERTON, Department of Physics and Astronomy, University of Utah — In this work, we investigate gallium nitride nanowires (NWs) as a potential system for solar-driven water splitting. Although bulk GaN has a UV bandgap, the synthesized NWs exhibit strong absorption and fluorescence emission across the visible spectrum. Density functional theory calculations suggest that this visible fluorescence originates from mid-gap surface-defect states along the triangular facets of the NWs. The orientation of the NWs can be controlled during MOCVD growth, leading to different exposed crystallographic surface terminations with different electronic structures. High resolution microscopy techniques using AFM and confocal hyper-spectral imaging show spectral inhomogeneity across the widths of the NWs, providing evidence that various crystallographic terminations produce different surface states. These NWs also exhibit wave guiding properties, leading to Fabry-Perot fringes and high intensity spectra and the ends of the wires. Photoluminescence excitation spectroscopy reveals a non-linear dependence of the emission spectral features on excitation wavelength, indicating a complex distribution of mid-gap defect states. Time-resolved spectroscopy reveals non-exponential decay dynamics through a complicated manifold of mid-gap states.

## Wednesday, March 16, 2016 11:15AM - 2:15PM —

Session L53 DFD GSOFD DPOLY: Flow of Complex Fluids, Polymers, Gels Hilton Inner Harbor Holiday Ballroom 4 -

**11:15AM L53.00001 Anomalous response of nematic platelets under LAOStress and Strain revealed by 3D RheoSAXS**, O. KORCULANIN, ICS-3, Forschungszentrum Juelich, Germany, H. HIRSEMANN, B. STRUTH, DESY, Hamburg, Germany, G. PORTALE, Uni. of Groningen and Dubble, ESRF, Grenoble, France, M. P. LETTINGA, ICS-3, Forschungszentrum Juelich, Germany and KU Leuven, Belgium — Dispersions of colloidal Gibbsite platelets in the nematic phase display a complex response to Large Amplitude Oscillatory Shear (LAOS) flow that strongly depends on the strain amplitude. [1] In this work we applied LAOStress and LAOStrain to the nematic dispersion and probed the structure with time-resolved SAXS measurements. By using plate-plate and couette geometry, we had access to both the flow-vorticity and flow-gradient plane, respectively, thus obtain full 3D rotational motion of the director. For LAOStress, we observe strong asymmetrical behavior both in the rheological and the microscopic response. This asymmetry is connected to the yielding behavior of the platelets. By increasing the stress amplitude we observed that the response becomes more symmetric; however, this strongly depends on the frequency, hence the time necessary for the system to yield. Softening of the response towards the center of the gap was observed by scanning the gap while performing LAOStrain. The structural response at low strain amplitude does not propagate throughout the gap, whereas at high strain amplitudes the response in the bulk emerges as erratic. [1] M. P. Lettinga, et al., Non-linear behavior of colloidal platelets in shear flow. Phys. Rev. Lett.(2012) Vol. 109, 246001

**11:27AM L53.00002 Distinctive viscoelastic and viscoplastic nanomechanics of ionically cross-linked polyelectrolyte complexes under intermittent relaxation and creep**, BIAO HAN, TIANZHU MA, Drexel University School of Biomedical Eng., Sci. and Health Systems, DAEYEON LEE, VIVEK SHENOY, University of Pennsylvania, School of Engineering and Applied Science, LIN HAN, Drexel University School of Biomedical Eng., Sci. and Health Systems — This study aims to reveal unique nanoscale viscoelastic and viscoplastic properties of ionically linked polyelectrolyte networks. Layer-by-layer PAH/PAA complexes were tested by four continuous loading cycles in aqueous solutions. In each cycle, AFM-nanoindentation via a microspherical tip ( $R=5\mu\text{m}$ ) was applied up to  $1\mu\text{N}$  force, followed by a 30-60 sec hold at either a constant indentation depth to measure relaxation, or a constant force to measure creep. At a highly cross-linked, net neutral state (0.01M, pH 5.5), instantaneous modulus increased by 2.7-fold from first to last cycle, while the degree of relaxation ( $>95\%$ ) remain consistent. These results indicate repeated loading increases local cross-link density, while relaxation is consistently dominated by cross-link breaking and re-formation. In contrast, under creep, modulus increased by a similar 3.5-fold, and degree of creep is significantly attenuated from  $\approx 50\%$  to  $45\%$  from first to last cycle. Results from creep suggest constant viscous flow of polymer chains in the absence of permanent anchorage. As a result, an irreversible deformation ( $\approx 370\text{nm}$ ) was observed after multiple creep cycles, suggesting the presence of viscoplasticity.

**11:39AM L53.00003 Non-equilibrium Stokes-Einstein relation via active microrheology of hydrodynamically interacting suspensions**, HENRY CHU, ROSEANNA ZIA, Cornell University — In our recently developed non-equilibrium Stokes-Einstein relation, we showed that, in the absence of hydrodynamic interactions, the stress in a suspension is given by a balance between fluctuation and dissipation. Here, we generalize our theory for systems of hydrodynamically interacting colloids, via active microrheology, where motion of a Brownian probe through the medium reveals rheological properties. The strength of probe forcing compared to the entropic restoring force defines a Peclet number,  $Pe$ . In the absence of hydrodynamics, the first normal stress difference and the osmotic pressure scale as  $Pe^4$  and  $Pe^2$  respectively when probe forcing is weak, and uniformly as  $Pe$  for strong probe forcing. As hydrodynamics become important, interparticle forces give way to lubrication interactions. Hydrodynamic coupling leads to a new low- $Pe$  scaling of the first normal stress difference and the osmotic pressure as  $Pe^2$ , and high- $Pe$  scaling as  $Pe^\delta$ , where  $0.799 \leq \delta \leq 1$  as hydrodynamics vary from strong to weak. For the entire range of the strength of hydrodynamic interactions and probe forcing, the new phenomenological theory is shown to agree with standard micromechanical definitions of the stress. We further draw a connection between the stress and the energy storage in a suspension, and the entropic nature of such storage is identified.

**11:51AM L53.00004 Sticky-probe active microrheology**, DEREK HUANG, ROSEANNA ZIA, Cornell University — We study the strongly nonlinear flow behavior of a sticky colloidal dispersion via active microrheology, where the motion of a Brownian probe driven by external forces through the suspension is tracked to infer material properties. Most prior work focused on repulsive hard spheres and the influence of Brownian and hydrodynamic forces on rheological behavior, but in many biological suspensions, particles exert attractive forces on one another. Previous attempts to model the effects of particle attractions on sheared suspensions show that interparticle attractions increase suspension stress and viscosity, but these results are limited to weak shearing flows in macroscopic systems. In our microrheological model, probe motion through the suspension distorts the configuration of particles; the Peclet number, probe forcing compared to thermal forces, gives the extent of this distortion. The equilibrium microstructure and its distortion under probe forcing are also influenced by the strength of interparticle attractions relative to thermal forces. We determine the equilibrium and non-equilibrium microstructure and examine the forcing and attraction contributions to particle motion and suspension stress.

**12:03PM L53.00005 Stress diffusion in models for shear banding**, ELIAN MASNADA, PETER OLMSTED, Georgetown Univ — Understanding shear banding is of utmost importance from both theoretical and experimental point of view and consequently it has been studied for several decades [1]. Despite this study numerous aspects of shear banding remains poorly understood. Because of the intrinsic inhomogeneity in the shear banded state, applicable constitutive models must include spatial inhomogeneities, leading to a so-called 'diffusive' term in the equation of motion for the slow variables that carry stress [2,3]. Such terms are also vital in describing the interaction of bulk shear banding flows with walls and incorporation of wall slip. In this work, we consider different sources of 'diffusion' in polymer models in which concentration degrees of freedom are negligible. The simplest models used are consistent with diffusive terms whose origin is intrinsically dissipative, such as due to hydrodynamic interactions. By contrast, models in which elastic effects such as finite chain stiffness contribute to stress diffusion are inconsistent with simple diffusive models, and we propose alternative consistent models. [1] P. D. Olmsted, Rheol. Acta, 47, 283-300 (2008). [2] C.-Y. D. Lu et al, Phys. Rev. Lett., 84, 642 (2000). [3] A. W. El-Kareh and L. G. Leal, J. Non-Newton. Fluid Mech., 33, 257 (1989).

**12:15PM L53.00006 Strength of self-pinning in coffee drops.**, ANDRZEJ LATKA, KIMBERLY KAWCZINSKI, SIDNEY NAGEL, James Franck Institute, University of Chicago — The equilibrium contact angle  $\theta_e$  of a liquid drop placed on a solid surface is uniquely determined by a balance of surface tension forces according to Young's Equation, yet is rarely observed in real systems. Due to contact angle hysteresis, liquids can make contact with a surface at any angle between the receding and advancing contact angle:  $\theta_R < \theta_e < \theta_A$ . A particularly striking example of this phenomenon is the familiar coffee stain. For coffee  $\theta_R = 0$ , thus as the drop evaporates the contact line remains pinned at its initial location. This results in the majority of the coffee being deposited in a characteristic ring at the drop's original boundary. We investigate how solid particles suspended in a liquid could so strongly influence contact angle hysteresis, by measuring the receding contact angle of a drop at various times during the evaporation process. For low solute concentrations,  $\theta_R$  slowly decreases as the drop evaporates, but remains positive. Surprisingly, we find that increasing the solute concentration results in  $\theta_R = 0$  and a fully pinned contact line almost immediately after the drop is deposited.

**12:27PM L53.00007 Microfluidics of soft granular gels**, RYAN NIXON, Univ of Florida - Gainesville, TAPOMOY BHATTACHARJEE, W. GREGORY SAWYER, THOMAS E. ANGELINI, University of Florida — Microfluidic methods for encapsulating cells and particles typically involve drop making with two immiscible fluids. The main materials constraint in this approach is surface tension, creating inherent instability between the two fluids. We can eliminate this instability by using miscible inner and outer phases. This is achieved by using granular micro gels which are chemically miscible but physically do not mix. These microgels are yield stress materials, so they flow as solid plugs far from shear gradients, and fluidize where gradients are generated – near an injection nozzle for example. We have found that tuning the yield stress of the material by varying polymer concentration, device performance can be controlled. The solid like behavior of the gel allows us to produce infinitely stable jets that maintain their integrity and configuration over long distances and times. These properties can be combined and manipulated to produce discrete particulate bunches of an inner phase, flowing inside of an outer phase, well enough even to print a Morse code message suspended within flow chambers about a millimeter in diameter moving at millimeters a second.

**12:39PM L53.00008 Lift-enhanced Electrical Pinched Flow Fractionation for Particle and Cell Separation.**<sup>1</sup>, CORY THOMAS, ANDREW TODD, XINYU LU, XIANGCHUN XUAN, Clemson University — Pinched flow fractionation (PFF) is a microfluidic technique that utilizes the laminar flow profile in microchannels to continuously separate particles or cells by size. The flow can be either pressure-driven or electric field-driven. We demonstrate in this work that the wall-induced electrical lift force can be exploited to significantly increase the particle or cell displacement in electrical PFF due to its strong size dependence. This enhanced particle and cell separation is implemented by a simple elongation of the pinched segment in electrical PFF. It is demonstrated through both a binary and a ternary separation of polymer particles and biological cells based on surface charge and/or size. We also develop a numerical model to predict and understand this lift-enhanced electrical PFF.

<sup>1</sup>This work was supported by the Honors and Creative Inquiry programs at Clemson University.

**12:51PM L53.00009 Particle Size Effect on Wetting Kinetics of a Nanosuspension Drop: MD Simulations**, BAIYOU SHI, EDMUND WEBB, Lehigh University — The behavior of nano-fluids, or fluid suspensions containing nanoparticles, has garnered tremendous attention recently for applications in advanced manufacturing. In our previous results from MD simulations, for a wetting system with different advancing contact angles, cases where self-pinning was observed were compared to cases where it was not and relevant forces on particles at the contact line were computed. To advance this work, the roles of particle size and particle loading are examined. Results presented illustrate how particle size affects spreading kinetics and how this connects to dynamic droplet morphology and relevant forces that exist nearby the contact line region. Furthermore, increased particle size in simulations permits a more detailed investigation of particle/substrate interfacial contributions to behavior observed at the advancing contact line. Based on changes in spreading kinetics with particle size, forces between the particle and liquid front are predicted and compared to those computed from simulations. At high loading, particle/particle interactions become relevant and forces computed between particles entrained to an advancing contact line will be presented.

**1:03PM L53.00010 Numerical Computation of Mass Transport in Low Reynolds Number Flows and the Concentration Boundary Layer**, NICHOLAS A. LICATA, NATHANIEL J. FULLER, University of Michigan-Dearborn — Understanding the physical mechanisms by which an individual cell interacts with its environment often requires detailed information about the fluid in which the cell is immersed. Mass transport between the interior of the cell and the external environment is influenced by the flow of the extracellular fluid and the molecular diffusivity. Analytical calculations of the flow field are challenging in simple geometries, and not generally available in more realistic cases with irregular domain boundaries. Motivated by these problems, we discuss the numerical solution of Stokes equation by implementing a Gauss-Seidel algorithm on a staggered computational grid. The computed velocity profile is used as input to numerically solve the advection-diffusion equation for mass transport. Special attention is paid to the case of two-dimensional flows at large Péclet number. The numerical results are compared with a perturbative analytical treatment of the concentration boundary layer.

**1:15PM L53.00011 Cell mechanics through analysis of cell trajectories in microfluidic channel**, SAMUEL BOWIE, ALEXANDER ALEXEEV, TODD SULCHEK, Georgia Institute of Technology — The understanding of dynamic cell behavior can aid in research ranging from the mechanistic causes of diseases to the development of microfluidic devices for cancer detection. Through analysis of trajectories captured from video of the cells moving in a specially designed microfluidic device, insight into the dynamic viscoelastic nature of cells can be found. The microfluidic device distinguishes cells viscoelastic properties through the use of angled ridges causing a series of compressions, resulting in differences in trajectories based on cell stiffness. Trajectories of cell passing through the device are collected using image processing methods and data mining techniques are used to relate the trajectories to cell properties obtained from experiments. Furthermore, numerical simulation of the cell and microfluidic device are used to match the experimental results from the trajectory analysis. Combination of the modeling and experimental data help to uncover how changes in cellular structures result in changes in mechanical properties.

**1:27PM L53.00012 New analysis method for passive microrheology**, KENGO NISHI, CHRISTOPH SCHMIDT, Univ Goettingen, FRED MACKINTOSH, Vrije Universiteit — Passive microrheology is an experimental technique used to measure the mechanical response of materials from the fluctuations of micron-sized beads embedded in the medium. Microrheology is well suited to study rheological properties of materials that are difficult to obtain in larger amounts and also of materials inside of single cells. In one common approach, one uses the fluctuation-dissipation theorem to obtain the imaginary part of the material response function from the power spectral density of bead displacement fluctuations, while the real part of the response function is calculated using a Kramers-Kronig integral. The high-frequency cut-off of this integral strongly affects the real part of the response function in the high frequency region. Here, we discuss how to obtain more accurate values of the real part of the response function by an alternative method using autocorrelation functions.

**1:39PM L53.00013 Effect of droplet shape on ring stains from dried liquid**, MELVIN SANTIAGO, Department of Physics, Case Western Reserve University, Cleveland, Ohio 44106-7079, KATHERINE BROWN, Department of Physics, Hamilton College, Clinton NY 13323, HARSH MATHUR, Department of Physics, Case Western Reserve University, Cleveland, Ohio 44106-7079 — A landmark experimental paper on coffee stains by Deegan et al included a simple theoretical analysis of circular droplets [1]. The analysis was based on a model informally called the Maxwell House equations. It describes the evolving height profile of the droplet, the evaporation of the solvent and the outflow of solute to the rim of the droplet. Since typical droplets are not circles, here we extend the analysis to more general shapes. We find that for thin droplets the height profile may be determined by solving Poisson's equation in a domain corresponding to the footprint of the droplet. Evaporation is treated in a simple approximation via an electrostatic analogy and is dominated by the sharp edges of the droplet. Assuming zero vorticity allows us to analyze the solvent flow in droplets of arbitrary shape. We compare circular droplets to other shapes including long linear droplets, ring shaped droplets and droplets with an elliptical footprint. [1] R.D. Deegan et al, Nature 389, 827 (1997).

**1:51PM L53.00014 Lie Algebraic Analysis of Thin Film Marangoni Flows: Multiplicity of Self-Similar Solutions**, ZACHARY NICOLAOU, SANDRA TROIAN, California Institute of Technology, 1200 E. California Blvd., MC 128-95, Pasadena, CA — The rapid advance of an insoluble surfactant monolayer on a thin liquid film of higher surface tension is controlled by distinct flow regimes characterized by the relative strength of viscous, Marangoni and capillary forces. Such flows play a critical role in human pulmonary and ocular systems. During the past quarter century, researchers have focused exclusively on self-similar solutions to the governing pair of nonlinear PDEs for the film thickness,  $H(r/t^a)$ , and surface concentration,  $\Gamma(r/t^a)/t^b$ , in the limit where the Marangoni or capillary terms vanish, where  $r$  denotes the spatial variable,  $t$  is time, and  $a$  and  $b$  are fractional exponents. Using Lie algebraic techniques, we demonstrate for the first time the existence of several embedded symmetries in this system of equations which yield multiple self-similar solutions describing more complex scaling behavior, even when all three forces are incorporated. A special and previously unrecognized subset of these solutions reveals the dynamical behavior of film thinning and surfactant distribution near the origin, which ultimately meters the downstream flow. Finite element simulations confirm the suite of scaling exponents obtained analytically.

**2:03PM L53.00015 Convective flows generated by evaporation: experiments, linear stability analysis and numerical simulations**, JOCELYN DUNSTAN, Postdoc, KYOUNG JIN LEE, Professor, SIMON PARK, Senior Lecturer, RAYMOND E. GOLDSTEIN, Professor — A novel form of convection was observed in a suspension of non-motile *Photobacterium phosphoreum* bacteria. The pattern resembles classical bioconvection, however this strain has limited if any motility, which excludes this possible explanation. After performing a series of control experiments we found that the convection was actually driven by the evaporation of the salty bacterial medium, and the same kind of plumes were observed using polystyrene beads suspended in water with salt added. A mathematical model was formulated for the process and studied using a linear stability analysis and finite element method simulations, reproducing most of the observed experimental features. From the linear stability analysis, a threshold in salt concentration to observe convective motion was obtained, as well as the wavelength of the pattern at the onset of the instability. This was complemented by finite element simulations, which produced plume dynamics remarkably similar to the experimental observations. Evaporation-driven convection on the millimeter scale has not been studied extensively, and its effect may have been underestimated in other experiments.

**Wednesday, March 16, 2016 11:15AM - 2:15PM —**

**Session L54 DCMP: Supersolids and Band Structure in Strongly Correlated Systems** Hilton  
Baltimore Holiday Ballroom 5 - William Cannon, Texas AM University

**11:15AM L54.00001 Re-investigating Solid Helium under DC Rotation with a Rigid Torsional Oscillator** , JAEWON CHOI, Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon, Republic of Korea, TOMOYA TSUIKI, Department of Physics, Keio University, Yokohama, Kanagawa, Japan, DAISUKE TAKAHASHI, Department of General Education, Ashikaga Institute of Technology, Ashikaga, Tochigi, Japan, KEIYA SHIRAHAMA, Department of Physics, Keio University, Yokohama, Kanagawa, Japan, KIMITOSHI KONO, Quantum Condensed Phase Research Team, RIKEN, Wako, Saitama, Japan, HYOUNGSOON CHOI, EUNSEONG KIM, Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon, Republic of Korea — The resonant period drop observed in a torsional oscillator (TO) containing solid helium first interpreted as the signature of supersolid is now generally accepted as the shear modulus change of solid helium at low temperature. However, there are still several aspects in solid helium that remain unresolved. For instance, the striking DC rotation effect on the TO experiments was observed without altering the shear modulus of solid helium. The DC rotation is not expected to change the elastic property of solid helium while it can destroy superfluidity. Therefore, the DC rotation effect was considered as the strong evidence of superfluidity in solid helium. Here, we re-examine the effect of DC rotation by utilizing a rigidly constructed TO. Previous DC rotation experiments were performed with a TO exhibiting high reduction ratio of the period, which can be attributed to non-ideal construction of the TO. It is plausible that the resonance period and dissipation of non-ideal TO can be more susceptible to environmental vibration caused by the DC rotation. The response of the rigid TO under DC rotation will be reported to test the validity of the previous interpretation thoroughly.

**11:27AM L54.00002 Mass Flux Measurements in Solid  $^4\text{He}$** <sup>1</sup> , VALENTYN RUBANSKYI, YEGOR VEKHOV<sup>2</sup>, ROBERT HALLOCK, Univ of Mass - Amherst — There has been considerable attention given to solid helium over the past decade. Our approach to study the solid has been to sandwich solid helium between two reservoirs of superfluid helium. With this approach, we found and explored the characteristics of mass flux that takes place from one reservoir to the other<sup>3</sup>. We observed flow that has the characteristics of one-dimensional conductivity<sup>4</sup> and we have documented the effects that various concentrations of  $^3\text{He}$  impurity have on the temperature dependence of the flow<sup>5</sup>. These experiments continue and we will report on this work and new results that may be available.

<sup>1</sup>Supported by NSF via DMR 12-05217

<sup>2</sup>Current address: Department of Materials Science and Engineering, Univ. of Maryland, College Park, MD.

<sup>3</sup>M.W. Ray and R.B. Hallock, Phys. Rev. Letters 100, 235301 (2008); 105, 145301 (2010); Phys. Rev. B 79, 224302 (2009).

<sup>4</sup>Ye. Vekhov and R.B. Hallock, Phys. Rev. Letters 109, 045303 (2012); Phys. Rev. B 90, 134511 (2014).

<sup>5</sup>Ye. Vekhov, W.J. Mullin and Hallock, Phys. Rev. Letters 113, 035302 (2014); Ye. Vekhov and R.B Hallock, Phys. Rev. B 92, 104509 (2015).

**11:39AM L54.00003 Mass flow in bulk solid  $^4\text{He}$** <sup>1</sup> , ZHI GANG CHENG, JOHN BEAMISH, University of Alberta — Experiments with solid  $^4\text{He}$  and liquid confined in vycor pores have shown an unexpected mass flow in both liquid-solid-liquid and solid-liquid-solid junctions. In both configurations, non-thermally activated flow emerges below 600 mK. The flow rate increases as the temperature decreases, then drops suddenly at a temperature around 100 mK. This drop in flow rate is related to the  $^3\text{He}$  impurity concentration in the samples and prevents us from studying the flows intrinsic behavior at the lowest temperatures. We have now modified our measurement technique, in which solid helium is compressed at one end of a cell and flow is observed as a pressure response at the opposite end. By removing the vycor from our cell, we have eliminated liquid  $^4\text{He}$  and the liquid-solid interfaces which complicated the interpretation of earlier experiments. We find that similar mass flow occurs with only bulk solid  $^4\text{He}$  present. When we reduced the  $^3\text{He}$  concentration to the level of a few parts per trillion, we were able to measure the intrinsic flow rate down to lower temperatures, with no evidence of a drop in flow down to at least 25 mK.

<sup>1</sup>This work was supported by a grant from NSERC Canada

**11:51AM L54.00004 Superclimbing instability in solid Helium-4**<sup>1</sup> , ANATOLY KUKLOV, CSI and the Graduate Center, CUNY — The accumulation of matter in solid  $^4\text{He}$  observed in the UMASS group and dubbed as the syringe effect is discussed within the model of dislocations with superfluid core beyond the linear approximation. Such dislocations are found to be unstable with respect to the syringe effect if biased by chemical potential above a threshold  $\mu_c \approx Gb^4/L$ , where  $G$  is the shear modulus,  $b$  - Burgers vector and  $L$  - free length of a dislocation. In almost perfect crystals, where  $L$  can be as long as several  $\mu\text{m}$  or even longer, the threshold is *macroscopically* small - corresponding to overpressures smaller than few mbar. This effect for edge dislocations has its high temperature analog - Bardeen-Herring instability of dislocations due to diffusive high temperature vacancy transport. For screw dislocations the instability develops through helix formation first observed in Si at high temperatures by W. C. Dash (1958). In solid  $^4\text{He}$  the vacancy diffusion is replaced by the supertransport along dislocation cores. The instability should cause formation of the superfluid dislocation forest leading to the superflow-through-solid effect first observed in the UMASS group. Several testable predictions with respect to the bias and time dependence for the syringe dynamics are made.

<sup>1</sup> This work was supported by the NSF grant PHY1314469.

**12:03PM L54.00005 Analysis of recent observations of ultrasound propagation in solid  $^4\text{He}$**  , HARRY KOJIMA, Rutgers University, IZUMI IWASA, Kanagawa University, JOHN GOODKIND, UCSD — Extensive measurements have been made on the propagation of 10 MHz ultrasound in solid  $^4\text{He}$ . When the sound excitation level is low, sudden shifts in both the sound propagation velocity and attenuation are observed below 100 mK but the sudden shifts disappear when the excitation level is sufficiently high. The detailed response depends on the ultrasound excitation level and thermal history. The observations are analyzed in terms of the Granato-Lücke theory on the effects of dislocation line motion on the propagation of sound. The effects of pinning of dislocation lines by  $^3\text{He}$  impurities are included in the analysis. Parameters such as the average dislocation length, the dislocation line density, the dissipation coefficient and the impurity binding energy that are extracted by fitting the data to theory will be discussed.

**12:15PM L54.00006  $^4\text{He}$  adsorption on a  $^3\text{He}$ -plated graphite surface** , YONGKYUNG KWON, JEONGHWAN AHN, Konkuk University — Path-integral Monte Carlo (PIMC) calculations have been performed for  $^4\text{He}$  atoms on top of the  $^3\text{He}$  first layer on graphite. For this we ignore Fermi statistics of solidified  $^3\text{He}$  adatoms while Bose statistics of  $^4\text{He}$  atoms are fully incorporated. We first find that the first  $^3\text{He}$  layer exhibits a 7/12 commensurate solid structure at the areal density of  $0.111 \text{ \AA}^{-2}$ , which turns out to be identical to the experimental value for its completion density. Additional adsorption of  $^4\text{He}$  atoms above the complete first  $^3\text{He}$  layer is found to sustain the underlying  $^3\text{He}$  commensurate structure and the second  $^4\text{He}$  layer is observed to display the 4/7 commensurate structure with respect to the first-layer commensurate  $^3\text{He}$  solid at the areal density of  $0.0636 \text{ \AA}^{-2}$ . Furthermore, it is found that the 4/7 commensurate structure of the second-layer  $^4\text{He}$  atoms can be formed above a mixture of the first-layer  $^3\text{He}$  and  $^4\text{He}$  atoms on graphite. These PIMC results suggest that the 4/7 commensurate structure of the second-layer  $^4\text{He}$  atoms on graphite, whose existence on top of the first  $^4\text{He}$  layer has long been in dispute, may be realized on a  $^3\text{He}$ -plated graphite surface. This could lead to a new approach to observe two-dimensional supersolidity in  $^4\text{He}$  on graphite.

**12:27PM L54.00007 Thermodynamics of the Noninteracting Bose Gas in a Two-Dimensional Box**, HEQIU LI, QIUJIANG GUO, JI JIANG, Zhejiang University, DAVID C. JOHNSTON, Iowa State Univ — Bose-Einstein condensation (BEC) of a noninteracting Bose gas of  $N$  particles in a two-dimensional (2D) box with Dirichlet boundary conditions is studied. Confirming previous work, we find that BEC occurs at finite  $N$  at low temperatures  $T$  without the occurrence of a phase transition. We further show that the crossover temperature between weak and strong increases in BEC upon cooling is  $T_E \sim 1/\log(N)$  at fixed area per boson, so in the thermodynamic limit there is no significant BEC in 2D at finite  $T$ . Calculations of thermodynamic properties versus  $T$  and area  $A$  are presented, including Helmholtz free energy, entropy  $S$ , pressure  $p$ , ratio of  $p$  to the energy density  $U/A$ , heat capacity at constant area  $C_V$  and at constant pressure  $C_p$ , isothermal compressibility  $\kappa_T$  and thermal expansion coefficient  $\alpha_p$ , obtained using both the grand canonical ensemble (GCE) and canonical ensemble (CE) formalisms. The GCE formalism gives acceptable predictions for  $S$ ,  $p$ ,  $p/(U/A)$ ,  $\kappa_T$  and  $\alpha_p$  at large  $N$ ,  $T$  and  $A$ , but fails when  $N$  is small or BEC is significant, whereas the CE formalism gives accurate results even at low  $T$  and/or  $A$  where BEC occurs.

**12:39PM L54.00008 Characterizing Featureless Mott Insulating State by Quasiparticle Interferences - A DMFT Prospect<sup>1</sup>**, SHANTANU MUKHERJEE, WEI-CHENG LEE, State Univ of NY - Binghamton — In this talk we discuss the quasiparticle interferences (QPIs) of a Mott insulator using a T-matrix formalism implemented with the dynamical mean-field theory (T-DMFT). In the Mott insulating state, the DMFT predicts a singularity in the real part of electron self energy  $s(w)$  at low frequencies [1], which completely washes out the QPI at small bias voltage. However, the QPI patterns produced by the non-interacting Fermi surfaces can appear at a critical bias voltage in Mott insulating state. The existence of this non-zero critical bias voltage is a direct consequence of the singular behavior of  $\text{Re}[s(w)]/\sim n/w$  with  $n$  behaving as the 'order parameter' of Mott insulating state. We propose that this reentry of non-interacting QPI patterns could serve as an experimental signature of Mott insulating state, and the 'order parameter' can be experimentally measured [2]. [1] A. Georges et al, Rev. Mod. Phys. 68, 13 (1996). [2] Shantanu Mukherjee, and Wei-Cheng Lee, Arxiv: 1504.05214 (2015).

<sup>1</sup>W.C.L acknowledges financial support from start up fund from Binghamton University.

**12:51PM L54.00009 Band Theory for the Electronic and Magnetic Properties of VO<sub>2</sub> Phases<sup>1</sup>**, XIAO SHEN, Vanderbilt University, University of Memphis, SHENG XU, Jiangsu University of Science and Technology, KENT HALLMAN, RICHARD HAGLUND, Vanderbilt University, SOKRATES PANTELIDES, Vanderbilt University, Oak Ridge National Lab — VO<sub>2</sub> is widely studied for the insulator-metal transition between the monoclinic M1 (insulator) and rutile R (metal) phases. Recent experiments show that in addition to the M1 and R phases, VO<sub>2</sub> has a rich phase diagram including a recently identified metallic monoclinic phase, making the material particularly intriguing. The origin of the band gap in the insulating phase of VO<sub>2</sub> has been a subject of debate. It was suggested that the insulating phase cannot be described by band theory and thus strong correlations must be invoked. However, recent band calculations using density functional theory (DFT) with a hybrid functional and standard pseudopotentials correctly obtains a band gap for the M1 insulating phase. Subsequent calculations, however, found that the magnetic properties of VO<sub>2</sub> phases are not correctly described by such calculations. Here we present DFT calculations using a tuned hybrid functional and hard pseudopotentials that reproduce both the band gaps and the magnetic properties of the known VO<sub>2</sub> phases. Thus, it is appropriate to use band theory to describe VO<sub>2</sub> phases without invoking strong correlations. Furthermore, using the band theory treatment, we identify a candidate for the metallic monoclinic phase.

<sup>1</sup>DOE DE-FG02-09ER46554, NSF EECS-1509740

**1:03PM L54.00010 A minimal model for the structural energetics of VO<sub>2</sub><sup>1</sup>**, CHANUL KIM, CHRIS MARIANETTI, Columbia Univ, THE MARIANETTI GROUP TEAM — Resolving the structural, magnetic, and electronic structure of VO<sub>2</sub> from the first-principles of quantum mechanics is still a forefront problem despite decades of attention. Hybrid functionals have been shown to qualitatively ruin the structural energetics. While density functional theory (DFT) combined with cluster extensions of dynamical mean-field theory (DMFT) have demonstrated promising results in terms of the electronic properties, structural phase stability has not yet been addressed. In order to capture the basic physics of the structural transition, we propose a minimal model of VO<sub>2</sub> based on the one dimensional Peierls-Hubbard model and parameterize this based on DFT calculations of VO<sub>2</sub>. The total energy versus dimerization in the minimal model is then solved numerically exactly using density matrix renormalization group (DMRG) and compared to the Hartree-Fock solution. We demonstrate that the Hartree-Fock solution exhibits the same pathologies as DFT+U, and spin density functional theory for that matter, while the DMRG solution is consistent with experimental observation. Our results demonstrate the critical role of non-locality in the total energy, and this will need to be accounted for to obtain a complete description of VO<sub>2</sub> from first-principles.

<sup>1</sup>The authors acknowledge support from FAME, one of six centers of STARnet, a Semiconductor Research Corporation program sponsored by MARCO and DARPA.

**1:15PM L54.00011 Ab Initio Infrared Spectra and Electronic Response Calculations for the Insulating Phases of VO<sub>2</sub><sup>1</sup>**, CHRISTOPHER HENDRIKS, TYLER HUFFMAN, ERIC WALTER, MUMTAZ QAZILBASH, HENRY KRAKAUER, William and Mary College — Previous studies have shown<sup>2</sup> that, under doping or tensile strain and upon heating, the well-known vanadium dioxide (VO<sub>2</sub>) transition from an insulating monoclinic (M1) to a metallic rutile (R) phase progresses through a triclinic symmetry (T) phase and a magnetic monoclinic phase (M2), both of which are insulating. Structurally, this progression from M1 to R through T and M2 can be characterized by the progressive breaking of the V dimers. Investigation of the effect of these structural changes on the insulating phases of VO<sub>2</sub> may help resolve questions surrounding the long-debated issue of the respective roles of electronic correlation and Peierls mechanisms in driving the MIT. We investigated electronic and vibrational properties of the insulating phases of VO<sub>2</sub> in the framework of DFT+U. We will present *ab initio* calculations of infrared spectra and optical electronic responses for the insulating phases and compare these to available experimental measurements<sup>3,4,5,6</sup>.

<sup>1</sup>Supported by ONR

<sup>2</sup>J. H. Park et al., Nature **500**, 431 (2013).

<sup>3</sup>T. J. Huffman et al., PRB **87**, 115121 (2013).

<sup>4</sup>A. S. Barker et al., PRL **17**, 1286 (1966).

<sup>5</sup>H. W. Verleur et al., PR **172**, 788 (1968).

<sup>6</sup>J. M. Tomczak and S. Biermann, PRB **80**, 085117 (2009).

### 1:27PM L54.00012 Role of non-local exchange in the electronic structure of correlated oxides

, FEDERICO IORI, Université Paris Sud - CNRS, MATTEO GATTI, Theoretical Spectroscopy Group LSI - CNRS Ecole Polytechnique & Synchrotron SOLEIL, ANGEL RUBIO SECADES, Theory Department, Max Planck Institute for the Structure and Dynamics of Matter, Max Planck Society — Transition-metal oxides (TMO) with partially filled d or f shells are a prototype of correlated materials. They exhibit very interesting properties, like metal-insulator phase transitions (MIT) [1]. In this work we consider several TMO insulators in which Kohn-Sham LDA band structures are metallic: VO<sub>2</sub>, V<sub>2</sub>O<sub>3</sub>, Ti<sub>2</sub>O<sub>3</sub>, LaTiO<sub>3</sub> and YTiO<sub>3</sub>. In the past, this failure of LDA has been explained in terms of its inadequacy to capture the strong interactions taking place between correlated electrons. In the spirit of the Hubbard model, possible corrections to improve onsite correlation are the LDA+U [2] and LDA+DMFT [3] approaches. Here we make use of the HSE06 hybrid functional [4]. We show that, without invoking strong-correlation effects, the contribution of the non-local Fock exchange is essential to correct the LDA results, by curing its delocalization error. In fact, HSE06 provides insulating band structures and correctly describes the MIT in all the considered compounds [5]. We further discuss the advantages and the limitations of the HSE06 hybrid functional in correlated TMO [1] M. Imada et al., Rev. Mod. Phys. 70, 1039 (1998) [2] V.I. Anisimov, et al., Phys. Rev. B 44, 943 (1991). [3] A. Georges et al., Rev. Mod. Phys. 68, 13 (1996). [4] J. Heyd et al., J. Chem. Phys. 118, 8207 (2003); J. Heyd et al., J. Chem. Phys. , 219906(E) (2006). [5] F. Iori, M. Gatti, and A. Rubio Phys. Rev. B , 115129 (2012)

### 1:39PM L54.00013 The electronic structure of the Mott insulator VO<sub>2</sub>: the strongly correlated metal state is screened by impurity band.

, HYUN-TAK KIM, MIT Center in ETRI — A Mott insulator VO<sub>2</sub> (3d<sup>1</sup>) has a direct gap ( $\Delta_{direct} \propto V_{direct}$ ) of 0.6 eV and an indirect gap of  $\Delta_{act} \propto V_{direct} \approx 0.15$  eV coming from impurity indirect band. At T<sub>c</sub>,  $\Delta_{direct} = \Delta_{act} = 0$  is satisfied and the insulator-to-metal transition (IMT) occurs. The metallic carriers near core region can be trapped when a critical onsite Coulomb U<sub>c</sub> exists. Then, a potential energy is defined as

$$V_g = (V_{direct} + U_c) + V_{indirect} \\ = -(2/3)E_F(1 + e(N_{tot}/n_{tot})(1 - \exp(-\Delta_{act}/k_B T))) + U_c, \quad (2)$$

where  $V_{direct} = -(2/3)E_F$  is the screened Coulomb pseudopotential at K = 0.  $\Delta\rho = N_{tot}/n_{tot} \approx 0.018\%$  [1] is defined as the critical doping quantity, where  $n_{tot}$  is the carrier density in the direct band and  $N_{tot}$  is the carrier density in the impurity band. In  $U_c < (2/3)E_F$  case, it sustains the insulator state. However, when both  $U_c > (2/3)E_F$  and  $\Delta_{act} = 0$  by excitation are satisfied, the IMT occurs in  $V_g \geq 0$ . This indicates that the excitation ( $\Delta_{act} = 0$ ) breaks the Coulomb equilibrium ( $V_g < 0$  and insulator sustaining  $U_c$ ) in Eq. (1); the Coulomb energy changes from  $U_c$  to a  $U < U_c$ . The IMT can be switched by the doping (excitation;  $\Delta_{act} = 0$ ) and the de-doping (de-excitation;  $\Delta_{act} = 0.15$  eV) of  $\Delta\rho = N_{tot}/n_{tot}$  to the conduction band, by applying external parameters such as heat, pressure, doping etc. The direct band gap (semiconductor gap) in the Mott insulator smaller than that of dielectric insulators can be explained by  $U_c$ . [1] NewJ.Phys.6(2004)52.

### 1:51PM L54.00014 Two-dimensional quantum percolation with binary non-zero hopping integrals

, BRIANNA DILLON THOMAS, HISAO NAKANISHI, Purdue Univ — In a previous work [Dillon and Nakanishi, Eur.Phys.J B 87, 286 (2014)], we calculated the transmission coefficient of the two-dimensional quantum percolation problem and mapped out in detail the three regimes of localization, i.e., exponentially localized, power-law localized, and delocalized which had been proposed earlier [Islam and Nakanishi, Phys.Rev. E 77, 061109 (2008)]. We now consider a variation on quantum percolation in which the hopping integral ( $V_{diluted}$ ) associated with bonds that connect to at least one diluted site is non-zero but a fraction of the hopping integral ( $V_{full}=1$ ) between non-diluted sites. We study the latter model by calculating quantities such as the transmission coefficient and the inverse participation ratio and find the original quantum percolation results to be stable over a wide range of energy. In particular, except in the immediate neighborhood of the band center (where increasing  $V_{diluted}$  to just  $0.02*V_{full}$  appears to eliminate localization effects), increasing  $V_{diluted}$  only shifts the boundaries between the 3 regimes but does not eliminate them until the  $V_{diluted}$  reaches 20

### 2:03PM L54.00015 Angle resolved photoemission study of the strongly correlated metal V<sub>2</sub>O<sub>3</sub><sup>1</sup>

, IRENE LO VECCHIO, Lawrence Berkeley National Laboratory, JONATHAN D. DENLINGER, OLEG KRUPIN, Advanced Light Source (Berkeley), BUMJOON KIM, Max Planck Institut for Solid State Research (Stuttgart), PATRICIA METCALF, Purdue University (Indiana), STEFANO LUPI, University of Rome "Sapienza" (Italy), JAMES W. ALLEN, University of Michigan, ALESSANDRA LANZARA, University of California Berkeley and LBNL — V<sub>2</sub>O<sub>3</sub> is often considered as the textbook example for the Mott metal-insulator transition. It has been the playground for multiple theoretical approaches and attempts to describe its metallic ground state for half a century. However, the experimental electronic structure is still unknown because of difficulties related to the three-dimensional character of the Fermi surface and the inhomogeneous cleavage of single crystals. Here we reveal for the first time the band structure of V<sub>2</sub>O<sub>3</sub> using angle resolved photoemission spectroscopy. Direct comparison with theory is presented highlighting the important role of electron correlation for the physics of this material.

<sup>1</sup>Experiments at the Advanced Light Source were supported by the U.S. DOE Basic Energy Sciences (DE-AC02-05CH11231)

## Wednesday, March 16, 2016 11:15AM - 2:15PM –

Session L55 GQI: 20 Years of Quantum Error Correction Hilton Baltimore Holiday Ballroom 6 - Steve Flammia, University of Sydney

### 11:15AM L55.00001 Stability, topology, holography: The many facets of quantum error correction

, JOHN PRESKILL, Caltech — Quantum error correction is a surprising and far-reaching concept, with many implications for science and technology. The theory of quantum error-correcting codes has bolstered our confidence that quantum computing is scalable, deepened our understanding of topological phases of matter, and spawned novel insights into the quantum structure of spacetime.

### 11:51AM L55.00002 Fault Tolerance in Small Experiments

, DANIEL GOTTESMAN, Perimeter Inst for Theo Phys — Experiments are finally reaching the size and level of precise control where we can hope to see a truly fault-tolerant experiment within the next few years. I will give a proposal for a 5-qubit fault-tolerant experiment and discuss how to evaluate if an experiment has successfully demonstrated fault tolerance. I will also consider the possibility of using future fault-tolerant experiments to answer important questions about the interaction of fault-tolerant protocols with real experimental errors.

**12:27PM L55.00003 Quantum Error Correction and the Future of Solid State Quantum Computing<sup>1</sup>**, DAVID DIVINCENZO, Forschungszentrum Juelich and RWTH Aachen — Quantum error correction (QEC) theory has provided a very challenging but well defined goal for the further development of solid state qubit systems: achieve high enough fidelity so that fault-tolerant, error-corrected quantum computation in networks of these qubits becomes possible. I will begin by touching on some historical points: initial work on QEC is actually more than 20 years old, and the landmark work of Kitaev in 1996 which established 2D lattice structures as a suitable host for effective error correction, has its roots in theoretical work in many-body theory from Wegner in the 1970s. I will give some perspective on current developments in the implementation of small fragments of the surface code. The surface-code concept has driven a number of distinct requirements, beyond the reduction of error rates below the 1% range, that are actively considered as experiments are scaled beyond the 10-qubit level.

<sup>1</sup>Support of JARA FIT is acknowledged.

**1:03PM L55.00004 Quantum error correction with trapped ions**, PHILIPP SCHINDLER, University of Innsbruck — Quantum computers promise exponential speed-up compared to their classical counterparts for certain problems. Unfortunately, the states required for quantum computation are fragile and lose their quantum properties with growing system size. In a milestone work, it has been shown that quantum error correction can overcome this problem and enable arbitrary long and arbitrary high quality quantum algorithms. However, current experiments are not able to fulfill the requirements to employ useful quantum error correction procedures. In this talk, I will first review past proof-of-principle experiments in trapped ion quantum information processors. Building on that, I will sketch a way towards a medium-sized trapped ion system that will be capable of running an error correction procedure that outperforms its constituents.

**1:39PM L55.00005 Quantum error correction in superconducting circuits<sup>1</sup>**, MICHEL DEVORET, Yale University — Can we prolong the coherence of a two-state manifold in a complex quantum system beyond the coherence of its longest-lived component? This question is the starting point of the main challenges in the construction of a scalable quantum computer, namely the implementation of quantum error correction. The presentation will review the experimental progress that recently occurred in the field of superconducting quantum circuits towards the correction, for a full logical qubit memory, of the combinations of bit flip and phase flip errors.

<sup>1</sup>Work supported by ARO and YINQE.

**11:30AM - 11:30AM –**  
Session M1 DPOLY DBIO GSOF GSNP DFD: Poster Session II (Wednesday, 11:30 am - 2:30 pm) Exhibit Hall EF -

## **M1.00001 POLYMER PHYSICS –**

**M1.00002 Morphology Evolution and Dynamic Viscoelastic Behavior of Ternary Elastomer Blends under Shear<sup>1</sup>**, XIA DONG, XIANGGUI LIU, CHARLES C HAN, DUJIN WANG, Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Engineering Plastics, Institute of Chemistry CAS — The influence of nanoparticle geometry, such as size and shape, on the phase morphology of partially miscible binary polymer blends under and after shear has been examined by rheological and rheo-optical techniques. The phase morphologies of the solution-polymerized styrene-butadiene rubber and low vinyl content polyisoprene (SSBR/LPI) blend systems were affected by the dispersion status of fillers which were determined by filler shapes and shear strength. Under weak shear flow, the domain morphology of the OMMT filled blend was much thinner than that of the SiO<sub>2</sub> filled blend. Under strong shear flow, the string-like phase interface of the OMMT filled blend was much blurred compared with that of the SiO<sub>2</sub> filled blend. After shear cessation, the orientation status of OMMT sheets determined the orientation of newborn domains. Combined morphology observation and rheological analysis showed that the anisotropic structure and the unfavorable bending energy of OMMT sheets played important roles on phase morphology and its evolution process during or after shear.

<sup>1</sup>The authors thank the financial support from National Natural Science Foundation of China (No.51173195).

**M1.00003 Selective crystallization of regioregularity controlled polythiophene for enhancing mechanical stability and electronic performance**, HYEONG JUN KIM, KAIST, HOJEONG YU, POESTECH, JAE-HAN KIM, JIN-SUNG KIM, TAEK SOO KIM, KAIST, JOON HAK OH, POESTECH, BUMJOON KIM, KAIST — Considering the many potential applications of organic electronics in portable electronic devices, it is of great importance to develop an electro-active material that possesses mechanical stability and high electronic performance. Coexistence of both properties, however, is very difficult to achieve because good electronic performance is associated with long conjugation length, and high crystallinity often results in stiffness and brittleness. Herein, we utilize P3HT with two different regioregularities: high RR (98) P3HT has high electronic properties but poor mechanical resilience, and low RR P3HT (68) exhibits high elasticity and ductility but poor electronic performance. Selective crystallization of high RR P3HT induced by solution assembly allows construction of percolated networks of high RR P3HT nanowires (NWs) embedded in low RR P3HT matrix. Only 5 wt high RR P3HT is required to reach a hole mobility comparable to that of high RR P3HT, and high RR NWs embedded in film exhibits 20 times higher elongation at break. Selective self-assembly allows us to overcome the fragile nature of highly crystalline conjugated polymers without losing their electronic properties.

**M1.00004 Development of flash nanoprecipitation as a scalable platform for production of hybrid polymer-inorganic Janus particles<sup>1</sup>**, VICTORIA E. LEE, ROBERT K. PRUD'HOMME, RODNEY D. PRIESTLEY, Princeton University — Polymer Janus particles, containing two or more distinct domains, can act as supports for inorganic nanoparticles, stabilizing them against aggregation and templating anisotropic functionalization of the microparticles. This anisotropy can be advantageous for applications such as biofuel upgrading, bionanosensors, and responsive materials. Here, we introduce flash nanoprecipitation (FNP) as a scalable, fast process to create hybrid polymer-inorganic Janus particles with control of particle size and anisotropy. During FNP, polymer Janus particles form by rapid intermixing of a polymer solution with a poor solvent, inducing polymer precipitation and phase separation. Inorganic nanoparticles are then adsorbed selectively onto one domain of the polymer support by exploiting electrostatic interactions between the charged particles. By tuning polymer concentration and ratio in the feed stream, the particle size and anisotropy can be controlled. We further demonstrate that these hybrid particles can simultaneously stabilize emulsions and selectively catalyze the degradation of dye in one phase.

<sup>1</sup>With support from the Princeton Imaging Analysis Center

**M1.00005 Control of dynamical self-assembly of strongly Brownian nanoparticles through convective forces induced by ultrafast laser.** , SERIM ILDAY, GURSOY B. AKGUC, ONUR TOKEL, GHAITH MAKEY, OZGUN YAVUZ, KORAY YAVUZ, IHOR PAVLOV, F. OMER ILDAY, OGUZ GULSEREN, Bilkent Univ — We report a new dynamical self-assembly mechanism, where judicious use of convective and strong Brownian forces enables effective patterning of colloidal nanoparticles that are almost two orders of magnitude smaller than the laser beam. Optical trapping or tweezing effects are not involved, but the laser is used to create steep thermal gradients through multi-photon absorption, and thereby guide the colloids through convective forces. Convective forces can be thought as a positive feedback mechanism that helps to form and reinforce pattern, while Brownian motion act as a competing negative feedback mechanism to limit the growth of the pattern, as well as to increase the possibilities of bifurcation into different patterns, analogous to the competition observed in reaction-diffusion systems. By steering stochastic processes through these forces, we are able to gain control over the emergent pattern such as to form-deform-reform of a pattern, to change its shape and transport it spatially within seconds. This enables us to dynamically initiate and control large patterns comprised of hundreds of colloids. Further, by not relying on any specific chemical, optical or magnetic interaction, this new method is, in principle, completely independent of the material type being assembled.

**M1.00006 Amphiphilic Soft Janus Particles as Interfacial Stabilizers** , WENDA WANG, SUNNY NIU, CHRIS SOSA, ROBERT PRUD'HOMME, RODNEY PRIESTLEY, Princeton Univ, PRIESTLEY POLYMER GROUP TEAM, PRUD'HOMME RESEARCH GROUP TEAM — Janus particles, which incorporate two or more “faces” with different chemical functionality, have attracted great attention in scientific research. Amphiphilic Janus particles have two faces with distinctly different hydrophobicity. This can be thought of as colloidal surfactants. Theoretical studies on the stabilization of emulsions using Janus particles have confirmed higher efficiency. Herein we synthesize the narrow distributed amphiphilic polymeric Janus particles via Precipitation-Induced Self-Assembly (PISA). The efficiency of the amphiphilic Janus particles are tested on different oil/water systems. Biocompatible polymers can also be used on this strategy and may potentially have wide application for food emulsion, cosmetics and personal products.

**M1.00007 Time-resolved SANS studies on block copolymer micelles with varying core-solvent interactions** , TYLER COOKSEY, AVANTIKA SINGH, MARIA MARQUEZ, MEGAN ROBERTSON, University of Houston — The self-assembly of block copolymer micelles occurs through a relaxation process dominated by the exchange of individual polymer chains. The objective of this work is to probe the single chain exchange of block copolymer micelles with varying core-solvent interactions, utilizing time-resolved neutron scattering (TR-SANS). The interactions between the core-forming polymer and the solvent has many implications for the micelle structure, including the aggregation number, micelle size, and interfacial tension. However, few studies have investigated the effect of the core polymer-solvent interactions on the dynamics of micelle formation. We will focus our study on poly(epsilon-caprolactone-block-ethylene oxide) block copolymers forming micelle structures in mixtures of water and tetrahydrofuran (THF). It was observed that changing the THF concentration, which varies the degree of repulsion between the core and solvent, greatly influences the single chain exchange rate in this system.

**M1.00008 Spectroscopic Analysis of 10MAG/LDAO Reverse Micelles to Determine Characteristic Properties and Behavioral Extrema** .<sup>1</sup> , JOSHUA BERG<sup>2</sup>, CARA MAWSON<sup>3</sup>, ZACH NORRIS, NATHANIEL NUCCI, Rowan University — Reverse micelles are spontaneously organizing complexes of surfactant that encapsulate a nanoscale pool of water in a bulk non-polar solvent. Reverse micelle (RM) mixtures have a wide range of applications, including biophysical investigation of protein systems. A new RM mixture composed of decyl-1-mono glycerol (10MAG) and lauryldimethylammonium-N-oxide (LDAO) was recently described. This mixture has the potential to prove more widely applicable for use of RMs in applications that involve encapsulation of macromolecules, yet little is known about the phase behavior or size of reverse micelles created by this mixture. Data describing such behaviors for this mixture are presented here. We have used dynamic light scattering (DLS) and fluorescence spectroscopy to investigate the size and partitioning behavior of RMs in varying mixtures of 10MAG, LDAO, water, pentane, and hexanol. These data demonstrate that the 10MAG/LDAO RM mixture exhibits markedly different phase and RM size behavior than that of commonly used RM surfactant mixtures. The implications of these findings for use of the 10MAG/LDAO mix for RM applications will also be addressed.

<sup>1</sup>Funding provided by Rowan University

<sup>2</sup>\*co-presenting author

<sup>3</sup>\*co-presenting author

**M1.00009 Photolithography and Fluorescence Correlation Spectroscopy used to examine the rates of exchange in reverse micelle systems** .<sup>1</sup> , ZACH NORRIS, CARA MAWSON, KYRON JOHNSON, SARAH KESSLER, ANNE REBECCA, NATHAN WOLF, MICHAEL LIM, NATHANIEL NUCCI, Rowan University — Reverse micelles are molecular complexes that encapsulate a nanoscale pool of water in a surfactant shell dissolved in non-polar solvent. These complexes have a wide range of applications, and in all cases, the degree to which reverse micelles (RM) exchange their contents is relevant for their use. Despite its importance, this aspect of RM behavior is poorly understood. Photolithography is employed here to create micro and nano scale fluidic systems in which mixing rates can be precisely measured using fluorescence correlation spectroscopy (FCS). Micro-channel patterns are etched using reactive ion etching process into a layer of silicon dioxide on crystalline silicon substrates. Solutions containing mixtures of reverse micelles, proteins, and fluorophores are placed into reservoirs in the patterns, while diffusion and exchange between RMs is monitored using a FCS system built from a modified confocal Raman spectrometer. Using this approach, the diffusion and exchange rates for RM systems are measured as a function of the components of the RM mixture.

<sup>1</sup>Funding provided by Rowan University

**M1.00010 Self-assembly of mixed lipids into bicelles and vesicles: molecular dynamics simulations.** , HARI SHARMA, ZILU WANG, ELENA DORMIDONTOVA, Department of Physics and Institute of Materials Science, University of Connecticut, Storrs, CT — Formation of complex supramolecular nanostructures, such as micelles, bicelles, vesicles (liposomes) etc. via self-assembly of simple molecules has provided a new pathway for the design and development of effective drug carriers. Solid nanoparticles or functional biopolymers, such as RNA, DNA, peptides can be encapsulated into these carriers for controlled delivery or selective targeting. We performed coarse grained molecular dynamics simulation using the MARTINI force field to study the self-assembly of a binary surfactant mixture composed of long and short phospholipids, DPPC and DHPC, in the ratio 3:1. We found that at low temperature lipids self-assemble into a bicelle (nanodisc) with the longer lipid mainly forming the interior and short lipid the rim of the bicelle. At higher temperature the nanodisc transforms into a vesicle with homogeneously distributed lipids. The structural changes of these nanodiscs and vesicles imposed by gold nanoparticle encapsulation and pegylation will be addressed.

**M1.00011 Directed Assembly of Gold Nanoparticles via Polymer Single Crystals** , SHAN MEI, HAO QI, TIAN ZHOU, CHRISTOPHER LI, None, SOFT MATERIAL LAB TEAM — Gold nanoparticles (AuNPs) have attracted great attention due to their unique properties and potential applications. In recent years, more efforts have been made to the assembly of AuNP into various of ordered structures such as AuNP wires and sheets in order to transfer their properties from nanoscale to macroscale, as well as exploring new properties. In this work we report a method to assemble AuNP into well defined, free standing frame structure using poly(ethylene oxide) (PEO) lamellar single crystal as the template. By controlling the single crystal size and functioning pattern, we are able to tune the width and size of the AuNP frame. We consider this approach to be an efficient and precise way to assemble AuNP and this methodology could be applied to other metal or semiconductor NPs.

**M1.00012 Synthesis of Poly(N-isopropylacrylamide) Microcapsules for Drug Delivery Applications via UV Aerosol Photopolymerization.**<sup>1</sup>, NICOLE ROBERSON, DANIEL DENMARK, SARATH WITANACHCHI, University of South Florida — Hybrid drug delivery systems composed of thermoresponsive polymers and magnetic nanoparticles have been developed using chemical methods to deliver controlled amounts of a biotherapeutic to target tissue. These methods can be expensive, time intensive, and produce impure composites due to the use of surfactants during polymer synthesis. In this study, UV aerosol photopolymerization is used to synthesize N-isopropylacrylamide (NIPAM) monomers, N,N-methylenebisacrylamide (MBA) crosslinker, and irgacure 2959 photoinitiator into the transporting microcapsule for drug delivery. The method of UV aerosol photopolymerization allows for the continuous, cost effective, and time efficient synthesis of a high concentration of pure polymers in a short amount of time; toxic surfactants are not necessary. Optimal NIPAM monomer, MBA crosslinker, and irgacure 2959 photoinitiator concentrations were tested and analyzed to synthesize a microcapsule with optimal conditions for controlled drug delivery. Scanning Electron Microscope (SEM) imaging reveals that synthesis of polymer microcapsules of about 30 micrometers in size is effective through UV aerosol photopolymerization. Findings will contribute greatly to the field of emergency medicine.

<sup>1</sup>This work was supported by the United States Army (Grant No. W81XWH1020101/3349)

**M1.00013 Tertiary phase diagram of cellulose, ionic liquid and organic solvent**, XIN ZHANG, DOUG HENDERSON, Department of Materials Science and Engineering, University of Maryland, MADHUSUDAN TYAGI, YIMIN MAO, NCNR, NIST, Gaithersburg, MD, ROBERT M. BRIBER, HOWARD WANG, Department of Materials Science and Engineering, University of Maryland — Cellulose is the most abundant natural polymer on earth, and widely used in products from clothing to paper. Fundamental understanding of molecular solutions of cellulose is the key to realize advanced technologies beyond cellulose fibers. It has been reported that certain ionic liquid/organic solvent mixtures dissolve cellulose. In this study, the tertiary phase diagram of microcrystalline cellulose, 1-Ethyl-3-methylimidazolium acetate (EMIMAc), and dimethylformamide (DMF) mixtures has been determined using optical cloud point method and small angle neutron scattering (SANS). Data indicate that a molar ratio of EMIMAc to cellulose repeating unit equal or greater than 3 is necessary but not sufficient in forming one-phase homogeneous solutions. A miscibility gap exists in the dilute regime, where a minimum of 5 mol% of EMIM Ac in DMF is needed to form homogenous solutions. SANS show that cellulose chains adopt Gaussian-like conformation in homogenous solutions. The solutions exhibit the characteristics of upper critical solution temperature. Clustering of cellulose chains occurs at low EMIMAc/DMF or EMIMAc/cellulose ratio, or at low temperatures. The mechanism of cellulose dissolution in tertiary mixture is discussed.

**M1.00014 Thin blend films of cellulose and polyacrylonitrile**, RUI LU, XIN ZHANG, Department of Materials Science and Engineering, University of Maryland, College Park, MD, YIMIN MAO, NCNR, NIST, Gaithersburg, MD, ROBERT BRIBER, HOWARD WANG, Department of Materials Science and Engineering, University of Maryland, College Park, MD — Cellulose is the most abundant renewable, biocompatible and biodegradable natural polymer. Cellulose exhibits excellent chemical and mechanical stability, which makes it useful for applications such as construction, filtration, bio-scaffolding and packaging. To further expand the potential applications of cellulose materials, their alloying with synthetic polymers has been investigated. In this study, thin films of cotton linter cellulose (CLC) and polyacrylonitrile (PAN) blends with various compositions spanning the entire range from neat CLC to neat PAN were spun cast on silicon wafers from common solutions in dimethyl sulfoxide / ionic liquid mixtures. The morphologies of thin films were characterized using optical microscopy, atomic force microscopy, scanning electron microscopy and X-ray reflectivity. Morphologies of as-cast films are highly sensitive to the film preparation conditions; they vary from featureless smooth films to self-organized ordered nano-patterns to hierarchical structures spanning over multiple length scales from nanometers to tens of microns. By selectively removing the PAN-rich phase, the structures of blend films were studied to gain insights in their very high stability in hot water, acid and salt solutions.

**M1.00015 Process Dependence of Cellulose Nanofiber Fabrication**, DOUG HENDERSON, XIN ZHANG, Department of Materials Science and Engineering, University of Maryland-College Park, MD, YIMIN MAO, NCNR, NIST, Gaithersburg, MD, SOO-HWAN JANG, LIANGBING HU, ROBERT BRIBER, HOWARD WANG, Department of Materials Science and Engineering, University of Maryland-College Park, MD — Cellulose nanofibers (CNF) are the most abundant natural nanomaterial on earth with potential applications in renewable energy, polymer nanocomposites and flexible electronics. CNF can be produced through TEMPO oxidation which separates the hierarchical structure of cellulose fibers into smaller micro- and nanofibers by altering their surface chemistry, inducing a repulsive electrostatic charge on the fibers. This work will examine the structural evolution of CNF during production. Samples were prepared by removing and quenching aliquots during the TEMPO reaction. The fibers were washed, filtered and re-dispersed into D2O for small angle neutron scattering (SANS) measurements. The SANS data was analyzed to track the changes in the CNF structure as a function of reaction time.

**M1.00016 Multi-scale Characterization of Cellulose TEMPO-Nanofiber Suspension**, YIMIN MAO, Dept. of Materials Sci. and Eng., Univ. of Maryland, College Park; NIST Center for Neutron Research, National Institute of Standards and Technology, KAI LIU, BENJAMIN HSIAO, Chemistry Department, Stony Brook University — Cellulose nanofiber (CNF) suspensions were characterized at multiple length scales. CNF suspension was prepared by applying 2,2,6,6-tetramethyl-1-piperidinyloxy (TEMPO) oxidation method to dry wood pulp. TEMPO method was able to produce fine fibers with a cross section dimension being in the order of magnitude of several nanometers, and length being several hundred nanometers. The surface was negatively charged. Charge density was characterized by Zeta-potential measurement. Both small-angle X-ray (SAXS) and small-angle neutron (SANS) methods were employed to examine fiber dimensions in solution. Data fitting indicated that newly-developed ribbon model was able to capture the essence of CNFs geometry, which is also computationally economic. The rectangular-shaped cross section was consistent to cellulose's crystal structure; and was able to provide insights into how cellulose crystals were biologically synthesized and packed in nature. Multi-angle dynamic light scattering (DLS) was used to study CNF's diffusion properties. A strong scattering-angle dependence of auto-correlation function was observed. The characterization is useful to understanding suspension quality of CNF, and can provide guideline for follow-up research aimed for a variety of applications.

**M1.00017 Controlling the structure and rheology of TEMPO-oxidized cellulose in zinc chloride aqueous suspensions for fabricating advanced nanopaper**, SHA WANG, XIN ZHANG, LIANGBING HU, ROBERT BRIBER, HOWARD WANG, Dept. Materials Science and Engineering, University of Maryland, College Park, LINXIN ZHONG, State Key Laboratory of Pulp and Paper Engineering, South China University of Technology — Due to its abundance, low-cost, biocompatibility and renewability, cellulose has become an attractive candidate as a functional material for various advanced applications. A key to novel applications is the control of the structure and rheology of suspensions of fibrous cellulose. Among many different approaches of preparing cellulose suspensions, zinc chloride addition to aqueous suspensions is regarded an effective practice. In this study, effects of ZnCl<sub>2</sub> concentration on TEMPO-oxidized cellulose (TOC) nanofiber suspensions have been investigated. Highly-transparent cellulose nanofiber suspension can be rapidly obtained by dissolving TOC in 65 wt.% zinc chloride aqueous solutions at room temperature, whereas a transparent zinc ion cross-linked TOC gel could be obtained with zinc chloride concentration as low as 10 wt. %. The structural and rheological characteristics of TOC/ZnCl<sub>2</sub> suspensions have been measured to correlate to the performance of transparent and flexible nanocellulose paper subsequently produced via vacuum filtration or wet-casting processes.

**M1.00018 All-or-none folding of a polymer in confinement<sup>1</sup>** , MARK TAYLOR, Hiram College — A flexible homopolymer chain with sufficiently short-range interactions undergoes a discontinuous transition from an expanded coil to a compact crystallite analogous to the all-or-none folding transition exhibited by fast-folding proteins. One anticipates that geometric confinement will reduce the entropy of the unfolded chain, thereby stabilizing the folded state and shifting the transition to higher temperature. In this work we study a flexible square-well N-mer chain (monomer diameter  $d$ ) located between two hard walls forming a slit-like pore (width  $W$ ) with the chain end-tethered to one wall. We carry out Monte simulations with Wang-Landau sampling to construct the single-chain density of states and use both microcanonical and canonical analyses to characterize phase transitions. When the slit width is similar to the size of the folded chain we observe a modest stabilization effect. Further reduction of the slit width geometrically prohibits the chain from folding into the free-chain ground state. However, a discontinuous all-or-none folding transition still occurs to a flattened crystallite that spans the pore. All-or-none folding persists even to the limit of a very narrow pore ( $W \rightarrow d$ ) where the ground-state structure is a quasi-two-dimensional crystal.

<sup>1</sup>Funding: NSF DMR-1204747

**M1.00019 Exploring the existence of two T<sub>g</sub>s in thin, supported polymer films<sup>1</sup>** , ERIC CHEN, ETHAN GLOR, GABRIEL ANGRAND, ZAHRA FAKHRAAI, Univ of Pennsylvania, FAKHRAAI GROUP TEAM — Ellipsometry has commonly been used to characterize the glass transition temperature ( $T_g$ ) and other properties of nanoscale thin films. In some ultra-thin films the glass transition broadens and even becomes two distinct transitions, as previously observed in free-standing polystyrene, thin films. However, for most polymers, the second, lower  $T_g$  is located below the condensation temperature of water, generating large errors in determining the lower  $T_g$ , which is associated with the layer close to the free interface. Here we designed a vacuum stage with a base pressure of  $<1E-4$  torr, equipped with a Linkam temperature stage with a temperature range of 153 K-873 K to study the properties of thin polymer films, supported on a substrate, in a broad temperature range and explore the existence of two  $T_g$ s in these systems. The stage was machined from aluminum and used infrasil quartz windows to allow the transmission of polarized light without distortion. The vacuum allows for accurate ellipsometry measurements of the properties of thin polymer films, such as expansion coefficient and  $T_g$ , at temperatures well below room temperature, without artifacts due to water condensation.

<sup>1</sup>MRSEC (NSF-DMR-11- 20901)

**M1.00020 Limits of single-molecule super-resolution microscopy in thin polymer films** , MUZHOU WANG, MARCELO DAVANCO, JAMES M. MARR, J. ALEXANDER LIDDLE, JEFFREY W. GILMAN, National Institute of Standards and Technology — Structural characterization by super-resolution microscopy has become increasingly widespread, particularly in the biological community. The technique is powerful because it can produce real-space images with resolutions of tens of nanometers, while sample preparation is relatively non-invasive. Previous studies have applied these techniques to important scientific problems in the life sciences, but relatively little work has explored the attainable limit of resolution using samples of known structure. In this work, we apply photo-activated localization microscopy (PALM) to polymer films that have been nanopatterned using electron-beam lithography. Trace amounts of a rhodamine spiroamide dye are dispersed into nanostructured poly(methyl methacrylate), and UV-induced switching of the fluorophores enables nanoscale localization of single molecules to generate a final composite super-resolution image. Features as small as 50 nm are clearly resolvable. To determine the ultimate resolution limit, we investigate sources of error in the system, particularly from systematic mislocalizations due to the effect of fluorophore orientation on the single-molecule point-spread function.

**M1.00021 Phase separated microstructure and dynamics of polyurethane elastomers under strain** , CIPRIAN IACOB, Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA 16802 USA, AJAY PADALGIKAR, Implantable Electronic Systems Division, St. Jude Medical, Rogers, MN, USA, JAMES RUNT, Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA 16802 USA — The molecular mobility of polyurethane elastomers is of the utmost importance in establishing physical properties for uses ranging from automotive tires and shoe soles to more sophisticated aerospace and biomedical applications. In many of these applications, chain dynamics as well as mechanical properties under external stresses/strains are critical for determining ultimate performance. In order to develop a more complete understanding of their mechanical response, we explored the effect of uniaxial strain on the phase separated microstructure and molecular dynamics of the elastomers. We utilize X-ray scattering to investigate soft segment and hard domain orientation, and broadband dielectric spectroscopy for interrogation of the dynamics. Uniaxial deformation is found to significantly perturb the phase-separated microstructure and chain orientation, and results in a considerable slowing down of the dynamics of the elastomers. Attenuated total reflectance Fourier transform infrared spectroscopy measurements of the polyurethanes under uniaxial deformation are also employed and the results are quantitatively correlated with mechanical tensile tests and the degree of phase separation from small-angle X-ray scattering measurements.

**M1.00022 Phase behavior of the thermoresponsive polymer Poly(N-isopropyl acrylamide) at variable pressure** , ALFONS SCHULTE, Department of Physics and College of Optics and Photonics, University of Central Florida, Orlando, FL 32817-2385, KORA-LEE CLAUDE, SIMON PINZEK, PETER MLLER-BUSCHBAUM, CHRISTINE PAPADAKIS, TU Munchen, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching — Stimuli-responsive such as Poly(N-isopropyl acrylamide) (PNIPAM) exhibit lower critical solution temperature (LCST) behaviour. At ambient pressure it is associated with the release of water and coil to globule transition of the polymer chains, leading to phase separation. Using turbidimetry we measure the P-T phase diagram over an extended range of pressure (0.1–400 MPa) and temperature (-10–40 °C). The phase boundary shows an elliptic profile, i.e. the cloud point temperature first increases and then decreases with pressure. This is reflected in the change in Gibbs free energy, isothermal compressibility, and isobaric heat capacity. The role of solvent-solvent interaction and addition of co-solvents is discussed.

**M1.00023 Complex Cure Kinetics of the Hydroxyl-Epoxy Reaction in DGEBA Epoxy Hardened with Diethanolamine** , WINDY ANCIPIK, JOHN MCCOY, New Mexico Institute of Mining and Technology, JAMIE KROPKA, MATHIAS CELINA, Sandia National Laboratories — The curing of a diglycidyl ether of bisphenol-A Epoxy (Epon 828) with diethanolamine (DEA) involves a fast amine-epoxide reaction followed by a slower hydroxyl-epoxide reaction. At curing temperatures below 100°C, the time scales of these two reactions are well separated, and the hydroxyl addition can be studied as an "isolated" reaction. The hydroxyl-epoxide reaction is of great interest due to the complex kinetics involved, which are brought about by competing reactions. The reaction kinetics are believed to be tertiary amine catalyzed and are well fit to a modified form of the Kamal-type equation. Here we study the complex long term reaction kinetics at various temperatures, by using isothermal modulated differential scanning calorimetry, micro calorimetry, and infrared spectroscopy. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

**M1.00024 Relaxation Characteristics of 828 DGEBA Epoxy Over Long Time Periods** , JASMINE HOO, RILEY C. REPROGLE, BRIAN WISLER, GABRIEL K. ARECHEDERRA, JOHN D. MCCOY, New Mexico Institute of Mining and Technology, JAMIE M. KROPKA, KEVIN N. LONG, Sandia National Laboratories — The mechanical relaxation response in uniaxial compression of a diglycidyl ether of bisphenol-A epoxy was studied over long time periods. The epoxy, 828DEA, was Epon 828 cured with diethanolamine (DEA). A sample was compressed at constant strain rate and held at various strain levels for days to allow the sample to relax. The sample was then compressed further and held once more. The relaxation curves were fit with a stretched exponential function. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

**M1.00025 Effect of Structure on Charge Mobility in Partially Ordered Polymeric Systems**, WAYLON LUO, KIRAN KHANAL, JUTTA LUETTNER-STRATHMANN, University of Akron — The performance of thin film organic semiconductor devices depends on the mobility of the charge carriers, which is strongly affected by the structure of the material. Accounting for these effects in device simulations is difficult since the size of the active layer is too large to generate realistic morphologies from molecular simulations of the constituents. In this work, we present Monte Carlo simulations of a coarse-grained lattice model for dense polymeric systems with a semiflexible component that undergoes a transition to (partially) ordered states at low temperatures. To investigate charge transport, the lattice polymer configurations become part of a model device, which consists of a layer of the material between two electrodes at different potentials. We determine the mobility from Monte Carlo simulations of charge carriers. To model the effect of polymer chain connectivity on charge transport we include an energetic barrier to hopping between sites on different chains; energetic disorder is taken into account by averaging over many polymer configurations. We find that ordering in the material leads to strong mobility anisotropies with increased mobility for transport parallel to the ordered domains and reduced mobility for perpendicular transport.

**M1.00026 Improved electrospinning processing of PU/PEDOT:PSS for electronic textile applications**<sup>1</sup>, ERIN EVKE<sup>2</sup>, Materials Engineering, AARON CLIPPINGER<sup>3</sup>, Biomedical Engineering, CLAYSON SPACKMAN, JOHN-SAMUEL, Mechanical, Aerospace and Nuclear Engineering, RAHMI OZISIK, Materials Engineering; Rensselaer Polytechnic Institute — Poly(3,4-ethylenedioxythiophene)/poly(4-styrenesulfonate), PEDOT:PSS, is an electrically conductive polymer used in electronic textile (e-textile) applications, such as electrochromic textiles, strain sensors, and resistive heaters. In the current study, PEDOT:PSS is blended with varying concentrations of polyurethane (PU) to investigate the flexibility of PU/PEDOT:PSS fibers that are produced via a modified electrospinning process where the jet is collected close to the tip of the needle, thereby, enabling the collection of straight fibers by a rotating spool. The electrical conductivity and mechanical properties of PU/PEDOT:PSS fibers are characterized to understand the effect of PU concentration and the processing parameters.

<sup>1</sup>This material is based upon work supported by the National Science Foundation under Grant No. CMMI-1538730

<sup>2</sup>Undergraduate Student

<sup>3</sup>Undergraduate Student

**M1.00027 Monte-Carlo simulations of a coarse-grained model for  $\alpha$ -oligothiophenes**, AMANI AL-MUTAIRI, JUTTA LUETTNER-STRATHMANN, Department of Physics, University of Akron — The interfacial layer of an organic semiconductor in contact with a metal electrode has important effects on the performance of thin-film devices. However, the structure of this layer is not easy to model. Oligothiophenes are small,  $\pi$ -conjugated molecules with applications in organic electronics that also serve as small-molecule models for polythiophenes.  $\alpha$ -hexithiophene (6T) is a six-ring molecule, whose adsorption on noble metal surfaces has been studied extensively (see, e.g., Ref. [1]). In this work, we develop a coarse-grained model for  $\alpha$ -oligothiophenes. We describe the molecules as linear chains of bonded, discotic particles with Gay-Berne potential interactions between non-bonded ellipsoids. We perform Monte Carlo simulations to study the structure of isolated and adsorbed molecules. [1] M. Kiel et al. Phys. Rev. B 75, 195439 (2007).

**M1.00028 Conductance Thin Film Model of Flexible Organic Thin Film Device using COMSOL Multiphysics**, CAROLYN CARRADERO-SANTIAGO, JOSEE VEDRINE-PAULUS, University of Puerto Rico at Humacao — We developed a virtual model to analyze the electrical conductivity of multilayered thin films placed above a graphene conducting and flexible polyethylene terephthalate (PET) substrate. The organic layers of poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) as a hole conducting layer, poly(3-hexylthiophene-2,5-diyl) (P3HT), as a p-type, phenyl-C61-butyric acid methyl ester (PCBM) and as n-type, with aluminum as a top conductor. COMSOL Multiphysics was the software we used to develop the virtual model to analyze potential variations and conductivity through the thin-film layers. COMSOL Multiphysics software allows simulation and modeling of physical phenomena represented by differential equations such as heat transfer, fluid flow, electromagnetism, and structural mechanics. In this work, using the AC/DC, electric currents module we defined the geometry of the model and properties for each of the six layers: PET/graphene/PEDOT:PSS/P3HT/PCBM/aluminum. We analyzed the model with varying thicknesses of graphene and active layers (P3HT/PCBM). This simulation allowed us to analyze the electrical conductivity, and visualize the model with varying voltage potential, or bias across the plates, useful for applications in solar cell devices.

**M1.00029 Photopatterned surface relief gratings in azobenzene-amorphous polycarbonate thin films**<sup>1</sup>, MORTEN VOLLMANN, Technical University Berlin, PETER GETEK, University of Applied Sciences Berlin, KELLIE OLEAR, CODY COMBS, BENJAMIN CAMPOS, EDMUND WITKOWSKI, The College of New Jersey, ERIN CAIN, Temple University, DAVID MCGEE, The College of New Jersey — Photoinduced orientation of azobenzene chromophores in polymeric host materials has been broadly explored for optical processing applications. Illumination of the chromophore with polarized light rotates the trans isomer perpendicular to the polarization, resulting in spatially modulated birefringence. The photoinduced anisotropy may also drive mass transport, with surface relief patterns being observed in a wide variety of systems. Here we report photoinduced birefringence in a guest-host system of Disperse Red 1- amorphous polycarbonate (DR1-APC). Birefringence was induced with a 490 nm laser and probed at 633 nm, with typical values of  $\Delta n = 0.01$  in 2 micron thick films. Illumination of DR1-APC with intensity and/or polarization gratings also resulted in sinusoidal surface relief patterns with periodicity 1- 3 micron as controlled by the interbeam crossing angle of the 490 nm writing beams; the surface modulation was  $\pm 20$  nm as measured by atomic force microscopy. Photopatterned DR1-APC is advantageous for applications given the ease of thin-film fabrication and the high glass transition temperature of APC, resulting in robust optically-induced surface gratings.

<sup>1</sup>We acknowledge support from NSF-DMR award No. 1138416

**M1.00030 Morphology of conjugated polymer/insulating polymer blends from inkjet printing and its correlation to the function of field-effect transistors**, HUIPENG CHEN, GUOCHEN ZHENG, LIQIN HU, HUIHUANG YANG, TAILIANG GUO, Fuzhou University — Printed electronics is a rapidly developing field of research which covers any electronic devices or circuits that can be processed using direct printing techniques. Among those printing techniques, inkjet printing is a technique of increasing interest for organic field-effect transistors (FETs) due to its fully data driven and direct patterning. In this work, the morphology of conjugated polymer/insulating polymer blends from inkjet printing and their FET properties has been investigated. The crystallinity and packing of conjugated polymer has been examined by synchrotron x-ray diffraction. The detailed information about the interface and domains of polymer blends were investigated by small angle neutron scattering. It is found that the domains and polymer interface were crucial to the FET properties. Finally, the relationship between morphology and function has been established for polymer blends FET from inkjet printing.

**M1.00031 Solvent-vapor concentration imparts selectivity on the propagation front during polymorphic transformation in molecular-semiconductor thin films**, GEOFFREY PURDUM, Dept. of Chemical and Biological Engineering, Princeton University, THOMAS GESSNER, R. THOMAS WEITZ, BASF SE, GMV 67056, Germany, YUEH-LIN LOO, Dept. of Chemical and Biological Engineering, Princeton University — Post-deposition processing allows precise control over the structural development of molecular-semiconductor thin films. In particular, solvent-vapor annealing converts thin films of a core-chlorinated naphthalene diimide from its triclinic polymorph to its monoclinic polymorph. By tuning the concentration of solvent vapor, we can simultaneously impact the morphology of the resulting monoclinic thin film. At low solvent-vapor concentrations, transformation in-plane is isotropic; we observe comparable transformation rates along the b- and c-axes, resulting in plate-like domains. At high solvent-vapor concentrations, transformation along the c-axis is instead favored, resulting in the formation of needle-like domains. Extended solvent-vapor annealing at these conditions can lead to isolated needles in the active channels of field-effect transistors; these devices exhibit electron mobilities exceeding  $1 \text{ cm}^2/\text{Vs}$ .

**M1.00032 Charge conduction in partially fluorinated discotic liquid crystals**, MITCHELL POWERS, ZHE LI, ROBERT TWIEG, BRETT ELLMAN, Kent State University — Motivated by the role of electrostatic interactions on stacking of partially fluorinated conjugated compounds, we present mobility measurements of, e.g., 1,4-difluoro-2,3,6,7,10,11-hexakis(pentaoxytriphenylene) (2F-HAT5) in discotic mesophases across a wide range of temperature and applied electric field. Charge conduction in this case is well described by a disorder driven hopping model. 2F-HAT5 exhibits a mobility of approximately  $2 \times 10^{-3} \text{ cm}^2/\text{Vs}$ , similar to the parent triphenylene, and has a weak temperature dependence throughout its discotic mesophase, which extends below room temperature. We compare results on this and related compounds to various theoretical models.

**M1.00033 Gated Seebeck Using Polymerized Ionic Liquid Gate Dielectrics**, ELAYNE THOMAS, BHOOSHAN POPPER, HAIYU FANG, MICHAEL CHABINYC, RACHEL SEGALMAN, Univ of California - Santa Barbara — Thermoelectric materials have the ability to convert a temperature gradient into usable electrical power via the Seebeck effect. This phenomenon is directly related to the material's Seebeck coefficient and electrical conductivity, which are in turn linked to its electron (or hole) mobility and carrier concentration. Organic semiconductors show promise for thermoelectric applications due to their flexibility and low-temperature manufacturing techniques; however, the role of ionized dopants on charge transport in these materials remains poorly understood. In this work, we use polymerized ionic liquids (PILs) as a gate dielectric in organic field-effect transistors to directly control the concentration of charges in the conducting channel. We report a method to tune the carrier concentration in the transistor channel via electrostatic gate modulation. We observe carrier concentration levels that are comparable to traditional doping methods with the added ability to precisely tune the concentration of charges induced. With this process, we aim to gather new information on the effect of ions on the performance of organic semiconductors in hopes of better understanding charge transport in conducting polymers on a molecular level.

**M1.00034 Electrospun Composite Nanofibers of Semiconductive Polymers for Coaxial PN Junctions**, WILLIAM SERRANO, SYLVIA THOMAS, University of South Florida at Tampa — The objective of this research is to investigate the conditions under P3HT and Activink, semiconducting polymers, form 1 dimension (1D) coaxial p-n junctions and to characterize their behavior in the presence of UV radiation and organic gases. For the first time, fabrication and characterization of semiconductor polymeric single fiber coaxial arrangements will be studied. Electrospinning, a low cost, fast and reliable method, with a coaxial syringe arrangement will be used to fabricate these fibers. With the formation of fiber coaxial arrangements, there will be investigations of dimensionality crossovers e.g., from one-dimensional (1D) to two-dimensional (2D). Coaxial core/shell fibers have been realized as seen in a recent publication on an electrospun nanofiber p-n heterojunction of oxides ( $\text{BiFeO}_3$  and  $\text{TiO}_2$ , respectively) using the electrospinning technique with hydrothermal method. In regards to organic semiconducting coaxial p-n junction nanofibers, no reported studies have been conducted, making this study fundamental and essential for organic semiconducting nano devices for flexible electronics and multi-dimensional integrated circuits.

**M1.00035 A novel Graphene Oxide film: Synthesis and Dielectric properties**, BETUL CANIMKURBEY, SAIT EREN SAN, Gebze Technical University, MUHAMMAD YASIN, National University of Science and Technology, MUHAMMET ERKAN KSE, Gebze Technical University — In this work, we used Hummers method to synthesize Graphene Oxide (GO) and its parallel plate impedance spectroscopic technique to investigate dielectric properties. Graphene Oxide films were coated using drop casting method on ITO substrate. To analyze film morphology, atomic force microscopy was used. Dielectrics measurements of the samples were performed using impedance analyzer (HP-4194) in frequency range (100 Hz to 10MHz) at different temperatures. It was observed that the films' AC conductivity  $\sigma_{ac}$  varied with angular frequency,  $\omega$  as  $\omega^S$ , with  $S < 1$ . The electrical properties of GO showed changes depending on both frequency and temperature. We observed GO film contains direct current (DC) and Correlated Barrier Hopping (CBH) conductivity mechanisms at low and high frequency ranges, respectively. Using solution processed Graphene Oxide will provide potential for organic electronic applications through its photon absorption and transmittance capability in the visible range and excellent electrical parameters.

**M1.00036 Synthesis and Characterization of Plant based Polythiophene Copolymers for Light Harvesting Applications**<sup>1</sup>, UDARI KODITHUWAKKU, PRASHANTHA MALAVI ARACHCHI, DILRU RATNAWEERA, University of Sri Jayewardenepura, Sri Lanka — Polythiophenes became more attractive in diverse applications due to some of their inherent properties including thermal and environmental stability as well as optical and electronic conductive properties. Commonly thiophene monomers are obtained from byproducts of crude oils. The current study discuss for the first time the synthesis and characterization of light harvesting polythiophenes copolymers from thiophene derivatives extracted from *Tagetes* species. There were mainly two thiophenes derivatives, 5-(3-buten-1-ynyl)-2, 2-bithienyl and 2, 2', 5, 2'-terthienyl (terthiophene), in the roots of the plant. Chemical oxidative radical polymerization was followed during the synthesis of copolymers with various block compositions of plant based terthiophenes and 3-hexyl terthiophenes. Structural characterization of the synthetic products was done using FTIR, NMR, Uv-vis, XRD and DSC techniques. Polythiophene homopolymers obtained from plant based terthiophenes have limited processability of solar cells due to poor solubility in common organic solvents. A significant solubility improvement was observed with copolymers having minor contributions of 3-hexylthiophenes.

<sup>1</sup>Research Grants, University of Sri Jayewardenepura, Sri Lanka

**M1.00037 Synthesis and Photoelectrochemistry Characterization of Polymer based on 4,7-Di(thiophen-2-yl)-benzo[c][1,2,5]thiadiazole, (DTBT).** , LUZ MARIA LAZO JIMENEZ<sup>1</sup>, Instituto de Ciencias Nucleares, UNAM., BERNARDO ANTONIO FRONTANA-URIBE<sup>2</sup>, Centro Conjunto de Investigación en Química Sustentable, CCIQS-UNAM-UAEM. — Poly[4,7-di-(thiophen-2-yl)-benzo[c]-[1,2,5] thiadiazole], P(DTBT), is used in polymer:PCMB blends as active layer on organic photovoltaic devices, (OPV); DTBT-based copolymers show well-reversible oxidation and reduction electrochemical processes. These processes indicate their high electrochemical stability suitable for n- and p-doping. This is a typical feature benzothiadiazole containing molecules. In the present study the synthesis conditions of the monomer, 4,7-di-(thiophen-2-yl)-benzo[c]-[1,2,5]-thiadiazole based on Stille coupling reactions has been investigated and its respectively polymer P(DTBT) was prepared by repetitive potential-sweep anodic oxidation of the corresponding monomer DTBT onto Pt disk or indium tin oxide (ITO) electrodes. Electrochemical cyclic voltammetry (CV) was performed to determine the HOMO and the LUMO energy levels of the conjugated DTBT and P(DTBT), both exhibit amphoteric redox properties, n- and p- doping process. The optical gap estimated from electrochemical measurements of the polymer P(DTBT) was found to be 1.77 eV, which is close to the reported band gap (1.1-1.2eV) determined by optical absorption technique . Photoelectrochemical characterization of P(DTBT) was realized from UV-Vis-NIR spectra recorded at different applied potentials. These result are correlated with the charge-transfer phenomena in the polymers applied as active layer on OPV's.

<sup>1</sup>Av. Universidad 3000. Coyoacán.C.P. 04510. México. D.F. MEXICO

<sup>2</sup>Km 14.4 Carretera Toluca-Atlaquilco. C.P. 50200, Toluca-, Estado de México. MEXICO

**M1.00038 Electrospinning Nanofiber Based Organic Solar Cell**<sup>1</sup> , ZHENHUA YANG, YING LIU, STONY BROOK UNIVERSITY, MARIA MOFFA, CNR-Istituto Nanoscienze, CHANG-YONG NAM, Brookhaven National lab, DARIO PISIGNANO, CNR-Istituto Nanoscienze, MIRIAM RAFAILOVICH, STONY BROOK UNIVERSITY — Bulk heterojunction (BHJ) polymer solar cells are an area of intense interest due to their potential to result in printable, inexpensive solar cells which can be processed onto flexible substrates. The active layer is typically spin coated from the solution of polythiophene derivatives (donor) and fullerenes (acceptor) and interconnected domains are formed because of phase separation. However, the power conversion efficiency (PCE) of BHJ solar cell is restricted by the presence of unfavorable morphological features, including dead ends or isolated domains. Here we MEH-PPV:PVP:PCBM electrospun nanofiber into BHJ solar cell for the active layer morphology optimization. Larger interfacial area between donor and acceptor is obtained with electrospinning method and the high aspect ratio of the MEH-PPV:PVP:PCBM nanofibers allow them to easily form a continuous pathway. The surface morphology is investigated with atomic force microscopy (AFM) and scanning electron microscopy (SEM). Electrospun nanofibers are discussed as a favorable structure for application in bulk-heterojunction organic solar cells.

<sup>1</sup>Electrospinning Nanofiber Based Bulk Heterojunction Organic Solar Cell

**M1.00039 Asymmetric Zinc Phthalocyanines as Dye-Sensitized Solar Cells.** , GULENAY TUNC, YUNUS YAVUZ, AYSEGUL GUREK, BETUL CANIMKURBEY, ARIF KOSEMIN, SAIT EREN SAN, VEFA AHSEN, Gebze Technical University — Dye-sensitized solar cells (DSSCs) have received increasing attention due to their high incident to photon efficiency, easy fabrication and low production cost . Tremendous research efforts have been devoted to the development of new and efficient sensitizers suitable for practical use. In TiO<sub>2</sub>-based DSSCs, efficiencies of up to 11.4% under simulated sunlight have been obtained with ruthenium polypyridyl complexes. However, the main drawback of ruthenium complexes is the lack of absorption in the red region of the visible light and the high cost. For this reason, dyes with large and stable p-conjugated systems such as porphyrins and phthalocyanines are important classes of potential sensitizers for highly efficient DSSCs. Phthalocyanines (Pcs) have been widely used as sensitizers because of their improved light-harvesting properties in the far red- and near-IR spectral regions and their extraordinary robustness [1]. In this work, a series of asymmetric Zn(II) Pcs bearing a carboxylic acid group and six hexylthia groups either at the peripheral or non-peripheral positions have been designed and synthesized to investigate the influence of the COOH group and the positions of hexylthia groups on the dye-sensitized solar cell (DSSC) performance.

**M1.00040 Highly conductive polymer electrolyte membranes modified with polyethylene glycol-bis-carbamate**<sup>1</sup> , GUOPENG FU, Univ of Akron, JANEL DEMPSEY, John Carroll University, THEIN KYU, Univ of Akron — By virtue of its non-flammability and chemical stability, polyethylene glycol (PEG) networks have shown potential application in all solid-state polymer electrolyte membranes (PEM). However, room temperature ionic conductivity of these PEG based PEMs is inherently low. Plasticization of these PEMs is needed to improve the ionic conductivity. It was demonstrated by this group that small-molecule plasticizers such as succinonitrile, ethylene carbonate, or urea-carbamate can boost ionic conductivity of solid-state polymer electrolyte membranes. Polyethylene glycol bis-carbamate (PEGBC) was synthesized via condensation reaction of polyethylene glycol diamine and ethylene carbonate. The PEGBC modified PEM has shown higher ionic conductivity relative to the unmodified PEM. Moreover, PEGBC modified PEM has a better thermal stability relative to ethylene carbonate based liquid electrolyte with enhanced ionic conductivity.

<sup>1</sup>Supported by NSF-DMR 1161070, 1502543 and REU 1359321

**M1.00041 Neutron Vibrational Spectroscopy and modeling of polymer/dopant interactions** , ADAM MOULE, THOMAS HARRELSON, University of California, Davis, YONGQIANG CHENG, ANIBAL RAMIREZ-CUESTA, Oak Ridge National Lab, ROLAND FALLER, University of California, Davis, DAVID HUANG, University of Adelaide, Australia — Neutron vibrational spectroscopy (VISION and ORNL) is a powerful technique to determine the configurations of organic species in amorphous samples. We apply this technique to samples of the semiconducting polymer regio-regular P3HT to determine the molecular configurations outside of the crystalline domains, which have never been investigated. Application of density functional theory modeling using crystal field theory and for the single molecule approach yield a variety of configurations of the polymer backbone and side chains. These results demonstrate that only 1% of the volume corresponds to the assumed crystal structure solved using x-ray diffraction. In addition we investigate the configurations of P3HT doped with the molecular dopant F4TCNQ and determine that the charging of the polymer backbone leads to increased side chain stiffness. These results have significant implications for design of organic electronic devices based on thiophenes.

**M1.00042 Single- and Multilayered Nanostructures via Laser-Induced Block Copolymer Self-Assembly**<sup>1</sup> , PAWEŁ MAJEWSKI, KEVIN YAGER, ATIKUR RAHMAN, CHARLES BLACK, Brookhaven Natl Lab — We present a novel method of accelerated self-assembly of block copolymer thin films utilizing laser light, called Laser Zone Annealing (LZA). In our approach, steep temperature transients are induced in block copolymer films by rastering narrowly focused laser line over the light-absorbing substrate. Extremely steep temperature gradients accelerate the process of self-assembly by several orders-of-magnitude compared to conventional oven annealing, and, when coupled to photo-thermal shearing, lead to global alignment of block copolymer domains assessed by GISXAS diffraction studies and real-space SEM imaging. We demonstrate monolithic alignment of various block-copolymer thin films including PS-b-PMMA, PS-b-PEO, PS-b-P2VP, PS-b-PI and observe different responsiveness to the shearing rate depending on the characteristic relaxation timescale of the particular material. Subsequently, we use the aligned polymeric films as templates for synthesis of single- and multi-layered arrays of inorganic, metallic or semiconducting nanowires and nanomeshes and investigate their anisotropic electro-optical properties.

<sup>1</sup>Research carried out in part at the Center for Functional Nanomaterials, Brookhaven National Laboratory, which is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886.

**M1.00043 Temperature dependent structural, elastic, and polar properties of ferroelectric polyvinylidene fluoride (PVDF) and trifluoroethylene (TrFE) copolymers**, FU-CHANG SUN, AVINASH DON-GARE, ALEXANDRU ASANDEI, University of Connecticut, PAMIR ALPAY, University of Connecticut, SERGE NAKHMANSON, University of Connecticut, UNIVERSITY OF CONNECTICUT TEAM — We use molecular dynamics to calculate the structural, elastic, and polar properties of crystalline ferroelectric  $\beta$ -poly(vinylidene fluoride), PVDF ( $-\text{CH}_2\text{-CF}_2-$ )<sub>n</sub> with randomized trifluoroethylene TrFE ( $-\text{CHF-CF}_2-$ )<sub>n</sub> as a function of TrFE content (0-50%) in the temperature range of 0-400 K. There is a very good agreement between the experimentally obtained and the computed values of the lattice parameters, thermal expansion coefficients, elastic constants, polarization, and pyroelectric coefficients. A continuous decrease in Young's modulus with increasing TrFE content was observed and attributed to the increased intramolecular and intermolecular repulsive interactions between fluorine atoms. The computed polarization displayed a similar trend, with the room temperature spontaneous polarization decreasing by 44% from 13.8  $\mu\text{C}/\text{cm}^2$  (pure PVDF) to 7.7  $\mu\text{C}/\text{cm}^2$  [50/50 poly(VDF-co-TrFE)]. Our results show that molecular dynamics can be used as a practical tool to predict the mechanical and polarization-related behavior of ferroelectric poly(VDF-co-TrFE). Such an atomistic model can thus serve as a guide for practical applications of this important multifunctional polymer.

**M1.00044 Understanding Nonlinear Dielectric Properties in a Biaxially Oriented Poly(vinylidene fluoride) Film at Both Low and High Electric Fields<sup>1</sup>**, YUE LI, College of Polymer Science and Engineering, Sichuan University, LEI ZHU, Department of Macromolecular Science and Engineering, Case Western Reserve University, CASE WESTERN RESERVE UNIVERSITY TEAM, SICHUAN UNIVERSITY TEAM — Understanding nonlinear dielectric behavior in polar polymers is crucial to their potential application as next generation high energy density and low loss dielectrics. In this work, we studied nonlinear dielectric properties of a biaxially oriented poly(vinylidene fluoride) (BOPVDF) film under both low and high electric fields. It was observed that the low-field dielectric nonlinearity for the BOPVDF disappeared above 10 Hz at room temperature, suggesting that the low-field dielectric nonlinearity originated from ionic migration of impurity ions rather than dipolar relaxation of the amorphous segments. Above the coercive field (EC  $\sim 70$  MV/m), bipolar electric displacement-electric field (D-E) loop tests were used to extract the nonlinear behavior for pure PVDF crystals, which had a clear origin of ferroelectric switching of polar crystalline dipoles and domains and nonpolar-to-polar ( $\alpha \rightarrow \delta \rightarrow \beta$ ) phase transformations. Using HVBDS, it was observed that the ferroelectric switching of polar crystalline dipoles and domains in BOPVDF above the EC always took place between 20 and 500 Hz, regardless of a broad range of temperature from -30 to 100 C. This behavior was drastically different from the amorphous PVDF dipoles, which had a strong dependence on frequency over orders of magnitude.

<sup>1</sup>This work is supported by NSF(DMR-1402733)

**M1.00045 Correlating Thin-Film Radical Density with Charge Transport in Open-Shell Conducting Macromolecules**, MARTHA HAY, ELIZABETH JERGENS, BRYAN BOUDOURIS, Purdue University — Within the class of radical polymers, stable open-shell species serve as the medium for charge transport by undergoing oxidation-reduction (redox) reactions. The kinetics of these reactions are rapid enough that they are not considered rate-limiting in the electronic interactions of these materials. Rather, the proximity of these radical sites is paramount as a synthetic handle. Unfortunately, controlling the density of radicals has proven challenging in radical polymer systems. Often radical functionality is imparted to a polymer, rather than polymerizing a radical-containing monomer unit. This can prove troublesome as longer reaction times, in the interest of higher radical functionality, can lead to the elimination of radicals. Thus, the consequential altering of the radical electronic interactions is not well understood. We have synthesized a series of polynorbornene-based radical monomers at controlled radical loadings such that the radical density was preserved from monomer to polymer synthesis. As such, we attribute any change in the macroscopic transport properties to a change in the spacing between radical sites. These results elucidate the role of radical site distribution on the electronic performance of nitroxide-based radical polymers.

**M1.00046 Polyvinylidene fluoride molecules in nanofibers, imaged at atomic scale by aberration corrected electron microscopy<sup>1</sup>**, DARRELL RENEKER, JOSEPH GORSE, DINESH LOLLA, The University of Akron, CHRISTIAN KISIELOWSKI, Lawrence Berkeley National Laboratory, JIAYUAN MIAO, PHILIP TAYLOR, Case Western Reserve University, GEORGE CHASE, The University of Akron — Atomic scale features of polyvinylidene fluoride molecules (PVDF) were observed. Electron micrographs of thin, self-supporting PVDF nanofibers showed conformations and relative locations of atoms in segments of polymer molecules. Rows of CF<sub>2</sub> atomic groups, at 0.25 nm intervals, marked the paths of segments of the PVDF molecules. The fact that an electron microscope image of a segment of a PVDF molecule depended upon the particular azimuthal direction, along which the segment was viewed, enabled observation of twist around the molecular axis. The 0.2 nm side-by-side distance between the two fluorine atoms attached to the same carbon atom was clearly resolved. Morphological and chemical changes produced by energetic electrons, ranging from no change to fiber scission, over many orders of magnitude of electrons per unit area, provide quantitative new insights into radiation chemistry. Relative movements of segments of molecules were observed. Synergism between high resolution electron micrographs and images created by molecular dynamic modeling was demonstrated. This paper is at the threshold of growing usefulness of electron microscopy to the science and engineering of polymer and other molecules.

<sup>1</sup>Support from Coalescence Filtration Nanofiber Consortium and from the Office of Basic Energy Sciences Contract No. DE-AC02-05CH11231

**M1.00047 Design of Free-Standing Microstructured Conducting Polymer Films for Enhanced Particle Removal from Non-uniform Surfaces**, JENNIFER LASTER, NICHOLAS DEOM, BRYAN BOUDOURIS, STEPHEN BEAUDOIN, Purdue University — Particle removal from surfaces is important for a wide range of industrial applications (e.g., microelectronics fabrication). One of the main forces of particle adhesion to a surface is the van der Waals attraction force, which will be the focus of this effort. The surface features of interacting bodies can play a controlling role in the adhesion of particles by increasing or decreasing the amount of mass within the range of strong van der Waals forces. In order to control these interactions, specific geometries can be designed in order to manipulate the micro- and nanostructure of a material, which can conform to the features of a corresponding substrate increasing the overall contact area between the two surfaces. In this work, microstructured films of the conducting polymer polypyrrole (PPy) were synthesized through template-assisted electropolymerization techniques. The removal of fluorescently-labeled polystyrene beads from aluminum surfaces of varying roughness was measured and compared for microstructured and flat PPy films. The microstructured films were found to have an overall increase in the amount of particles removed from the aluminum surfaces; this demonstrates the ability to manipulate particle adhesion through advanced nanostructured polymer templating.

**M1.00048 Out-of-plane Block Copolymer Microdomains in High Aspect-Ratio Templates**, KARIM GADELRAH, WUBIN BAI, ALFREDO ALEXANDER-KATZ, CAROLINE ROSS, Massachusetts Inst of Tech-MIT — Directed self-assembly DSA of block copolymers BCP proved to be a power approach for nanoscale fabrication. In addition, BCP with highly incompatible blocks (high Flory-Huggins interaction parameter ( $\chi$ )) offer improvement in resolution of the BCP patterns. Unfortunately, high- $\chi$  BCPs usually exhibit large differences in surface affinity between the two blocks, forming a surface layer of the lower surface energy block and favoring in-plane orientation of lamellae or cylindrical microdomains. Here, we explore the conditions under which a high  $\chi$  BCP creates an out-of-plane lamellar structure using high aspect ratio trenches with preferential walls. We employ self-consistent field theory SCFT and single mode expansion of Ginzburg-Landau free energy expression in the weak segregation limit to analytically construct a phase diagram of the in- and out-of-plane lamellae as a function of aspect ratio and surface affinity. It is found that achieving an out of plane lamellar structure necessitates a coupling between aspect ratio and surface functionality. In particular, strong side wall attraction results in out-of-plane lamellae when the trench aspect ratio is greater than unity. The results are validated for a polystyrene-block-polydimethylsiloxane (PS-b-PDMS) system within trenches made using interference lithography.

**M1.00049 Vertically Aligned Nanoplate Particles Directed by Block Copolymer Domains for Anisotropic Properties**, NADIA KROOK, University of Pennsylvania, JEFFREY METH, DuPont, CHRISTOPHER MURRAY, ROBERT RIG-  
GLEMAN, RUSSELL COMPOSTO, University of Pennsylvania — During common processing methods, anisotropic fillers in polymer nanocomposites align in the direction of flow, parallel to the surfaces, thus enhancing properties in the plane of the substrate. This research aims to create thin film nanocomposites with perpendicularly aligned anisotropic particles to improve properties in the out-of-plane direction. The demonstrated work explores vertical orientation of rare-earth fluoride nanoplates in lamellar-forming poly(styrene-*b*-methyl methacrylate) to establish a platform that controls the alignment of any planar particle. Currently, gadolinium fluoride (GdF<sub>3</sub>) rhombus nanoplates with the longest and shortest diagonal dimensions of ~30 nm and ~25 nm, respectively, have been specially synthesized with the potential to intercalate the block copolymer (BCP) domains. By employing a ternary brush blend layer to neutralize silicon substrates to both BCP domains, vertical lamellae orientation has been enabled with an optimum film thickness of ~110 nm. The GdF<sub>3</sub> surfaces are chemically modified to drive the plates to a specific BCP domain. After surface modification, the dispersion of GdF<sub>3</sub> in homopolymer will first be shown followed by morphology results from integrating GdF<sub>3</sub> into the BCP using scanning and transmission electron microscopy.

**M1.00050 The role of ultra-fast solvent evaporation on the directed self-assembly of block polymer thin films**, CHLOE DRAPES, G. NELSON, M. GRANT, J. WONG, A. BARUTH, Creighton University — The directed self-assembly of nano-structures in block polymer thin films *via* solvent vapor annealing is complicated by several factors, including evaporation rate. Solvent vapor annealing exposes a disordered film to solvent(s) in the vapor phase, increasing mobility and tuning surface energy, with the intention of producing an ordered structure. Recent theoretical predictions reveal the solvent evaporation affects the resultant nano-structuring. In a competition between phase separation and kinetic trapping during drying, faster solvent removal can enhance the propagation of a given morphology into the bulk of the thin film down to the substrate. Recent construction of a purpose-built, computer controlled solvent vapor annealing chamber provides control over forced solvent evaporation down to 15 ms. This is accomplished using pneumatically actuated nitrogen flow into and out of the chamber. Furthermore, *in situ* spectral reflectance, with 10 ms temporal resolution, monitors the swelling and evaporation. Presently, cylinder-forming polystyrene-*block*-polylactide thin films were swollen with 40% (by volume) tetrahydrofuran, followed by immediate evaporation under a variety of designed conditions. This includes various evaporation times, ranging from 15 ms to several seconds, and four unique rate trajectories, including linear, exponential, and combinations. Atomic force microscopy reveals specific surface, free and substrate, morphologies of the resultant films, dependent on specific evaporation conditions. Funded by the Clare Boothe Luce Foundation and Nebraska EPSCoR.

**M1.00051 Towards ultra-fast solvent evaporation, the development of a computer controlled solvent vapor annealing chamber**, GUNNAR NELSON, J. WONG, C. DRAPES, M. GRANT, A. BARUTH, Creighton Univ, Omaha, NE — Despite the promise of cheap and fast nanoscale ordering of block polymer thin films *via* solvent vapor annealing, a standardized, scalable production scheme remains elusive. Solvent vapor annealing exposes a nano-thin film to the vapors of one or more solvents with the goal of forming a swollen and mobile state to direct the self-assembly process by tuning surface energies and mediating unfavorable chain interactions. We have shown that optimized annealing conditions, where kinetic and thermal properties for crystal growth are extremely fast (<1s), exist at solvent concentrations just below the order-disorder transition of the film. However, when investigating the propagation of a given morphology into the bulk of a film during drying, the role of solvent evaporation comes under great scrutiny. During this process, the film undergoes a competition between two fronts; phase separation and kinetic trapping. Recent results in both theory and experiment point toward this critical element in controlling the resultant morphologies; however, no current method includes a controllable solvent evaporation rate at ultra-fast time scales. We report on a computer-controlled, pneumatically actuated chamber that provides control over solvent evaporation down to 15 ms. Furthermore, *in situ* spectral reflectance monitors solvent concentration with 10 ms temporal resolution and reveals several possible evaporation trajectories, ranging from linear to exponential to logarithmic. Funded by Dr. Randolph Ferlic Summer Research Scholarship and NASA Nebraska Space Grant.

**M1.00052 Directed Self-Assembly of Block Copolymers in Thin Films on Polymer Nano-Stripes**, DONG-EUN LEE, HO-JONG KANG, DONG HYUN LEE, Dankook University, NANO FUNCTIONAL MATERIALS LAB. TEAM — In this study, we report directed self-assembly (DSA) of block copolymers in thin films on nano-stripes of polymers. Unique nano-stripes of poly(tetrafluoro ethylene) (PTFE) having ~20 nm of amplitude and ~200 nm of pitch were simply generated by physically rubbing a PTFE bar on various substrates like Si wafers, glass, and polyimide due to its low friction coefficient and high wear rate. The resulting nano-stripes were extremely oriented along the rubbing direction. Then, various asymmetric polystyrene-*block*-poly(2-vinylpyridine) copolymers (PS-*b*-P2VP) were directly self-assembled on the nano-stripes of PTFE by solvent-annealing in vapor of tetrahydrofuran (THF). As a result, PS-*b*-P2VP exhibited extremely ordered P2VP cylinders oriented normal to the surface in large area on the underlying nano-stripes of PTFE. In addition, as utilizing the BCPs as templates, hexagonal arrays of metal nanoparticles were generated in large area for further application. BCP thin films and arrays of metal nanoparticles were characterized by atomic force microscopy (AFM) and scanning electron microscopy (SEM).

**M1.00053 Perpendicular Orientation of Nanodomains on Versatile Substrates through Self-Neutralization Induced by Star-Shaped Block Copolymers**, MOOSEONG KIM, SANGSHIN JANG, KYU SEONG LEE, HONG CHUL MOON, JONGHEON KWAk, JICHEOL PARK, GUMHYE JEON, JIN KON KIM, POSTECH — A novel self-neutralization concept is introduced by designing molecular architecture of a block copolymer. Star-shaped 18 arm poly(methyl methacrylate)-*block*-polystyrene copolymers ((PMMA-*b*-PS)<sub>18</sub>) exhibiting lamellar and PMMA cylindrical nanodomains are synthesized. When a thin film of (PMMA-*b*-PS)<sub>18</sub> is spin-coated on a substrate, vertically aligned lamellar and cylindrical nanodomains are obtained without any pre- or post-treatment, although thermal annealing for a short time (less than 30 min) is required to improve the spatial array of vertically aligned nanodomains. This result is attributed to the star-shaped molecular architecture that overcomes the difference in the surface affinity between PS and PMMA chains. Moreover, vertical orientations are observed on versatile substrates, for instance, semiconductor (Si, SiO<sub>x</sub>), metal (Au), PS or PMMA-brushed substrate, and a flexible polymer sheet of polyethylene naphthalate.

**M1.00054 The morphology of A2B miktoarm polymer in thin film**, HYEYOUNG KIM, Univ of Mass - Amherst, BEOM-GOO KANG, University of Tennessee, ZHIWEI SUN, JAEWON CHOI, THOMAS RUSSELL, Univ of Mass - Amherst — The morphologies of A2B mikto-arm polymer consisted of poly(2-vinyl pyridine) and polystyrene ((P2VP)2PS) in thin film were examined. Solvent vapor annealing produces films with lamellae perpendicular to the substrate within a very short time. The change in the morphology for different periods of time, corresponding to different swelling ratios was observed by grazing incidence small angle x-ray scattering and scanning force microscopy. This morphology showed the smaller height difference between PS and P2VP microdomains, when compared to the corresponding diblock copolymer. We also observed the long-range ordering formed on the saw-tooth pattern. Thermal annealing, on the other hand, resulted in the lamellae being oriented parallel to the substrate, where unusual behavior was depending on the film thickness and surface energy of substrate.

**M1.00055 Simple, generalizable route to highly aligned block copolymer thin films<sup>1</sup>**, ZHE QIANG, KEVIN CAVICCHI, BRYAN VOGT, University of Akron, UNIVERSITY OF AKRON TEAM — Macroscopic alignment of block copolymer domains in thin films is desired for many applications, such as cell responsive surfaces or optical polarizers. Alignment generally requires specialized tools that apply external fields, shear force gradient, or produce topological patterned substrates. This requirement limits the broad academic application of aligned BCPs. Here, we describe a simple modification of commonly utilized solvent vapor annealing (SVA) process for macroscopic alignment of BCPs. Adhering a flat, crosslinked elastomer pad to the BCP film leads to differential swelling between the elastomer pad and BCP to produce a shear force that aligns the ordered BCP domains. The role of elastomer properties, solvent quality, drying rate and degree of segregation of the block copolymer will be discussed to provide generalized rules for alignment with this technique. Cylindrical nanostructures formed in polystyrene-block-polydimethylsiloxane can be transformed into arrays of silica lines and increasing the thickness from a monolayer to bilayer can effectively halve the spacing of the lines. These results illustrate a generalized method for BCP alignment and a potential route for the generation of complex hierarchical assembled structures.

<sup>1</sup>A generalized method for block copolymer thin film alignment: solvent vapor annealing with shear

**M1.00056 Sulfation effect on levan polysaccharide chains structure with molecular dynamics simulations<sup>1</sup>**, BINNAZ COSKUNKAN, Yeditepe University, DENIZ TURGUT, DENIZ RENDE, Rensselaer Polytechnic Institute, SEYDA MALTA, Yeditepe University, NIHAT BAYSAL, RAHMI OZISIK, Rensselaer Polytechnic Institute, EBRU TOKSOY-ONER, Marmara University — Diversity in conformations and structural heterogeneity make polysaccharides the most challenging biopolymer type for experimental and theoretical characterization studies. Levan is a biopolymer chain that consists of fructose rings with  $\beta(2-6)$  linkages. It is a glycan that has great potential as a functional biopolymer in foods, feeds, cosmetics, pharmaceutical and chemical industries. Sulfated polysaccharides are group of macromolecules with sulfated groups in their hydroxyl parts with a range of important biological properties. Sulfate groups and their positions have a major effect on anticoagulant activity. It is reported that sulfate modified levan has anticoagulant activity such as heparin. In the current study, the effect of sulfation on the structure and dynamics of unmodified and sulfate modified levan are investigated via fully atomistic Molecular Dynamics simulations in aqueous media and varying salt concentrations at 310 K.

<sup>1</sup>This material is based upon work supported by the National Science Foundation under Grant No. CMMI-1538730.

**M1.00057 The Effects of pH and Temperature on the Nanostructure of Chitosan Films<sup>1</sup>**, RAMONA LUNA, AHMED TOUHAMI, University of Texas Rio Grande Valley — Developing a matrix that can mimic tissue-like environment for cell cultures and molecular studies can help reduce the loss of some cell functions that occur when investigations are performed in vitro. Of particular interest is chitosan (CS): abundant and renewable biopolymer that is also biodegradable and non-toxic. The present study focuses on synthesizing CS films under various conditions and for multiple applications. We are using several techniques to characterize the physicochemical properties of the synthesized films. The contact angle technique is used to determine the hydrophobicity, hydrophilicity, and the surface free energy. The atomic force microscopy is used to determine the nanostructure, and nanomechanical properties. Here we specifically investigated the effect of the pH and the temperature on the nanostructure of the CS films. AFM images showed remarkable changes in the surface nanostructures that increase the roughness of the films when the pH of the solution increases. However, the surface free energy of these films has not shown any significant changes with the pH. By investigating the properties of these films, the needed biomaterial platform for a specific biological system can be designed and manipulated to increase its performance and lifetime.

<sup>1</sup>Supported by: NSF and MBRS RISE Program

**M1.00058 Characterization of Nanoparticle Aggregation in Biologically Relevant Fluids**, KATHLEEN MCENNIS, JOERG LAHANN, University of Michigan — Nanoparticles (NPs) are often studied as drug delivery vehicles, but little is known about their behavior in blood once injected into animal models. If the NPs aggregate in blood, they will be shunted to the liver or spleen instead of reaching the intended target. The use of animals for these experiments is costly and raises ethical questions. Typically dynamic light scattering (DLS) is used to analyze aggregation behavior, but DLS cannot be used because the components of blood also scatter light. As an alternative, a method of analyzing NPs in biologically relevant fluids such as blood plasma has been developed using nanoparticle tracking analysis (NTA) with fluorescent filters. In this work, NTA was used to analyze the aggregation behavior of fluorescent polystyrene NPs with different surface modifications in blood plasma. It was expected that different surface chemistries on the particles will change the aggregation behavior. The effect of the surface modifications was investigated by quantifying the percentage of NPs in aggregates after addition to blood plasma. The use of this characterization method will allow for better understanding of particle behavior in the body, and potential problems, specifically aggregation, can be addressed before investing in in vivo studies.

**M1.00059 Ring Structure of Center of Spacetime, DNA, and Extraterrestrial Being**, DAYONG CAO, AEEA — There is a balance of the flat universe between the stellar matter and the dark massenergy (include dark matter and dark energy) which make of dark hole which has the center of the spacetime. The Einstein's equation has the other formula of the structure of the center of spacetime. There are also balance system between the solar system and its companion dark hole, and between the Milky Way galaxy and its center of the huge dark hole. The model of stellar matter can explain of the structure of molecule by electromagnetic interaction (of the spacetime effect). The ring structure both the nucleic acid and protein is like the structure of the center of the spacetime. It produced by an interaction of double helix between dark massenergy and stellar matter when the companion dark hole of sun seasonal impacted near solar system, and took dark comets and dark massenergy on the earth, and made extinctions while they were producing new DNA of lives, broke the old one to the petroleum, natural gas, and coal. DNA of extraterrestrial being who live on system of the companion dark hole maybe have special ring structure with the double helix. A new big extinction is coming for human being and extraterrestrial being. <http://meetings.aps.org/link/BAPS.2015.APR.H14.8> <http://meetings.aps.org/link/BAPS.2012.APR.K1.79>

**M1.00060 Coacervate Core Micelles for the Dispersion and Stabilization of Organophosphate Hydrolase in Organic Solvents.**, CAROLYN MILLS, ALLIE OBERMEYER, XUEHUI DONG, BRADLEY D. OLSEN, Massachusetts Institute of Technology — Bulk organophosphate (OP) nerve agents are difficult to decontaminate on site and dangerous to transport. The organophosphate hydrolase (OPH) enzyme is an efficient catalyst for hydrolyzing, and thus decontaminating, these compounds, but suffers from poor stability in the hydrophobic bulk OP environment. Here, we exploit the complex coacervation phase separation phenomenon to form complex coacervate core micelles (C3Ms) that can protect this OPH enzyme under these conditions. Stable C3Ms form when mixing a charged-neutral block copolymer methyl-quaternized poly(4-vinylpyridine)-*block*-poly(oligo(ethylene glycol) methacrylate) (Qp4vp-*b*-POEGMA), a homopolymer poly(acrylic acid) (PAA), and OPH under a certain conditions. The C3Ms are then transferred into two organic solvents, ethanol and dimethyl methylphosphonate (DMMP), which is a good simulant for the physical properties of the OP compounds. The C3Ms retain their nanostructures in the organic solvents. The activity test of OPH indicates that the C3Ms successfully protect OPH activity in organic solvents.

**M1.00061 Fluorescence Recovery after Photobleaching in Confined Polymer Thin Films**, LAURA A. G. GRAY, CLIFFORD P. BRANGWYNNE, RODNEY D. PRIESTLEY, Princeton Univ, Dept. of Chemical and Biological Engineering — Over the past twenty years many studies have shown a reduction in the glass transition temperature ( $T_g$ ) of thin polymer films confined on the nanoscale when supported on non-attractive substrates or free-standing. The depth dependence of  $T_g$  has been measured using thin layers of fluorescently tagged polymer to localize the dye within a larger polymer film stack, revealing a decrease in local  $T_g$  tens of nanometers into the film. These results have been explained by the propagation of enhanced mobility from the free-surface into the polymer film. Fewer direct measurements of molecular mobility have been made in confined polymer systems. Here, we present the results of fluorescence recovery after photobleaching (FRAP) experiments investigating the mobility of fluorescently doped and labeled methacrylate-based polymers confined in thin film geometries. Bleaching and recovery was monitored using a laser-scanning confocal microscope that enabled us to bleach arbitrary micron-sized shapes to monitor diffusion in polymer melts.

**M1.00062 Using Atomistic Molecular Dynamics Simulations to Guide Development of Coarse-Grained Models of Polyethylene glycol (PEG), Elastic-like peptides (ELP) and Collagen-like peptides (CMP) For Biomaterial Design**, FRANCESCA STANZIONE, Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE 19716., ARTHI JAYARAMAN, Department of Chemical and Biomolecular Engineering, Department of Materials Science and Engineering, University of Delaware, Newark, DE 19716. — Molecular dynamics (MD) is a well established technique to study the structure and dynamics of biomolecular systems. While atomistic simulations maintain chemical details, they are computationally intensive, thus limiting the accessible time, the length scales and the sampling. To overcome these limitations, coarse-grained (CG) models have proven to be successful in reproducing experimentally relevant length and time scales with reasonable computational expense. CG models can be developed to be phenomenological by effectively reproducing experimental results or can be developed by mapping rigorously to structural information provided by atomistic MD simulations. The latter method is recommended for biomolecules and biomaterials since atomistic simulations capture the detailed effect of the medium on interactions that affect the structure, dynamics and functional properties of the biomolecules, and that can be programmed into the CG models. In this poster we highlight three different cases where atomistic MD simulations provide such essential information to guide CG models: Polyethylene glycol, Elastic-like peptides and Collagen-like peptides based biomaterials.

**M1.00063 The influence of ionic strength on DNA diffusion in gel networks<sup>1</sup>**, YUANXI FU, AH-YOUNG JEE, HYEONG-JU KIM, STEVE GRANICK, Institute for Basic Science — Cations are known to reduce the rigidity of the DNA molecules by screening the negative charge along the sugar phosphate backbone. This was established by optical tweezer pulling experiment of immobilized DNA strands. However, little is known regarding the influence of ions on the motion of DNA molecules as they thread through network meshes. We imaged in real time the Brownian diffusion of fluorescent labeled lambda-DNA in an agarose gel network in the presence of salt with monovalent or multivalent cations. Each movie was analyzed using home-written program to yield a trajectory of center of the mass and the accompanying history of the shape fluctuations. One preliminary finding is that ionic strength has a profound influence on the slope of the trace of mean square displacement (MSD) versus time.

<sup>1</sup>The influence of ionic strength on DNA diffusion in gel networks

**M1.00064 Active microrheology of entangled blends of DNA and Actin link polymer flexibility to induced molecular deformations and stress propagation**, ROBERT FITZPATRICK, RAE ROBERTSON-ANDERSON, University of San Diego, ANDERSON RESEARCH TEAM — Actin is a ubiquitous structural protein in the cytoskeleton that gives cells shape and rigidity, and plays important roles in mechanical processes such as cell motility and division. Actins diverse roles stem from its ability to polymerize into semiflexible filaments that are less than one persistence length ( $\sim 17$  nm) in length, and form entangled networks that display unique viscoelastic properties. We previously found that entangled actin networks propagate microscale forces over several persistence lengths ( $\sim 60$  nm) and takes minutes to relax. DNA, oppositely, has thousands of persistence lengths (50 nm) per chain, exhibits minimal force propagation, and takes only seconds to re-equilibrate. To directly determine the role of flexibility in mechanical response and force propagation of entangled networks, we use optical tweezers and fluorescence microscopy to investigate blends of actin and DNA. We use optically driven microspheres to perturb the network far from equilibrium and measure the force the network creates in response to the induced force. We simultaneously track partially labeled actin filaments during the perturbation and subsequent relaxation period. We characterize filament deformation and show explicitly how induced microscale forces propagate through the network.

**M1.00065 Deep image analysis of entangled ring-shaped DNA**, HYEONGJU KIM, AH-YOUNG JEE, STEVE GRANICK, Institute for Basic Science — Ring-shaped DNA entangled in aqueous actin networks and observed by super-resolution microscopy (STED; stimulated emission depletion) offers rich data for comparison with unresolved questions of polymer physics. Using home-written software, we calculated not only the center of mass (CoM) and CoM trajectories of hundreds of molecules, but also analyzed conformation dynamics with statistical analysis including wavelet transformation and a correlation matrix approach. The analysis reveals some surprising aspects unanticipated by classical theories.

**M1.00066 Quantifying the effects of cyclic defects on the mechanical properties of polymer gels**, RUI WANG, MINGJIANG ZHONG, KEN KAWAMOTO, JEREMIAH JOHNSON, BRADLEY OLSEN, Massachusetts Institute of Technology — Understanding the correlation between the topology and properties of polymer gels is an outstanding challenge in polymer science. Classical theories of gel elasticity assume acyclic tree-like network topology; however, all polymer gels inevitably possess cyclic defects: loops that have profound, yet previously unpredictable, effect on gel properties. Here, we develop a modified phantom network theory that describes the effects of loops on the modulus of polymer gels. We demonstrate that small loops (primary and secondary loops) have vital effect on the modulus; whereas this negative impact decreases rapidly as the loop order increases, especially for networks with higher junction functionalities. Loop effect is non-local, which can propagate to its neighborhood strands. We show that adjacent loops weaken the network cooperatively, resulting in the nonlinear decrease of the dimensionless modulus ( $G/vkT$ , where  $v$  is the total density of polymer strands) with the loop fraction. The theory is in good agreement with the experimental data without any fitting parameters.

**M1.00067 Degrafting of polymer brushes from substrates enables insight about the brush structure and facilitates surface patterning.**, ROHAN PATIL, North Carolina State Univ, SALOMON TURGMAN-COHEN, Kettering University, JIRI SROGL, North Carolina State Univ, DOUGLAS KISEROW, US Army Research Office, JAN GENZER, North Carolina State Univ — Polymers end-grafted to surfaces or interfaces, commonly referred to as polymer brushes, enable tailoring physico-chemical properties of material surfaces. Many applications of polymer brushes require information about the molecular weight (MW) and grafting density (GD) of polymer brushes. For brushes synthesized by surface initiated polymerization (SIP) determining these attributes was always a challenge. We have developed a simple method of measuring MW and GD of these systems by degrafting SIP from silica-based surfaces by using tetrabutyl ammonium fluoride (TBAF), which attacks selectively Si-O bonds and enables complete degrafting of poly(methyl methacrylate) (PMMA) brushes from silica based substrates without damaging the backbone. The rate of PMMA degrafting decreases with reaction time and depends on the concentration of TBAF, temperature, and the initial GD of the system. The molecular weight distribution of the degrafted PMMA was measured using size exclusion chromatography. The GD was calculated from known MW and dry thickness of the PMMA brush. Spatial patterns of degrafted regions on the substrate can be prepared by either localizing the TBAF to certain regions or by gradually immersing homogeneous samples into TBAF solution.

**M1.00068 Driving Organic Molecule Crystallization with Surface Reconstructions**, JESSICA BICKEL, GIANFRANCO TROVATO, Cleveland State University — This work examines how surface reconstructions can drive crystallization of organic molecules via self-assembly. Organic electronic molecules have low conductivities compared to inorganic materials, but crystallizing these polymers increases their conductivity. This project uses surface reconstructions with periodically repeating topographies to drive the crystallization process. The samples are grown by placing a drop of a dilute PEDOT solution on the clean Si(001)-(2x1) or Si(111)-(7x7) surface reconstruction and heating the surface up to both evaporate the solvent and promote diffusion of the polymer to the thermodynamically defined lowest energy position. The resulting samples are characterized by scanning tunneling microscopy (STM) with respect to their crystallinity and electronic properties. Of particular interest is whether there is a preferential location for the PEDOT molecule to adsorb and whether there are any conformational changes upon adsorption that modify the HOMO-LUMO gap. This work is being done in a new pan-style RHK-STM enclosed in a glovebox at Cleveland State University. The glovebox has O<sub>2</sub> and H<sub>2</sub>O levels of less than 1ppm. This allows for sample preparation and imaging in a controlled environment that is free from contamination.

**M1.00069 The Study of Interpenetration Length between dPS Films and PS-grafted Layers**, HOYEON LEE, SEONGJUN JO, Yonsei University, TOYOAKI HIRATA, Kyushu University, NORIFUMI L. YAMADA, J-PARC, KEIJI TANAKA, Kyushu University, DU YEOL RYU<sup>1</sup>, Yonsei University — In polymer thin film system, the type of interfacial interaction is a critical parameter to determining the thermal and physical properties of polymer films. Interestingly, the interfacial energy of grafted substrates with polymer chains is remarkably altered by simply controlling grafting density, which has been referred to as autophobicity. In this study, we investigated the interpenetrating interfaces between deuterated polystyrene (dPS) and grafted substrates with the same chemical identity. PS-grafted substrates were prepared using a grafting-to approach with hydroxyl end-functionalized polystyrene (PSOH) in a dry brush regime, where the brush thickness and grafting density were determined based on the chain length (or molecular weight,  $M_n$ ) of PSOHs. The interpenetration lengths ( $\xi$ ) at interfaces between dPS and PS-grafted layers were characterized using neutron reflectivity (NR) measurements (performed at the SOFIA beam-line at J-PARC, Japan).

<sup>1</sup>academic adviser

**M1.00070 Glass transition dynamics and charge carrier mobility in conjugated polyfluorene thin films**, HUI QIN, DAN LIU, TAO WANG, Wuhan University of Technology — Conjugated polymers are commonly used in organic optoelectronic devices, e.g. organic photovoltaics (OPVs), light-emitting diodes (LEDs) and field effect transistors (FETs). In these devices, the conjugated polymers are prepared as thin films with thicknesses in the range of tens to hundreds of nanometers, and are interfaced with different function layers made from organic or inorganic materials. We have studied the glass transition temperature ( $T_g$ ) of poly(9, 9-dioctylfluorene)-co-N-(1, 4-butylphenyl)diphenylamine (TFB) thin films supported on different substrates, as well as their SCLC charge carrier mobility in photodiodes. Both Monotonic and non-monotonic  $T_g$  deviations are observed in TFB thin films supported on Si/SiO<sub>2</sub> and PEDOT:PSS, respectively. With low to moderate thermal crosslinking, the thickness dependent  $T_g$  deviation still exists, which diminishes in TFB films with a high crosslinking degree. The vertical charge carrier mobility of TFB thin films extracted from the SCLC measurements is found increase with film thickness, a value increases from 1 to 50  $\times 10^{-6}$  cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup> in the thickness range from 15 to 180 nm. Crosslinking was found to reduce the carrier mobility in TFB thin films. The  $T_g$  deviations are also discussed using the classic layered models in the literature. Our results provide a precise guide for the fabrication and design of high performance optoelectronic devices.

**M1.00071 Bending and Fracture in Thin Polymer Films during Capillary Origami Assembly.**, TIMOTHY TWOHIG, ANDREW CROLL, North Dakota State Univ — Capillary origami uses liquid tension to bend thin films into useful shapes and structures. The ability to scale this process to the microscopic range has led to growing interest in capillary origami and many potential applications. Clearly, the creation of three dimensional structures from flat sheets depends deeply on a combination of properties: fluid tensions, film thickness, film modulus and importantly the films fracture properties. Fractures in a film are a critical component of macroscopic origami but macroscopic methods for creating these fractures are not possible at the microscopic scale. We present an experimental investigation of the interplay of capillary forces and material properties in the creation of controlled fractures in thin polymer films. Specifically, we use capillary forces to lift and bend a thin polymer film to the point of fracture using a variety of film thicknesses and material properties and attempt to model the basic underlying physics. We observe the creation of delaminations and fractures at pre-determined sites that can be tailored to specific shapes to be utilized in capillary origami.

**M1.00072 Confinement Effect on the Effective Viscosity of Plasticized Polymer Films**<sup>1</sup>, FEI CHEN, D. PENG, Boston University Physics Department, Y. OGATA, K. TANAKA, Kyushu University Department of Applied Chemistry, Z. YANG, Soochow University Department of Polymer Science and Engineering, Y. FUJII, National Institute for Materials Science (Japan), N. L. YAMADA, Neutron Science Laboratory High Energy Accelerator Research Organization (Japan), C. H. LAM, Hong Kong Polytechnic University Department of Applied Physics, OPHELIA K. C. TSUI, Boston University Physics Department — We have measured the effective viscosity of polystyrene films with a small (4 wt%) added amount of dioctyl phthalate (DOP) deposited on silica. A broad range of molecular weights,  $M_w$ , from 13.7 to 2,100 kg/mol was investigated. Our result shows that for the thin films with  $M_w < 100$  kg/mol, the addition of DOP causes the effective viscosity to decrease by a factor of ~4, independent of  $M_w$ . But for the higher  $M_w$  films, the effective viscosity of the DOP added films creeps towards that of the neat films with increasing  $M_w$ . A model assuming the effective viscosity to be dominated by enhanced surface mobility for the lower  $M_w$  films, but surface-promoted interfacial slippage for the higher  $M_w$  films is able to account for the experimental observations.

<sup>1</sup>We are grateful to the support of National Science Foundation through the project DMR-1310536.

**M1.00073 Adhesion and Wetting in Soft Polymeric Systems**<sup>1</sup>, ANDREY DOBRYNIN, ZHEN CAO, Univ of Akron, MARK STEVENS, Sandia National Laboratories — We have developed a generalized model of particle/surface interactions describing adhesion and wetting phenomena. We show that for an elastic nanoparticle with radius  $R_p$  and shear modulus  $G_p$  interacting with an elastic substrate having shear modulus  $G_s$  the crossover between adhesion and wetting-like behavior is determined by a dimensionless parameter  $\beta \propto \gamma^*(G^*R_p)^{-2/3}W^{-1/3}$ . In the limit of small values of the parameter  $\beta \ll 1$ , our model reproduces JKR model for particle adhesion on elastic substrates (adhesion regime). However, in the opposite limit,  $\beta \gg 1$ , the capillary forces play a dominant role and determine particle/substrate interactions (wetting regime). We extended our approach to describe the detachment of rigid nanoparticles from elastic surfaces. Simulation results confirm that the detachment force,  $f^*$ , depends on a dimensionless parameter  $\delta \propto \gamma_s(G_sR_p)^{-1/3}W^{-2/3}$ , which corresponds to the ratio of the surface energy of the neck and the substrate elastic energy. In the case when  $\delta \ll 1$ , the critical detachment force approaches a critical value calculated in the framework of the JKR model,  $f^* = 1.5\pi WR_p$  (JKR regime). However, in the opposite limit, the critical detachment force scales as  $f^* \propto \gamma_s^{3/2}R_p^{1/2}G_s^{-1/2}$  (necking regime). All simulation data can be described by a crossover function  $f^* \propto \gamma_s^{3/2}R_p^{1/2}G_s^{-1/2}\delta^{-1.89}$ .

<sup>1</sup>NSF DMR-1409710

**M1.00074 Novel adhesion properties of irreversibly adsorbed polymer chains<sup>1</sup>**, ZHIZHAO CHEN, MANI SEN, JUSTIN CHEUNG, DEBORAH BARKLEY, NAISHENG JIANG, WENDUO ZENG, MAYA K. ENDOH, TADANORI KOGA, Stony Brook University — The stability of thin polymer films on solids is of vital interest in traditional technologies and in new emerging nanotechnologies. We recently found that nanoscale structures of polymer chains adsorbed onto a silicon (Si) substrate (“adsorbed nanolayers”) play a crucial role in the thermal stability of the film. To understand the adhesion mechanism at the adsorbed polymer-free polymer interface, we mimicked the interface by preparing bilayers where a 200 nm-thick polymer film and an adsorbed nanolayer, both prepared on Si, were pressed together at high temperature. The bilayers were then subjected to an adhesion test by measuring the critical normal force required to separate the two films. Polystyrene was used as a model. The results are intriguing as they show an absence of adhesion between the “flattened” adsorbed chains, which lie flat on the solid, and the chemically identical free chains. On the other hand, the “loosely adsorbed” polymer chains, which are formed as a result of limited adsorption space on the solid surface, do display a degree of adhesion with the bulk polymer. We postulate that the loosely adsorbed chains act as “connectors” which promote adhesion effectively across the solid-polymer interface.

<sup>1</sup>We acknowledge the financial support from NSF Grant No. CMMI-1332499.

**M1.00075 Entropic Segregation of Short Polymers to the Surface of a Polydisperse Blend<sup>1</sup>**, PENDAR MAHMOUDI, MARK MATSEN, University of Waterloo — Surface effects become particularly important for micro-sized and even more so for nano-sized objects. Naturally, enthalpic preferences will cause certain components of a multi-component material to segregate to a surface, but in polymeric materials this can also happen as a result of purely entropic reasons. To demonstrate this, we consider the effect of a surface on a binary blend of chemically identical long and short polymers, using self-consistent field theory. Despite the absence of any enthalpic preference, the short polymers are found to segregate to the surface. We investigate how the amount of the surface excess and its decay length depends on the polymeric model, the molecular weights of the two polymers and the blend composition.

<sup>1</sup>This work was supported by NSERC of Canada.

**M1.00076 Effect of tacticity on the structure and glass transition temperature of polystyrene thin films**, YERGOU TATEK, SOLOMON NEGASH, Addis Ababa University, MESFIN TSIGE, The University of Akron — Detailed atomistic Molecular Dynamics simulations are performed to explore the effect of tacticity on the glass transition temperature as well as other pertinent structural properties of films of polystyrene (PS) chains adsorbed onto two distinct types of solid substrates. The investigated systems consist of thin films made of isotactic, syndiotactic and atactic PS chains adsorbed on graphite and hydroxylated silica surfaces. The structure of the films is investigated in terms of film density profiles and side chains and backbone orientations. Simulations results reveal a marked dependence of the film structure on substrate type while the absence of a strong correlation between structure and tacticity is observed. Moreover, it is found that the glass transition temperature is also substrate dependent and takes larger values for films adsorbed on graphite surface, irrespective of chain tacticity.

**M1.00077 Capillary wrinkling of thin bilayer polymeric sheets<sup>1</sup>**, JOOYOUNG CHANG, NARAYANAN MENON, THOMAS RUSSELL, Univ of Mass - Amherst — We have investigated capillary force induced wrinkling on a floated polymeric bilayer thin sheet. The origin of the wrinkle pattern is compressional hoop stress caused by the capillary force of a water droplet placed on the floated polymeric thin sheet afore investigated. Herein, we study the effect of the differences of surface energy arising from the hydrophobicity of Polystyrene (PS Mw: 97 K, Contact Angle: 88 °) and the hydrophilicity of Poly(methylmethacrylate) (PMMA Mw: 99K, Contact Angle: 68 °) on two sides of a bilayer film. We measure the number and the length of the wrinkles by broadly varying the range of thicknesses of top (9 nm to 550 nm) and bottom layer (25 nm to 330 nm). At the same, there is only a small contrast in mechanical properties of the two layers (PS E = 3.4 GPa, and PMMA E = 3 GPa). The number of the wrinkles is not strongly affected by the composition (PS(Top)/PMMA(Bottom) or PMMA(Top)/PS(Bottom)) and the thickness of each and overall bilayer system. However, the length of the wrinkle is governed by the contact angle of the drop on the top layer of bilayer system. We also compare this to the wrinkle pattern obtained in monolayer systems over a wide range of thickness from PS and PMMA (7 nm to 1 μm).

<sup>1</sup>W.M. Keck Foundation

**M1.00078 Role of monomer sequence and backbone structure in polypeptoid and polypeptide polymers for anti-fouling applications**, ANASTASIA PATTERSON, GEORGIOS RIZIS, UC Santa Barbara, BRANDON WENNING, Cornell University, JOHN FINLAY, Newcastle University, CHRISTOPHER OBER, Cornell University, RACHEL SEGALMAN, UC Santa Barbara — Polymeric coatings rely on a fine balance of surface properties to achieve biofouling resistance. Bioinspired polymers and oligomers provide a modular strategy for the inclusion of multiple functionalities with controlled architecture, sequence and surface properties. In this work, polypeptoid and polypeptide functionalized coatings based on PEO and PDMS block copolymers were compared with respect to surface presentation and fouling by *Ulva linza*. While polypeptoids and polypeptides are simple isomers of each other, the lack of backbone chirality and hydrogen bonding in polypeptoids leads to surprisingly different surface behavior. Specifically, the polypeptoids surface segregate much more strongly than analogous polypeptide functionalized polymers, which in turn affects the performance of the coating. Indeed, polypeptoid functionalized surfaces were significantly better both in terms of anti-fouling and fouling release than the corresponding polypeptide-bearing polymers. The role of specific monomer sequence and backbone chemistry will be further discussed in this poster.

**M1.00079 Conformation and hydration of surface grafted and free polyethylene oxide chains in solutions.<sup>1</sup>**, UDAYA DAHAL, Department Dept. of Physics and Institute of Materials Science, Univ. of Connecticut, ZILU WANG, Dept. of Physics and Institute of Materials Science, Univ. of Connecticut, ELENA DORMIDONTOVA, DDept. of Physics and Institute of Materials Science, Univ. of Connecticut — Due to the wide application of polyethylene oxide (PEO), ranging from biomedicine to fuel cells, it is one of the most studied polymers in the scientific world. In order to elucidate detailed molecular-level insights on the impact of surface grafting on PEO conformation, we performed atomistic molecular dynamics simulations of PEO chains in solution and grafted to a flat gold surface in different solvents. We examined the hydration as well as conformation of the free chain compared to the grafted polymer in pure water and mixed solvents. We find that grafted chains are stiffer and have a stronger tendency to form helical structures in isobutyric acid or mixture of isobutyric acid and water solution than the free chains in corresponding solutions. For grafted chains exposed to pure water the random coil conformation is retained at low grafting density, but becomes stretched and more dehydrated as the grafting density or temperature increases.

<sup>1</sup>This research is supported by NSF (DMR-1410928)

**M1.00080 Charge transport and structural dynamics in ultra-thin films of polymerized ionic liquids**<sup>1</sup>, MAXIMILIAN HERES, TYLER COSBY, Univ of Tennessee, Knoxville, STEFAN BERDZINSKI, VERONICA STREHMEL, Department of Chemistry and Institute for coatings and surface chemistry, Hochschule Niederrhein University of Applied Sciences, ROBERTO BENSON, JOSHUA SANGORO, Univ of Tennessee, Knoxville — Ion conduction and structural dynamics in a series of ultra-thin films of imidazolium based polymerized ionic liquids are investigated using broadband dielectric spectroscopy, atomic force microscopy, and ellipsometry. No alteration in the characteristic charge transport rate is observed between bulk sample and films as thin as 12nm. These results are discussed within the recent approaches proposed to explain the confinement effects on structural dynamics in polymers and low molecular weight ionic liquids.

<sup>1</sup>NSF DRM Polymers Program

**M1.00081 Molecular dynamics simulations and morphology analysis of TEM imaged PVDF nanofibers**<sup>1</sup>, JIAYUAN MIAO, Case Western Reserve University, DARRELL RENEKER, MESFIN TSIGE, University of Akron, PHILIP TAYLOR, Case Western Reserve University — With the goal of elucidating the structure of polyvinylidene fluoride (PVDF) nanofibers, all-atom molecular dynamics simulations were performed, and the results compared with structures observed in high resolution transmission electron microscopy (TEM) at the molecular level. Simulation shows that the stability of the  $\beta$ -phase component in a PVDF nanofiber is influenced by its thickness and processing history. When exposed to irradiation, as in a TEM observation, the structure is then further modified by the effects of chain scission. The transformation from the  $\beta$  phase into a paraelectric phase can explain the spindle formation and serpentine motion of molecular segments observed by Zhong et al. (Polymer, 54, 2013, 3745-3756) in irradiated PVDF nanofibers. From a comparison between simulated and experimental TEM images it was possible to identify numerous features that are useful in unveiling the inherent structure of PVDF nanofibers. The experimental TEM images appear to match well with those predicted by a model based on  $\alpha$ -phase PVDF, while also being consistent with an alternative model (Nanoscale 2015, DOI: 10.1039/c5nr01619c).

<sup>1</sup>Work supported by the Petroleum Research Fund of the ACS

**M1.00082 Processing and characterization of natural fiber reinforced thermoplastic composites using micro-braiding technique**, SATOSHI KOBAYASHI, Tokyo Metropolitan Univ, SHINJI OGIHARA, Tokyo University of Science — In the present study, we investigate fatigue properties of green composites. A hemp fiber yarn reinforced poly(lactic acid) composite was selected as a green composite. Unidirectional (UD) and textile (Textile) composites were fabricated using micro-braiding technique. Fatigue tests results indicated that fatigue damages in UD composites was splitting which occurred just before the final fracture, while matrix crack and debonding between matrix and fiber yarn occurred and accumulated stably in Textile composites. These results were consistent with modulus reduction and acoustic emission measurement during fatigue tests.

**M1.00083 Deformation Behavior during Processing in Carbon Fiber Reinforced Plastics**, SHINJI OGIHARA, Tokyo University of Science, SATOSHI KOBAYASHI, Tokyo Metropolitan University — In this study, we manufacture the device for measuring the friction between the prepreg curing process and subjected to pull-out tests with it. The prepreg used in this study is a unidirectional carbon/epoxy, produced by TORAY designation of T700SC/2592. When creating specimens 4-ply prepreps are prepared and laminated. The 2-ply prepreps in the middle are shifted 50mm. In order to measure the friction between the prepreg during the cure process, we simulate the environment in the autoclave in the device, and we experiment in pull-out test. Test environment simulating temperature and pressure. The speed of displacement should be calculated by coefficient of thermal expansions (CTE). By calculation, 0.05mm/min gives the order of magnitude of displacement speed. In this study, 3 pull-out speeds are used: 0.01, 0.05 and 0.1mm/min. The specimen was heated by a couple of heaters, and we controlled the heaters with a temperature controller along the curing conditions of the prepreg. We put pressure using 4 bolts. Two strain gages were put on the bolt. We can understand the load applied to the specimen from the strain of the bolt. Pressure was adjusted the tightness of the bolt according to curing conditions. By using such a device, the pull-out test performed by tensile testing machine while adding temperature and pressure. During the 5 hours, we perform experiments while recording the load and stroke. The shear stress determined from the load and the stroke, and evaluated.

**M1.00084 Localized Memory Effect of Elastomers Filled with Nanoparticles**, SHOUBO LI, XIAORONG WANG, Chemical Engineering, Tongji University, Shanghai — When a filler-reinforced elastomer compound is oscillatory sheared or pressed at a small fixed strain (e.g., 2%) for a period of time, it can produce a localized memory perturbation in its dynamic spectrum. Typically, a localized memory appears near the applied strain amplitude in the loss modulus spectrum. Sequential holding the system at two strains can produce one or two holes depending on the deformation histories. While this discovery of localized memory effect seems to be significant and compelling, its generality in vulcanized elastomers containing various fillers has not yet been tested extensively. In this work, we intend to expand on our previous work of a colloidal silica-filled model system to carbon black-filled real rubbers. We also examine the effect of filler volume fraction in rubber compounds on the spectral memory phenomenon.

**M1.00085 Mechanical Properties of Cellulose Microfiber Reinforced Polyolefin**, SATOSHI KOBAYASHI, HIROYUKI YAMADA, Tokyo Metropolitan Univ — Cellulose microfiber (CeF) has been expected as a reinforcement of polymer because of its high modulus and strength and lower cost. In the present study, mechanical properties of CeF/polyolefin were investigated. Tensile modulus increased with increasing CeF content. On the other hand, tensile strength decreased. Fatigue properties were also investigated with acoustic emission measurement. Stiffness of the composites gradually decreased with loading. Drastic decrease in stiffness was observed just before the final fracture. Based on the Mori-Tanaka's theory, the method to calculate modulus of CeF were proposed to evaluate dispersion of CeF.

**M1.00086 Soft composites with the twisted plywood microstructure, a lesson from nature.**<sup>1</sup>, YONGJIN KIM, ALFRED CROSBY, Univ of Mass - Amherst, CROSBY RESEARCH GROUP TEAM — The twisted plywood microstructure, consisting of rigid structural units within a continuous matrix, is known to be prevalent in many natural materials, including exoskeletons of crustacean, scales of fish, and even bones of mammals. Although it is yet to be resolved whether this structure is a product of evolution or an inevitable consequence of chirality of building blocks, nature utilizes the structure extensively to create various components. Previous studies have focused on fabricating and characterizing synthetic composites with similar structures; however, these composites have been based on a rigid matrix, e.g. an epoxy resin, and hard fibers, e.g. carbon fibers. For this combination of materials, it has been difficult to deconvolute the specific roles of each component. For a better understanding of the advantage of the structure, we have developed flexible composites, comprising a soft matrix and hard fiber bundles at two different size scales. Macroscopic engineered samples were created by combining elastomer and hard fibers, while sub-micron composites are fabricated from self-assembled nanoparticle ribbons and hydrogel matrices. The advantageous mechanical response of these flexible twisted plywood composites is characterized and presented.

<sup>1</sup>This material is based upon work supported by, or in part by, the U. S. Army Research Laboratory and the U. S. Army Research Office under contract/grant number W911NF-15-1-0358

**M1.00087 Modeling heterogeneous polymer-grafted nanoparticle networks having biomimetic core-shell structure**, BADEL L. MBANGA, VICTOR V. YASHIN, Chemical Engineering Department, University of Pittsburgh, Pittsburgh, PA 15261, USA, NIELS HOLTEN-ANDERSEN, Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, ANNA C. BALAZS, Chemical Engineering Department, University of Pittsburgh, Pittsburgh, PA 15261, USA — Inspired by the remarkable mechanical properties of such biological structures as mussel adhesive fibers, we use 3D computational modeling to study the behavior of heterogeneous polymer-grafted nanoparticle (PGN) networks under tensile deformation. The building block of a PGN network is a nanoparticle with grafted polymer chains whose free ends' reactive groups can form both permanent and labile bonds with the end chains on the nearby particles. The tunable behavior of cross-linked PGN networks makes them excellent candidates for designing novel materials with enhanced mechanical properties. Here, we consider the PGN networks having the core-shell structures, in which the type and strength of the inter-particle bonds in the outer shell differ from those in the core. Using the computer simulations, we obtain and compare the ultimate tensile properties (strength, toughness, ductility) and the strain recovery properties for the uniform samples and various core-shell structures. We demonstrate that the core-shell structures could be designed to obtain highly resilient self-healing materials

**M1.00088 Effects of Dimensionality and Flexibility of Conductive Fillers in Nanocomposites on Percolating Network Formation and Electrical Conductivity**, SEULKI KWON, HYUN WOO CHO, BONG JUNE SUNG, Department of Chemistry, Sogang University, Seoul 121-742, Republic of Korea — We conduct extensive Langevin dynamics (LD) simulation to explore how the dimensionality and flexibility of conductive fillers in polymer nanocomposites influence their percolation network formation and electrical conductivity. The percolation network formation of nanoparticles in polymer matrices is critical to obtaining desired properties of polymer nanocomposites. Some nanofillers such as carbon nanotubes (CNTs) and graphene nanosheets, are so flexible that they become either wavy or crumpled. Such a variability in nanofiller conformation brings a change to the percolation network, but has been often ignored in the theoretical and computational investigation. We consider three kinds of nanofillers of different dimensionality: zero-dimensional (0D) nanospheres, one-dimensional (1D) nanorods, and two-dimensional (2D) nanoplates. We estimate the percolation network concentration ( $\varphi_c$ ) and electrical conductivity with careful finite-size scaling. When the sizes of nanofillers are comparable, the dimensionality of nanofillers influences on  $\varphi_c$  and electrical conductivity of nanocomposites significantly. The effect of flexibility of nanofillers is less significant than that of dimensionality.

**M1.00089 Structure, Nanomechanics and Dynamics of Dispersed Surfactant-Free Clay Nanocomposite Films**, XIAO ZHANG, JING ZHAO, University of Akron, CHAD SNYDER, National Institute of Standards and Technology, ALAMGIR KARIM, University of Akron, NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY COLLABORATION — Natural Montmorillonite particles were dispersed as tactoids in thin films of polycaprolactone (PCL) through a flow coating technique assisted by ultra-sonication. Wide angle X-ray scattering (WAXS), Grazing-incidence wide angle X-ray scattering (GI-WAXS), and transmission electron microscopy (TEM) were used to confirm the level of dispersion. These characterization techniques are in conjunction with its nanomechanical properties via strain-induced buckling instability for modulus measurements (SIEBIMM), a high throughput technique to characterize thin film mechanical properties. The linear strengthening trend of the elastic modulus enhancements was fitted with Halpin-Tsai (HT) model, correlating the nanoparticle geometric effects and mechanical behaviors based on continuum theories. The overall aspect ratio of dispersed tactoids obtained through HT model fitting is in reasonable agreement with digital electron microscope image analysis. Moreover, glass transition behaviors of the composites were characterized using broadband dielectric relaxation spectroscopy. The segmental relaxation behaviors indicate that the associated mechanical property changes are due to the continuum filler effect rather than the interfacial confinement effect.

**M1.00090 Influence of Surface Coating of Magnetic Nanoparticles on Mechanical Properties of Polymer Nanocomposites<sup>1</sup>**, ECEM YARAR, GIZEM KARAKAS, Yeditepe University, DENIZ RENDE, RAHMI OZISIK, Rensselaer Polytechnic Institute, SEYDA MALTA, Yeditepe University — Polymer nanocomposites have emerged as promising materials due to improved properties when compared with conventional bulk polymers. Nanofillers are natural or synthetic organic/inorganic particles that are less than 100 nm in at least one dimension. Even the addition of trace amounts of nanofillers to polymers may lead to unique combinations of properties. Among variety of inorganic nanofillers, iron oxide magnetic nanoparticles are of great interest due to their unique physical and chemical properties, such as low toxicity, biocompatibility, large magnetization and conductivity, owing to their extremely small size and large specific surface area. In this study, approximately 8-10 nm magnetic nanoparticles coated with either citric acid or oleic acid are synthesized and blended with poly(methyl methacrylate) (PMMA) or poly(ethylene oxide) (PEO). The hydrophobicity/hydrophilicity of the polymer and the surface coating on the iron oxide nanoparticles are exploited to control the dispersion state of nanoparticles, and the effect of dispersion on mechanical and thermal properties of the nanocomposite are investigated via experimental methods such as dynamic mechanical analysis and differential scanning calorimetry.

<sup>1</sup>This material is based upon work partially supported by the National Science Foundation under Grant No. CMMI-1538730 and TUBITAK 112M666

**M1.00091 Wide Angle X-Ray Scattering Investigations on Irradiated iPP-VGCF Nanocomposites.**, ARNOLD FONSECA, DORINA CHIPARA, KAREN LOZANO, MIRCEA CHIPARA, The University of Texas Rio Grande Valley — Isotactic Polypropylene (iPP) has been loaded by various amounts of Vapor Grown Carbon Nanofiber (VGCF), ranging between 0 and 20 % wt., via melt mixing. The as obtained nanocomposites were gamma irradiated in air, at room temperature, at a dose rate of about 1 kGy/h and various integral doses ranging between 0 and 28 kGy. by using a <sup>60</sup>Co source. Wide Angle X-Ray Spectroscopy has been used to quantify the changes in the crystalline structure and the degree of crystallinity of iPP-VGCF nanocomposites. The measurements have been carried out by a Bruker Discover 8 spectrometer. Additional measurements have been performed by Raman spectroscopy using a Renishaw InVia microscope system operating at 532 and 785 nm. The experimental spectra of the nanocomposite were fitted by assuming a superposition of extended Breit-Wigner-Fano line shapes. It is concluded that the observed modifications noticed in these nanocomposites are dominated by the radiation-induced degradation of the polymeric matrix. Differential Scanning calorimetry data provided additional information regarding the effect of the nanofiller on the degree of crystallinity.

**M1.00092 Designing a gel-fiber composite to extract nanoparticles from solution**, YA LIU, University of Pittsburgh, OLGA KUKSENOK, Clemson University, ANNA BALAZS, University of Pittsburgh — Using DPD simulations, we proposed the design of a gel-fiber coating where the components of the system act in concert to extract particles from solution and localize these solids in the underlying gel layer. We model an array of flexible fibers that are embedded in a lower critical solution temperature (LCST) thermo-responsive gel, which swells at lower temperatures and collapses at higher temperatures. The system is immersed in a solution containing dispersed nanoparticles and this fluid is driven to flow by an imposed shear. When the gel is heated, it collapses to expose the fibers, and thereby, triggers the "catch" process. Namely, the fibers can act like "arms" that wrap around the nanoparticle and bring it from the outer solvent into the gel layer. Moreover, we show that depending on the flexibility and hydrophobicity of the fibers, as well as the imposed shear, we can position the nanoparticles at the desired height within the gel layer. Our approach can be utilized for the detection and separation of components in fluids and for the controlled insertion of nanoparticles within a hydrogel at a particular distance from the gel interface

**M1.00093 ABSTRACT WITHDRAWN —**

**M1.00094 Viscoelastic Analysis of Thermally Stiffening Polymer Nanocomposites<sup>1</sup>**, ANDREW EHLERS\*, DENIZ RENDE, Rensselaer Polytechnic Institute, ERKAN SENSES, PINAR AKCORA, Stevens Institute of Technology, RAHMI OZISIK, Rensselaer Polytechnic Institute — Poly(ethylene oxide), PEO, filled with silica nanoparticles coated with poly(methyl methacrylate), PMMA, was shown to present thermally stiffening behavior above the glass transition temperature of both PEO and PMMA. In the current study, the viscoelastic behavior of this nanocomposite system is investigated via nanoindentation experiments to complement on going rheological studies. Results were compared to neat polymers, PEO and PMMA, to understand the effect of coated nanoparticles.

<sup>1</sup>This material is based upon work supported by the National Science Foundation under Grant No. CMMI-1538730. \*Undergraduate student.

**M1.00095 Controlling the Degradation of Bioresorbable Polymers<sup>1</sup>**, ISTVAN MORITZ, BRIAN CROWLEY\*, ELIZABETH BRUNDAGE\*, Materials Science and Engineering, Rensselaer Polytechnic Institute, DENIZ RENDE, Center for Materials, Devices and Integrated Systems, RAHMI OZISIK, Materials Science and Engineering, Rensselaer Polytechnic Institute — Bioresorbable polymers play a vital role in the development of implantable materials that are used in surgical procedures, controlled drug delivery systems; and tissue engineering scaffolds. The half-life of common bioresorbable polymers ranges from 3 to over 12 months and slow bioresorption rates of these polymers restrict their use to a limited set of applications. The use of embedded enzymes was previously proposed to control the degradation rate of bioresorbable polymers, and was shown to decrease average degradation time to about 0.5 months. In this study, electromagnetic actuation of iron oxide magnetic nanoparticles embedded in an encapsulant polymer, poly(ethyleneoxide), PEO, was employed to initiate enzyme assisted degradation of bioresorbable polymer poly(caprolactone), PCL. Results indicate that the internal temperature of iron oxide magnetic nanoparticle doped PEO samples can be increased via an alternating magnetic field, and temperature increase depends strongly on nanoparticle concentration and magnetic field parameters. The temperature achieved is sufficient to relax the PEO matrix and to enable the diffusion of enzymes from PEO to a surrounding PCL matrix. Current studies are directed at measuring the degradation rate of PCL due to the diffused enzyme.

<sup>1</sup>This material is based upon work supported by the National Science Foundation under Grant No. CMMI-1538730. \*Undergraduate student.

**M1.00096 Interfacial slip in nano filled polymer blends**, JOHN MIKHAIL, DI XU, JOSEPH ORTIZ, DILIP GERSAPPE, Stony Brook University — The ability to control the interfacial slip in polymer blends is key to strengthening the material. Here, we look at how nano fillers can be used to strengthen the interface. By designing nano fillers with the appropriate surface energy we show how nano fillers can localize at the interface between the two polymer blends. We examine the role that the aspect ratio of the nano filler has on its ability to reduce the interfacial slip, and look to understand the mechanisms by which the slip is reduced. We look for network formation near the interface as a possible strengthening mechanism.

**M1.00097 Nanocellulose Composite Materials Synthesizes with Ultrasonic Agitation**, TIMOTHY KIDD, ANDREW FOLKEN, BYRON FRITCH, DEREK BRADLEY, University of Northern Iowa — We have extended current techniques in forming nanocellulose composite solids, suspensions and aerogels to enhance the breakdown of cellulose into its molecular components. Using only mechanical processing which includes ball milling, using a simple mortar and pestle, and ultrasonic agitation, we are able to create very low concentration uniform nanocellulose suspensions in water, as well as incorporate other materials such as graphite, carbon nanotubes, and magnetic materials. Of interest is that no chemical processing is necessary, nor is the use of nanoparticles, necessary for composite formation. Using both graphite and carbon nanotubes, we are able to achieve conducting nanocellulose solids and aerogels. Standard magnetic powder can also be incorporated to create magnetic solids. The technique also allows for the creation of an extremely fine nanocellulose suspension in water. Using extremely low concentrations, less than 1% cellulose by mass, along with careful control over processing parameters, we are able to achieve highly dilute, yet homogenous nanocellulose suspensions. When air dried, these suspensions have similar hardness and strength properties to those created with more typical starting cellulose concentrations (2-10%). However, when freeze-dried, these dilute suspensions form aerogels with a new morphology with much higher surface area than those with higher starting concentrations. We are currently examining the effect of this higher surface area on the properties of nanocellulose aerogel composites and how it influences the impact of incorporating nanocellulose into other polymer materials.

**M1.00098 Predicting  $\chi$  for polymers with stiffness mismatch from simulations**, DANIEL KOZUCH, WENLIN ZHANG, ENRIQUE GOMEZ, SCOTT MILNER, Department of Chemical Engineering, Penn State University — The Flory-Huggins  $\chi$  parameter describes the excess free energy of mixing and governs phase behavior for polymer blends and block copolymers. For chemically distinct polymers, the value of  $\chi$  is dominated by the mismatch in cohesive energy densities of the monomers. For blends of chemically similar polymers, the entropic portion of  $\chi$ , arising from non-ideal local packing, becomes more significant. Using polymer field theory, Fredrickson, Liu, and Bates predict that a difference in backbone stiffness can result in a positive  $\chi$  for chains consisting of chemically identical monomers. To quantitatively investigate this phenomenon, we perform molecular dynamic (MD) simulations for bead-spring chains which differ only in stiffness. From the simulations, we apply a novel thermodynamic integration to extract  $\chi$  as low as  $10^{-3}$  per monomer for blends with mild stiffness mismatch. By introducing a standardized effective monomer, we map real polymers to our bead-spring chains and show that the predicted entropic portion of  $\chi$  are consistent with experimental data.

**M1.00099 Comparative Study of Silk-Silk Alloy Materials**, YE XUE, Rowan University; Nanjing University, DAVE JAO, Rowan University, WENBING HU, Nanjing University, NATHAN WOLF, EVA-MARIE ROCKS, XIAO HU, Rowan University — Silk fibroin materials can be used for various kinds of biomedical applications. We report a comparative study of silk-silk blend materials using thermal analysis and infrared spectroscopy. Four groups of silk-silk blend films: Mori-Tussah, Mori-Muga, Mori-Eri and Mori-Thai, were fabricated from aqueous solutions and blended at different weight ratios, respectively. These silk-silk blend systems exploit the beneficial material properties of both silks. DSC and temperature-modulated DSC were used to measure the transition temperatures and heat capacity of these water-based silk-silk blend films. Fourier transform infrared spectrometer was used to characterize secondary structures of silk-silk blends. This study demonstrates that Mori silk are fully miscible with Tussah, Muga, Eri and Thai silk at different weight ratios without phase separation. Glass transition temperatures, degradation temperatures and the contents of alpha-helix and random coils of those silk-silk blend films can be controlled by changing the contents of different silks in the blend system. The features of Mori silk combined with the attributes of Tussah, Muga, Eri and Thai silk offer a useful suite of materials for a variety of applications in the future.

**M1.00100 Compatibility and Impact Resistance of Biodegradable Polymer Blends Using Clays and Natural Nanotubes**, YICHEN GUO, XUE YUAN, XIANGHAO ZUO, MIRIAM RAFAILOVICH, Stony Brook University — Montmorillonite clays and Halloysite nanotubes (HNTs) were modified by surface adsorption of resorcinol di (phenyl phosphate) (RDP) oligomers. Biodegradable poly (lactic acid) (PLA) and poly (butylene adipate-co-butylene terephthalate) (PBAT) polymers were blended together with RDP coated clays and tubes. TEM images of thin sections indicated that even though both RDP coated clay nanotubes and platelets located on the interfacial region between two immiscible polymers, only the platelets, having the larger aspect ratio, were able to reduce the PBAT domain sizes. The ability of clay platelets to partially compatibilize the blend was further confirmed by the dynamic mechanical analysis (DMA) which showed that the glass transition temperatures of two polymers tend to shift closer. Izod impact testing demonstrated that the rubbery PBAT phase greatly increased the impact strength of the unfilled blend, but addition of only 5% of clay filler decrease the impact strength by nearly 50% while a small increase was observed with nanotubes at that concentration. A simple model is proposed. The clay platelets are observed to cover the interfacial area. Although they are effective at reducing the interfacial tension, they block the entanglements between two polymer phase and increase the overall brittleness. On the other hand, the HNTs are observed to lie perpendicular to the interface, which makes them less effective in reducing interfacial tension, but far more effective at retarding micro-crack propagation.

**M1.00101 Hybrid Simulation Strategy for Simulating Self-Assembled Morphologies at the Atomistic Length Scales<sup>1</sup>**, VAIDYANATHAN SETHURAMAN, VENKAT GANESAN, Univ of Texas, Austin — In the context of Lithium-ion batteries, an enhancement in both ionic conductivity and mechanical properties, were observed for block copolymer electrolytes with increasing MW. On the contrary, when homopolymers were used as electrolytes, the ionic conductivity decreased with increasing MW. However, the origins of such increase in conductivity are unclear and are speculated to be tied to both the morphology and the atomistic details of the copolymer themselves. Motivated by such issues, we present a strategy to create ordered morphologies of block copolymers at the atomistic level using a combination of coarse-graining and inverse coarse-graining techniques. A mapping which is developed using the long-ranged structural mapping in the disordered phases will be utilized to generate self-assembled morphologies. In particular we focus on generating self-assembled morphologies of PS-PEO at the atomistic length scales. Statics and dynamics of such self-assembled morphologies will be presented and the effect of self assembly on the transport properties of ions will also be explored.

<sup>1</sup>Funded by NSF

**M1.00102 Controlling Miscibility in Polyethylene-Polynorbornene Block Copolymers via Side-Group Chemistry.**, WILLIAM MULHEARN, RICHARD REGISTER, Princeton University — Block copolymers containing a crystallizable block, such as polyethylene (PE), and an amorphous block with high glass transition temperature ( $T_g$ ) are an interesting class of materials since the rigid glassy block can improve the mechanical response of the article under strain by reinforcing the crystal fold surface. However, to prepare an easily processable PE-containing block copolymer it is necessary to avoid microphase separation in the melt by selection of amorphous blocks with weak repulsive interactions against PE (low Flory interaction parameter  $\chi$  or interaction energy density  $X$ ). Most such low- $\chi$  polymers are chemically similar to PE, such as copolymers of ethylene and a small amount of an  $\alpha$ -olefin, and therefore exhibit similarly low glass transition temperatures. This work investigates a series of low- and high- $T_g$  polymers based on substituted norbornene monomers, polymerized via ring-opening metathesis polymerization (ROMP). Hydrogenated polynorbornene derivatives possess a wide range of glass transition temperatures, and miscibility with PE can be readily tuned by the choice of substituents on the monomers (e.g. aromatic vs. aliphatic groups). Two species investigated, hydrogenated poly(cyclohexyl norbornene) and hydrogenated poly(norbornyl norbornene), have high  $T_g$  and also remain miscible with polyethylene to high molecular weight. Furthermore, we develop a set of mixing rules to qualitatively predict the solubility behavior of substituted ROMP polynorbornenes as a function of their side-groups.

**M1.00103 Influence of Homopolymers on the Microdomain Behavior of Block Copolymers in 2D Confinement**, YOUNGKEOL KIM, SUNGYOUL HWANG, GUIDUK YU, KOOKHEON CHAR, Seoul Natl Univ — Constraints imposed by nanometer scale confinement lead to changes in bulk equilibrium behavior of block copolymers (BCPs). Cylindrical pores with diameters corresponding to the length equivalent of several copolymer chains have been employed to investigate the influence of two-dimensional confinement on the behavior of BCPs. In this study, we expand the scope to homopolymer-BCP binary blends. Given fraction of homopolymers, the phase behavior of blends is dependent on molecular weight ( $M_w$ ) of homopolymers. Lamella- and cylinder-forming poly(styrene-*b*-butadiene) (PS-*b*-PBD) and PS homopolymers (hPS) were drawn into the pores of anodized aluminum oxide (AAO) membranes in the melt by capillary forces. Based on the detailed observation of the morphologies within porous columns, we analyzed the structural transition of BCPs induced by the presence of hPS and confinement. The effect of hPS on the micro-domain of BCPs is greatly accentuated in nanoscale confinement compared to the bulk state due to the entropic loss of polymer chains. Pore diameters of AAO and  $M_w$  of the PS-*b*-PBD are also controlled so as to examine the effects of confinement on the phase transition of PS-*b*-PBD/hPS blends.

**M1.00104 Tunable Surface Energy Interlayer Coating to Control the Phase Behavior of Block Copolymers in 2D Confinement**, SUNGYOUL HWANG, YOUNGKEOL KIM, DOKYEONG KWON, KOOKHEON CHAR, Seoul Natl Univ — There have been many studies to investigate the phase behavior of block copolymers (BCPs) in cylindrical confinement. In the nanometer scale 2D confinement, the phase behavior of BCPs is mainly dependent upon commensurability and interfacial interaction. However, most studies have focused only on the effects of commensurability on the microdomains of BCP. In this study, we employed organosilicate (OS) which has tunable surface energy upon adjusting curing temperature as interlayer to examine the phase behavior of BCPs as a function of interfacial energy. The OS interlayer was coated in the inner surface of anodized aluminum oxide (AAO) pores by template-wetting method and cured in a range of temperature to control the surface energy of the interlayer. Lamellae-forming poly(styrene-*b*-methyl methacrylate) (PS-*b*-PMMA) (SMA) in the melt was injected into the OS-coated AAO pores by capillary forces. With the detailed analysis, we note that the self-assembly of SMA within 2D confinement is competitively affected by both entropic and enthalpic effects as the contact interfacial energy is varied. Simply by controlling the curing temperature of the OS interlayer, various morphologies arising from both preferential and neutral wetting were identified.

**M1.00105 Bottlebrush Copolymer Morphology Transition: Influence of Side Chain Length and Block Volume Fraction<sup>1</sup>**, YUE GAI, DONG-PO SONG, JAMES WATKINS, Univ of Mass - Amherst — Brush block copolymers synthesized via living ring-opening metathesis polymerization (ROMP) offer unique advantages as templates for functional hybrid materials. Unlike linear block copolymer, the bottlebrush polymer phase transition not only depends on volume fractions of the two blocks but also on side chain length. Here we report the morphology transitions of PS-*b*-PEO bottlebrush copolymer (BBCP) as a function of PEO side chain length and block volume fraction. For the BBCPs with similar side chain lengths, highly ordered lamellar morphologies were observed with PEO volume fractions in a wide range from 32 vol% to 72 vol%, which is significantly different from that of traditional linear block copolymers. This study will lay the groundwork for nanostructure fabrications using the BBCPs and provides new insights into the phase behavior of the new type of materials.

<sup>1</sup>This work was supported by NSF center for Hierarchical Manufacturing at the University of Massachusetts, Amherst.

**M1.00106 Microwave Irradiation on Graphene Dispersed Within Polymeric Matrices.**, JORGE CISNEROS, BRIAN YUST, MIRCEA CHIPARA, Univ of Texas Rio Grande Valley — Graphene is a two dimensional nanomaterial with high thermal and electric conductivity and Young modulus. These features make graphene an ideal reinforcement for polymeric matrices. However, the mechanical features of polymer-carbon nanostructured composites are limited by the dispersion of the filler and by the delamination or microcracks initiated at the interface between the polymeric matrix and nanofiller. This last weakness can be addressed by improving the interface via chemical and physical methods. Microwave heating of graphite is a very efficient approach if the polymeric matrix does not also have a strong absorption. During the irradiation, the nanofiller is preferentially heated; the local melting of the polymer at the interface improves the interface by filling the microcracks and delaminations. Nanocomposites of polystyrene-poly(ethylene-*ran*-butylene)-polystyrene loaded by various amounts of graphene ranging from 0 % to 20 % wt. have been prepared by solution mixing using chloroform as solvent. The as obtained nanocomposites have been subjected to microwave irradiation in an Anton Paar Monowave 300 system operating at 75 W, for various irradiation times 5, 10, 15, 30, 45, and 60 minutes. The effect of microwave irradiation has been studied by Raman spectroscopy.

**M1.00107 Acoustic and Ultrasonic Spectral Evolution in Pre- and Post-Damage Self-Healing Poly (Ethylene Co-Methacrylic Acid) Ionomer Samples** , JONATHAN BUCKLEY, KENNETH PESTKA II, Longwood University, STEPHEN KALISTA, Department of Biomedical Engineering, Rensselaer Polytechnic Institute — We measured the pre- and post-damage resonant spectra of several self-healing ionomer samples composed of poly (ethylene co-methacrylic acid) (EMAA). The post-damage results indicate significant time-dependent variation in the acoustic and ultrasonic resonant spectral waveforms of these self-healing samples. These results are consistent with other recent experiments that demonstrate time evolution of resonant frequencies and associated quality factors within samples of post-damage EMAA ionomers. However, in our experiments it was found that, in some circumstances, the quality factors and associated resonant frequencies can exhibit time-dependent variation both before and after external damage. By quantifying time-dependent variations in the spectra of undamaged samples, including quality factor, resonant frequency and spectral waveform, we demonstrate a method to isolate changes in the resonant spectra that are present solely due to the post-damage healing behavior of these EMAA ionomers.

**M1.00108 Effect of charge density in chain extension reactions involving complexes of 4, 4'-diaminodiphenylmethane and various alkali metal salts** , SUBRAJEET DESHMUKH, KATHERINE CARRASQUILLO , FANG CHANG TSAI, LINA WU, SHAW LING HSU, University of Massachusetts Amherst, UNIVERSITY OF MASSACHUSETTS AMHERST TEAM — Controlling the reaction of methylene diphenyl diisocyanate (MDI)-terminated polyester prepolymer and 4, 4'-diaminodiphenylmethane (MDA) is extremely important in many large scale applications. The ion-diamine complex has the advantage of blocking the instantaneous reaction between the diamine and isocyanate from taking place until it is released at elevated temperatures. We synthesized complexes of MDA with various alkali metal salts. These complexes create a barrier between the diamine and isocyanate thus preventing the premature reaction. We compared the complexes in terms of their dissociation and the subsequent curing with the prepolymer. Charge density had a tremendous effect. DSC showed that Na complexes dissociated at a lower temperature and needed less energy to dissociate than the Li complexes. The effect of change in cation on complex dissociation was more pronounced compared to the change in anion. Also, the ionic liquid introduced greatly altered the dissociation behavior. Temperature and time resolved IR spectroscopy was used to monitor the urea and NH band. By DSC and IR, we showed that NaCl complex is best suited for the curing of prepolymer with regards to curing temperature and energy.

**M1.00109 Structural dynamics in polystyrene-b-polyisoprene copolymers with varying molecular architectures** , THOMAS KINSEY, MAXIMILIAN HERES, JIMMY MAYS, ROBERTO BENSON, JOSHUA SANGORO, Univ of Tennessee, Knoxville — A series of polystyrene-polyisoprene block copolymers with different molecular architectures are investigated by broadband dielectric spectroscopy and temperature modulated differential scanning calorimetry. The influence of copolymer composition on segmental and normal mode relaxation dynamics is analyzed. These results are discussed with respect to the current understanding of copolymer dynamics and interactions.

**M1.00110 How to Improve Ion Transport in Polymer Nanocomposites? Insights from Atomistic Simulations** , SANTHOSH MOGURAMPALLY, VENKAT GANESAN, Univ of Texas, Austin — We present different strategies to enhance ion conducting properties of polymer nanocomposite electrolytes and their implications by varying the surface chemistries of the nanoparticles and interactions between nanoparticle and components of polymer-salt mixture. Our molecular dynamics simulations suggest that the ionic mobilities and conductivities correlate with the combined effects of the changes in polymer segmental dynamics and the modifications in the local environment of ionic species arising from the introduction of nanoparticles. In the presence of  $\alpha$ ,  $\beta$  and  $\gamma$ - $\text{Al}_2\text{O}_3$  nanoparticles, we observe a monotonic decrease of ionic conductivities and mobilities with the nanoparticle loading due to the corresponding slowing of polymer dynamics. However, with the introduction of the repulsive interactions between nanoparticle and components of polymer-salt mixture, we find an increase in the mobility and conductivity of the polymer nanocomposites. However, the repulsive interactions seem to decrease the elastic moduli in contrast to the moduli enhancing effects by attractive interactions.

**M1.00111 STRUCTURE OF ANION-CONDUCTING POLYMERS FROM WAXS AND MD SIMULATIONS** , BARBARA FRISKEN, SEPEHR TAHMASEBI, ERIC SCHIBLI, STEVEN HOLDCROFT, Simon Fraser University — The structure of novel polymers for anion exchange membranes (AEMs) is investigated using wide angle X-ray scattering (WAXS) combined with molecular dynamics (MD) simulations using a united-atom force field model based on the DREIDING force field. The polymers being studied are poly(benzimidazole) (PBI) derivatives including poly(dimethylbenzimidazole) (PDMBI), mesitylene poly(benzimidazole) (mes-PBI), and mesitylene poly(dimethylbenzimidazole) (mes-PDMBI). WAXS reveals an amorphous structure with two main length scales. By comparing simulation results to WAXS data, we attribute features observed in the scattering data to side-to-side spacing between polymer chains and to the parallel-ring stacking of the benzimidazole rings. Overall, we are able to validate the interpretation of scattering data by combining MD simulations and scattering experiments.

**M1.00112 Charge Transport and Dynamics in Confined Phosphonium-based Ionic Liquids<sup>1</sup>** , TYLER COSBY, University of Tennessee, Knoxville, KATSUHIKO TSUNASHIMA, National Institute of Technology, Wakayama College, JOSHUA SANGORO, University of Tennessee, Knoxville — Charge transport and structural dynamics in a homologous series of phosphonium-based ionic liquids confined in silica nanopores are investigated by broadband dielectric spectroscopy and Fourier transform infrared spectroscopy. The impact of alkyl chain length and hydrophobic aggregation on the physicochemical properties as well as the interplay between confinement effects and pore-wall interactions through silica surface silanization are investigated. The results are discussed within the framework of current understanding of confinement effects in ionic liquid systems, especially in comparison to imidazolium-based ionic liquids.

<sup>1</sup>NSF DMR Polymers Program

**M1.00113 Charge Transport and Dynamics in Confined Ammonium and Phosphonium-based Ionic Liquids** , MATTHEW HARRIS, TYLER COSBY, Univ of Tennessee, Knoxville, KATSUHIKO TSUNASHIMA, National Institute of Technology, Wakayama College, JOSHUA SANGORO, Univ of Tennessee, Knoxville — Charge transport and structural dynamics in a homologous series of ammonium and phosphonium ionic liquids confined in silica nanopores are investigated by broadband dielectric spectroscopy and Fourier transform infrared spectroscopy. The impact of the central atom of the cation on the physicochemical properties as well as the interplay between confinement effects and pore-wall interactions through silica surface silanization are investigated. The results are discussed within the framework of current understanding of confinement effects in ionic liquid systems, especially in comparison to imidazolium-based ionic liquids.

**M1.00114 Amphiphilic Zwitterionic Coatings for Marine Anti-Biofouling Applications.** , EDWIN WALKER JR, C. K. PANDIYARAJAN, KIRILL EFIMENKO, JAN GENZER, North Carolina State Univ — Marine biofouling is a problem plaguing the surfaces of cargo ships, military ships and submarines. Previous approaches have relied primarily on the use of Cu-based coatings, which have deleterious effects on aquatic life. Recently, the vast majority of research efforts have focused on the use of polymer brushes synthesized by controlled radical polymerization to create either, the commonly used PEG/PEO materials, amphiphilic alternatives or promising zwitterionic-based moieties. Our approach is based on copolymerizing N, N'-2-dimethylaminoethyl methacrylate (DMAEMA) and propargyl methacrylate (PgMA) in different molar ratios (typically, 1:1 and 3:1) using AIBN-based free radical initiator. The copolymers are then benzitized with 1, 3- propane sultone to obtain zwitterionic macromolecules. We create substrate-anchored hydrogels by casting the copolymers as films onto polystyrene-based substrates and crosslink them using a photo-active reagent benzophenone. We investigate the cross-linking reaction with IR, the thickness and swelling as a function of ionic strength and electrolyte using spectroscopic ellipsometry and the wettability using water contact angle. We study the resistance of the coatings towards non-specific protein adsorption using fibrinogen and BSA.

### M1.00115 How does the molecular network structure influence PDMS elastomer wettability?

, MATTHEW MELILLO, JAN GENZER, North Carolina State University — Poly(dimethylsiloxane) (PDMS) is one of the most common elastomers, with applications ranging from medical devices to absorbents for water treatment. Fundamental understanding of how liquids spread on the surface of and absorb into PDMS networks is of critical importance for the design and use of another application - microfluidic devices. We have systematically studied the effects of polymer molecular weight, loading of tetra-functional crosslinker, end-group chemical functionality, and the extent of dilution of the curing mixture on the mechanical and surface properties of end-linked PDMS networks. The gel and sol fractions, storage and loss moduli, liquid swelling ratios, and water contact angles have all been shown to vary greatly based on the aforementioned variables. Similar trends were observed for the commercial PDMS material, Sylgard-184. Our results have confirmed theories predicting the relationships between modulus and swelling. Furthermore, we have provided new evidence for the strong influence that substrate modulus and molecular network structure have on the wettability of PDMS elastomers. These findings will aid in the design and implementation of efficient microfluidics and other PDMS-based materials that involve the transport of liquids.

### M1.00116 The effects of elastocapillary length on the surface creasing instability of hydrogels

, TETSU OUCHI, Univ of Mass - Amherst, QIHAN LIU, ZHIGANG SUO, Harvard University, RYAN HAYWARD, Univ of Mass - Amherst — Creasing is a mode of surface instability induced by compressing elastomers or gels. Formation of creases is known to proceed by a nucleation and growth process, and the critical nucleus size is thought to be determined by the elastocapillary length (defined by the ratio of surface tension to elastic modulus). Here, we vary the elastocapillary length over the range of 0.008 to 0.4 mm by preparing a series of soft hydrogels with different compositions and contacting them with humidified air. By rapidly applying compression, we are able to achieve strains that exceed the Maxwell strain (where creases become favorable compared to a flat surface) by more than 0.10, and which approach Biot's prediction for linear instability of a compressed half-space. Regardless of the conditions, however, we observe formation of creases only by nucleation and growth, although the density of nucleation sites is found to be sensitive to elastocapillary length. Interestingly, fast propagation of creases (at velocities similar to the speed of sound in the material) are found at strains approaching Biot's point.

### M1.00117 Computer Simulations of Bottlebrush Melts and Soft Networks<sup>1</sup>

, ZHEN CAO, Univ of Akron, JAN-MICHAEL CARRILLO, Oak Ridge National Laboratory, SERGEI SHEIKO, Univ of NC - Chapel Hill, ANDREY DOBRYNIN, Univ of Akron — We have studied dense bottlebrush systems in a melt and network state using a combination of the molecular dynamics simulations and analytical calculations. Our simulations show that the bottlebrush macromolecules in a melt behave as ideal chains with the effective Kuhn length  $b_K$ . The bottlebrush induced bending rigidity is due to redistribution of the side chains upon backbone bending. Kuhn length of the bottlebrushes increases with increasing the side-chain degree of polymerization  $n_{sc} \propto b_K \propto n_{sc}^{0.46}$ . This model of bottlebrush macromolecules is extended to describe mechanical properties of bottlebrush networks in linear and nonlinear deformation regimes. In the linear deformation regime, the network shear modulus scales with the degree of polymerization of the side chains as  $G_0 \propto (n_{sc} + 1)^{-1}$  as long as the ratio of the Kuhn length to the size of the fully extended bottlebrush backbone between crosslinks,  $R_{max}$ , is smaller than unity,  $b_K/R_{max} \ll 1$ . Bottlebrush networks with  $b_K/R_{max} \propto 1$  demonstrate behavior similar to that of networks of semiflexible chains with  $G_0 \propto n_{sc}^{0.5}$ . In the nonlinear deformation regime, the deformation dependent shear modulus is a universal function of the first strain invariant  $I_1$  and bottlebrush backbone deformation ratio  $\beta$  describing stretching ability of the bottlebrush backbone between crosslinks.

<sup>1</sup>NSF DMR-1409710 DMR-1436201

### M1.00118 Modeling polymer gel that strengthen under tension

, SANTIDAN BISWAS, VICTOR V. YASHIN, ANNA C. BALAZS, Univ of Pittsburgh — We develop a constitutive model of a responsive polymer gel, which can reversibly form additional crosslinks when under tension. We assume that the polymer chains incorporate the folded domains encompassing the reactive functional groups (cryptic sites). Under extension of the network, the domains unfold and expose the cryptic sites, which can then form labile bonds with the linker chains grafted to the network. Once the deformation is removed, the linkers detach from the cryptic sites, and unfolded domains go back to the folded configuration thus hiding the cryptic sites. The gel behavior under applied force is described by the equations of elasticity of the polymer network coupled to the kinetic equations for the folding and binding transitions. The developed model could be used for designing new polymer gel-based materials that exhibit self-strengthening in response to a mechanical action.

### M1.00119 Modeling thermal-mechanical behavior of networks with reconfigurable crosslinks<sup>1</sup>

, JE-CHANG YANG, YUAN MENG, MITCHELL ANTHAMATTEN, University of Rochester — Actively moving polymers nearly always involve the storage or release of mechanical energy using external stimuli. Thermomechanical experiments were conducted on well-defined chemical networks bearing both permanent and light-reconfigurable covalent junctions. Experimental data include stress relaxation and mechanical creep during photoinduced network reconfiguration as well as equilibrium stress-strain behavior of reprogrammed networks. Physical models of elastic networks were applied to describe thermomechanical behavior during and after bond re-formation while under external stress. The role of dangling ends in influencing competitive network mechanics is evaluated to explain observed phenomena and discrepancies between theory and data. Understanding how process path is related to the equilibrium thermomechanics of such reprogrammed networks is important to engineering shape actuator driven by crystallization.

<sup>1</sup>NSF ECCS-1530540

### M1.00120 Imparting large macroscopic changes with small changes in polypeptide composition

, MICHELLE SING, GARETH MCKINLEY, BRADLEY OLSEN, Massachusetts Institute of Technology — Block copolymers composed of polypeptides provide an excellent platform for exploring the underlying physics surrounding macroscopic associative network behavior. Previous work in our group has elucidated a difference in the mechanical properties of two nearly identical elastin-like polypeptide (ELP) endblocks. In poly(ELP)s, this substitution is known to result in tighter beta turns. These beta turns exhibit slower responses to changes in temperature within the material. Under shear, the modulus for the alanine-containing ELP triblock is almost three times higher than the glycine-containing ELP. Additionally, preliminary tensile tests show higher stress and strain at break for the alanine ELP triblock. We are able to explain the reasons for this behavior using a variety of spectroscopic and analytical techniques. Small angle neutron and x-ray scattering indicate differences in ordering between the alanine and glycine containing ELP materials both in shear and in stagnant flow.

### M1.00121 Effect of Temperature and Strain on a Self-assembled Gel

, SATISH MISHRA, SANTANU KUNDU, Mississippi State University — Gels are widely used in food industry and biomedical field. For physically associating gels, mechanical properties depend on the nature of association between the polymer and the solvent. A thermoreversible, physically associating gel is considered here, which consists of 10% (v/v) poly (methyl methacrylate) - poly (n-butyl acrylate) - poly (methyl methacrylate) in butanol, a midblock selective solvent. Below gelation temperature, the end blocks collapse and form aggregates, and the mid-blocks act as bridges between those aggregates. Rheo-SANS experiments were conducted on these samples where small angle neutron scattering (SANS) and shear-rheology experiments are combined. SANS data were collected over a wide temperature range, from 65C to -10C with and without strain. Near the gelation temperature, SANS data can be fitted with hard sphere model. However, with decrease of temperature, structural changes, due to clustering of aggregates, are observed. The SANS and rheological results in combination provide insight in structural changes of the gel with strain and temperature, respectively.

**M1.00122 Rubber Elasticity for percolation network consisting of Gaussian Chains**, KENGO NISHI, Georg-August-Universitt Gttingen, MITSUHIRO SHIBAYAMA, TAKAMASA SAKAI, The University of Tokyo — A theory describing the elastic modulus for percolation networks of Gaussian chains on general lattices such as square and cubic lattices is proposed and its validity is examined with simulation and mechanical experiments on well-defined polymer networks. The theory was developed by generalizing the effective medium approximation for Hookian spring network (EMA) to Gaussian chain networks. From EMA theory, we found that the ratio of the elastic modulus at  $p, G$  to that at  $p = 1, G_0$ , must be equal to  $G/G_0 = (p - 2/f)/(1 - 2/f)$  if the position of sites can be determined so as to meet the force balance, where  $p$  is the degree of cross-linking reaction. However, the EMA prediction cannot be applicable near its percolation threshold because EMA is a mean field theory. Thus, we combine real-space renormalization and EMA, and propose a theory called real-space renormalized EMA, i.e., REMA. The elastic modulus predicted by REMA is in excellent agreement with the results of simulations and experiments of near-ideal diamond lattice gels.

Please set this talk on Mon, Tue, or Wed (March 14-16) just after its accompanying talk, MAR16-2015-000773.

**M1.00123 Nonlinear Stress Relaxation of “Quasi-monodisperse Polyisoprene and Poly(*ptert*-butylstyrene)**, HIROSHI WATANABE, YUMI M.

Viscoelastic relaxation was examined for entangled miscible blends of *cis*-polyisoprene (PI) and poly(*ptert*-butylstyrene) (PtBS) therein,  $\tau_{PI}$  and  $\tau_{PtBS}$ , changed with the composition  $w_{PI}$  and the molecular weights  $M_{PI}$  and  $M_{PtBS}$ .  $w_{PI}$ ,  $M_{PI}$ , and  $M_{PtBS}$  values were chosen adequately. For example, in a blend with  $w_{PI} = 0.75$ ,  $M_{PI}/\tau_{PtBS} = 1$  and  $M/M_e = 55$  and  $8.3$  for PI and PtBS. Under small strains, this blend exhibited a single relaxation peak, thereby behaving as a “quasi-monodisperse” material. Under large step strains, the blend showed two relaxation peaks, known as the type-A damping for entangled monodisperse homopolymers. Nevertheless, PI had  $M/M_e = 55$  and PtBS had  $M/M_e = 8.3$ . Large  $M/M_e$  ratio exhibit very strong type-C damping. Thus, as compared to homopolymers, the nonlinear relaxation of the blend with large  $M/M_e$  ratio. This suppression is discussed in relation to the slow Rouse retraction of the coexisting PtBS chains.

(I have to take off on Thursday).

**M1.00124 Bidirectional Control of Flow in Thin Polymer Films by Photochemically Manipulating Surface Tension**, CHAE BIN KIM, DUSTIN JAMES, SUNSHINE ZHOU, AUSTIN DULANEY, CHRISTOPHER ELLISON, The University of Texas at Austin — The Marangoni effect causes transport of liquids in response to surface tension gradients. In a thin polymer film, such flow results in formation of topographic features that could be exploited as a practically useful route to manufacture patterned surfaces. An especially versatile material for this application should be able to be spatially programmed to possess regions of higher or lower relative surface tension so that the direction of flow into or out of those regions can be directed with precision. To this end, we describe here a photopolymer whose melt-state surface tension can be selectively raised or lowered in light exposed regions depending on the wavelength and dose of applied light. The direction of Marangoni flow into or out of irradiated regions agrees with expected surface tension changes associated with each photochemical transformation. We believe this patterning methodology will be potentially useful for high throughput fabrication environments such as roll-to-roll processing that can exploit contact-free and solvent-free topography development.

**M1.00125 Dynamics of associating polymers and the sticky Rouse model: a study by combined dielectric and dynamic mechanical techniques**, YANGYANG WANG, Oak Ridge National Laboratory, TYLER COSBY, JOSHUA SANGORO, University of Tennessee, Knoxville — Reversible association through non-covalent bonding is ubiquitous in the soft matter world. Despite decades of studies, the dynamics of associating polymers have not been well understood. Here we examine the dynamics of butadiene- and isoprene-based polymeric systems with pairwise association through hydrogen bonding. Compared to ionomers, where reversible crosslinks are typically not well defined, these hydrogen bonding polymers are associated through strictly binary contacts and thus provide a better opportunity to test theoretical ideas. By combining dielectric spectroscopy and dynamic mechanical measurement, we are able to identify both chain and junction dynamics and analyze their motional coupling mechanism. The results are discussed in the context of the sticky Rouse model.

**M1.00126 Evolution of Yield Stress during Structural Relaxation for the Epoxy 828DEA<sup>1</sup>**, GABRIEL ARECHEDERRA, JOHN MCCOY, New Mexico Tech, JAMIE KROPKA, Sandia National Laboratories — The evolution of yield stress from structural relaxation of diethanolamine cured diglycidyl ether of bisphenol-A, 828DEA, was tracked using uniaxial compression experiments. Samples were aged isothermally for up to 3 months at 5 temperatures ranging from deep in the glass to above  $T_g$ . Since 828DEA has remaining reactive potential, it is anticipated that the  $T_g$  will continue to evolve throughout the course of the study as new chemical crosslinks are formed. Consequently, it is important to track the evolution of  $T_g$  as well as the progression of the fictive temperature in order to interpret the evolution of yield stress.

<sup>1</sup>Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energys National Nuclear Security Administration under contract DE-AC04-94AL85000.

**M1.00127 Can Stress Relaxation Experiments be Used to Assess Deformation Induced Mobility in Glassy Polymers?**, JAMIE KROPKA, KEVIN LONG, Sandia National Laboratories — The observance of an increase in glassy polymer relaxation rates under a mechanical deformation is often referred to as deformation induced mobility (DIM). It has been argued that stress relaxation experiments can provide indirect evidence of this phenomenon. Recently, stress relaxation experiments have been interpreted as demonstrating a mobility decrease with increased deformation when very slow strain rates,  $1.2 \times 10^{-5} \text{ s}^{-1}$ , are used to apply the deformation. This would suggest against generality of DIM and would have significant implications to constitutive models founded on this principle. Here, a mathematical exercise is performed to evaluate the implications of DIM on stress relaxation response. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energys National Nuclear Security Administration under contract DE-AC04-94AL85000.

**M1.00128 Chain networking revealed by molecular dynamics simulation**, YEXIN ZHENG, MESFIN TSIGE, SHI-QING WANG, Department of Polymer Science, University of Akron — Based on Kremer-Grest model for entangled polymer melts, we demonstrate how the response of a polymer glass depends critically on the chain length. After quenching two melts of very different chain lengths (350 beads per chain and 30 beads per chain) into deeply glassy states, we subject them to uniaxial extension. Our MD simulations show that the glass of long chains undergoes stable necking after yielding whereas the system of short chains is unable to neck and breaks up after strain localization. During ductile extension of the polymer glass made of long chain significant chain tension builds up in the load-bearing strands (LBSs). Further analysis is expected to reveal evidence of activation of the primary structure during post-yield extension. These results lend support to the recent molecular model<sup>1</sup> and are the simulations to demonstrate the role of chain networking. This work is supported, in part, by a NSF grant (DMR-EAGER-1444859)

<sup>1</sup>Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energys National Nuclear Security Administration under contract DE-AC04-94AL85000.

**M1.00127 Can Stress Relaxation Experiments be Used to Assess Deformation Induced Mobility in Glassy Polymers?**, JAMIE KROPKA, KEVIN LONG, Sandia National Laboratories — The observance of an increase in glassy polymer relaxation rates under a mechanical deformation is often referred to as deformation induced mobility (DIM). It has been argued that stress relaxation experiments can provide indirect evidence of this phenomenon. Recently, stress relaxation experiments have been interpreted as demonstrating a mobility decrease with increased deformation when very slow strain rates,  $1.2 \times 10^{-5} \text{ s}^{-1}$ , are used to apply the deformation. This would suggest against generality of DIM and would have significant implications to constitutive models founded on this principle. Here, a mathematical exercise is performed to evaluate the implications of DIM on stress relaxation response. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energys National Nuclear Security Administration under contract DE-AC04-94AL85000.

**M1.00128 Chain networking revealed by molecular dynamics simulation**, YEXIN ZHENG, MESFIN TSIGE, SHI-QING WANG, Department of Polymer Science, University of Akron — Based on Kremer-Grest model for entangled polymer melts, we demonstrate how the response of a polymer glass depends critically on the chain length. After quenching two melts of very different chain lengths (350 beads per chain and 30 beads per chain) into deeply glassy states, we subject them to uniaxial extension. Our MD simulations show that the glass of long chains undergoes stable necking after yielding whereas the system of short chains is unable to neck and breaks up after strain localization. During ductile extension of the polymer glass made of long chain significant chain tension builds up in the load-bearing strands (LBSs). Further analysis is expected to reveal evidence of activation of the primary structure during post-yield extension. These results lend support to the recent molecular model<sup>1</sup> and are the simulations to demonstrate the role of chain networking. This work is supported, in part, by a NSF grant (DMR-EAGER-1444859)

**M1.00129 How plasticizer makes a ductile polymer glass brittle?**<sup>1</sup>, YUE ZHAO, XIAOXIAO LI, SHI-QING WANG, Univ of Akron — During uniaxial extension, a polymer glass of high molecular weight is ductile at high temperatures (still below  $T_g$ ) and turns brittle when the temperature is sufficiently lowered. Incorporation of small-molecular additives to polymer glasses can speed up segmental relaxation considerably. The effect of such plasticization should be to make the polymers more ductile. We examined the effect of blending a few weight percent of either triphenyl phosphate (TPP) or a mineral oil to a commercial-grade PS and PMMA. Our Instron tests show that the plasticized PS is less ductile. Specifically, at 70 °C, the original PS is ductile at an extensional rate of 0.02 s<sup>-1</sup> [1] whereas the PS with 4 wt. % TPP turns brittle. Mechanical spectroscopic measurements show that the alpha relaxation time is shortened by more than two orders of magnitude with 4 wt. % TPP. On the other hand, such anomalous behavior did not occur in PMMA. We need to go beyond the conventional description to rationalize these results. [1] Li, X.; Wang, S. Q. ACS Macro Letters 2015, 1110-1113.

<sup>1</sup>This work is supported, in part, by a NSF grant (DMR-EAGER-1444859)

**M1.00130 Surface diffusion of molecular glasses: Material dependence and impact on physical stability**<sup>1</sup>, SHIGANG RUAN, WEI ZHANG, LIAN YU, University of Wisconsin-Madison — Surface diffusion coefficients have been measured for molecular glasses tris-naphthylbenzene (TNB) and PMMA oligomers by surface grating decay. Surface diffusion on TNB is vastly faster than bulk diffusion, by a factor of  $10^7$  at  $T_g$ , while the process is very slow on PMMA. Along with the previous results on *o*-terphenyl, nifedipine, indomethacin, and polystyrene oligomers, we find that surface diffusion slows down with increasing molecular size and intermolecular forces, whereas bulk diffusion has a weaker material dependence. The molecular glasses studied show fast crystal growth on the free surface. A general correlation is observed between the coefficient of surface diffusion and the velocity of surface crystal growth, indicating surface crystallization is supported by surface mobility. (Zhu, L., et al. *Phys. Rev. Lett.* 106 (2011): 256103; Zhang, W., et al. *J. Phys. Chem. B* 119 (2015): 5071-5078)

<sup>1</sup>NSF

**M1.00131 Liquid Crystalline Phases of Polymer Brushes**<sup>1</sup>, KIANA AMINI, NASSER ABUKHDEIR, MARK MATSEN, University of Waterloo — The phase behavior of liquid-crystal polymeric brushes in solvent are investigated using self-consistent field theory. The polymers are modeled as freely-jointed chain consisting of  $N$  rigid segments. The isotropic interactions between the polymer and the solvent are treated using the standard Flory-Huggins theory, while the anisotropic liquid-crystalline (LC) interactions between rigid segments are taken into account using the Mayer-Saupe theory. For weak LC interactions, the brush exhibits the conventional parabolic-like profile, while for strong LC interactions, the polymers crystallize into a dense brush with a step-like profile. At intermediate interaction strengths, we find the microphase-segregated phase observed previously for lattice-model calculations.<sup>2</sup> In this phase, the brush exhibits a crystalline layer next to the grafting surface with an external layer similar to the conventional brush.

<sup>1</sup>This work was supported by NSERC of Canada.

<sup>2</sup>V. M. Amoskov, T. M. Birshtein, and V. A. Pryamitsyn, *Macromolecules*, **31**, 3720 (1998).

**M1.00132 Thermal Characterization of Thermotropic Nematic Liquid-Crystalline Elastomers**, DAVID THOMAS, MATT CARDARELLI, Tufts University, ANTONI SANCHEZ-FERRER, ETH Zurich, BADEL L. MBANGA, TIMOTHY J. ATHERTON, PEGGY CEBE, Tufts University — Nematic Liquid-Crystalline Elastomers (LCEs) are weakly crosslinked polymeric networks that exhibit rubber elasticity and liquid-crystalline orientational order due to the presence of mesogenic groups. Three end-on side-chain nematic LCEs were investigated using real-time synchrotron wide-angle X-ray scattering (WAXS), differential scanning calorimetry (DSC), and thermogravimetry (TG) to correlate thermal behavior with structural and chemical differences among them. The elastomers differed in crosslinking density and mesogen composition. Thermally reversible glass transition temperature,  $T_g$ , and nematic-to-isotropic transition temperature,  $T_{ni}$ , were observed upon heating and cooling for all samples. By varying the heating rate,  $T_g^0$  and  $T_{ni}^0$  were determined at zero heating rate. The temperature dependence of the orientational order parameter was determined from the anisotropic azimuthal angular distribution of the equatorial reflection seen during real-time WAXS experiments. Our results show that the choice of crosslinking unit, its shape, density, as well as the structure of co-monomers, all influence the temperature range over which the thermal transitions take place.

**M1.00133 Crystal Growth Theory for Random Copolymers of Crystallizable and Non-crystallizable Units**, HERVE MARAND, HADI MOHAMMADI, Virginia Tech, Department of Chemistry — While the presence of randomly distributed non-crystallizable units (e.g. short branches in metallocene linear low density polyethylene) has been carefully considered in the thermodynamics of copolymers crystallization, it has been mostly ignored in the analysis of crystal growth rate data. In this work, we present an extension of the Lauritzen-Hoffman (LH) secondary nucleation theory that considers crystal growth processes for random copolymers of crystallizable and non-crystallizable units. Concentrating on the distribution of crystallizable unit sequence lengths rather than the whole polymer chain, rate equations in the LH theory are modified to account for the population of crystallizable sequences able to form a specific number of folds. We then calculate the flux over the nucleation barrier for each lamellar thickness, the secondary nucleation rate,  $i$ , the substrate completion rate,  $g$ , and derive the crystal growth rate,  $G$ , as a function of crystallization temperature. The model also allows prediction of the lamellar thickness distribution as a function of crystallization temperature. In qualitative agreement with literature data, our model predicts lower crystal growth rates and higher average lamellar thicknesses for m-LLDPE than for linear polyethylene at the same undercooling.

**M1.00134 Flow-induced Crystallization of Long Chain Aliphatic Polyamides under a Complex Flow Field**<sup>1</sup>, XIA DONG, YUNYUN GAO, LILI WANG, DUJIN WANG, Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Engineering Plastics, Institute of Chemistry CAS — The present work deals with the flow-induced multiple orientations and crystallization structure of polymer melts under a complex flow field. This complex flow field is characteristic of the consistent coupling of extensional pulse and closely followed shear flow in a narrow channel. Utilizing an ingenious combination of an advanced micro-injection device and long chain aliphatic polyamides, the flow-induced crystallization morphology was well preserved for ex-situ synchrotron micro-focused wide angle X-ray scattering as well as small angle X-ray scattering. The experimental results clearly indicate that the effect of extensional pulse on the polymer melt is restrained and further diminished due to either the transverse tumble of fountain flow or the rapid retraction of stretched high molecular weight tails. However, the residual shish-kebab structures in the core layer of the far-end of channel suggest that the effect of extensional pulse should be considered in the small-scaled geometries or under the high strain rate condition.

<sup>1</sup>The authors thank the financial support from MOST (2013BAE02B02, 2014CB643600) and NSFC(21574140).

**M1.00135 Effects of mechanical strain and heat on the strain-induced crystalline  $\beta$  to  $\alpha$  structural transition of syndiotactic polystyrene.** , FUYUAKI ENDO, ATSUSHI HOTTA, Department of Mechanical Engineering, Keio University — The polymorphic behavior of syndiotactic polystyrene (sPS) during the  $\beta$  to  $\alpha$  form transition was investigated. sPS presents complex polymorphism with five crystalline forms. Quite a few crystalline structural transitions have also been reported, including our recent discovery of the structural transition from  $\beta$  to  $\alpha$  forms induced by tensile deformation at around 200C. In this study, we analyzed the individual effects of mechanical strain and heat on the  $\beta$  to  $\alpha$  crystalline structural transformation caused by the mechanical deformation. sPS film samples containing  $\beta$  form crystals were prepared and stretched at 130C (near the glass transition temperature of sPS), followed by the annealing process of the samples below the melting temperature. X-ray analyses revealed that the stretched sample possessed mesomorphic  $\alpha$  forms, indicating that the mechanical strain could invoke the destruction of  $\beta$  form crystals by producing mesomorphic  $\alpha$  forms. Interestingly, the annealed samples exhibited sharp X-ray reflections typical of  $\alpha$  forms, which became even sharper by the increase in the annealing temperature. It was therefore concluded that the heat could induce the structural transitions from mesomorphic  $\alpha$  forms to perfect  $\alpha$  forms.

**M1.00136 Tracing Poly(ethylene-oxide) Crystallization using Atomic Force Microscopy<sup>1</sup>** , XAVIER CAPALDI, SAMUEL AMANUEL, None — The early stages of nucleation and crystallization of Poly(ethylene-oxide) have been studied using Atomic Force Microscopy equipped with a heating and cooling stage. Effects of molecular weight and sample preparation techniques were studied using amplitude and frequency modulation. Mapping the viscoelastic behavior at different temperatures and has enabled the development of a relatively new technique for following the evolution of crystallization and melting of a semi-crystalline polymer.

<sup>1</sup>Tracing Poly(ethylene-oxide) Crystallization using Atomic Force Microscopy

**M1.00137 Viscoelastic Properties of Fluorinated Ethylene-Propylene (FEP) Random Copolymers<sup>1</sup>** , MEGAN CURTIN\*, BENJAMIN WRIGHT\*, Chemical and Biological Engineering, RAHMI OZISIK, Materials Science and Engineering, Rensselaer Polytechnic Institute — Fluorinated ethylene-propylene (FEP) random copolymers contain tetrafluoroethylene (TFE) and hexafluoropropylene (HFP) repeat units. FEP is an excellent alternative to poly(tetrafluoroethylene), PTFE, which cannot be melt processed due to its high molecular weight and extensive crystallinity. On the other hand, FEP is a melt processible polymer and offers similar if not the same properties as PTFE. Many studies have been performed on FEP over the years, however, the properties of these polymers strongly depend on the HFP concentration and molecular weight (distribution). Just like PTFE, FEP cannot be dissolved in many solvents, therefore, obtaining molecular weight distribution of these polymers is not possible with commonly used methods. In the current study, we perform rheological analysis of various FEPs and obtain their molecular weight distributions by employing the Tuminello method.

<sup>1</sup>This material is based upon work supported by the National Science Foundation under Grant No. CMMI-1538730. \*Undergraduate students .

**M1.00138 Thermal Properties of Trogamid by Conventional and Fast Scanning Calorimetry<sup>1</sup>** , PEGGY CEBE, JOHN MERFELD, BIN MAO, Tufts University, ANDREAS WURM, EVGENY ZHURAVLEV, CHRISTOPH SCHICK, University of Rostock — We use conventional slow scan rate differential scanning calorimetry, and fast scanning chip-based calorimetry (FSC), to investigate the crystallization and melting behavior of Trogamid, a chemical relative of nylon. Fundamental thermal properties of Trogamid were studied, including the melt crystallization kinetics, heat of fusion, and the solid and liquid state heat capacities. Using slow scan DSC (at 5 K/min), Trogamid displays a glass transition relaxation process at ~133 C, melting endotherm peak at 250 C, and is stable upon repeated heating to 310 C. When using slow scan DSC, the isothermal melt crystallization temperatures were restricted to 225 C or above. Trogamid crystallizes rapidly from the melt and conventional calorimetry is unable to cool sufficiently fast to prevent nucleation and crystal growth prior to stabilization at lower crystallization temperatures. Using FSC we were able to cool nano-gram sizes samples at 2000 K/s to investigate a much lower range of melt crystallization temperatures, from 205-225 C. The experimental protocol for performing FSC on semicrystalline polymers to obtain liquid state heat capacity data will be presented.

<sup>1</sup>National Science Foundation, Polymers Program DMR-1206010; DAAD; Tufts Faculty Supported Leave

**M1.00139 Polymer crystallization in thin films: morphology and physical properties** , GIOVANNI KELLY, JULIE ALBERT, Tulane University — Polymer crystallization has been studied both computationally and experimentally for decades, elucidating many of the mysteries surrounding crystallization kinetics and thermodynamics. However, many unanswered questions remain pertaining to the relationships between crystallization phenomena and material properties needed for specific applications that range from drug delivery and tissue engineering to optical devices and mechanically robust membranes. One of the especially interesting facets of polymer crystallization is the behavior observed when these long chain molecules are spatially confined in thin and ultrathin films. Confined geometry leads to chain configurations, and therefore thermal, mechanical, and optical properties, sometimes far removed from reported bulk values. This project aims to study the phenomena exhibited by linear semi-crystalline polymers in thin films as well as the way in which blending with homopolymers, block copolymers, and novel polymer chain architectures affect morphology, biodegradation, optical, thermal, and mechanical properties.

**M1.00140 Morphological Evolution During Tensile Deformation in Semi-Crystalline Precise Functional Copolymers via Fitting of *In Situ* Xray Scattering** , EDWARD B. TRIGG, L. ROBERT MIDDLETON, University of Pennsylvania, BRIAN S. AITKEN, University of Florida, JASON AZOULAY, DUSTIN MURTAGH, Sandia National Laboratories, KENNETH B. WAGENER, University of Florida, JOSEPH CORDARO, Sandia National Laboratories, KAREN I. WINEY, University of Pennsylvania — Morphological evolution during tensile deformation of semi-crystalline polymers is often described qualitatively. The layered crystal structures of precise copolymers, in which functional groups are bonded at precise intervals along the polymer backbone, allow for quantitative fitting of oriented X-ray scattering peaks to provide additional information. The crystallites in precise poly(ethylene-co-acrylic acid) align with the acid group layers' normal vector *parallel* to the tensile direction, while those in precise poly(ethylene-co-imidazolium bromide) align with the layers' normal vector *perpendicular* to the tensile direction. We present fits of *in situ* X-ray scattering during tensile deformation of semi-crystalline precise copolymers, to quantify the size, shape, and degree of orientation of the crystallites during the deformation process. Mathematical descriptions of the X-ray scattering in these two cases is explored, and a physical explanation for the difference in alignment direction is proposed.

**M1.00141 Probing polyethylene crystallization via simultaneous Raman scattering, rheology and microscopy** , KALMAN MIGLER, ANTHONY KOTULA, ANGELA HIGHT WALKER, NIST — The structure and rheology of polyolefins during crystallization is of critical importance to the polymer processing industry. Here we present simultaneous Raman scattering, rheological and optical microscopy measurements of crystallizing high density polyethylenes during quiescent and slow flow conditions. Raman scattering measurements during quiescent crystallization allow us to quantify three different mass fractions of chain conformers: an amorphous fraction, an orthorhombic crystalline fraction, and a fraction of chains that contain many consecutive trans bonds but are not part of the orthorhombic crystal. These non-crystalline consecutive trans (NCCT) conformers are generated as a precursor to crystallinity. Slow steady shear rates ( $1 \leq \dot{\gamma} \leq 1$ ) applied during isothermal crystallization experiments dramatically increase the crystallization rate as well as the amount of NCCT conformers produced. Optical measurements of sheared samples during crystallization reveal the formation of fiber structures that compositionally contain more NCCT conformers than the surrounding melt. The increase in the complex shear modulus commonly measured for crystallizing polyethylenes correlates with the growth of chain conformers and the appearance of spherulites within the melt.

**M1.00142 Molecular simulations of the formation of semi-crystalline structure from super-cooled polyethylene melt**, PENG YI, Johns Hopkins Univ — Formation of semi-crystalline structure is important for industrial processing, but it is scientifically poorly understood due to the strong anisotropy and the conformational flexibility of polymer chains. In this work we report the results of molecular dynamics simulations of homogeneous crystallization from polyethylene melts. A realistic united atom model was used. At room temperature (~30% supercooling), the crystal nucleation and growth lead to a stable semi-crystalline structure, with crystal lamellae separated by amorphous regions. Entanglement in the amorphous region prevents further crystal growth. The crystal-amorphous interface migrates with changing annealing temperature. Chain segments in the amorphous region adopt loop, bridge and tail conformations. Their populations and lengths were calculated and analyzed.

**M1.00143 Engineering Multi-scale Electrospun Structure for Integration into Architected 3-D Nanofibers for Cimex Annihilation: Fabrication and Mechanism Study.**, SHAN HE, LINXI ZHANG, stony brook university, YING LIU, Advanced Energy Research and Technology Center, MIRIAM RAFAILOVICH, Stony Brook University, GARCIA CENTER FOR POLYMERS AT ENGINEERED INTERFACES TEAM — In this study, engineered electrospun scaffolds with fibers oriented with designed curvature in three dimensions (3D) including the looped structure were developed based on the principle of electrostatic repulsion. Here we illustrate that 3D electrospun recycled polystyrene fibers could closely mimic the unique architectures of multi-direction and multi-layer nano-spiderweb. In contrast to virgin PS, the recycled PS (Dart Styrofoam) are known to contain zinc stearate which acts as a surfactant resulting in higher electrical charge and larger fiber curvature, hence, lower modulus. The surfactant, which is known to decrease the surface tension, may have also been effective at decreasing the confinement of the PS, where chain stretching was shown to occur, in response to the high surface tension at the air interface. Three dimensional flexible architecture with complex structures are shown to be necessary in order to block the motion of Cimex lectularius. Here we show how an engineered electrospun network of surfactant modified polymer fibers with calculated dimensions can be used to immobilize the insects. The mechanical response of the fibers has to be specifically tailored so that it is elastically deformed, without fracturing or flowing. Carefully controlling and tailoring the electrospinning parameters we can now utilize architected 3D nanofiber to create an environmental-friendly Cimex immobilization device which can lead to annihilation solution for all the other harmful insects.

**M1.00144 From Non-equilibrium to Equilibrium: Micellar Kinetics seen by Time-resolved Small-angle Scattering**, REIDAR LUND, Department of Chemistry, University of Oslo — The kinetic pathways of self-assembled nanostructures are not fully understood. Time-resolved small-angle X-ray/neutron scattering (TR-SAXS/SANS) is powerful technique<sup>1</sup> that allows kinetics processes such as nucleation processes<sup>2,3</sup> and morphological transitions<sup>4,5</sup> to be followed with structural resolution over time scales starting from milliseconds. Neutrons offer the additional advantage of facile contrast variation through H/D substitution schemes, which also allow equilibrium processes such as molecular exchange and diffusion to be studied<sup>1,6,7</sup>. Here we will highlight the current capabilities of TR-SAS and show results on the kinetics of polymeric micelles. We will address how the understanding of kinetic pathways can be used control the nanostructure.

1. Lund, R.; Willner, L.; Richter, D. Adv Polym Sci. 2013, 259, 51–158.
2. Lund, R.; et al. Phys Rev Lett. 2009, 102, 188301.
3. Jensen, et al J. S. J. Am. Chem. Soc. 2013, 135, 7214–7222.
4. Lund, R. et al . ACS Macro Lett. 2013, 2, 1082–1087.
5. Jensen, et al Angew. Chem. Int. Ed. 2014, 53, 11524–11528.
6. Lund, R. et al Phys Rev Lett. 2006, 96, 068302.
7. S. H. Choi, et al Phys Rev Lett. 2010, 104, 47802.

**M1.00145 Characterization and Molecular Simulation of Poly(p-phenylene/m-phenylene) Copolymers.**<sup>1</sup>, ROBERT BUBECK, Michigan State University, STEVEN KEINATH, Michigan Molecular Institute - Retired — Characterization and molecular simulation of the molecular structure and microstructure of poly(p-phenylene/m-phenylene) copolymers were carried out. Tensile modulus, yield stress, and entanglement molecular weight were modeled as amorphous polymers as a function of m-phenylene content. Significant biphasic character, however, was observed for two copolymers in the melt near 300°C using variable temperature synchrotron-based WAXS. The biphasic nature of the melt may be a contributor to difficulty in melt processing. Precise experimental determinations of entanglement molecular weights were frustrated by the occurrence of significant amounts of nematic mesophasic order in the rubbery and melt regimes of two commercial poly(p-phenylene/m-phenylene) examples. Nonetheless, entanglement molecular weights obtained by molecular modeling can be useful for experimental guidance because the level of order in the glassy phase near ambient temperature was found to be low (5 %) regardless of melt processing history. Based on both the modeling and WAXS measurements, it is believed that increasing m-phenylene content reduces modulus, and improves toughness and processibility.

<sup>1</sup> Beamtime at the Cornell High Energy Synchrotron Source is gratefully acknowledged.

**M1.00146 Thermal Conductivity behavior of MWCNT based PMMA and PC composites**, GIRIJA DUBEY, York College-CUNY, NY11451, PRASHANT JINDAL, University Institute of Engineering & Technology, Panjab University, 160014, India, RAJIV BHANDARI, NEHA DHIMAN, CHETAN BAJAJ, VIJAY JINDAL, Department of Physics, Panjab University, Chandigarh 160014, India — Poly methyl methacrylate (PMMA) and Polycarbonate (PC) are low cost polymer materials which can be easily transformed into desired shapes for various applications. However they have poor mechanical, thermal and electrical properties which are required to be enhanced to widen their scope of applications specifically where along with high strength, rapid heat transfer is essential. Multi Walled Carbon nanotubes (MWCNTs) are excellent new materials having extraordinary mechanical and transport properties. We will report results of fabricating composites of varying compositions of MWCNTs with PMMA and PC and their thermal conductivity behaviour using simple transient heat flow methods. The samples in disk shapes of around 2 cm diameters and 0.2 cm thickness with MWCNT compositions varying up to 10 wt% were fabricated. We found that both PMMA and PC measured high thermal conductivity with increase in the composition of CNTs. The thermal conductivity of 10wt% MWCNT/PMMA composite increased by nearly two times in comparison to pure PMMA.

**M1.00147 Rheological Properties of a Polybutadiene/Clay Nano-Composite Crosslinked via Thiol-ene Click Chemistry** , VIJESH TANNA, H. HENNING WINTER, Univ of Mass - Amherst — We have created an industrially feasible processing method to create a novel polybutadiene/clay nanocomposite. The fabrication step was designed such the final composite would be chemically crosslinked with exfoliated clay sheets dispersed randomly throughout the polymer matrix. Due to the polybutadiene's high functionality, the composite's storage modulus was shown to increase by several orders of magnitude due to crosslinking. In addition, the effect of reinforcements due to clay was shown to double the storage modulus of the composite due to the high elasticity of individual clay sheets. Surprisingly, we observed a critical crossover frequency,  $w_c$ , below which the mechanical properties, complex modulus, of the neat crosslinked polymer slightly exceed that of the composite. This transition may be due to the large lateral dimensions of the individual clay sheets, hundreds of microns, preventing a small number of crosslinks from forming. We have shown that reinforcement from both chemical crosslinks and clay significantly improves the mechanical properties of the polybutadiene/clay composite and have quantified this reinforcement over a wide range of temperatures and frequencies.

**M1.00148 Quantum Molecular Dynamics Validation of Nanocarbon Synthesis by High-Temperature Oxidation of Nanoparticles<sup>1</sup>** , CHUNYANG SHENG, KENICHI NOMURA, RAJIV KALIA, AIICHIRO NAKANO, Collaboratory for Advanced Computing and Simulations, KOHEI SHIMAMURA, FUYUKI SHIMOJO, Department of Physics, Kumamoto University, PRIYA VASHISHTA, Collaboratory for Advanced Computing and Simulations, DEPARTMENT OF PHYSICS, KUMAMOTO UNIVERSITY COLLABORATION, CACS USC COLLABORATION — High-temperature oxidation of silicon-carbide nanoparticles (nSiC) underlies a wide range of technologies from high-power electronic switches for efficient electrical grid, thermal protection of space vehicles, to self-healing ceramic nanocomposites. Here, multimillion-atom reactive molecular dynamics simulations validated by *ab initio* quantum molecular dynamics simulations predict unexpected condensation of large graphene flakes during high-temperature oxidation of nSiC. In the validation process Small nSiC in oxygen environment is chosen to perform QMD simulation, then the QMD results provide the number of Si-O and C-O bonds as a function of time and high temperature. Same RMD simulation is simultaneously performed. We compare the time evolution of different bonds, and observe the condensation of large number of C-cluster nuclei into larger carbon clusters. We further provide the QMD simulation results as an input to a genetic algorithm, which trains the RMD force field parameters, the output force field produce results that are closer to the ground truth QMD simulation results.

<sup>1</sup>This research was supported by the Department of Energy (DOE)

**M1.00149 Role of Entropic Barriers in Controlling Polymer Diffusion in Polystyrene Nanocomposites** , PHILIP GRIFFIN, WEI-SHAO TUNG, University of Pennsylvania, JEFFREY METH, Dupont, NIGEL CLARKE, University of Sheffield, RUSSELL COMPOSTO, KAREN WINEY, University of Pennsylvania — Polymer diffusion in polymer nanocomposites (PNCs) is significantly modified relative to the neat state. While it is suspected that nanoparticle-induced confinement plays a key role in the diffusion process, a detailed understanding of this process remains nonetheless elusive. We present recent studies of the temperature dependent polymer center-of-mass tracer diffusion coefficient in an athermal PNC comprising polystyrene and phenyl-capped, spherical silica NPs using elastic recoil detection. We find that the polymer tracer diffusion coefficient in the PNC relative to the bulk decreases with increasing nanoparticle concentration and is unexpectedly more strongly reduced at higher temperatures. This unusual temperature dependence of polymer diffusion in PNCs cannot be explained by the reptation model or a modified version incorporating an effective tube diameter, but instead it is the direct result of entropic free energy barriers imposed on polymer chains under confinement.

**M1.00150 Morphology and Transport Properties of Novel Polymer Nanocomposites Resulted from Melt Processing of Polyvinylacetate Substrates Coated with Layer-by-Layer Assemblies** , IMAN SOLTANI, RICHARD J. SPONTAK, North Carolina State Univ — Novel polymer nanocomposites (PNCs) were processed through layer-by-layer (LBL) deposition of clay and polyethylene terephthalate ionomer layers on polyvinylacetate (PVAc) substrates, followed by repetitive melt pressing of coated samples to crush LBL assemblies into the polymeric matrix. The increase in the clay content in resulted PNCs prepared through similar LBL coatings, relative to previously studied hydrophobic polystyrene-based nanocomposites, postulated superiority of PVAc, with relatively higher hydrophilicity, to interact with LBL assemblies. Also, these PNCs showed relatively good barrier improvement against transport of oxygen and carbon dioxide gases, proposing the scavenging effect of LBL assemblies crushed portions as highly tortuous labyrinths with high aspect ratios, comprising edge-edge flocculated exfoliated clay platelets, observed through transmission electron micrographs. However, combinative morphological investigations through optical microscopy, x-ray diffractometry, and transmission electron microscopy proposed low global dispersion of clay throughout polymeric matrix, conjecturing insufficient intensity of stress applied through cyclic melt pressing, and/or slight thermal degradation of samples via extended times of processing at high temperatures.

**M1.00151 Polymer Dynamics by Dielectric Spectroscopy** , JENNIFER ZEHNER, KARIN BICHLER, GERALD SCHNEIDER, Louisiana State University Chemistry Department — Theoretical modeling of polymer dynamics is fundamentally important to describe experimental results and to develop new materials. There are many different processes in polymers covering a very broad time range. Dielectric spectroscopy is able to cover a broad frequency range, around 10 decades. Thus many different processes can be studied and it provides a unique means to explore the processes and the time-scales. In our presentation, we emphasize how the line-shape permits to derive information on certain mechanisms. We use entangled melts and demonstrate the influence of entanglements, contour length-fluctuations and constraint release on the spectra and describe it by a theory. Furthermore, we compare it to rheology experiment and demonstrate those parts which are complimentary. We use this knowledge to achieve an advanced understanding of polymer dynamics in nanocomposites.

**M1.00152 Polymer Dynamics in Blends** , KARIN BICHLER, JENNIFER ZEHNER, GERALD SCHNEIDER, Louisiana State University Chemistry Department — Depending on their miscibility mixtures of polymers or polymers and nanoparticles tend to phase separate. Such systems are of fundamental interest. For example, in case of a blend of two polymer melts a dynamic asymmetry may be generated. It could slow down the chains in one phase or accelerate the chains in the other phase. Due to their heterogeneity these systems are of fundamental interest. Using a certain technique it is very challenging to access all of the information necessary to understand the materials and the interplay between different phases. In order to enhance our understanding, we apply dielectric spectroscopy, scattering experiments and atomic force microscopy to reveal both structure and dynamics and to unravel the fascinating processes.

**M1.00153 Nonadiabatic Dynamical Studies of Lead Chalcogenide Quantum Dots (Pb<sub>16</sub>X<sub>16</sub>; X = S, Se, Te) Passivated with thin Cadmium Chalcogenide Shells** , PATRICK TAMUKONG, SVETLANA KILINA, North Dakota State University — DFT and TDDFT studies of Pb<sub>16</sub>X<sub>16</sub>/Cd<sub>52</sub>Y<sub>52</sub> (X, Y = S, Se, Te) Core/Shell quantum dots (QDs) have been performed to assess their ground (i.e., the optimized geometries, density of states, projected density of states, and optical absorption spectra), and excited state properties. Most of the heterostructures were analyzed for the first time (e.g., Pb<sub>16</sub>S<sub>16</sub>/Cd<sub>52</sub>Te<sub>52</sub> and Pb<sub>16</sub>Te<sub>16</sub>/Cd<sub>52</sub>Se<sub>52</sub>). The thin shell core/shell QDs proved to be largely borderline type II with much similarity between QDs containing Cd<sub>52</sub>S<sub>52</sub> and Cd<sub>52</sub>Se<sub>52</sub> shells, whereas core/shell QDs with a Cd<sub>52</sub>Te<sub>52</sub> shell appeared to be borderline type-I. Nonadiabatic DFT-based dynamics, coupled with the surface hopping method, have been done to investigate fates of excited electrons or holes in these systems.

**M1.00154 Emergent Magnetism in Mesoporous Materials**, SHER ALAM, KEK Accelerator Lab, AJAYAN VINU, University of Queensland — We discuss the emergence of magnetism in Mesoporous Materials. We have obtained experimental results showing a variety of magnetic behaviors arising, by using different types of mesoporous or nanoporous templates. Since the templates allow different magnetic properties to arise naturally we have dubbed this as dynamic templating method. Our procedure and realization incidentally demonstrates the idea of Nanoarchitectonics proposed by Aono, as a MANA concept. Which, simply means to allow different nano-blocks to interact to obtain a certain desired structure and properties.

**M1.00155 Using Self-Similarity to Simulate Meniscus Evolution Around TMV Due to Surface Diffusion**<sup>1</sup>, RICHARD POTTER, YUE ZHANG<sup>2</sup>, ZAHRA FAKHRAAI<sup>3</sup>, Univ of Pennsylvania — It has been hypothesized that enhanced surface diffusion allows the formation of stable molecular glasses during physical vapor deposition. The improved properties of these glasses, such as increased density and kinetic stability can help improve material properties in pioneering fields of technology such as organic electronics and pharmaceutical drug delivery. While surface diffusion has been measured previously on the surfaces of organic glasses, direct measurements on the surface of vapor-deposited stable glasses has proven more challenging. This research focuses on a straightforward method for measuring the surface diffusion coefficients of molecular glasses through the use of tobacco mosaic virus (TMV) nanorods as probe particles. In conjunction, mathematical models based on the thin film equation were used to simulate fast meniscus formation around the nanorods on the glassy surface. The evolution of the meniscus is self-similar, which allows quick quantification of the diffusion coefficient, by solving the time evolution for a single experiment. Experimental data were compared and fit to these simulations to derive a quantity for the surface diffusion coefficient,  $D_s$ .

<sup>1</sup>NSF-CAREER DMR-1350044

<sup>2</sup>Co-author

<sup>3</sup>Corresponding Author

**M1.00156 Interfacial damping properties of polymeric composites: Effect of interfacial strength**, YAPING HUANG, Nanyang Institute of Technology — Experimental studies on interfacial properties of polymeric composites, such as glass transition temperature, showed that the interfacial strength was critical. Numerical studies could also predict interfacial properties based on interfacial strength. In this study, interfacial damping properties and interfacial strength of fiber based polymeric composites were measured by dynamic mechanical tests and micro-bond tests, respectively, with the objective of quantitative analysis. Properties of polymers, varying from polar to non-polar, from amorphous to semi-crystalline, from low molecular weight to high molecular weight, were investigated. The results showed supportive predictions about interfacial damping properties of fiber based polymeric composites.

**M1.00157 Equilibrium flattening process of irreversibly adsorbed polymer chains on a solid**<sup>1</sup>, MANI SEN, Materials Science and Engineering (MSE), Stony Brook University (SBU), NY, NAISHENG JIANG, MAYA ENDOH, TADANORI KOGA, MSE, SBU, DAISUKE KAWAGUCHI, KEIJI TANAKA, Kyushu University, Japan — We here report the equilibrium process of adsorbed polymer chains on a solid by sum frequency generation (SFG) spectroscopy. Polystyrene (PS,  $M_w = 290$  kDa) thin films prepared onto quartz prisms (a weakly attractive system) were used as a model system. Spin-cast PS 50 nm films on quartz surface (QS) were annealed at  $150\text{ }^\circ\text{C} > T_g$  for up to 100 h and subsequently rinsed with chloroform to derive the “flattened chains” that lie flat onto the substrate surface. The SFG results for the “matured” flattened chains after annealing for 96 h revealed the strong interfacial orientation of the backbone chains and weak orientation of PS phenyl rings at the QS which is in contrast to a PS spin-cast film annealed at  $150\text{ }^\circ\text{C}$  for 1 h: the phenyl rings were strongly directed toward the QS, while the backbone chains were weakly orientated at the QS. We postulate that the increase in the number of solid/segment contacts of the backbone chains is the driving force for this equilibrium flattening process. We will also discuss the generality of this flattening process by using solvent-cast PS thin films where the chains are randomly oriented near the QS.

<sup>1</sup>Acknowledgement: NSF Grant No. CMMI-1332499.

**M1.00158 Phase Transitions of 2-Decanol in Nano Pores**<sup>1</sup>, SAMUEL AMANUEL, JASON TURNER, CALEB NOVINS, ALEXANDER CLAIN, Dept. of Phys & Astro., Union College — We studied the melting of 2-decanol confined in nano pores, 10-100 nm, using a power-compensated Differential Scanning Calorimeter (DSC). The melting temperature of the nano confined 2-decanol decreases as pore size decreases and a linear relationship is observed between the melting temperature and the inverse of the pore size. This is in agreement with the Gibbs-Thomson prediction. In addition, the apparent heat of fusion of the 2-decanol confined in the nano pores appears to decrease as the size of the pores decreases. However, the apparent heat of fusion of the nano confined 2-decanol may not necessarily be its true heat of fusion. Annealing, for instance, increases the apparent heat of fusion by as much as 26%. A correction or alternate procedure should be employed to extract the true heat of fusion from DSC measurements, especially when the physical size of the sample is in nano scale or the sample possesses a large surface area to volume ratio.

<sup>1</sup>This work was partially supported by NSF-DMR: 1229142.

**M1.00159 Heat of fusion of primary alcohol confined in Nano pores.**<sup>1</sup>, HARRISONN GRIFFIN, SAMUEL AMANUE, Dept. of Phys. & Astro., Union College — Melting behavior of physically confined 1-decanol in nano porous silica was probed using a Differential Scanning Calorimeter (DSC). In agreement with the Gibbs-Thompson prediction, we observe that the melting temperature of the confined 1-decanol scales inversely with the physical size of the pores. Contrary to the assumption used in developing the Gibbs-Thompson equation, however, the apparent heat of fusion decreases as the pore size decreases. Previously, several models have been proposed where the interfacial layer/s of molecules do not participate in the phase transition and thereby would not contribute to the heat of fusion. While these could reconcile the seeming contradiction, annealing the nano confined materials enables some of the interfacial layers to be incorporated into an existing crystal. This leads to an increase in the apparent heat of fusion and a systematic relationship exists between the annealing temperature and the increase in the apparent heat of fusion.

<sup>1</sup>This work was partially supported by NSF-DMR: 1229142.

**M1.00160 Structure and Dynamics of Polymers in Cylindrical Nanoconfinement: A Molecular Dynamics Study**, JAMES PRESSLY, ROBERT RIGGLEMAN, KAREN WINEY, Univ of Pennsylvania — The structure and dynamics of polymers under nanoconfinement is critical for understanding how polymers behave in applications from hydraulic fracking to fabricating integrated circuits. We previously used simulations to explore the effect of the diameter of cylindrical pores ( $d = 10-40\sigma$ , where  $\sigma$  is the unit length in reduced units) on polymer end-to-end distance ( $R_{ee,perp}$ ,  $R_{ee,par}$ ), entanglement density, melt diffusion coefficient ( $D$ ), and local relaxation time ( $\tau_{perp}$ ,  $\tau_{par}$ ) at fixed polymer chain length ( $N = 350$ ). These studies found  $D$ ,  $R_{ee,par}$ , and  $\tau_{perp}$  increased with increasing confinement while entanglement density,  $R_{ee,perp}$ , and  $\tau_{par}$  decreased. Experiments also found that  $D$  increased but to a lesser extent. Here, we examine the molecular weight dependence of these properties using  $N = 25, 50, 100, 200, 350$ , and 500 confined to pores of diameter  $14\sigma$  to examine a range of confinements. Our preliminary results show that as  $N$  increases  $D$  and  $R_{ee,par}$  increase as well, relative to the unconfined state, while entanglement density and  $R_{ee,perp}$  decrease, consistent with our previous work. Interestingly,  $\tau$  is shown to be independent of chain length indicating the impact of confinement imposed by reducing pore diameter is distinct from that imposed by increasing chain length.

## **M1.00161 Man-made Earthquakes & Multifractals in Neutral Fluid Turbulence/Injection<sup>1</sup>**

WH- MAKSOED<sup>2</sup>, Prodi of Physics UI, Depok 16424- INDONESIA — Man-made earthquakes coincides with induced seismicity: "typically minor earthquakes & tremors that are caused by human activity that alters the stresses & Strains on the earth crust" [Wikipedia: "induced seismicity"]. For these, RD Andrews wrote: "Based on observed seismicity rate & geographical trends following major oil & gas plays with large amounts of produced water, the rates & trends in seismicity are very unlikely to represent a naturally occurring process". "The Prague, Oklahoma, earthquake sequence of 2011, along the Wilzetta faults zone, included the significant foreshock, a main shock of magnitude 5.7, it has been suggested that this sequence represent earthquakes triggered by fluid injection/natural fluid turbulence shows multifractal characteristics, of [405]-325-7968 of Dr. G. Randy Keller to UI tuitions of @ Rp. 29, 405, 000.00.

<sup>1</sup>Acknowledgements to HE. Mr. H. TUK SETYOHADI, Jl. Sriwijaya Raya 3, South-Jakarta, INDONESIA

<sup>2</sup>of Rabi & Heisenberg hamiltonian oughts to relates to Chris King: "Neurofractal dynamics"

## **M1.00162 FLUIDS —**

### **M1.00163 Chemically generated convective transport in microfluidic system**

OLEG SHKLYAEV, Department of Chemical Engineering, The University of Pittsburgh, SAMBEETA DAS, ALICIA ALTEMOSE, Department of Chemistry, The Pennsylvania State University, HENRY SHUM, ANNA BALAZS, Department of Chemical Engineering, The University of Pittsburgh, AYUSMAN SEN, Department of Chemistry, The Pennsylvania State University — High precision manipulation of small volumes of fluid, containing suspended micron sized objects like cells, viruses, and large molecules, is one of the main goals in designing modern lab-on-a-chip devices which can find a variety of chemical and biological applications. To transport the cargo toward sensing elements, typical microfluidic devices often use pressure driven flows. Here, we propose to use enzymatic chemical reactions which decompose reagent into less dense products and generate flows that can transport particles. Density variations that lead to flow in the assigned direction are created between the place where reagent is fed into the solution and the location where it is decomposed by enzymes attached to the surface of the microchannel. When the reagent is depleted, the fluid motion stops and particles sediment to the bottom. We demonstrate how the choice of chemicals, leading to specific reaction rates, can affect the transport properties. In particular, we show that the intensity of the fluid flow, the final location of cargo, and the time for cargo delivery are controlled by the amount and type of reagent in the system.

### **M1.00164 Flow reversal in enzymatic microfluidic pumps**

HENRY SHUM, University of Pittsburgh, ISAMAR ORTIZ-RIVERA, ARJUN AGRAWAL, AYUSMAN SEN, Pennsylvania State University, ANNA BALAZS, University of Pittsburgh — A chemical reaction occurring at an enzyme-covered patch in a closed fluid chamber generates local solute concentration gradients and, hence, fluid density gradients. This has recently been shown to drive fluid flows with speeds of the order of microns per second. We develop and analyze a model that accounts for fluid density changes due to consumption of the reaction substrate and accumulation of products for such a fluid pump based on the enzyme urease. Hydrolysis of urea by urease produces ammonium bicarbonate, which leads to a net increase in solution density. Higher density fluid is expected to sink and spread horizontally away from the pump. Modeling reveals, however, that the local fluid density is not necessarily greatest near the pump and fluid flow can even reverse in direction after some time. The qualitative behavior depends on two dimensionless parameters, the ratio of solutal expansion coefficients and the ratio of diffusion coefficients for the reaction substrate and product. The predicted reversal of pumping direction is experimentally verified and we show that the direction of pumping also depends on the amount of enzyme present on the patch. A better understanding of these pumps will aid in the design of responsive, chemically powered microfluidic flow control.

### **M1.00165 Phase transitions analogy for cavity flows.**

PETRU FODOR, MIRON KAUFMAN, Physics, Cleveland State University — The fluid flow in cavity type systems, in which one of the walls is moving while the others are stationary, is analyzed using computational modeling, under the assumption of no-slip boundary conditions. By iteratively adapting the mesh used, we are able to map with high spatial resolution the complex flow structures that form at the two types of corners of the cavity, i.e. (i) corners defined by stationary walls, and (ii) corners defined by a stationary and the moving wall, respectively. For the structures that form in the vicinity of the fixed points defined by the corners, we observe that the flow magnitudes and spatial distributions follow scaling laws similar with critical phenomena. In particular, the behavior at the first type of corner is analogous to a first-order transition (discontinuity) point, while the behavior at the second one is analogous to a thermodynamic critical point (second-order transition). These results provide a unique insight into the solution to Navier-Stokes equations for cavity flows.

### **M1.00166 A Statistical investigation of sloshing parameters for multiphase offshore separators**

MD MAHMUD<sup>1</sup>, Lamar University, RAFIQU KHAN<sup>2</sup>, Cameron Corp, QIANG XU<sup>3</sup>, Lamar University — Liquid sloshing in multiphase offshore separators has been the subject of intense investigations for last several decades both by experiments and simulations. Large number scientists have worked to minimize sloshing impacts and others have developed new methods to describe the sloshing patterns. In addition, complex mathematical models are developed to characterize sloshing phenomenon. However, a comprehensive statistical study of the input parameters and output results is yet to be done. In this study, statistical approaches will be considered to determine the significant parameters for liquid sloshing. The factor analysis and principal component analysis techniques are considered to identify the significant parameters for liquid sloshing. Numerical experiments are carried out through Computation Fluid Dynamics (CFD) technique using ANSYS Fluent software. The input parameters considered here are liquid depth/length ratio, acceleration, wave frequencies, amplitudes in various sea state conditions. The measured variables include hydrodynamic force, pressure, moments, turbulent kinetic energy, height of interfaces. Mathematical correlations may be developed from the data analysis.

<sup>1</sup>Graduate Student Dept of Chemical Eng, Lamar University, Beaumont, TX 77710

<sup>2</sup>ETCL Principal Engineer Cameron Corp, 4901 W Sam Houston Pkway, Houston, TX

<sup>3</sup>Associate Prof Dept of Chemical Eng Lamar University

### **M1.00167 Efficient Combustion Simulation via the Adaptive Wavelet Collocation Method**

KEVIN LUNG, ERIC BROWN-DYMKOSKI, VICTOR GUERRERO, ERIC DORAN, KEN MUSETH, JO BALME, BOB URBERGER, ANDRE KESSLER, STEPHEN JONES, BILLY MOSES, ANTHONY CROGNALE, Space Exploration Tech (SpaceX) — Rocket engine development continues to be driven by the intuition and experience of designers, progressing through extensive trial-and-error test campaigns. Extreme temperatures and pressures frustrate direct observation, while high-fidelity simulation can be impractically expensive owing to the inherent multi-scale, multi-physics nature of the problem. To address this cost, an adaptive multi-resolution PDE solver has been designed which targets the high performance, many-core architecture of GPUs. The adaptive wavelet collocation method is used to maintain a sparse-data representation of the high resolution simulation, greatly reducing the memory footprint while tightly controlling physical fidelity. The tensorial, stencil topology of wavelet-based grids lends itself to highly vectorized algorithms which are necessary to exploit the performance of GPUs. This approach permits efficient implementation of direct finite-rate kinetics, and improved resolution of steep thermodynamic gradients and the smaller mixing scales that drive combustion dynamics. Resolving these scales is crucial for accurate chemical kinetics, which are typically degraded or lost in statistical modeling approaches.

**M1.00168 Dual-Mode Measurement and Theoretical Analysis of Evaporation Kinetics of Binary Mixtures**<sup>1</sup>, HANYU SONG, Mechanical Engineering, University of Connecticut, CHI-RUEI HE, Chemical Engineering, National Chung Hsing University, CARL BASDEO, JI-QIN LI, DEZHUANG YE, Mechanical Engineering, University of Connecticut, DEVENDRA KALONIA, School of Pharmacy, University of Connecticut, SI-YU LI, Chemical Engineering, National Chung Hsing University, TAI-HSI FAN, Mechanical Engineering, University of Connecticut — Theoretical and experimental investigations are presented for the precision measurement of evaporation kinetics of binary mixtures using a quartz crystal resonator. A thin layer of light alcohol mixture including a volatile (methanol) and a much less volatile (1-butanol) components is deployed on top of the resonator. The normal or acoustic mode is to detect the moving liquid-vapor interface due to evaporation with a great spatial precision on the order of microns, and simultaneously the shear mode is used for in-situ detection of point viscosity or concentration of the mixture near the resonator. A one-dimensional theoretical model is developed to describe the underlying mass transfer and interfacial transport phenomena. Along with the modeling results, the transient evaporation kinetics, moving interface, and the stratification of viscosity of the liquid mixture during evaporation are simultaneously measured by the impedance response of the shear and longitudinal waves emitted from the resonator. The system can be used to characterize complicated evaporation kinetics involving multi-component fuels.

<sup>1</sup>American Chemical Society Petroleum Research Fund, NSF CMMI-0952646

## **M1.00169 SOFT CONDENSED MATTER —**

**M1.00170 Spin-resolved conductance of Dirac electrons through multibarrier arrays**, DIPENDRA DAHAL, Graduate Center and Hunter College of City University of New York, 695 Park Avenue, New York, NY 10065, USA, GODFREY GUMBS, Hunter College of City University of New York, 695 Park Avenue, New York, NY 10065, USA, ANDRII IUROV, Center for High Technology Materials, University of New Mexico, Albuquerque, NM 87106, USA — We use a transfer matrix method to calculate the transmission coefficient of Dirac electrons through an arbitrary number of square potential barrier in gapped monolayer graphene (MLG) and bilayer graphene (BLG). The widths of barriers may not be chosen equal. The shift in the angle of incidence and the width of the barrier required for resonance are investigated numerically for both MLG and BLG. We compare the effects due to energy gap on these two transmission coefficient for each of these two structures (MLG and BLG). We present our results as functions of barrier width, height as well as incoming electron energy as well as band gap and examine the conditions for which perfect reflection or transmission occurs. Our transmission data are further used to calculate conductivity.

**M1.00171 Dielectric Screening Response of a Plasmonic "Sandwich"**, N.J.M. HORING, Department of Physics and Engineering Physics, Stevens Institute of Technology, Hoboken, NJ 07030, GODFREY GUMBS, DIPENDRA DAHAL, Department of Physics and Astronomy, Hunter College, CUNY, New York, NY 10065, ANDRII IUROV, Center for High Technology Materials, University of New Mexico, Albuquerque, NM 87106 — We have formulated the RPA integral equation for a system composed of two identical semi-infinite metallic plasmas with planar bounding surfaces at  $z = \pm d/2$ . The gap between the two metallic bulk plasmas contains a two-dimensional semiconductor plasma at  $z=0$ . This equation for the inverse dielectric function is solved analytically in position representation for a narrow gap, yielding an explicit formula for the inverse dielectric screening function in terms of the nonlocal 2D semiconductor polarizability and the bulk metallic polarizability, the latter well approximated in the local limit. Based on this solution, we have evaluated the nonlocal plasmon dispersion relation computationally, taking Graphene as the 2D semiconductor plasma. The associated nonlocal Graphene plasmon spectrum coupled to the sandwich system is exhibited in 3D plots, which show a linear mode and another displaced from the bulk plasma frequency.

**M1.00172 EM Wave Transmission through a Nano-hole in a Plasmonic Layer**, DESIRE DESIRE MIESSEIN, NORMAN J. MORGENSTERN HORING, HARRY LENZING, Department of Physics and Engineering Physics, Stevens Institute of Technology, Hoboken, NJ 07030, GODFREY GUMBS, Department of Physics and Astronomy, Hunter College, CUNY, New York, NY 10065 — We examine the role of the angle of incidence of an incoming EM wave in its transmission through a subwavelength nano-hole in a thin semiconductor plasmonic layer. Fully detailed calculations and results are exhibited for p- and s-polarizations of the incident wave for a variety of incident angles in the near, middle and far zones of the transmitted radiation. Our dyadic Greens function formulation includes both (1) the electromagnetic field transmitted directly through the 2D plasmonic layer and (2) the radiation emanating from the nano-hole. Interference fringes due to this superposition are explicitly exhibited. Based on an integral equation formulation, this dyadic Greens function approach does not involve any appeal to metallic boundary conditions. It incorporates the role of the 2D plasmon of the semiconductor layer, which is smeared due to its lateral wave number dependence. We find that the interference fringes, which are clustered near the nano-hole, flatten to a uniform level of transmission directly through the sheet alone at large distances from the nano-hole.

**M1.00173 Modeling heterogeneous polymer-grafted nanoparticle networks**, TAO ZHANG, BADEL MBANGA, VICTOR YASHIN, ANNA BALAZS, Chemical Engineering Department, University of Pittsburgh, Pennsylvania 15261, USA — Via a dynamic 3D computational approach, we simulate the heterogeneous polymer-grafted nanoparticle networks. The nanoparticles rigid cores are decorated with a corona of grafted polymers, which contain reactive functional groups at the chain ends. With the overlap of grafted polymers, these reactive groups can form weak labile bonds, which can reform after breakage, or stronger bonds, which rupture irreversibly and thus, the nanoparticles are interconnected by dual cross-links. Previous work has been done on homogeneous networks, while we introduce the heterogeneity by considering two types of particles having different reactive functional groups, so that the labile bond energy varies depending on types of the two end reactive groups. We study the effect of tensile and rotational deformations on the network morphology, and observe, in particular, the phase separation of two types of particles. Our results will provide guidelines for designing transformable material that can controllably change structure under mechanical action.

**M1.00174 Adhesion of Particulate Materials to Mesostructured Polypyrrole**, DARBY HOSS, Purdue University, ROBERT KNEPPER, PETER HOTCHKISS, ALEXANDER TAPPAN, Sandia National Laboratories, BRYAN BOUDOURIS, STEPHEN BEAUDOIN, Purdue University — Interactions based on van der Waals (vdW) forces will influence the performance and reliability of mesostructured polypyrrole swabs used for the collection and detection of trace particles. The vdW adhesion force between materials is described by the Hamaker constant, and these constants are measured via optical and dielectric properties (i.e., according to Lifshitz theory), inverse gas chromatography (IGC), and contact angle measurements. Here, contact angle measurements were performed on films of several common materials and used to estimate Hamaker constants. This, in turn, will allow for the tuning of the design properties associated with the polypyrrole swabs. A comparison of these results to Hamaker constants estimated using Lifshitz Theory and IGC reveals the fundamental behavior of the materials. The Hamaker constants were then used in a new computational vdW adhesion model. The idealized model describes particle adhesion to an array of mesostructures. This model elucidates the importance of where the particle makes contact with the mesostructure and the independence of vdW forces generated by each mesostructure. These results will facilitate the rational design of polypyrrole swabs optimized for harvesting microscale particles of trace materials.

**M1.00175 Droplet Dynamics of a Flowing Emulsion System**, OLIVIA CYPULL, KLEBERT FEITOSA, James Madison University — The inner workings of glassy systems have long been a topic of interest for soft material scientists. Similarities between the jamming behavior of emulsions and the glass transition of glassy systems have prompted the conjecture that they might share the same underlying mechanism. Here we study a dense oil-in-water emulsion system forced to flow through a narrow microchannel. By matching the index of refraction of the two phases, we image the internal dynamics of the droplets in a confocal microscope. At low velocity speeds, we find that the velocity along the edge of the microchannel was not significantly different than then the average droplet velocity in the bulk suggesting a near plug flow. By contrast the droplets near the edge experienced more movement perpendicular to the flow indicating the fluidization effect of the confining walls.

**M1.00176 Self-assembly in Dipolar Fluids<sup>1</sup>**, MICHELA RONTI, SOFIA KANTOROVICH, Univ of Vienna — We are studying low temperature structural transitions in dipolar hard spheres (DHS), combining grand-canonical Monte Carlo simulations and direct analytical theoretical calculations. DHS is characterized by long-range anisotropic interactions: it consists of a point dipole at the center of a hard sphere. We are interested in low temperature and low density phase behaviour of DHS systems. From a theoretical point of view the process of self-assembly is not responsible for a phase transition; this belief was completely reverted by theoretical studies showing that the process of self-assembly is alone capable to induce phase transition. On the other hand in the last years it was proved that no sign of critical behaviour is observed, implementing efficient and tailored Monte Carlo algorithms. Moreover a theoretical approach based on Density Functional Theory was developed: a series of structural transitions were discovered providing evidence of a hierarchy in the structures on cooling. We are performing free-energy calculations in order to draw the phase diagram of DHS model. Comparing the numerical results with the theoretical ones shed light on the scenario of temperature induced structural transitions in magnetic nanocolloids.

<sup>1</sup>ETN-COLLDENSE (H2020-MCSA-ITN-2014, Grant No. 642774)

**M1.00177 Deconvolution of the role of metal and pH in metal coordinating polymers.<sup>1</sup>**, SETH CAZZELL, NIELS HOLTEN-ANDERSEN, Massachusetts Inst of Tech-MIT — Nature uses metal binding amino acids to engineer both mechanical properties and structural functionality. Some examples of this metal binding behavior can be found in both mussel foot protein and DNA binding protein. The mussel byssal thread contains reversible intermolecular protein-metal bonds, allowing it to withstand harsh intertidal environments. Zinc fingers form intramolecular protein-metal bonds to stabilize the tertiary structure of DNA binding proteins, allowing specific structural functionality. Inspired by both these metal-binding materials, we present mechanical and spectroscopic characterization of a model polymer system, designed to mimic this bonding. Through these studies, we are able to answer fundamental polymer physics questions, such as the role of pH and metal to ligand ratio, illuminating both the macroscopic and microscopic material behavior. These understandings further bio-inspired engineering techniques that are used to design viscoelastic soft materials.

<sup>1</sup>I was supported by the Department of Defense (DoD) through the National Defense Science & Engineering Graduate Fellowship (NDSEG) Program.

**M1.00178 Optically induced thermal response of Chlorophyll for biomedical applications**, CHIAWEI TU, SADAT MD EHSAN, YUAN ZHAO, DONGLU SHI, DAVID MAST, Univ of Cincinnati — The heating behavior of Chlorophyll was investigated for possible use in hyperthermia cancer treatments. One measure of hyperthermia effectiveness is the Specific Absorption Rate (SAR) defined as the initial slope of the sample heating behavior, however, for nanoparticle (NP) loaded samples, this initial heating rate is often limited by heat transfer mechanisms from the NPs to the surrounding material and not the initial NP heating. This is especially true for water-based, NP loaded tissue surrogates. Organic solvent dispersed NP loaded samples face the additional problem of heating rate variations due to solvent evaporation effects. We report on measurements of the initial optical heating rates of Chlorophyll and deposited directly on small, Pt thin film resistance temperature detectors (RTDs). Solid state lasers (638 nm and 655 nm) were used to illuminate these samples at different intensities and at specific wavelengths associated with peaks (662 nm) in Chlorophyll's UV-VIS optical absorption spectra while recording the RTD resistance at 0.1 second intervals. This technique significantly reduce evaporation errors we had experienced and has the potential to directly measure the heating behavior of Chlorophyll based NP materials.

**M1.00179 Directed percolation identified as equilibrium pre-transition towards non-equilibrium arrested gel states**, MARCO LAURATI, RONJA CAPELLMANN, MATTHIAS KOHL, STEFAN EGELHAAF, MICHAEL SCHMIEDEBERG, University of Düsseldorf — The macroscopic properties of gels arise from their slow dynamics and load bearing network structure, which are exploited by nature and in numerous industrial products. However, a link between these structural and dynamical properties has remained elusive. Here we present confocal microscopy experiments and simulations of gel-forming colloid-polymer mixtures with competing interactions. They reveal that gel formation is preceded by continuous and directed percolation. Both transitions lead to system spanning networks, but only directed percolation results in extremely slow dynamics, ageing and a shrinking of the gel that resembles syneresis. Therefore, dynamical arrest in gels is found to be linked to a structural transition, namely directed percolation, which is quantitatively associated with the mean number of bonded neighbours. Directed percolation is a universality class of transitions out of equilibrium, our study hence connects gel formation to a well-developed theoretical framework which now can be exploited to achieve a detailed understanding of arrested gels.

**M1.00180 Novel coarse-graining approach for Star polymer and linear Homopolymer mixtures**, EMANUELE LOCATELLI, CHRISTOS LIKOS, University of Vienna — We present a novel coarse-graining approach, suitable for star polymer mixtures. The approach is based on the calculation of the effective interaction between a star polymer and a single monomer, which can be used to coarse-grain the interaction between a star and a complex object. The effective interaction has been calculated numerically for star polymers of different functionalities  $f$  and for different degrees of polymerization  $N$ . We find that these potentials can be scaled following the star polymer scaling laws. We test our approach, calculating the effective interaction between a star polymer and a linear homopolymer, comparing the results obtained from coarse graining and monomer resolved simulations. We employ this technique to study star - linear homopolymer mixtures, focusing on the limit of very long homopolymers.

**M1.00181 A simple depth-averaged model for dry granular flow**, CHI-YAO HUNG, National Taiwan University, COLIN P. STARK, Lamont-Doherty Earth Observatory, Columbia University, HERVÉ CAPART, National Taiwan University — Granular flow over an erodible bed is an important phenomenon in both industrial and geophysical settings. Here we develop a depth-averaged theory for dry erosive flows using balance equations for mass, momentum and (crucially) kinetic energy. We assume a linearized GDR-Midi rheology for granular deformation and Coulomb friction along the sidewalls. The theory predicts the kinematic behavior of channelized flows under a variety of conditions, which we test in two sets of experiments: (1) a linear chute, where abrupt changes in tilt drive unsteady uniform flows; (2) a rotating drum, to explore steady non-uniform flow. The theoretical predictions match the experimental results well in all cases, without the need to tune parameters or invoke an ad hoc equation for entrainment at the base of the flow. Here we focus on the drum problem. A dimensionless rotation rate (related to Froude number) characterizes flow geometry and accounts not just for spin rate, drum radius and gravity, but also for grain size, wall friction and channel width. By incorporating Coriolis force the theory can treat behavior under centrifuge-induced enhanced gravity. We identify asymptotic flow regimes at low and high dimensionless rotation rates that exhibit distinct power-law scaling behaviors.

**M1.00182 A Computational Study of the Growth of Hexagonal Ice.**, MAXWELL FULFORD, King's College London, UK, MATTEO SALVALAGLIO, UCL, UK, MICHELE PARRINELLO, ETH Zurich; USI Lugano, CARLA MOLTENI, King's College London, UK — Hexagonal ice (Ih) has two distinct crystallographic surfaces; a basal and prism surface. At low vapour pressures, Ih forms thin plates and elongated prisms, depending on the temperature. The macroscopic shape depends on the relative rate of growth of the basal and prism surfaces. The aim of our research is to estimate the relative rate of growth of the two surfaces for a range of temperatures and ultimately predict the shape of Ih, using computer simulations. Our simulations show the well-known phenomenon that the surface of ice lowers its interfacial free energy by forming a stable quasi-liquid layer (QLL). The QLL mediates crystal growth and has a thickness which varies with temperature and crystallographic surface. We use a combination of Molecular Dynamics and Metadynamics to study how the interfacial structure at the ice/quasi-liquid and quasi-liquid/vapour interfaces influence the adsorption potential, surface transport properties and growth shape..

**M1.00183 The mystery of Coulomb friction in sediment transport**<sup>1</sup>, THOMAS PHTZ, Ocean College, Zhejiang University, ORENCIO DURAN, MARUM-Center for Marine Environmental Sciences, University of Bremen — Nearly all analytical models of sediment transport in Newtonian fluid (e.g., air or water) are based on Bagnold's assumption of a constant Coulomb friction coefficient (particle-shear-pressure-ratio,  $\mu$ ) at the interface ( $z_b$ ) between sediment bed and transport layer. In fact, this assumption is the main reason why these models predict the sediment load (and subsequently the sediment transport rate) to be proportional to the excess shear stress ( $\tau - \tau_t$ ), a scaling which has been confirmed in many wind-tunnel and flume experiments. Attempts to explain why  $\mu(z_b)$  is constant have usually been based on the sliding-friction analogy or rheology arguments. However, here we analytically derive  $\mu(z_s) \approx \sqrt{3} - 1$ , where  $z_s$  is the location at which the production rate of particle fluctuation energy is maximal. Our derivation is based on the assumption that the rate of collisional transfer of horizontal into vertical kinetic energy is typically much larger than the rate of energy dissipation. Using state-of-the-art numerical simulations of sediment transport in Newtonian fluid, we validate all assumptions and approximation involved in our derivation. Interestingly, the location  $z_s$  can significantly deviate from  $z_b$  depending on the simulated conditions.

<sup>1</sup>We acknowledge support from grants National Natural Science Foundation of China (Nos. 1151101041 and 41376095) and Natural Science Foundation of Zhejiang Province (No. LR16E090001).

**M1.00184 Core formation by porous flow allowed by hysteresis in melt network topology**, SOHEIL GHANBARZADEH, MARC HESSE, MASHA PRODANOVIC, The University of Texas at Austin — The formation of the core via percolation is an attractive process to form planetary cores early in the planets evolution. There is currently a debate whether the ratio of interfacial forces between solid-solid and solid-liquid interfaces, imposing the dihedral angle between the solid grains and the pore fluid, in an olivine-melt matrix allows the formation of a percolating network. We present first computations of equilibrium melt distributions in realistic irregular grains and show that the percolation threshold at dihedral angles above 60 degrees is significantly larger than those previously reported for simple geometries. However, given typical compositions of the terrestrial planets initial porosities after the onset of melting of iron are large, 20-40threshold to form a connected melt network. As the porosity decreases due to melt segregation the network remains connected and allows core formation by porous flow. Only as the porosities approach 1and the iron become isolated in pockets along triple junctions. This residual iron may provide an explanation for the formation of dense layers near the core mantle boundary such as "

**M1.00185 Spontaneous Pattern Formation of Surface Nanodroplets from Competitive Growth**, DETLEF LOHSE, University of Twente, SHUHUA PENG, XUEHUA ZHANG, RMIT, Melbourne — Nanoscale droplets on a substrate are of great interest because of their relevance for droplet-based technologies for light manipulation, lab-on-chip devices, miniaturised reactors, encapsulation and many others. In this work, we establish a basic principle for the symmetrical arrangement of surface nanodroplets during their growth under simple flow conditions. In our model system, nanodroplets nucleate at the rim of spherical cap microstructures on a substrate, due to a pulse of oversaturation is supplied by a solvent exchange process. We find that, while growing at the rim of the microcap, the nanodroplets self-organise into highly symmetric arrangements, with respect to position, size, and mutual distance. The angle between the neighbouring droplets is four times the ratio between the base radii of the droplets and the spherical caps. We show and explain how the nanodroplets acquire the symmetrical spatial arrangement during their competitive growth and why and how the competition enhances the overall growth rate of the nucleated nanodroplets. This mechanism behind the nanodroplet self-organisation promises a simple approach for the location control of droplets with a volume down to attoliters.

**M1.00186 Decoupling between Diffusivity and Effective Viscosity in Poly(isobutyl methacrylate) Films with a Thickness-Independent Glass Transition**<sup>1</sup>, KUN GENG, Boston University Physics Department, REIKA KATSUMATA, University of Texas at Austin, McKetta Department of Chemical Engineering, XUANJI YU, Boston University Division of Materials Science and Engineering, HEONJOO HA, AUSTIN R. DULANEY, CHRISTOPHER J. ELLISON, University of Texas at Austin, McKetta Department of Chemical Engineering, OPHELIA K.C. TSUI, Boston University Physics Department, Division of Materials Science and Engineering — We report measurements of self-diffusion ( $D$ ) and effective viscosity ( $\eta_{\text{eff}}$ ) on silica-supported poly(isobutyl methacrylate) (PiBMA) thin films. These films had been found to exhibit thickness ( $h_0$ ) independence in the glass transition temperature,  $T_g$  ( $= 58^\circ\text{C}$ ). At  $T = 106^\circ\text{C}$ ,  $D$  was independent of  $h_0$ , consistent with  $T_g$ . On the other hand,  $\eta_{\text{eff}}$  decreased with decreasing  $h_0$ , indicating decoupling between  $D$  and  $\eta_{\text{eff}}$ . We contemplate that the decoupling is caused by dynamic heterogeneity in the film and that  $D$  and  $\eta_{\text{eff}}$  are different dynamic averages. Specifically, by using a layer model, where the film is divided into sub-layers with thickness  $h_i$  and local viscosity  $\eta_i$ , and assuming that  $D \sim k_B T / \langle \eta_i \rangle$  and  $\eta_{\text{eff}} \sim \langle h_i^3 / (3\eta_i) \rangle$ , we are able to account for all the measurements.

<sup>1</sup>We are grateful to the support of NSF through the project DMR-1310536 and DMR-1053293.

**M1.00187 Interfacial Bubble Deformations**<sup>1</sup>, BRIAN SEYMOUR, James Madison University, PARVIS SHABANE, Virginia Tech, OLIVIA CYPULL, James Madison University, SHENGFENG CHENG, Virginia Tech, KLEBERT FEITOSA, James Madison University — Soap bubbles floating at an air-water experience deformations as a result of surface tension and hydrostatic forces. In this experiment, we investigate the nature of such deformations by taking cross-sectional images of bubbles of different volumes. The results show that as their volume increases, bubbles transition from spherical to hemispherical shape. The deformation of the interface also changes with bubble volume with the capillary rise converging to the capillary length as volume increases. The profile of the top and bottom of the bubble and the capillary rise are completely determined by the volume and pressure differences.

<sup>1</sup>James Madison University Department of Physics and Astronomy, 4VA Consortium, Research Corporation for Advancement of Science

**M1.00188 Temperature-dependent neutron diffraction measurements from D<sub>2</sub>O hydrating single-supported lipid bilayers of DMPC**<sup>1</sup>, Z. N. BUCK, J. TORRES, A. MAZZA, H. KAISER, H. TAUB, Univ. of Missouri - Columbia, F. Y. HANSEN, Technical University of Denmark, A. MISKOWIEC, Oak Ridge National Lab, M. TYAGI, NIST Center for Neutron Research — The freezing point depression of water associated with biological membranes, studied principally by NMR, has been of interest for decades. Here we have used neutron diffraction measurements at the University of Missouri Research Reactor (MURR) to investigate the freezing behavior of water associated with single-supported zwitterionic lipid bilayers composed of DMPC. Diffraction patterns obtained as a function of temperature reveal that water freezes abruptly into its hexagonal phase at 270 K with no evidence of amorphous ice. Following the initial crystallization of the membrane-associated water there is a region of continuous hexagonal crystal growth, which is believed to occur in the interfacial water closest to the membrane. The temperature-dependent intensity of the observed Bragg peaks have been compared with that of incoherently elastically-scattered neutrons collected on the High-Flux Backscattering Spectrometer at NIST from an identical sample hydrated with H<sub>2</sub>O [2]. We find excellent agreement between the two data sets, suggesting the absence of amorphous solid water and that all the water hydrating a DMPC membrane eventually freezes into the hexagonal crystalline phase. <sup>2</sup>M. Bai *et al.*, Europhys. Lett. **98**, 48006 (2012).

<sup>1</sup>Supported by NSF Grant Nos. DMR-0944772 and DGE-1069091

**M1.00189 Elasticity and Extensibility Determine Printability and Spinnability of Polymer Solutions** , JELENA DINIC, LEIDY JIMENEZ, VIVEK SHARMA, Univ of Illinois - Chicago — Many advanced manufacturing technologies like inkjet and 3D printing, nano-fiber spinning involve complex free-surface flows, and the formation of columnar necks that undergo spontaneous capillary-driven thinning and pinch-off. The progressive self-thinning of neck is often characterized by self-similar profiles and scaling laws that depend on the relative magnitude of capillary, inertial and viscous stresses for simple (Newtonian and inelastic) fluids. Stream-wise velocity gradients that arise within the thinning columnar neck create an extensional flow field that can orient and stretch macromolecules, contributing extra elastic stresses and extensional viscosity that change thinning and pinch-off dynamics for polymeric complex fluids. Characterizing the filament thinning and break-up kinetics in jetting, dripping and stretching liquid bridge provides invaluable insight into the interplay of elastic, viscous, capillary and inertial stresses relevant for these applications. We elucidate how polymer composition, flexibility and molecular weight determine the thinning and pinch-off kinetics in our experiments. Both effective relaxation time and transient extensional viscosity are found to be strongly concentration dependent even for dilute solutions.

**M1.00190 Patterns, Instabilities, Colors, and Flows in Vertical Foam Films** , SUBINUER YILIXIATI , YIRAN ZHANG , EWELINA WOJCIK , VIVEK SHARMA , Univ of Illinois - Chicago — Understanding and controlling the drainage kinetics of thin films is an important problem that underlies the stability, lifetime and rheology of foams and emulsions. We follow the drainage kinetics of vertical foam films using imaging and color science. Interference between light reflected from two surfactant-laden surfaces that are 100 nm - 10 micron apart leads to thickness-dependent iridescent colors in the visible region. Below 50 nm the thin films appear as black. In this study, we utilize the thin film interference colors as markers for identifying patterns, instabilities and flows within vertical foam films. We study the emergence of thickness fluctuations near the borders (i.e. marginal regeneration) and within thinning films. Finally, we elucidate how buoyancy, capillarity, convection and gravity-driven instabilities and flows, are affected by the choice and concentration of constituents. We find fascinating examples of two-dimensional hydrodynamics and unexplained, if not unprecedented, drainage kinetics.

**M1.00191 Effects of aspect ratio on the phase diagram of spheroidal particles<sup>1</sup>** , SONGUL KUTLU, JASON HAAGA, JEFFREY RICKMAN, JAMES GUNTON, Lehigh University — Ellipsoidal particles occur in both colloidal and protein science. Models of protein phase transitions based on interacting spheroidal particles can often be more realistic than those based on spherical molecules. One of the interesting questions is how the aspect ratio of spheroidal particles affects the phase diagram. Some results have been obtained in an earlier study by Odriozola (J. Chem. Phys. 136:134505 (2012)). In this poster we present results for the phase diagram of hard spheroids interacting via a quasi-square-well potential, for different aspect ratios. These results are obtained from Monte Carlo simulations using the replica exchange method. We find that the phase diagram, including the crystal phase transition, is sensitive to the choice of aspect ratio.

<sup>1</sup>G. Harold and Leila Y. Mathers Foundation

**M1.00192 Coarse-grained simulation of dynamin-mediated fission** , MARCUS MULLER, GUOJIE ZHANG, MARC FUHRMANS, Georg-August University, Goettingen, Germany — Fission is a process in which a region of a lipid bilayer is deformed and separated from its host membrane, so that an additional, topologically independent compartment surrounded by a continuous lipid bilayer is formed. It is a fundamental process in the compartmentalization of living organisms and carefully regulated by a number of membrane-shaping proteins. An important group within these is the dynamin family of proteins that are involved in the final severance of the hourglass-shaped neck, via which the growing compartment remains connected to the main volume until the completion of fission. We present computer simulations testing different hypotheses of how dynamin proteins facilitate fission by constriction and curvature. Our results on constraint-induced fission of cylindrical membrane tubes emphasize the importance of the local creation of positive curvature and reveal a complex picture of fission, in which the topological transformation can become arrested in an intermediate stage if the proteins constituting the fission machinery are not adaptive.

**M1.00193 Coarse grained modeling of transport properties in monoclonal antibody solution** , JAMES SWAN, GANG WANG, Massachusetts Inst of Tech-MIT — Monoclonal antibodies and their derivatives represent the fastest growing segment of the bio pharmaceutical industry. For many applications such as novel cancer therapies, high concentration, sub-cutaneous injections of these protein solutions are desired. However, depending on the peptide sequence within the antibody, such high concentration formulations can be too viscous to inject via human derived force alone. Understanding how heterogeneous charge distribution and hydrophobicity within the antibodies leads to high viscosities is crucial to their future application. In this talk, we explore a coarse grained computational model of therapeutically relevant monoclonal antibodies that accounts for electrostatic, dispersion and hydrodynamic interactions between suspended antibodies to predict assembly and transport properties in concentrated antibody solutions. We explain the high viscosities observed in many experimental studies of the same biologics.

**M1.00194 Hierarchical Cluster Formation in Concentrated Monoclonal Antibody Formulations** , P. DOUGLAS GODFRIN, University of Delaware, JONATHAN ZARZAR, ISIDRO (DAN) ZARRAGA, Genentech, Inc., LIONEL PORCAR, PETER FALUS, Institute Laue-Langevin, NORMAN WAGNER, University of Delaware, YUN LIU, NIST Center for Neutron Research, University of Delaware — Reversible cluster formation has been identified as an underlying cause of large solution viscosities observed in some concentrated monoclonal antibody (mAb) formulations. As high solution viscosity prevents the use of subcutaneous injection as a delivery method for some mAbs, a fundamental understanding of the interactions responsible for high viscosities in concentrated mAb solutions is of significant relevance to mAb applications in human health care as well as of intellectual interest. Here, we present a detailed investigation of a well-studied IgG1 based mAb to relate the short time dynamics and microstructure to significant viscosity changes over a range of pharmaceutically relevant physiochemical conditions. Using a combination of experimental techniques, it is found that upon adding Na<sub>2</sub>SO<sub>4</sub>, these antibodies dimerize in solution. Proteins form strongly bounded reversible dimers at dilute concentrations that, when concentrated, interact with each other to form loosely bounded, large, transient clusters. The combined effect of forming strongly bounded dimers and a large transient network is a significant increase in the solution viscosity. Strongly bounded, reversible dimers may exist in many IgG1 based mAb systems such that these results contribute to a more comprehensive understanding of the physical mechanisms producing high viscosities in concentrated protein solutions.

**M1.00195 Probing matrix and tumor mechanics with *in situ* calibrated optical trap based active microrheology** , JACK RORY STAUNTON, WILFRED VIEIRA, KANDICE TANNER, NIH, TISSUE MORPHODYNAMICS UNIT TEAM — Aberrant extracellular matrix deposition and vascularization, concomitant with proliferation and phenotypic changes undergone by cancer cells, alter mechanical properties in the tumor microenvironment during cancer progression. Tumor mechanics conversely influence progression, and the identification of physical biomarkers promise improved diagnostic and prognostic power. Optical trap based active microrheology enables measurement of forces up to 0.5 nN within a sample, allowing interrogation of *in vitro* biomaterials, *ex vivo* tissue sections, and small organisms *in vivo*. We fabricated collagen I hydrogels exhibiting distinct structural properties by tuning polymerization temperature T<sub>p</sub>, and measured their shear storage and loss moduli at frequencies 1-15k Hz at multiple amplitudes. Lower T<sub>p</sub> gels, with larger pore size but thicker, longer fibers, were stiffer than higher T<sub>p</sub> gels; decreasing strain increased loss moduli and decreased storage moduli at low frequencies. We subcutaneously injected probes with metastatic murine melanoma cells into mice. The excised tumors displayed storage and loss moduli 40 Pa and 10 Pa at 1 Hz, increasing to 500 Pa and 1 kPa at 15 kHz, respectively.

**M1.00196 Dynamics of Micropipette Vibration During Piezo-assisted Microinjection<sup>1</sup>**, MEHDI KARZAR-JEDDI<sup>2</sup>, NEJAT OLGAC, TAI-HSI FAN, Department of Mechanical Engineering, University of Connecticut, Storrs, Connecticut 06269-3139, USA — Microinjection is a well-accepted method to introduce materials such as sperm, DNA materials, or nucleus into a living cell for biomedical applications. The conventional microinjection procedure consists of immobilizing the cell by applying suction through a holding pipette, and then an injecting micropipette penetrates through the cell membrane and introduces the materials into the cell. To assist the penetration process a piezo-generated pulse train is applied to the injecting pipette, which causes an undesirable lateral vibration at the injecting pipette tip. In this research we provide an analytical model to study the response of micropipette to the piezo-pulse train using the Duhamel integral method. Our results show that filling the micropipette tip with mercury causes a larger amplitude stroke vibration in micropipette tip than that of empty micropipette when it is submerged in the viscous medium surrounding the cell. The mercury introduced larger stroke vibration can cause a larger shear force and assist the penetration of micropipette through the cell membrane.

<sup>1</sup>This work is supported by NSF CBET-0828733 and NIH R24RR018934-01

<sup>2</sup>Current affiliation: Department of Civil Environmental and Geo- Engineering, University of Minnesota

**M1.00197 Characterizing the mechanical behavior of the zebrafish germ layers**, DAVID KEALHOFER, FRIEDHELM SERWANE, ALESSANDRO MONGERA, PAYAM ROWGHANIAN, ADAM LUCIO, OTGER CAMPÀS, University of California, Santa Barbara — Organ morphogenesis and the development of the animal body plan involve complex spatial and temporal control of tissue- and cell-level mechanics. A prime example is the generation of stresses by individual cells to reorganize the tissue. These processes have remained poorly understood due to a lack of techniques to characterize the local constitutive law of the material, which relates local cellular forces to the resulting tissue flows. We have developed a method for quantitative, local in vivo study of material properties in living tissue using magnetic droplet probes. We use this technique to study the material properties of the different zebrafish germ layers using aggregates of zebrafish mesendodermal and ectodermal cells as a model system. These aggregates are ideal for controlled studies of the mechanics of individual germ layers because of the homogeneity of the cell type and the simple spherical geometry. Furthermore, the numerous molecular tools and transgenic lines already developed for this model organism can be applied to these aggregates, allowing us to characterize the contributions of cell cortex tension and cell adhesion to the mechanical properties of the zebrafish germ layers.

**M1.00198 A finite element study of the stability of spontaneous curling of thin shells**, XIAOMIN HAN, Thayer School of Engineering, Dartmouth College, QIAOHANG GUO, College of Material Science and Engineering, Fuzhou University, KEVIN CHU, Serendipity Research, IAN TRASE, NAN HU, ZI CHEN, Thayer School of Engineering, Dartmouth College — Thin shells are of great interest in engineering due to their ubiquity in nature. The mechanical instabilities of thin shells are a key factor in understanding many real world phenomena, such as the closure of a Venus flytrap or the curling of a dried leaf. Given the analytical theory that quantitatively described the stability of thin shells subject to surface stress, we are able to identify a dimensionless parameter that controls the stability of thin shells. Finite element analyses are employed to numerically examine the predictions. Bi-layer plates are fabricated where one layer is pre-stretched and has much smaller Young's modulus than the other layer to examine mechanical instability. By measuring the two principle curvatures on the plate, the onset of bifurcation can be determined. Different initial conditions and material properties are taken into account in the FEA, including initial curvature, Poisson's ratio, and the magnitude of surface stress. The numerical experiments agree well with the theory.

**M1.00199 Diffusion of micrometer-sized soft particles in confinement<sup>1</sup>**, BENJAMIN JORDAN, KEVIN APTOWICZ, West Chester University — We investigate the diffusion of micrometer sized poly(N-isopropylacrylamide) (PNIPAM) gel particles in confinement. The influence of confinement on the transport of small particles is becoming increasingly important for microfluidics and bio-fluidics. Analytical solutions to this problem are limited to very unique geometries or gross approximations. Computational methods have provided more insight into the problem as well as experimental investigations. However, most research has focused on the hard-sphere problem. In this work, we will explore the diffusion of soft particles in confinement. The dynamics of the particles confined between two parallel walls is captured with video-microscopy. In addition, we use a recently developed technique to measure confinement of particles in-situ with a precision of 1%. This poster will present some preliminary results of how confinement affects the diffusion of these soft particles.

<sup>1</sup>We acknowledge support from grant DMR-1206231.

**M1.00200 Electric Double Layer electrostatics of spherical polyelectrolyte brushes with pH-dependent charge density**, HAO LI, GUANG CHEN, SHAYANDEV SINHA, SIDDHARTHA DAS, Univ of Maryland-College Park, SOFT MATTER, INTERFACES, AND ENERGY LABORATORY (SMIEL) TEAM — Understanding the electric double layer (EDL) electrostatics of spherical polyelectrolyte (PE) brushes, which are spherical particles grafted with PE layers, is essential for appropriate use of PE-grafted micro-nanoparticles for targeted drug delivery, oil recovery, water harvesting, emulsion stabilization, emulsion breaking, etc. Here we elucidate the EDL electrostatics of spherical PE brushes for the case where the PE exhibits pH-dependent charge density. This pH-dependence necessitates the consideration of explicit hydrogen ion concentration, which in turn dictates the distribution of monomers along the length of the grafted PE. This monomer distribution is shown to be a function of the nature of the sphere (metallic or a charged or uncharged dielectric or a liquid-filled sphere). All the calculations are performed for the case where the PE electrostatics can be decoupled from the PE elastic and excluded volume effects. Initial predictions are also provided for the case where such decoupling is not possible.

**M1.00201 Unraveling the Nanostructure and Chain Conformation of Peptide-polymer Conjugates in Solution using Small-angle X-ray Scattering**, REIDAR LUND, Department of chemistry, University of Oslo, TING XU, UC-Berkeley, HE DONG, Clarkson University — For therapeutics, polymer functionalization, often by poly(ethylene glycol), PEG ("PEGylation"), is an effective method to improve the solubility, increase the life time and protect the proteins from the immune system[1]. However it is essential that the proteins maintain their structural integrity in solution- thus the role of the polymer and their interactions with proteins needs to be understood. In this work we show how small-angle X-ray scattering (SAXS) can be used as a powerful technique to characterize the structural components of peptide-polymer conjugates in solution [2,3]. We specifically show that by applying detailed modelling very detailed structural features can be revealed, including the PEG chain conformation. In the presentation we will provide an overview of the methodology, specifically addressing peptides that form either alpha-helical bundles [2,3] or beta-sheet structures [4,5] and relate their structure in solution to their crystal structure.

1. Harris JM and Chess RB. 2003 *Nat Rev Drug Discov* 2(3):214
2. Shu J, Lund R, and Xu T. 2012. *Biomacromolecules* 13(6): 1945.
3. Lund R, Shu J, and Xu T T. 2013. *Macromolecules* 46(4):1625
4. Yang, M.; et al *Chem. Commun.* 2014, 50, 4827.
5. Xu, D. et al. *Chem. Commun.* 2014, 51, 1289.

**M1.00202 Geometric Frustration Selects Morphology in Chiral Filament Bundles<sup>1</sup>**, DOUGLAS HALL, ISAAC BRUSS, UMass Amherst, JUSTIN BARONE, Virginia Tech, GREGORY GRASON, UMass Amherst — Assemblies of twisted filaments appear in a range of biological contexts, from extracellular filament bundles to amyloid fibrils. Owing to numerous distinctions in molecular structures and interactions underlying these diverse assemblies, a framework to predict and classify the basic mechanisms of structure formation in twisted filament assemblies is still lacking. In this study, we model how the size and shape of self-assembled fibers are controlled by competition between the elastic costs of inter-filament frustration, bending deformation of filaments and bundle surface energy. Exploiting a geometric mapping between inter-filament packing in twisted bundles and packing on positively-curved 2D surfaces, we show that the anisotropy of the bundle cross-section is determined by a single parameter describing the competition between elastic and bending costs. We compare the continuum model's predictions for stability of cylindrical and tape-like twisted morphologies to numerical simulations of cohesive filament bundles and observations of micron-scale amyloid fibers assembled from hydrolyzed protein fragments.

<sup>1</sup>NSF (CAREER) DMR-0955760

**M1.00203 Controlling the Size and Shape of the Elastin-Like Polypeptide based Micelles**, KIRIL STRELETZKY, HANNAH SHUMAN, ADAM MARASCHKY, NOLAN HOLLAND, Cleveland State University — Elastin-like polypeptide (ELP) trimer constructs make reliable environmentally responsive micellar systems because they exhibit a controllable transition from being water-soluble at low temperatures to aggregating at high temperatures. It has been shown that depending on the specific details of the ELP design (length of the ELP chain, pH and salt concentration) micelles can vary in size and shape between spherical micelles with diameter 30-100 nm to elongated particles with an aspect ratio of about 10. This makes ELP trimers a convenient platform for developing potential drug delivery and bio-sensing applications as well as for understanding micelle formation in ELP systems. Since at a given salt concentration, the headgroup area for each foldon should be constant, the size of the micelles is expected to be proportional to the volume of the linear ELP available per foldon headgroup. Therefore, adding linear ELPs to a system of ELP-foldon should result in changes of the micelle volume allowing to control micelle size and possibly shape. The effects of addition of linear ELPs on size, shape, and molecular weight of micelles at different salt concentrations were studied by a combination of Dynamic Light Scattering and Static Light Scattering. The initial results on 50 M ELP-foldon samples (at low salt) show that Rh of mixed micelles increases more than 5-fold as the amount of linear ELP raised from 0 to 50 M. It was also found that a given mixture of linear and trimer constructs has two temperature-based transitions and therefore displays three predominant size regimes.

**M1.00204 Directed Assembly of Hierarchically Ordered Clusters from Anisotropic Microparticles<sup>1</sup>**, KOOHEE HAN, BHUVNESH BHARTI, North Carolina State Univ, C. WYATT SHIELDS IV, GABRIEL P. LOPEZ, Duke University, ORLIN D. VELEV, North Carolina State Univ — The directed assembly of colloidal particles with specific connectivity, symmetry, and directional response requires controlled interactions and means of programmable binding force. We will show how patchy microparticles can be hierarchically assembled into ordered clusters, resulting from directional interactions between metal-coated facets. First, we introduce lipid mediated capillary bridging as a new class of binding force for directed assembly of metallo-dielectric patchy microspheres. Iron oxide surface patches on latex microspheres were selectively wetted with liquid lipids, guiding the particle assembly into well-defined 2D and 3D clusters. The temperature driven fluid-to-gel phase transition of the fatty acids acts as a thermal switch for cluster assembly and disassembly. Secondly, we used external fields to bind patchy microcubes based on their polarization configuration and interparticle interaction. We present assembled clusters of cobalt-coated patchy microcubes that can be dynamically reconfigured using external magnetic field. The residual polarization of ferromagnetic cobalt patches allows for preserving the assembled sequence even in the absence of the field and drives dynamic reconfiguration of assembled clusters.

<sup>1</sup>NSF Grant DMR-1121107

**M1.00205 Aging and nonlinear rheology of thermoreversible colloidal gels**, NORMAN WAGNER, MELISSA GORDON, CHRISTOPHER KLOXIN, University of Delaware — Colloidal dispersions are found in a wide variety of consumer products such as paint, food and pharmaceuticals. We investigate gel formation and aging in a thermoreversible gel consisting of octadecyl-coated silica nanoparticles suspended in n-tetradecane. In this system, the octadecyl brush can undergo a phase change allowing the attractions between particles to be tuned by temperature (1,2). By probing the system with steady shear and large amplitude oscillatory shear, we have studied the effect of thermal history and shear history on gel formation and gel mechanical properties during aging. Gels were formed by approaching a common temperature from above and below to determine a reference state from which creep tests were conducted. Creep ringing was observed as expected for the viscoelastic gel. The rheological aging is interpreted in terms of the gel microstructure formed with differing thermal and shear histories to determine how processing affects structure. Recently proposed scaling laws for the rheology and structure under flow are explored within the context of gel aging (3). Through rheological and microstructural measurements, we will further the understanding of gel formation and aging in this model system which may be applied to processing conditions in an industrial setting. 1. Eberle, A.P.R., Wagner, N. J., Akgun, B. & Satija, S. K. Langmuir 26, 3003–3007 (2010). 2. Eberle, A.P.R., Castañeda-Priego, R., Kim, J. M. & Wagner, N. J. Langmuir 28, 1866–1878 (2012). 3. Eberle, A.P.R., et al., Physical Review E, 89, 050302 (2014).

**M1.00206 Dissolution of a Colloidal Particle in an Oscillatory Fluid Medium**, DEZHUANG YE, JI-QIN LI, Mechanical Engineering, University of Connecticut, ROBIN BOGNER, Pharmaceutical Sciences, University of Connecticut, TAI-HSI FAN, Mechanical Engineering, University of Connecticut — Understanding dissolution kinetics of a colloidal particle in an aqueous solution is of great importance in many pharmaceutical and biochemical applications. We present theoretical analysis of low Reynolds number transient dynamics and mass transfer of a dissolving spherical particle in a unidirectional oscillatory flow. The coupling of fluid flow and passive motion of the particle are resolved analytically, and the transient mass transfer associated with the oscillation of the particle is numerically computed. The flow patterns, diffusive and convective transport phenomena, and the dissolution kinetics under various saturation concentrations and flow conditions are characterized by the frequency parameter, Schmidt number, and Peclet number. The result serves as a basic case in determining the efficiency of drug dissolution or reconstitution that depends on various shaking methods.

**M1.00207 Effective temperatures and the breakdown of the Stokes-Einstein relation for particle suspensions<sup>1</sup>**, CARLOS MENDOZA, Materials Research Institute UNAM, IVAN SANTAMARA-HOLEK, UMDI-J Facultad de Ciencias UNAM, AGUSTIN PREZ-MADRID, Departament de Física Fonamental, Universitat de Barcelona — The short- and long-time breakdown of the classical Stokes-Einstein relation for colloidal suspensions at arbitrary volume fractions is explained here by examining the role that confinement and attractive interactions play in the intra- and inter-cage dynamics executed by the colloidal particles. We show that the short-time diffusion coefficient is larger than the one predicted by the classical Stokes-Einstein relation due to a non-equilibrated energy transfer between kinetic and configuration degrees of freedom. This transfer can be incorporated in an effective temperature that replaces the bath temperature in a Generalized Stokes-Einstein relation (GSER). This relation then allows to obtain the diffusion coefficient once the viscosity is known. On the other hand, the temporary cluster formation induced by confinement and attractive interactions of hydrodynamic nature, makes the long-time diffusion coefficient to be smaller than the corresponding one obtained from the classical Stokes-Einstein relation. Additionally, we provide a simple expression based on a differential effective medium theory (DEMT) that allows to calculate the diffusion coefficient at short and long times. Comparison of our results with experiments and simulations for suspensions of hard and porous spheres shows an excellent agreement in all cases.

<sup>1</sup>UNAM DGAPA IN-110613

**M1.00208 Hydrodynamic interactions in colloidal systems confined to linear geometries with a singular corner.**<sup>1</sup> , BINHUA LIN, RYAN ZARCONI, STUART A. RICE, University of Chicago — Here we investigate the question of whether or not the requirement that particles diffuse around a corner affects their hydrodynamic coupling. We report the results of studies of the collective diffusion coefficients of particles in quasi-one-dimensional linear channels of widths 3 and 5  $\mu\text{m}$ , each with a singular central corner of angle: 60-, 90-, 120-, and 180-degrees. We find that for large angles, the channels are so close in their geometry to 180-degrees that the corner has very little to no effect on the hydrodynamic coupling of particles on opposite sides of the apex. For small angles, the corner's effect is to increase the particle separation at which the maximum hydrodynamic coupling occurs.

<sup>1</sup> U Chicago MRSEC (NSF-DMR-1420709), Dreyfus Foundation (Agency award : SI-14-014)

**M1.00209 Effect of Salts on Drainage of Foam** , SOUMYADIP SETT, University of Illinois at Chicago, STOYAN KARAKASHEV, University of Sofia, Bulgaria, STOYAN SMOUKOV, University of Cambridge, UK, ALEXANDER YARIN, University of Illinois at Chicago — Gravitational drainage from thin planar vertical sodium dodecyl sulfate (SDS) films in the presence of inorganic salts was experimentally studied. Strong ion-specific effects of the counter ions were found to affect the stability and the rate of drainage of the planar foam films as a function of concentration of the inorganic salts. The counter-ions can either stabilize (below the critical concentration) or destabilize the foam films. We found that the strongest foam stabilizer salt became the strongest foam destabilizer beyond its critical concentration.

**M1.00210 The role of the anchoring conditions in the electro rheological behavior of a nematic constrained by two coaxial cylinders and submitted by a pressure drop** , DANIEL MARTNEZ SNCHEZ, Universidad Autonoma de la Ciudad de Mxico, JUAN ADRIN REYES CERVANTES, Universidad Nacional Autonoma de Mxico — We study a nematic liquid crystal (LC) filling the region between two coaxial cylinders subjected to the simultaneous action of both a pressure gradient applied parallel to the axis of the cylinders and a radial low frequency electric field. For the LC 4'-n-pentyl-4-cyanobiphenyl (5CB), we consider soft anchoring boundary conditions to obtain the configuration of the director and the velocity profile and the pressure gradient for nonslip boundary conditions. Finally, we calculate the effective viscosity, the first normal stress difference, and the dragging forces on the cylinders.

**M1.00211 Colloidal particles embedded in liquid crystal droplets** , DREW MELCHERT, MONIRO SADAT, YE ZHOU, JUAN J. DE PABLO<sup>1</sup>, Institute for Molecular Engineering, University of Chicago — In this work, we encapsulate polystyrene and silica particles in nematic liquid crystal (LC) droplets dispersed in water using microfluidic glass capillary devices. While polystyrene particles induce planar anchoring on the surface, silica particles, treated with DMOAP, create homeotropic anchoring of the LC molecules at their surface. Sodium dodecyl sulfate (SDS) is added to the aqueous phase to stabilize LC droplets and promote a radial configuration with point defect in the center of LC droplet. Our experimental and computational studies show that, when trapped inside the LC droplets, particles with both anchoring types become mostly localized at the defect point (at the center) and interact with the radial configuration. Interestingly, a twisting structure is observed for polystyrene particle with strong planar anchoring. Although localization of the particles at the droplet center is the most stable state and with the lowest free energy, off-center positions also emerge, displacing the defect point from the center to near the surface of a radial droplet.

<sup>1</sup> - corresponding author - Second affiliation: Argonne National Laboratory, Argonne, IL 60439, USA

**M1.00212 Coarse-Grained Molecular Monte Carlo Simulations of Liquid Crystal-Nanoparticle Mixtures**<sup>1</sup> , RYAN NEUFELD, GRIGORIY KIMAEV, FRED FU, NASSER M. ABUKHDEIR, University of Waterloo — Coarse-grained intermolecular potentials have proven capable of capturing essential details of interactions between molecule molecules, while substantially reducing the number of degrees of freedom of the system under study. In the domain of liquid crystals, the Gay-Berne (GB) potential has been successfully used to model the behavior of rod-like and disk-like mesogens. However, only ellipsoid-like interaction potentials can be described with GB, making it a poor fit for many real-world mesogens. In this work, the results of Monte Carlo simulations of liquid crystal domains using the Zewdie-Corner (ZC) potential are presented. The ZC potential is constructed from an orthogonal series of basis functions, allowing for potentials of essentially arbitrary shapes to be modeled. We also present simulations of mixtures of liquid crystalline mesogens with nanoparticles. Experimentally these mixtures have been observed to exhibit microphase separation and formation of long-range networks under some conditions. This highlights the need for a coarse-grained approach which can capture salient details on the molecular scale while simulating sufficiently large domains to observe these phenomena. We compare the phase behavior of our simulations with that of a recently presented continuum theory.

<sup>1</sup> This work was made possible by the Natural Sciences and Engineering Research Council of Canada and Compute Ontario.

## **M1.00213 ABSTRACT WITHDRAWN —**

**M1.00214 Magnetic domains and defects in ferromagnetic liquid crystal colloids realized with optical patterning**<sup>1</sup> , ANDREW HESS, QINGKUN LIU, IVAN SMALYUKH, University of Colorado Boulder — A promising approach in designing composite materials with unusual physical behavior combines solid nanostructures and orientationally ordered soft matter at the mesoscale. Such composites not only inherit properties of their constituents but also can exhibit emergent behavior, such as ferromagnetic ordering of colloidal metal nanoparticles forming mesoscopic magnetization domains when dispersed in a nematic liquid crystal. Here we demonstrate the optical patterning of domain structures and topological defects in such ferromagnetic liquid crystal colloids which allows for altering their response to magnetic fields. Our findings reveal the nature of the defects in this soft matter system which is different as compared to non-polar nematic and ferromagnetic systems alike.

<sup>1</sup> This research was supported by the NSF grant DMR-1420736.

**M1.00215 Conformation of charged vesicles: the Debye Huckel and the low curvature limit** , KUMARI PRITI SINHA, PROF. ROCHISH M. THAKKAR, Indian Inst of Tech-Bombay — The shape as well as tension and pressure inside an uncharged vesicle are determined by the reduced volume. These parameters are important for a vesicle or a biological cell, since it can affect bio-physical processes such as osmosis and permeation, interaction with external agents such as bio- macromolecules and thermal fluctuations of the bilayer membrane of a vesicle. Charged membranes are ubiquitous in nature, most biological cell bio-membranes are charged, and therefore the knowledge of shape, tension and pressure of charged vesicles is critical. Additionally, the distribution of charges in the inner and outer leaflets is also important as it can affect the spatial interaction of a bilayer membrane with proteins. This work addresses these issues in the low charge and curvature limit. Our analysis indicates that despite a very strong two-way coupling between the charge and the curvature, the shapes of charged vesicles remain similar to that of uncharged vesicles at comparable reduced volumes, even for reasonable values of total charge. However, the tension and pressure values are higher, and are accurately estimated. Similarly the charge distribution on the outer and inner leaflet is strongly affected by the curvature. The value of spontaneous curvature due to charge redistribution is estimated. The insensitivity of the shape to charges persists even when only the outer leaflet is charged instead of charged inner and outer leaflets

**M1.00216 Emergence of DNA-encapsulating liposomes from a DNA-lipid blend film<sup>1</sup>**, SHUN-SUKE SHIMOBAYASHI, Department of Physics, Kyoto University, MAFUMI HISHIDA, Department of Chemistry, Tsukuba University, TOMO KURIMURA, MASATOSHI ICHIKAWA, Department of Physics, Kyoto University — A Micro-scale giant unilamellar vesicle (GUV) densely encapsulating molecular systems is one of the simplest life-mimicking model systems. The dehydration-rehydration process proposed by Deamer et al. more than 30 years ago generates vesicles to satisfy the constraints of micro-scale size, unilamellarity and densely polymer-encapsulation [1]. Nevertheless, the physico-chemical mechanism of a set of dehydration-rehydration process has been poorly understood. The present study reveals crucial factors on the process through fluorescent microscopic observation [2] and small angle x-ray scattering. From the results, we propose a plausible physical mechanism for the process, making it possible to optimize the encapsulation of any agent. [1] D. W. Deamer, G. L. Barchfield, J. Mol. Evol, 18, 203-206 (1982). [2] S. F. Shimobayashi and M. Ichikawa, J. Phys. Chem. B 118, 10688-10694 (2014).

<sup>1</sup>This work was supported by Grant-in-Aid for JSPS Fellows Grant (No. 25-1270) and by KAKENHI (Nos. 26707020, 25103012, and 26115709).

**M1.00217 Lipid transfer energetics between free-standing and solid supported membranes: reconciling discrepancies.**, BENNY WAH, JOSEPH ADAMS, JEFFREY BREIDIGAN, LI GE, PIOTR HORBAL, Univ of Illinois - Chicago, LIONEL PORCAR, University of Delaware, SUMIT GARG, URSULA PEREZ-SALAS, Univ of Illinois - Chicago — The membranes of animal cells have significant variation in the lipid and protein composition. If it weren't for the active work of proteins that maintain most of these variations, membranes would ultimately homogenize throughout by mixing. It has been long been recognized that the study of the passive movement of lipids between and within membranes can provide insight into this energetic toll. Using small angle neutron scattering, a non-invasive in situ technique, we recently demonstrated that tags or small structure changes in the lipids can have a huge effect on their transport characteristics. In the present study we compare lipid transfer and energetics between supported free standing membranes. We find that exchange and flipping process are comparable while the presence of the surface slightly increases inter and intra-membrane transport rates. The activation energies for exchange appear to be nearly unaffected by the presence of the surface while for flip-flop it slightly increases. The increase in the rates due to the presence of the surface may possibly explain the apparent contradicting behavior previously reported on supported flat membrane systems and in free-standing membranes.

**M1.00218 Photo-Regeneration of Severed Gel Using Photo-Controlled Radical Polymerization**, AWANEESH SINGH, Univ of Pittsburgh, OLGA KUKSENOK, Clemson University, JEREMIAH A. JOHNSON, Massachusetts Institute of Technology, ANNA C. BALAZS, Univ of Pittsburgh — Using the framework of dissipative particle dynamics (DPD) simulation, we developed a novel computational model that enables photo-regeneration of the gel matrix when a significant portion of the material is severed. We considered photo-controlled radical polymerization (photo-CRP) within polymer networks with embedded iniferters (initiators for the photo-CRP reaction). These iniferters turn on the polymerization process in the presence of light with monomers and cross-linkers in the solution. This "photo-growth" allow us to effectively regenerate severed gels under the application of light. The growth process can be turned off once the polymerization is near completion, which forms a new cross-linked gel that resembles the uncut material. The polymerization rate can be modulated by altering the light intensity.

**M1.00219 Frictional Properties of UV illuminated ZnO Thin Films Grown by Pulsed Laser Deposition<sup>1</sup>**, HSIANG-CHIH CHIU, HUAN-PU CHANG, FANG-YU LO, YU-TING YEH, Department of Physics, National Taiwan Normal University, DEPARTMENT OF PHYSICS, NATIONAL TAIWAN NORMAL UNIVERSITY COLLABORATION — Zinc Oxide (ZnO) nanostructures have potential applications in nano-electro-mechanical systems (NEMS) due to their unique physical properties. ZnO is also an excellent lubricant and hence a promising candidate for protective coatings in NEMS. By means of atomic force microscopy (AFM), we have investigated the frictional properties of ZnO thin films prepared by pulsed laser deposition technique. In addition, UV illumination is used to convert the surface wettability of ZnO thin films from being more hydrophobic to superhydrophilic via the photo-catalyst effect. We found that the frictional properties of the UV illuminated, superhydrophilic ZnO surface are strongly dependent on the environment humidity. While for hydrophobic ZnO, no such dependence is found. The observed frictional behaviors can be explained by the interplay between the surface roughness, environmental humidity and the presence of nanoscale capillary condensation forming between surface asperities at the tip-ZnO contact. Our results might find applications in future ZnO related NEMS.

<sup>1</sup>Frictional Properties of UV illuminated ZnO Thin Films Grown by Pulsed Laser Deposition

**M1.00220 Fracture of molecular glasses under tension and fracture-induced crystallization**, YINSHAN CHEN, TRAVIS POWELL, LIAN YU, University of Wisconsin-Madison — Molecular glasses are formed and fractured by cooling a liquid on a less thermally expansive substrate. In-plane tension is created by the mismatch of thermal expansion coefficients and accumulates to cause catastrophic network fracture. This simple experiment allowed the measurement of fracture toughness and the heat of fracture of molecular glasses for the first time. For the systems studied (*o*-terphenyl, indomethacin, and sucrose benzoate), the fracture condition is well described by recent theories and a material-specific energy release rate (fracture toughness) approximately 1 J/m<sup>2</sup>. The heat of fracture was found to be anomalously high relative to the value expected for the energy release rate and the surface area created. The large release of heat is caused by the reduction of heat capacity for a glass film constrained on a rigid substrate. Rapid crystal growth was observed along fracture surfaces. (Ref.: Powell, C. T.; Chen, Y.; Yu, L. J. Non-Crystalline Solids 2015, 429, 122–128)

**M1.00221 Supramolecular Hydrogels from Self-Assembly of di-Fmoc-L-lysine**, SEYED MEYSAM HASHEMNEJAD, KINSEY NAAS, SANTANU KUNDU, Mississippi State University — Mechanical properties and nanostructure of a supramolecular hydrogel formed by self-assembly of di-fluorenylmethyloxycarbonyl-lysine (di-Fmoc-L-lysine) are reported here. Hydrogels were prepared by solvent switch technique in which water was added to a solution of di-Fmoc-L-lysine in dimethyl sulfoxide (DMSO). Mechanical properties of the gels were investigated using shear and cavitation rheology. The gels display strain-softening behavior at moderate strain values. Morphological investigations of the samples were conducted using FTIR and CD spectroscopy, electron microscopy, and atomic force microscopy (AFM). Self-assembled fibers with lateral dimensions ranging from 10 to 50 nm were captured in microscopy studies. FTIR results indicate  $\beta$ -sheet-like conformation of the peptides in the hydrogel.

**M1.00222 Predicting out-of-Equilibrium Phase Behavior in the Dynamic Self-Assembly of Colloidal Crystals**, JAMES SWAN, ZACHARY SHERMAN, Massachusetts Inst of Tech-MIT — Crystals self-assembled from colloidal particles are useful in an array of well demonstrated applications. During fabrication however, gelation and glassification often leave these materials arrested in defective or disordered metastable states. We show how time-dependent, pulsed interparticle interactions can avoid kinetic barriers and yield well-ordered crystalline domains for a suspension of hard, spherical colloidal particles interacting through short-range attractions. This dynamic self-assembly process is analogous to the flashing Brownian ratchet. Although this is an inherently unsteady, out-of-equilibrium process, we can predict its outcome using appropriate time averages of equilibrium equations of state. The predicted phase behavior is tested and validated by examining the fluid/crystal coexistence of such dynamically self-assembling dispersions in Brownian dynamics simulations of sedimentation equilibrium and homogeneous nucleation. We also show that our dynamic self-assembly scheme offers control and tunability over the crystal growth kinetics and can even stabilize nonequilibrium structures.

**M1.00223 Achieving synchronization with active hybrid materials: Coupling self-oscillating gels and piezoelectric films.** , VICTOR V. YASHIN, Department of Chemical Engineering, University of Pittsburgh, STEVEN P. LEVITAN, Department of Electrical and Computer Engineering, University of Pittsburgh, ANNA C. BALAZS, Department of Chemical Engineering, University of Pittsburgh — Our goal is to develop materials that compute by using non-linear oscillating chemical reactions to perform spatio-temporal recognition tasks. The material of choice is a polymer gel undergoing the oscillatory Belousov-Zhabotinsky reaction. The novelty of our approach is in employing hybrid gel-piezoelectric micro-electro-mechanical systems (MEMS) to couple local chemo-mechanical oscillations over long distances by electrical connection. Our modeling revealed that (1) interaction between the MEMS units is sufficiently strong for synchronization; (2) the mode of synchronization depends on the number of units, type of circuit connection (serial or parallel), and polarity of the units; (3) each mode has a distinctive pattern in phase of oscillations and generated voltage. The results indicate feasibility of using the hybrid gel-piezoelectric MEMS for oscillator based unconventional computing.

**M1.00224 Rheological Characterization of Bioinspired Mineralization in Hydrogels** , ABIGAIL REGITSKY, NIELS HOLTEN-ANDERSEN, Massachusetts Institute of Technology — With increasing amounts of CO<sub>2</sub> in the atmosphere linked to potentially catastrophic climate change, it is critical that we find methods to permanently sequester and store CO<sub>2</sub>. Inspired by the natural biomineralization of calcium carbonate (CaCO<sub>3</sub>), one future goal of this project is to understand the mechanisms of CaCO<sub>3</sub> mineralization in order to ultimately optimize a bioinspired hydrogel system, which produces high value industrial powders that consume CO<sub>2</sub> as a feedstock. Along the way, we are developing a rheological technique to study mineral nucleation and growth events by measuring the modulations in mechanical properties of a hydrogel system during mineralization. Our initial system consists of a gelatin hydrogel matrix, which is preloaded with calcium ions, and an aqueous solution of carbonate ions, which are allowed to diffuse through the gel to initiate the mineralization process. In order to monitor how the growth of minerals affects the mechanical properties of the gel network, we measure the storage (G') and loss (G'') moduli of the system in situ. Future work will focus on modifying the properties of the minerals formed by changing the polymer used in the hydrogel network and adding other organic molecules into the system.

**M1.00225 Hardening and yielding in colloidal gels** , EMANUELA DEL GADO, JADER COLOMBO, MEHDI BOUZID, Georgetown University — Attractive colloidal gel networks are disordered elastic solids that can form even in extremely dilute particle suspensions. With interaction strengths comparable to the thermal energy, their stress-bearing network can locally restructure via breaking and reforming inter-particle bonds. We use molecular dynamics simulations of a model system to investigate the strain hardening and the yielding process. During shear start up protocol, the system exhibits strong localization of tensile stresses that may be released through the breaking and formation of new bonds. In this regime, the small amplitude oscillatory shear analysis shows that the storage and the loss modulus follow a power law behavior that are closely reminiscent of experimental observations. At large accumulated strains, the strain-induced reorganization of the gel may trigger flow heterogeneities and eventually lead to the yielding of the gel via a quasi brittle damage of its structure.

**M1.00226 Agglomerate Breakdown in Shear Thickening Fluids by Large Amplitude Oscillatory Shear (LAOS)** , RAN TAO, KIRK D. RICE, GALE A. HOLMES, NIST - Natl Inst of Stds & Tech — Amorphous fumed silica and polypropylene glycol (PPG) suspensions were investigated using both steady shear and oscillatory shear rheology. As-mixed and sonicated silica/PPG suspensions show different shear thickening behavior with different critical shear rates as analyzed by the MITLAOS framework as well as the Fourier Transform approach. The as-mixed suspensions show a pronounced decrease in viscosity or modulus over the course of measurement, which is ascribed to an irreversible breakdown of silica-PPG agglomerates induced by shear. We also extend research to study colloidal silica/PPG dispersions under the same LAOS framework. In particular, we seek to understand the impact of the nanoparticle's structure, i.e., fractal vs. non-fractal, on the oscillatory STF response.

## M1.00227 STATISTICAL AND NONLINEAR PHYSICS —

**M1.00228 Three Dimensional Observations of Quantum Vortex Dynamics in Superfluid Helium** , PETER MEGSON, DANIEL LATHROP, University of Maryland, College Park — Liquid helium, when cooled below 2.17 K, becomes a superfluid with exotic physical properties such as flow without friction. Superfluid flow is irrotational except about line-like topological phase defects with quantized circulation, known as quantum vortices. The dynamics of these vortices include events such as reconnection, wherein vortices meet and exchange tails, and Kelvin wave propagation, a possible mechanism for energy dissipation. We observe the dynamics of fluorescent nanoparticles trapped on the vortices using a newly developed 3D stereographic system. This talk will present new observations of reconnection events and analysis comparing vortex reconnection behavior in three dimensions to previous work that observed such events in two-dimensional projection. In particular, we discuss the power law scaling of vortex separation as a function of time and the effect of the initial angle of separation between the vortex filaments.

**M1.00229 Tension-induced tunable corrugation in bio-inspired two-phase soft composite materials: mechanisms and implications** , AHMED ELBANNA, QIANLI CHEN, University of Illinois Urbana Champaign — We numerically investigate the elastic deformation response of a two-phase bio-inspired soft composite material under externally applied concentric tension using the finite element method. We show that by carefully designing the inclusion pattern it is possible to induce corrugations normal to the direction of stretch. By stacking 1D composite fibers to form 2D membranes, these corrugations collectively lead to the formation of membrane channels with shapes and sizes that are tunable by the level of stretch. Furthermore, we show that by using specific inclusion patterns in laminated plates, it is possible to create pop-ups and troughs enabling the development of complex 3D geometries from planar construction. We have found that the corrugation amplitude increases with the stiffness of inclusion and its eccentricity from the tension axis. We discuss the mechanisms leading to the development of corrugations as well as its different implications. We discuss applications for this design in a variety of fields including tunable band gap formation, surface roughness controllability, auxetic materials and toughness enhancement via programmable evolving geometrical effects..

**M1.00230 Phase correlation in the eigenfunctions of a class of quantum chaotic systems** , JIAOZI WANG, WENGE WANG, Univ of Sci & Tech of China — The random matrix theory predicts vanishing correlation function for eigenfunctions. In this work, we study an important class of quantum chaotic systems, whose Hamiltonians have a sparse structure in unperturbed bases. It is shown that, contrary to the prediction of the random matrix theory, components of the eigenfunctions in such systems have interesting phase correlations, giving non-vanishing correlation functions. Explicit expressions for some of the correlation functions are derived and checked by numerical simulations. As an application, a relation between a type of transition probability and a survival probability amplitude is derived.

**M1.00231 Harnessing geometric and magnetic nonlinearities in phononic meta-plates** , OSAMA BILAL, ANDRE FOEHR, CHIARA DARAIO, Department of Mechanical and Process Engineering, ETH-Zurich — Owing to their physical realization, locally resonant metamaterials retain narrow subwavelength band gaps. Moreover, the fixed geometry and dimensions of the unit cell set a hardbound on the central frequency of the operational bandwidth. Real-time tunable metamaterials extend the range of applications and further enable the realization of new sensors, filters, and switches. Our work harnesses the interaction between geometric nonlinearity and nonlinear magnetic potentials to engineer frequency-agile subwavelength band gaps. The concept is general and applicable to various metamaterials systems. Both numerical simulations and experimental realization of the proposed concept will be presented.

**M1.00232 Propagation of mechanical waves through a stochastic medium with spherical symmetry** , CARLOS AVENDANO, Universidad Autonoma de la Ciudad de Mexico, ADRIAN REYES, Universidad Nacional Autonoma de Mexico — We analyze the propagation of mechanical waves through an anisotropic and inhomogeneous medium with spherical symmetry. We assume that both its elastic and density properties, are random functions of spatial coordinates with specific statistical properties, which allow us to represent media whose properties are not completely determined. We compute the expected value of this system.

**M1.00233 A network model of human aging: Limits, errors, and information** , SPENCER FARRELL, ARNOLD MITNITSKI, KENNETH ROCKWOOD, ANDREW RUTENBERG, Dalhousie University — The Frailty Index (FI) quantifies human aging using the fraction of accumulated age-related deficits. The FI correlates strongly with mortality and accumulates non-linearly and stochastically with age. Clinical data shows a nearly universal limit of  $FI \leq 0.7$ . We computationally model an aging population using a network model of interacting deficits. Deficits damage and repair at rates that depend upon the average damage of connected nodes. The model is parametrized to fit clinical data. We find that attribution errors, especially false negative, allow the model to recover the frailty limit. Mutual information allows us to assess how well the FI can predict mortality. Mutual information provides a non-parametric measure of how the FI predicts mortality. We find that attribution errors have a small effect on the mutual information when many deficits are included in the model. The mutual information of our model and of the clinical data are comparable.

**M1.00234 Changes in the Distribution of Avalanches on a Conical Bead Pile with Cohesion<sup>1</sup>** , JUSTINE WALKER, SUSAN LEHMAN, College of Wooster, KARIN DAHMEN, MICHAEL LEBLANC, University of Illinois at Urbana-Champaign, JONATHAN UHL, Retired — The probability distributions for avalanches of varying size are experimentally determined for a slowly driven, conical bead pile. The pile is composed of roughly 20 000 steel spheres, 3 mm in diameter, atop a circular base; it is driven by adding one bead at a time to the apex of the pile. We investigate the dynamic response of the pile by recording avalanches off the pile over the course of tens of thousands of bead drops. The avalanching behavior is studied at different drop heights and different amounts of cohesion between the beads. The level of cohesion is tuned through use of an applied uniform magnetic field. Smaller, local avalanches are distinguished from larger, non-local avalanches and the moments of the avalanche distribution are calculated separately for these different populations. The resulting moments scale with cohesion differently, and the results are compared to the scaling predictions from an analytic mean-field model and corresponding simulation of slip avalanches in a shear system [Dahmen, Nat Phys 7, 554 (2011)].

<sup>1</sup>Research supported by NSF CBET 1336116 and 1336634

**M1.00235 Improving detection of avalanches on a conical bead pile<sup>1</sup>** , AVI VAJPEYI, SUSAN LEHMAN, College of Wooster, KARIN DAHMEN, MICHAEL LEBLANC, University of Illinois at Urbana-Champaign, JONATHAN UHL, Retired — A conical bead pile subject to slow driving and an external magnetic field is used as a simple system to investigate the variations in the avalanche size probability distribution function. Steel beads are dropped onto the pile from different heights and at different strengths of applied magnetic field. Avalanches are recorded by the change in mass as beads fall off the pile. Experimentally we observe an increasing deviation from power law behavior as the field and thus cohesion between the beads increases. We compare our experimental results for the probability distribution function to the results of an analytic theory from a mean-field model of slip avalanches [Dahmen, Nat Phys 7, 554 (2011)]. The model also makes predictions for avalanche duration, which is not measurable with the existing system. To more fully characterize the avalanching behavior of the pile over time, a high-speed camera has been added to the system to record the largest avalanches and allow more detailed analysis. The conical pile geometry presents a challenge for observation and particle tracking over the full pile. Our implementation scheme and preliminary results from the video analysis are presented.

<sup>1</sup>Research supported by NSF CBET 1336116 and 1336634

**M1.00236 Effects of sudden density changes in disordered superconductors and semiconductors<sup>1</sup>** , HIBA ASSI, HARSHWARDHAN CHATURVEDI, MICHEL PLEIMLING, UWE TÄUBER, Department of Physics, Virginia Tech — Vortices in type-II superconductors in the presence of extended, linear defects display the strongly pinned Bose glass phase at low temperatures. This disorder-dominated thermodynamic state is characterized by suppressed lateral flux line fluctuations and very slow structural relaxation kinetics: The vortices migrate between different columnar pinning centers to minimize the mutual repulsive interactions and eventually optimize the system's pinning configuration. To monitor the flux lines' late-time structural relaxations, we employ a mapping between an effectively two-dimensional Bose glass system and a modified Coulomb glass model, originally developed to describe disordered semiconductors at low temperatures. By means of Monte Carlo simulations, we investigate the effects of the introduction of random bare site energies and sudden changes in the vortex or charge carrier density on the soft Coulomb gap that appears in the density of states due to the emerging spatial anticorrelations. The non-equilibrium relaxation properties of the Bose and Coulomb glass states and the ensuing aging kinetics are studied through the two-time density autocorrelation function and its various scaling forms.

<sup>1</sup>Research supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02-09ER46613.

**M1.00237 Autonomous Brownian motors driven by nonadiabatic variation of internal parameters** , ALEX PLYUKHIN, Saint Anselm College — We study a family of autonomous motors based on a Brownian particle driven from thermal equilibrium by periodic in time variation of the internal potential through which the particle interacts with molecules of the surrounding thermal bath. We demonstrate for such motors the absence of a linear response regime: The average driving force and drift velocity are shown to be quadratic in both the frequency and amplitude of the variation. The adiabatic approximation (of an infinitely slow variation) and the leading correction to it (linear in the variation's frequency) lead to zero drift and are insufficient to describe the motor's operation.

**M1.00238 Modeling the Earth: Climate on an Icosphere** , STEPHANIE FOUTS, Washington and Lee University, L. JONATHAN COOK, Roanoke College — The totally asymmetric simple exclusion process with Langmuir kinetics is a one-dimensional transport model used to study the motion of particles through a lattice. Its applications include systems in the fields of biology, climatology, mathematics, civil engineering, and physics. In our research, we examine the temporal dynamics through the power spectra, as well as the time-averaged particle distribution on the lattice via Monte Carlo simulations. We have applied our particle transport model to an icosahedron in an attempt to model Earth's changing climate. In our research, we examine the temporal dynamics of the particle distribution on the lattice, as they correspond to seasonal heat fluctuations in the polar and equatorial regions of the globe. Using Monte Carlos simulations, we alter the input parameters of the system to explore the resultant actions of the Earth-system model. Our findings include seasonal oscillations consistent with those seen in reality. We also built a mathematical framework for our model which, when solved numerically, matches the oscillations seen in our physical system.

**M1.00239 Directed Nanopatterning with Nonlinear Laser Lithography** , ONUR TOKEL, OZGUN YAVUZ, EMRE ERGECEN, IHOR PAVLOV, GHAITH MAKEY, FATIH OMER ILDAY, Bilkent University — In spite of the successes of maskless optical nanopatterning methods, it remains extremely challenging to create any isotropic, periodic nanopattern. Further, available optical techniques lack the long-range coverage and high periodicity demanded by photonics and photovoltaics applications. Here, we provide a novel solution with Nonlinear Laser Lithography (NLL) approach [1]. Notably, we demonstrate that self-organized nanopatterns can be produced in all possible Bravais lattice types. Further, we show that carefully chosen defects or structured noise can direct NLL symmetries. Exploitation of directed self-organization to select or guide to predetermined symmetries is a new capability. Predictive capabilities for such far-from-equilibrium, dissipative systems is very limited due to a lack of experimental systems with predictive models. Here we also present a completely predictive model, and experimentally confirm that the emergence of motifs can be regulated by engineering defects, while the polarization of the ultrafast laser prescribes lattice symmetry, which in turn reinforces translational invariance. Thus, NLL enables a novel, maskless nanofabrication approach, where laser-induced nanopatterns can be rapidly created in any lattice symmetry. [1] Nature Photonics, 7, 897 (2013)

**M1.00240 purohit@seas.upenn.edu** , XIAOJUN LIANG, PRASHANT PUROHIT, University of Pennsylvania — The thermal fluctuations of lipid bilayer membranes are key to their interaction with cellular components as well as the measurement of their mechanical properties. Typically, membrane fluctuations are analyzed by decomposing into normal modes or by molecular simulations. Here we propose a new approach to calculate the partition function of a membrane. We view the membrane as a fluctuating von Karman plate and discretize it into triangular elements. We express its energy as a function of nodal displacements, and then compute the partition function and covariance matrix using Gaussian integrals. We recover well-known results for the dependence of the projected area of the membrane on the applied tension and recent simulation results on the dependence of membrane free energy on geometry, spontaneous curvature and tension. As new applications we compute the fluctuations of the membrane of a malaria infected cell and analyze the effects of boundary conditions on fluctuations. We also compare our calculation with some simulation method to show our time efficiency as well as accuracy.

**M1.00241 Back-and-forth micromotion of aqueous droplets in a dc electric field** , TOMO KURIMURA, MASATOSHI ICHIKAWA, Kyoto University, MASAHIRO TAKINOUE, Tokyo Institute of Technology, KENICHI YOSHIKAWA, Doshisha University — Recently, it was reported that an aqueous droplet in an oil phase exhibited rhythmic back-and-forth motion under stationary dc voltage on the order of 100 V. Here, we demonstrate that the threshold voltage for inducing such oscillation is successfully decreased to the order of 10 V through downsizing of the experimental system [1]. Notably, the threshold electric field tends to decrease with a nonlinear scaling relationship accompanied by the downsizing. We derive a simple theoretical model to interpret the system size dependence of the threshold voltage. This model equation suggests the unique effect of additional noise, which is qualitatively characterized as a coherent resonance by an actual experiment as a kind of coherent resonance. Our result would provide insight into the construction of micrometer-sized self-commutating motors and actuators in microfluidic and micromechanical devices. [1] TK, MI, MT and KY, Phys.Rev.E 88, 042918 (2013).

**M1.00242 Phase Transitions in a Model of Y-Molecules Abstract** , DANIELLE HOLZ, DONOVAN RUTH, Lehigh University, RAUL TORAL, Institute for Cross-Disciplinary Physics and Complex Systems, JAMES GUNTUN, Lehigh University — Immunoglobulin is a Y-shaped molecule that functions as an antibody to neutralize pathogens. In special cases where there is a high concentration of immunoglobulin molecules, self-aggregation can occur and the molecules undergo phase transitions. This prevents the molecules from completing their function. We used a simplified model of 2-Dimensional Y-molecules with three identical arms on a triangular lattice with 2-dimensional Grand Canonical Ensemble. The molecules were permitted to be placed, removed, rotated or moved on the lattice. Once phase coexistence was found, we used histogram reweighting and multicanonical sampling to calculate our phase diagram.

## M1.00243 ABSTRACT WITHDRAWN —

**M1.00244 Social Network Influence and Personal Financial Status** , SHAOJUN LUO, FLAVIANO MORONE, City College of CUNY, CARLOS SARRAUTE, Grandata, Buenos Aires, Argentina, HERNAN MAKSE, City College of CUNY — Networks of social ties emerging from individual economic needs display a highly structured architecture. In response to socio-economic demands, people reshape their circle of contacts for maximizing their social status, and ipso facto, the pattern of their interconnections is strongly correlated with their personal financial situation. In this work we transform this qualitative and verbal statement into an operative definition, which allows us to quantify the economic wellness of individuals through a measure of their collective influence. We consider the network of mobile phone calls made by the Mexican population during three months, in order to study the correlation of person's economic situation with her network location. Notably, we find that rich people tend to be also the most influential nodes, i.e., they self-organize to optimally position themselves in the network. This finding may be also raised at the level of a principle, a fact that would explain the emergence of the phenomenon of collective influence itself as the result of the local optimization of socio-economic interactions. Our method represents a powerful and efficient indicator of socio-economic robustness, which may be applied to maximize the effect of large scale economic intervention and stimulus policies

**M1.00245 Statistical Mechanics of Japanese Labor Markets** , HE CHEN<sup>1</sup>, Hokkaido University — We introduce a probabilistic model to analyze job-matching processes of recent Japanese labor markets, in particular, for university graduates by means of statistical physics. To make a model of the market efficiently, we take into account several hypotheses. Namely, each company fixes the (business year independent) number of opening positions for newcomers. The ability of gathering newcomers depends on the result of job matching process in past business years. This fact means that the ability of the company is weakening if the company did not make their quota or the company gathered applicants too much over the quota. All university graduates who are looking for their jobs can access the public information about the ranking of companies. By assuming the above essential key points, we construct the local energy function of each company and describe the probability that an arbitrary company gets students at each business year by a Boltzmann-Gibbs distribution. We evaluate the relevant physical quantities such as the employment rate and Gini index. We discuss social inequalities in labor markets, and provide some ways to improve these situations, such as the informal job offer rate, the job-worker mismatch between students and companies.

<sup>1</sup>Graduate School of Information Science and Technology

**M1.00246 Agitated granular rod monolayers: Tetratic or uniaxial nematic?**<sup>1</sup> , THOMAS MUELLER, Experimentalphysik V, University of Bayreuth, DANIEL DE LAS HERAS, Theoretische Physik II, University of Bayreuth, INGO REHBERG, KAI HUANG, Experimentalphysik V, University of Bayreuth — The ordering of granular rod monolayers under vertical agitations against gravity is investigated experimentally and compared quantitatively with equilibrium Monte Carlo simulations and density functional theory. At sufficiently high number density, short rods form a tetratic state and long rods form a uniaxial nematic state. The ordering transitions are found to be independent of the agitation frequency and strength, suggesting that the detailed nature of energy injection into such a nonequilibrium system does not play a crucial role. Interestingly, the length-to-width ratio at which the order changes from tetratic to uniaxial is around 7.3 in both experiments and simulations. This quantitative agreement indicates that, despite of driven far from thermodynamic equilibrium, agitated granular systems may share similar features with corresponding equilibrium systems. Finally, we summarize the universal and non-universal aspects between nonequilibrium granular rod and equilibrium liquid crystal systems in a state diagram.

<sup>1</sup>TM and KH acknowledge the support from the DFG through Grant No. HU1939/2-1

**M1.00247 Buckling of Patterned Top Films**, DOKYEONG KWON, Seoul Natl Univ, HYO SEON SUH, University of Chicago, KOOKHEON CHAR, Seoul Natl Univ — Buckling of thin films on elastomeric substrates such as polydimethylsiloxane (PDMS) is the well-known phenomenon in buckling instability originating from the moduli mismatch between a substrate and a thin film placed on the top. Recently, many studies on the microstructure created by the buckling with flat top films have been reported and physics behind them has almost been well received. However, only a few work has been done for the buckling structure with micro- or nano-patterned top films and buckling mechanics for patterned top film-PDMS bilayers has not yet been established in detail. Here, we present the buckling of various patterned top films placed on top of elastomeric PDMS substrates. Geometrical patterns were prepared by unconventional lithography techniques such as thermal imprinting of polystyrene (PS) films. Buckling instability was induced by applying mechanical stress to the patterned top surface-PDMS bilayers. Resulting buckled structures showed different mechanical structures as shape and structural parameters of the top thin films were varied. The structural changes were analyzed by introducing a beam theory or a plate theory for the simple modeling of the top surfaces, giving insights on the buckling mechanics of top films with complicated patterns placed on PDMS substrates.

**M1.00248 Triggered Snap-Through of Bistable Shells**<sup>1</sup>, YIJIE CAI, Wuhan University of Technology, SHICHENG HUANG, IAN TRASE, NAN HU, ZI CHEN, Dartmouth College — Elastic bistable shells are common structures in nature and engineering, such as the lobes of the Venus flytrap or the surface of a toy jumping poppers. Despite their ubiquity, the parameters that control the bistability of such structures are not well understood. In this study, we explore how the geometrical features of radially symmetric elastic shells affect the shape and potential energy of a shell's stable states, and how to tune certain parameters in order to generate a snap-through transition from a convex semi-stable state to concave stable state. We fabricated a series of elastic shells with varying geometric parameters out of silicone rubber and measured the resulting potential energy in the semi-stable state. Finite element simulations were also conducted in order to determine the deformation and stress in the shells during snap-through. It was found that the energy of the semi-stable state is controlled by only two geometric parameters and a dimensionless ratio. We also noted two distinct transitions during snap-through, one between monostability and semi-bistability (the state a popper toy is in before it snaps-through and jumps), and a second transition between semi-bistability and true bistability. This work shows that it is possible to use a set of simple parameters to tailor the energy landscape of an elastic shell in order to generate complex trigger motions for their potential use in smart applications.

<sup>1</sup>Z.C. acknowledge support from Society in Science-Branco Weiss Fellowship, administered by ETH Zurich.

**M1.00249 Cook-Levin Theorem Algorithmic-Reducibility/Completeness = Wilson Renormalization-(Semi)-Group Fixed-Points; "Noise"-Induced Phase-Transitions (NITs) to Accelerate Algorithmics ("NIT-Picking") REPLACING CRUTCHES!!!: Models: Turing-machine, finite-state-models, finite-automata.**, FREDERIC YOUNG, EDWARD SIEGEL, FUZZYICS=CATEGORYICS=ANALOGYICS=PRAGMATICS/CATEGORY-SEMANTICS ONTOLOGY COGNITION ANALYTICS — Cook-Levin theorem algorithmic computational-complexity(C-C) algorithmic-equivalence reducibility/completeness equivalence to renormalization-(semi)-group phase-transitions critical-phenomena statistical-physics universality-classes fixed-points, is exploited via Siegel FUZZYICS=CATEGORYICS=ANALOGYICS=PRAGMATICS/CATEGORY-SEMANTICS ONTOLOGY COGNITION ANALYTICS-Aristotle "square-of-opposition" tabular list-format truth-table matrix analytics predicts and implements "noise"-induced phase-transitions (NITs) to accelerate versus to decelerate Harel [Algorithmics (1987)]-Sipser[Intro.Thy. Computation('97)] algorithmic C-C: "NIT-picking"(!!!), to optimize optimization-problems optimally(OOPO). Versus iso-"noise" power-spectrum quantitative-only amplitude/magnitude-only variation stochastic-resonance, "NIT-picking" is "noise" power-spectrum QUALitative-type variation via quantitative critical-exponents variation. Computer-"science"/SEANCE algorithmic C-C models: Turing-machine, finite-state-models, finite-automata,..., discrete-maths graph-theory equivalence to physics Feynman-diagrams are identified as early-days once-workable valid but limiting IMPEDING CRUTCHES(!!!), ONLY IMPEDE latter-days new-insights!!!

**M1.00250 Thermodynamics and Phase Transitions of Ising Model on Inhomogeneous Stochastic Recursive Lattice**<sup>1</sup>, RAN HUANG, Shanghai Jiao Tong Univ — As one of the few exactly solvable thermodynamic models, the Ising model on recursive lattice is featured by its impressive advantages and successful applications in various thermodynamic and statistical researches. However this model was considered that, since the recursive calculation demands homogeneous structure, it can only describe the bulk and even systems with narrow utilization. In this work we figured out a practical methodology to extend the conventional homogeneous structure of single-unit Husimi lattice to be random inhomogeneous lattices with variable units and structures, while keeping the feature of exact calculation. Three designs of inhomogeneous recursive lattices: the random-angled rhombus lattice, the Husimi lattice of variable units, and the randomly multi-branched Husimi square lattice; and the corresponding exact recursive calculations based on the partial partition function algorithm, which is derived from the Bethe Cavity method, have been investigated and developed. With the "total-symmetry assumption" and the "iterative-replica trick" we were able to exactly solve the classical ferromagnetic spin-1 Ising models on these lattices, to describe the complex systems that can only be solved by approximations or simulations on regular lattices. Our work may enhance the application of the exact calculation on recursive lattices in various fields of materials science and applied physics, especially it may serve as a powerful tool to explore the cross-dimensional thermodynamics and phase transitions.

<sup>1</sup> National Natural Science Foundation of China (Grant No. 11505110)

**M1.00251 Nonlinear dynamics of Bohmian trajectories in a double-well potential**, O. F. DE ALCAN-TARA BONFIM, Univ of Portland, JOAO FLORENCIO, Universidade Federal Fluminense, RJ-Brazil — We investigate the dynamics of a quantum particle in a one-dimensional double-well potential within the framework of Bohm's quantum mechanics. We find that the behavior of the trajectories is linked to the degree of complexity of the initial wave packet. By increasing the complexity of the wave packet we obtain trajectories that are either periodic, quasiperiodic, or chaoticlike.

**M1.00252 Nematic-columnar phase transition in oriented hard rectangles**, TRISHA NATH, The Institute of Mathematical Sciences, C.I.T. Campus, Taramani, Chennai 600113, India, DEEPAK DHAR, Department of Theoretical Physics, Tata Institute of Fundamental Research, Homi Bhabha Road, Mumbai, 400005, India, R. RAJESH, The Institute of Mathematical Sciences, C.I.T. Campus, Taramani, Chennai 600113, India — We consider an assembly of monodispersed hard rectangles of size  $2 \times d$  on a square lattice with only hard core interactions amongst them. The long axes of the rectangles can be oriented along the horizontal or vertical directions. For large enough aspect ratio, it is known that this system undergoes three phase transitions as the density ( $\rho$ ) of rectangles is increased: first an isotropic-nematic transition (at  $\rho_1^*$ ), second a nematic-columnar transition (at  $\rho_2^*$ ), and third a columnar-sublattice transition (at  $\rho_3^*$ ). In the nematic phase, only the orientational symmetry is broken. The columnar and sublattice phases correspond to additional broken translational symmetries along one (perpendicular to the nematic orientation) and both directions respectively. Interestingly, the critical value  $\rho_2^*$  remains finite, approximately 0.73, even as  $d \rightarrow \infty$ . We develop a systematic high density expansion for the surface tension between two differently-ordered columnar phases. Keeping only the first order perturbative correction term and setting this surface tension to zero, we get an estimate of  $\rho_2^*$  in excellent agreement with estimates from Monte Carlo simulations, for all  $d \geq 2$ .

**M1.00253 BIOLOGICAL PHYSICS** —

**M1.00254 Single-molecule studies of collagen mechanics** , NANCY FORDE, NAGHMEH REZAEI, Department of Physics, Simon Fraser University, MICHAEL KIRKNESS, Department of Molecular Biology and Biochemistry, Simon Fraser University — Collagen is the fundamental structural protein in vertebrates. Its triple helical structure at the molecular level is believed to be strongly related to its mechanical role in connective tissues. However, the mechanics of collagen at the single-molecule level remain contentious. Estimates of its persistence length span an order of magnitude, from 15-180 nm for this biopolymer of 300 nm contour length. How collagen responds to applied force is also controversial, with different single-molecule studies suggesting one of three different responses: extending entropically, overwinding, or unwinding, all at forces below 10 pN. Using atomic force microscopy to image collagens deposited from solution, we find that their flexibility depends strongly on ionic strength and pH. To study force-dependent structural changes, we are performing highly parallelized enzymatic cleavage assays of triple helical collagen in our new compact centrifuge force microscope. Because proteolytic cleavage requires a locally unwound triple helix, these experiments are revealing how local collagen structure changes in response to applied force. Our results can help to resolve long-standing debates about collagen mechanics and structure at the molecular level.

**M1.00255 Population Dynamics of Viral Inactivation<sup>1</sup>** , KRISTA FREEMAN, DONG LI, Carnegie Mellon University, MANJA BEHRENS, Lund University, KIRIL STRELETZKY, Cleveland State University, ULF OLSSON, Lund University, ALEX EVILEVITCH, Carnegie Mellon University — We have investigated the population dynamics of viral inactivation *in vitro* using time-resolved cryo electron microscopy combined with light and X-ray scattering techniques. Using bacteriophage  $\lambda$  as a model system for pressurized double-stranded DNA viruses, we found that virions incubated with their cell receptor eject their genome in a stochastic triggering process. The triggering of DNA ejection occurs in a non synchronized manner after the receptor addition, resulting in an exponential decay of the number of genome-filled viruses with time. We have explored the characteristic time constant of this triggering process at different temperatures, salt conditions, and packaged genome lengths. Furthermore, using the temperature dependence we determined an activation energy for DNA ejections. The dependences of the time constant and activation energy on internal DNA pressure, affected by salt conditions and encapsidated genome length, suggest that the triggering process is directly dependent on the conformational state of the encapsidated DNA. The results of this work provide insight into how the *in vivo* kinetics of the spread of viral infection are influenced by intra- and extra cellular environmental conditions.

<sup>1</sup>This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. DGE-1252522.

**M1.00256 Theory of sequence-dependent scaling and confinement of viral RNA molecules<sup>1</sup>** , JOSHUA KELLY, Univ of California - Los Angeles — We present a general theory for the fractal dimensions of the genomic viral RNA molecules of small RNA viruses and apply the theory as well to RNA encapsidation competition experiments.

<sup>1</sup>Work supported by NSF

**M1.00257 Convex Lens-induced Confinement to Visualize Biopolymers and Interaction Parameters** , FRANK STABILE, DANIEL BERARD, GIL HENKIN, MARJAN SHAYEGAN, FRANOIS MICHAUD, SABRINA LESLIE, McGill University — In this poster, we present a versatile CLiC (Convex Lens-induced Confinement) microscopy system to access a broad range of biopolymer visualization and interaction parameters. In the CLiC technique, the curved surface of a convex lens is used to deform a flexible coverslip above a glass substrate, creating a nanoscale gap that can be tuned during an experiment to load and confine molecules into nanoscale features, both linear and circular, embedded in the bottom substrate. We demonstrate and characterize massively parallel DNA nanochannel-based stretching, building on prior work. Further, we demonstrate controlled insertion of reagent molecules within the CLiC imaging chamber. We visualize real-time reaction dynamics of nanoconfined species, including dye/DNA intercalation and DNA/DNA ligation reactions, demonstrating the versatility of this nanoscale microscopy platform.

**M1.00258 Slow Domain Motions of an Oligomeric Protein from Deep-Sea Hyperthermophile probed by Neutron Spin Echo** , DEBSINDHU BHOWMIK, UTSAB SHRESTHA, GURPREET DHINDSA, Wayne State University, MELISSA SHARP, European Spallation Source, LAURA R. STINGACIU, Oak Ridge National Laboratory, XIANG-QIANG CHU, Wayne State University, XIANG-QIANG CHU TEAM — Deep-sea microorganisms have the ability to survive under extreme conditions, such as high pressure and high temperature[1]. In this work, we used the combination of the neutron spin-echo (NSE) and the small angle neutron scattering (SANS) techniques to study the inter-domain motions of the inorganic pyrophosphate (IPPase) enzyme derived from thermostable microorganisms *Thermococcus thioreducens*. The IPPase has hexameric quaternary structure with molecular mass of approx. 120kDa (each subunit of 20kDa), which is a large oligomeric structure. The understanding of its slow inter-domain motions can be the key to explain how they are able to perform catalytic activity at higher temperature compared to mesophilic enzymes, thus leading to adapt to extreme environment present at the seabed [1]. The NSE can probe these slow motions directly in the time domain up to several tens of nanoseconds at the nanometers length scales, while the corresponding structural change can be explored by the SANS [2]. Our results provide a better picture of the local flexibility and conformational substates unique to these types of proteins, which will help us better understand the relation between protein dynamics and their biological activities. [1] U. R. Shrestha, et. al, PNAS (2015); X.-Q. Chu, et. al, JPCB 116, 9917 (2012). [2] R. Biehl, et. al, Soft Matt. 7, 1299 (2011)

**M1.00259 Replica-exchange Wang-Landau simulations of the HOP lattice protein model<sup>1</sup>** , GUANGJIE SHI, Center for Simulation Physics, The University of Georgia, THOMAS WÜST, ID Scientific IT Services, ETH Zürich, Switzerland, YING WAI LI, National Center for Computational Sciences, Oak Ridge National Laboratory, DAVID P. LANDAU, Center for Simulation Physics, The University of Georgia — The hydrophobic-polar (HP) lattice protein model has been the subject of intensive investigation in an effort to aid our understanding of protein folding. However, the high ground state degeneracies caused by its simplification stands in contrast to the generally unique native states of natural proteins. Here we proposed a simple modification, by introducing a new type of “neutral” monomer, 0, i.e. neither hydrophobic nor polar, thus rendering the model more realistic without increasing the difficulties of sampling significantly<sup>2</sup>. With the replica exchange Wang-Landau (REWL) scheme<sup>3</sup> we investigated several widely studied HP proteins and their HOP counterparts. Dramatic differences in both ground state and thermodynamic properties have been found. For example, the HOP version of Crambin shows more clear two-step folding and 3 order of magnitudes less ground state degeneracy than its HP counterpart.

<sup>1</sup>Supported by NSF

<sup>2</sup>G. Shi, T. Wüst, Y. W. Li and D. P. Landau J. Phys.: Conf. Ser. 640, 012017 (2015)

<sup>3</sup>T. Vogel, Y. W. Li, T. Wüst, and D. P. Landau, Phys. Rev. Lett., 110, 210603 (2013)

**M1.00260 Identifying paths of allosteric communication in the protein BirA through simulations** , GREGORY CUSTER, DOROTHY BECKETT, SILVINA MATYSIAK, University of Maryland — Biotin ligase/repressor (BirA) is a bifunctional enzyme which adenylates biotin and transfers the product, biotinyl-5-AMP (bio-5-AMP) to biotin carboxyl carrier protein (BCCP). In the absence of BCCP, bio-5-AMP promotes the dimerization of BirA. In dimer form, the BirA bio-5-AMP complex is able to bind to the biotin operator and prevents further synthesis of biotin. The bio-5-AMP binds away from the dimer interface, so it is acting as an allosteric activator. We perform all-atom molecular dynamics simulations with BirA to look at fluctuations within the protein at equilibrium. We simulate apoBirA, liganded BirA, as well as two mutants, M211A and V219A. In agreement with experimental observations, several loops of the protein become stabilized for the liganded BirA when compared to the apo protein. In addition, changes in the dimer interface are observed for the M211A and V219A mutations, which are located in the ligand binding region. Using inter-residue correlation coefficients and pair energies a communication network through the protein is constructed. With this network we have identified paths which have the potential to be important in allosteric activation of BirA. These paths and the methods we use to identify them will be presented.

**M1.00261 Modeling Hand-Over-Hand and Inchworm Steps in Myosin VI**, AMANDA JACK, Denison University, IAN LOWE, University of Pennsylvania, RIINA TEHVER, Denison University — Myosin VI is a molecular motor protein that moves along actin filaments to transport cargo within a cell. There is much experimental evidence that the myosin VI dimer moves “hand-over-hand” along actin; however, recent experiments suggest that the protein can also move via an “inchworm” mechanism. We created a mechanochemical kinetic model to predict myosin VI's behavior under different ATP, ADP, and force conditions, taking these alternative mechanisms into account. Our model's calculations agree well with experimental results and can also be used to predict myosin VI's behavior outside experimentally tested regimes, such as under forward force. We also predict an optimized motor function for the protein around physiological (-2 pN) load and anchoring under -3 pN load. By using our model to predict myosin VI's response to environmental change, we can gain insight into the behavior of a protein that can be difficult to observe experimentally.

**M1.00262 Synchrotron radiation circular dichroism spectroscopy study of recombinant T $\beta$ 4 folding**<sup>1</sup>, YUNG-CHIN HUANG, HSUEH-LIANG CHU, PENG-JEN CHEN, CHIA-CHING CHANG, Natl Chiao Tung Univ — Thymosin beta 4 (T $\beta$ 4) is a 43-amino acid small peptide, has been demonstrated that it can promote cardiac repair, wound repair, tissue protection, and involve in the proliferation of blood cell precursor stem cells of bone marrow. Moreover, T $\beta$ 4 has been identified as a multifunction intrinsically disordered protein, which is lacking the stable tertiary structure. Owing to the small size and disordered character, the T $\beta$ 4 protein degrades rapidly and the storage condition is critical. Therefore, it is not easy to reveal its folding mechanism of native T $\beta$ 4. However, recombinant T $\beta$ 4 protein (rT $\beta$ 4), which fused with a 5-kDa peptide in its amino-terminal, is stable and possesses identical function of T $\beta$ 4. Therefore, rT $\beta$ 4 can be used to study its folding mechanism. By using over-critical folding process, stable folding intermediates of rT $\beta$ 4 can be obtained. Structure analysis of folding intermediates by synchrotron radiation circular dichroism (SRCD) and fluorescence spectroscopies indicate that rT $\beta$ 4 is a random coil major protein and its hydrophobic region becomes compact gradually. Moreover, the rT $\beta$ 4 folding is a two state transition. Thermal denaturation analysis indicates that rT $\beta$ 4 lacks stable tertiary structure. These results indicated that rT $\beta$ 4, similar to T $\beta$ 4, is an intrinsically disordered protein.

<sup>1</sup>Research is supported by MOST, Taiwan. MOST 103-2112-M-009 -011 -MY3. Corresponding author: Chia-Ching Chang; cc-chang01@faculty.nctu.edu.tw

**M1.00263 Structural Properties of Human CaMKII Ca<sup>2+</sup>/Calmodulin-Dependent Protein Kinase II using X-ray Crystallography**, YUMENG MELODY CAO, Smith College, ETHAN MCSPADDEN, JOHN KURIYAN, U.C. Berkeley, DEPARTMENT OF MOLECULAR AND CELL BIOLOGY AND DEPARTMENT OF CHEMISTRY TEAM — To this day, human memory storage remains a mystery as we can at most describe the process vaguely on a cellular level. Switch-like properties of Calcium/Calmodulin-Dependent Protein Kinase II make it a leading candidate in understanding the molecular basis of human memory. The protein crystal was placed in the beam of a synchrotron source and the x-ray crystallography data was collected as reflections on a diffraction pattern that undergo Fourier transform to obtain the electron density. We observed two drastic differences from our solved structure at 2.75Å to a similar construct of the mouse CaMKII association domain. Firstly, our structure is a 6-fold symmetric dodecamer, whereas the previously published construct was a 7-fold symmetric tetradecamer. This suggests the association domain of human CaMKII is a dynamic structure that is triggered subunit exchange process. Secondly, in our structure the N-terminal tag is docked as an additional beta-strand on an uncapped beta-sheet present in each association domain protomer. This is concrete evidence of the involvement of the polypeptide docking site in the molecular mechanism underlining subunit exchange. In the future, we would like to selectively inhibit the exchange process while not disrupting the other functionalities of CaMKII.

**M1.00264 Nanomechanics of Protein Unfolding outside Protease Nanopores**, BINQUAN LUAN, RUHONG ZHOU, IBM T J Watson Res Ctr — Protein folding and unfolding have been the subject of active research for decades. Most of previous studies in protein unfolding were focused on temperature, chemical and/or force (such as in AFM) induced denaturations. Recent studies on the functional roles of proteasomes (such as ClpXP) revealed a novel unfolding process in cell, during which a target protein is mechanically unfolded and pulled into a confined, pore-like geometry for degradation. While the proteasome nanomachine has been extensively studied, the mechanism for unfolding proteins with the proteasome pore is still poorly understood. Here, we investigate the mechanical unfolding process of ubiquitin with (or really outside) an idealized proteasome pore, and compare such process with that in the AFM pulling experiment. Unexpectedly, the required force by a proteasome can be much smaller than that by the AFM. Simulation results also unveiled different nanomechanics, tearing fracture vs. shearing friction, in these two distinct types of mechanical unfoldings.

**M1.00265 Coarse Graining to Investigate Membrane Induced Peptide Folding of Anticancer Peptides**, SAI GANESAN, HONGCHENG XU, SILVINA MATYSIAK, Univ of Maryland-College Park — Information about membrane induced peptide folding mechanisms using all-atom molecular dynamics simulations is a challenge due to time and length scale issues. We recently developed a low resolution Water Explicit Polarizable PROtein coarse-grained Model by adding oppositely charged dummy particles inside protein backbone beads. These two dummy particles represent a fluctuating dipole, thus introducing structural polarization into the coarse-grained model. With this model, we were able to achieve significant  $\alpha$ - $\beta$  secondary structure content de novo, without any added bias. We extended the model to zwitterionic and anionic lipids, by adding oppositely charged dummy particles inside polar beads, to capture the ability of the head group region to form hydrogen bonds. We use zwitterionic POPC and anionic POPS as our model lipids, and a cationic anticancer peptide, SVS1, as our model peptide. We have characterized the driving forces for SVS1 folding on lipid bilayers with varying anionic and zwitterionic lipid compositions. Based on our results, dipolar interactions between peptide backbone and lipid head groups contribute to stabilize folded conformations. Cooperativity in folding is induced by both intra peptide and membrane-peptide interaction.

**M1.00266 Group transfer theory of single molecule imaging experiments in the F-ATPase biomolecular motor**<sup>1</sup>, SANDOR VOLKAN-KACSO, RUDOLPH MARCUS, California Institute of Technology — I describe a chemo-mechanical theory to treat single molecule imaging and “stalling” experiments on the F-ATPase enzyme. This enzyme is an effective stepping biomolecular rotary motor with a rotor shaft and a stator ring. Using group transfer theoretical approach the proposed structure-based theory couples the binding transition of nucleotides in the stator subunits and the physics of torsional elasticity in the rotor. The twisting of the elastic rotor domain acts as a perturbation upon the driving potential, the Gibbs free energy. In the theory, without the use of adjustable parameters, we predict the rate and equilibrium constant dependence of steps such as ATP binding and phosphate release as a function of manipulated rotor angle. Then we compare these predictions to available data from stalling experiments. Besides treating experiments, the theory can provide guides for atomistic simulations, which could calculate the reorganization parameter and the torsional spring constant. The framework is generic and I discuss its application to other single molecule experiments, such as controlled rotation and other biomolecular motors, including motor-DNA complexes and linear motors. [PNAS, Early Edition, Oct. 19, 2015, doi: 10.1073/pnas.1518489112]

<sup>1</sup>The authors would like to acknowledge support from the Office of the Naval Research, the Army Research Office, and the James W. Glanville Foundation.

**M1.00267 Molecular Dynamics Simulation and Statistics Analysis Reveals the Defense Response Mechanism in Plants**, ZHICHAO LIU, YUNJIE ZHAO, CHEN ZENG, Department of Physics, The George Washington University, COMPUTATIONAL BIOPHYSICS LAB TEAM — As the main protein of the bacterial flagella, flagellin plays an important role in perception and defense response. The newly discovered locus, FLS2, is ubiquitously expressed. FLS2 encodes a putative receptor kinase and shares many homologies with some plant resistance genes and even with some components of immune system of mammals and insects. In Arabidopsis, FLS2 perception is achieved by the recognition of epitope flg22, which induces FLS2 heteromerization with BAK1 and finally the plant immunity. Here we use both analytical methods such as Direct Coupling Analysis (DCA) and Molecular Dynamics (MD) Simulations to get a better understanding of the defense mechanism of FLS2. This may facilitate a redesign of flg22 or de-novo design for desired specificity and potency to extend the immune properties of FLS2 to other important crops and vegetables.

**M1.00268 Multiscale modeling of three-dimensional genome**, BIN ZHANG, PETER WOLYNES, Rice University — The genome, the blueprint of life, contains nearly all the information needed to build and maintain an entire organism. A comprehensive understanding of the genome is of paramount interest to human health and will advance progress in many areas, including life sciences, medicine, and biotechnology. The overarching goal of my research is to understand the structure-dynamics-function relationships of the human genome. In this talk, I will be presenting our efforts in moving towards that goal, with a particular emphasis on studying the three-dimensional organization, the structure of the genome with multi-scale approaches. Specifically, I will discuss the reconstruction of genome structures at both interphase and metaphase by making use of data from chromosome conformation capture experiments. Computationally modeling of chromatin fiber at atomistic level from first principles will also be presented as our effort for studying the genome structure from bottom up.

**M1.00269 Quantifying the DNA binding characteristics of ruthenium based threading intercalator  $\Lambda\text{-}\Lambda$ -P with optical tweezers**, NICHOLAS BRYDEN, Bridgewater State University, MA, MICAH MCCAULEY, Northeastern University, MA, FREDRIK WESTERLUND, PER LINCOLN, Chalmers University of Technology, Sweden, IOULIA ROUZINA, Ohio State University, OH, MARK WILLIAMS, Northeastern University, MA, THAYAPARAN PARAMANATHAN, Bridgewater State University, MA — Utilizing optical tweezers, biophysics researchers have been able to study drug-DNA interactions on the single molecule level. Binuclear ruthenium complexes are a particular type of drug molecule that have been found to have potential cancer-fighting qualities, due to their high binding affinity and low dissociation rates. These complexes are threading intercalators, meaning that they must thread their bulky side chains through DNA base pairs to allow the central planar moiety to intercalate between the bases. In this study, we explored the binding properties of the binuclear ruthenium complex,  $\Lambda\Lambda$ -P ( $\Lambda\Lambda$ -[ $\text{bidppz}(\text{phen})_4\text{Ru}_2$ ] $^{4+}$ ). A single DNA molecule is held at a constant force and the  $\Lambda\Lambda$ -P solution introduced to the system in varying concentrations until equilibrium is reached. DNA extension data at various concentrations of  $\Lambda\Lambda$ -P recorded as a function of time provide the DNA binding kinetics and equilibrium binding affinity. Preliminary data analysis suggests that  $\Lambda\Lambda$ -P exhibits fast binding kinetics compared to the very similar  $\Delta\Delta$ -P. These complexes have the same chemical structure and only differ in their chirality, which suggests that the left handed ( $\Lambda\Lambda$ ) threading moieties require less DNA structural distortion for threading compared with the right handed ( $\Delta\Delta$ ) threading moieties.

**M1.00270 Temperature Dependent Rotational Correlation in Lipids<sup>1</sup>**, CHRISTINA OTHON, NEDA DADASH-VAND, EDUARDO VEGA LOZADA, Wesleyan University — The lateral heterogeneity of lipid dynamics is explored in free standing lipid monolayers. As the temperature is lowered the lipids exhibit increasingly broad and heterogeneous rotational correlation. This increase in heterogeneity appears to exhibit a critical onset, similar to those observed for glass forming fluids. We explore this heterogeneous relaxation by measuring the rotational diffusion of a fluorescent probe (NBD-PC) using wide-field time-resolved fluorescence anisotropy microscopy, in single constituent lipid monolayer of DMPC. The observed relaxation exhibits a narrow, liquid-like distribution at high temperatures ( $\tau \sim 2.4$  ns), consistent with previous experimental measures by different methods. However, as the temperature is quenched, the distribution broadens, and we observe the appearance of a long relaxation population (16.5 ns). This demonstrates that the nanoscale diffusion and reorganization in lipid structures can be significantly complex, even in the simplest unstructured architectures. This result can have a significant impact on the organization, permeability and energetics of natural membrane structures.

<sup>1</sup> Temperature Dependent Rotational Correlation in Lipids

**M1.00271 A study of the eigenvectors of low frequency vibrational modes in crystalline cytidine via high pressure infrared absorption and molecular dynamics simulations.**, CARL STARKEY, University of Toledo, KRISTINA WOODS, Carnegie-Mellon University, SCOTT LEE, University of Toledo — High-pressure infrared absorption experiments and molecular dynamics simulations have been used to study the eigenvectors and eigenvalues of the vibrational modes of crystalline cytidine at 295 K by evaluating the logarithmic derivative of the vibrational frequency with respect to pressure:  $\frac{1}{\omega} \frac{d\omega}{dP}$ . Crystalline samples of molecular materials such as cytidine have vibrational modes that are localized within a molecular unit ("internal" modes) as well as modes in which the molecular units vibrate against each other ("external" modes). The value of the logarithmic derivative is a diagnostic probe of the nature of the eigenvector of the vibrational modes, making high pressure experiments a very useful probe for such studies. Internal stretching modes have low logarithmic derivatives while external as well as internal torsional and bending modes have higher logarithmic derivatives. Modes at about 503, 757, 795, 3093 and 3351  $\text{cm}^{-1}$  are found to have negative logarithmic pressure derivatives, indicating a weakening of the effective force constants associated with those modes. The two modes above 3000  $\text{cm}^{-1}$  are hydrogen-bond-stretching modes. The identity of all of these modes will be determined via molecular dynamical simulations.

**M1.00272 Computational Study of Pseudo-phosphorylation of the Microtubule associated Protein Tau**, DMITRIY PROKOPOVICH, LUCA LARINI, Rutgers University-Camden — This computational study focuses on the effect of pseudo-phosphorylation on the aggregation of the microtubule associated protein tau. In the axon of the neuron, tau regulates the assembly of microtubules in the cytoskeleton. This is important for both stabilization of and transport across the microtubules. One of the hallmarks of the Alzheimer's disease is that tau is hyper-phosphorylated and aggregates into neurofibrillary tangles that lay waste to the neurons. It is not known if hyper-phosphorylation directly causes the aggregation of tau into tangles. Experimentally, pseudo-phosphorylation mimics the effects of phosphorylation by mutating certain residues of the protein chain into charged residues. In this study, we will consider the fragment called PHF43 that belongs to the microtubule binding region and has been shown to readily aggregate.

**M1.00273 Quantum Computational Calculations of the Ionization Energies of Acidic and Basic Amino Acids: Aspartate, Glutamate, Arginine, Lysine, and Histidine.**<sup>1</sup>, C. P. DE GUZMAN, M. ANDRIANARI-JAONA, Y. S. LEE, V. ANDRIANARIJAONA, Department of Physics, Pacific Union College, Angwin, CA, 94508 — An extensive knowledge of the ionization energies of amino acids can provide vital information on protein sequencing, structure, and function. Acidic and basic amino acids are unique because they have three ionizable groups: the C-terminus, the N-terminus, and the side chain. The effects of multiple ionizable groups can be seen in how Aspartate's ionizable side chain heavily influences its preferred conformation (*J Phys Chem A*. 2011 April 7; 115(13): 2900–2912). Theoretical and experimental data on the ionization energies of many of these molecules is sparse. Considering each atom of the amino acid as a potential departing site for the electron gives insight on how the three ionizable groups affect the ionization process of the molecule and the dynamic coupling between the vibrational modes. In the following study, we optimized the structure of each acidic and basic amino acid then exported the three dimensional coordinates of the amino acids. We used ORCA to calculate single point energies for a region near the optimized coordinates and systematically went through the x, y, and z coordinates of each atom in the neutral and ionized forms of the amino acid. With the calculations, we were able to graph energy potential curves to better understand the quantum dynamic properties of the amino acids.

<sup>1</sup>The authors thank Pacific Union College Student Association for providing funds.

**M1.00274 Aggregation propensity of critical regions of the protein Tau**, MICAH MUTHEE, AZKA AHMED, LUCA LARINI, Rutgers University-Camden — The Alzheimer's disease is an irreversible, progressive brain disorder that slowly destroys memory and thinking skills, which eventually leads to the inability to carry out the simplest tasks. The Alzheimer's disease is characterized by the formation of protein aggregates both within and outside of the brain's cells, the neurons. Within the neurons, the aggregation of the protein tau leads to the destruction of the microtubules in the axon of the neuron. Tau belongs to a group of proteins referred to as Microtubule-Associated Proteins. It is extremely flexible and is classified as an intrinsically unstructured protein due to its low propensity to form secondary structure. Tau promotes tubulin assembly into microtubules thereby stabilizing the cytoskeleton of the axon of the neurons. The microtubule binding region of tau consists of 4 pseudo-repeats. In this study, we will focus on the aggregation propensity of two fragments. In this study we will focus on the PHF43 fragment that contains the third pseudo-repeat and has been shown experimentally to aggregate readily. Another fragment that contains the second pseudo-repeat will be considered as well. Mutations in this region are associated with various forms of dementia and for this reason we will consider the mutant P301L.

**M1.00275 A Novel Approach for Computing Cross-Sections in Ion-Mobility Measurements**, LUCA LARINI, OSCAR MARIN, Rutgers University - Camden — Mass spectrometry allows the identification of molecules based on their mass to charge ratio. One of the advantages of this technique is that it is able to distinguish molecules that differ for a small value of the mass. In addition, once the molecule of interest has been selected by the mass spectrometer, it can be further analyzed in an ion mobility tube that can characterize the conformations adopted by the molecule. This is extremely useful when dealing with unstructured proteins that populate multiple conformations. However, ion mobility distinguishes structures based on their cross-section. In order to associate a well-defined tridimensional structure to a specific cross-section, molecular dynamics simulations must be performed first, and then the theoretical cross-section compared to the experimental one. Computing a cross-section starting from molecular dynamics data is extremely computationally expensive. For this reason, we have developed a software that takes advantage of the multicore and multimode architecture of modern computer clusters.

**M1.00276 Single molecule fluorescence studies of transition paths in DNA hairpin folding**, KATHERINE TRUEX, HOI SUNG CHUNG, JOHN LOUIS, WILLIAM EATON, National Institutes of Health — DNA hairpins are the simplest structures for investigating fundamental aspects of nucleic acid folding mechanisms. For two-state hairpins, all of the mechanistic information on how the hairpin folds is contained in the transition path (TP), the rare event in single molecule trajectories when the free energy barrier between folded and unfolded states is actually crossed. The only previous experimental study of TPs in nucleic acids used optical tweezer measurements and Szabo's analytical theory for diffusive barrier crossing to reconstruct the free energy surface for an indirect determination of average TP times (Neupane *et al.* *PRL* 2012). We used confocal single molecule FRET and maximum likelihood analysis of photon trajectories to determine an upper bound of 2.5  $\mu$ s for the average TP time of a DNA hairpin (Truex *et al.*, *PRL* 2015), compared to the value of 4  $\mu$ s predicted by Neupane *et al.*, providing an important test of energy landscape theory. Current experiments are aimed at eventually characterizing structural changes during TPs, which will provide a very demanding test of mechanisms predicted by both theoretical models and simulations.

**M1.00277 Electrical Heart Defibrillation with Ion Channel Blockers**, ERIN FEENEY, COURTNEY CLARK, STEFFAN PUWAL, Oakland University — Heart disease is the leading cause of mortality in the United States. Rotary electrical waves within heart muscle underlie electrical disorders of the heart termed fibrillation; their propagation and breakup leads to a complex distribution of electrical activation of the tissue (and of the ensuing mechanical contraction that comes from electrical activation). Successful heart defibrillation has, thus far, been limited to delivering large electrical shocks to activate the entire heart and reset its electrical activity. In theory, defibrillation of a system this nonlinear should be possible with small electrical perturbations (stimulations). A successful algorithm for such a low-energy defibrillator continues to elude researchers. We propose to examine in silico whether low-energy electrical stimulations can be combined with antiarrhythmic, ion channel-blocking drugs to achieve a higher rate of defibrillation and whether the antiarrhythmic drugs should be delivered before or after electrical stimulation has commenced. Progress toward a more successful, low-energy defibrillator will greatly minimize the adverse effects noted in defibrillation and will assist in the development of pediatric defibrillators.

**M1.00278 Dynamics of driven transitions between minima of a complex energy landscapes**, SAI TEJA PUSULURI, Department of physics, Ohio University, ALEX H LANG, Computational Neurobiology Laboratory, Salk Institute, PANKAJ MEHTA, Department of physics, Boston University, HORACIO E CASTILLO, Department of physics, Ohio University — We recently modeled cellular interconversion dynamics[1] by using an epigenetic landscape model[2] inspired by neural network models. Given an arbitrary set of patterns, the model can be used to construct an energy landscape in which those patterns are the global minima. Here we study the transitions between stable states of the landscapes thus constructed, under the effect of an external driving force. We consider three different cases: i) choosing the patterns to be random and independently distributed ii) choosing a set of patterns directly derived from the experimental cellular transcription factor expression data for a representative set of cell types in an organism and iii) choosing randomly generated trees of hierarchically correlated patterns, inspired by biology. For each of the three cases, we study the stability of the global minima against thermal fluctuations and external driving forces, and the dynamics of the driven transitions away from global minima. We compare the results obtained in the three cases defined above, and in particular we explore to what degree the correlations between patterns affect the transition dynamics.

References

[1] Pusuluri *et al.* (2015) arXiv:1505.03889.

[2] Lang *et al.* (2014) *PLoS computational biology* 10, e1003734.

**M1.00279 Anomalous motor mediated cargo transport in microtubule networks**, STEVEN VANDAL, Worcester Polytechnic Institute, Dept of Physics, DANIEL MACVEIGH-FIERRO, ZHIYUAN SHEN, Worcester Polytechnic Institute, Dept of Biology and Biotechnology, KYLE LEMOI, Worcester Polytechnic Institute, Dept of Physics, LUIS VIDALI, Worcester Polytechnic Institute, Dept of Biology and Biotechnology, JENNIFER ROSS, University of Massachusetts Amherst, Dept of Physics, ERKAN TUZEL, Worcester Polytechnic Institute, Dept of Physics — Cargo transport is an important biological mechanism by which cells locomote, self-organize, and actively transport organelles. This transport is mediated by the cytoskeletal network and molecular motors; however, it is not known how network self-organization and dynamics affect these transport processes. In order to develop a mechanistic understanding of cargo transport, we use a coarse-grained Brownian dynamics model that incorporates the dynamics of these networks, as well as experimentally determined motor properties. We will test these models with two experimental systems: (1) in vitro microtubule networks with kinesin-1 motors, and quantum dot cargos on recreated microtubule networks, and (2) an excellent model organism, the moss *Physcomitrella patens*, in which chloroplasts are transported via the microtubule network by means of kinesin-like proteins. Phenomenological network characterizations are made, both in vivo and in vitro, and cargo motility is characterized using Mean Squared Displacement (MSD) measurements. Our simulations shed light on the role of network density and motor properties on the observed transport behavior, and improve our understanding of cargo transport in cells.

**M1.00280 Water - Based  $\text{TiO}_2$  Suspensions: A Raman Study**, ROBERTO RANGEL, DORINA CHIPARA, BRIAN YUST, DESIREE PADILLA, MIRCEA CHIPARA, The University of Texas Rio Grande Valley — The antibacterial features of  $\text{TiO}_2$  are under scrutiny due to the UV radiation, which contributes to the generation of reactive oxygen species, mainly in water environments. A study of  $\text{TiO}_2$  suspensions in water and broth is reported.  $\text{TiO}_2$  has a low solubility in water.  $\text{TiO}_2$  (anatase), with average diameter of 15 nm from Nanostructured & Amorphous Materials, Inc. has been added to the fluid (water, broth) and the mixture was stirred for 1-10 h, followed by a 10-60 minutes sonication. The suspension was left to sediment for 1 day before measurements. Quasistable suspensions of  $\text{TiO}_2$  in water and broth were investigated by Raman spectroscopy using a Renishaw InVia spectrometer operating at 532 and 785 nm. The spectra of the nanofiller have been simulated by a collection of Breit-Wigner Fano line shapes and the effect of the preparation conditions (stirring and sonication time) on the parameters of Raman lines are reported. The differences are explained by observing that the sonication destroys the agglomerates of anatase resulting in a better dispersion of nanoparticles and consequently a longer sedimentation time. Sample preparation/storage have been done both under dark and UV light conditions.

**M1.00281 The broadcasting mechanism of master regulator  $NF\kappa B$  switches.**, DAVIT POTOYAN, Rice University — The transcription factor  $NF\kappa B$  is involved in many cellular responses. Therefore there is a large number of sites in the genome to which  $NF\kappa B$  binds thereby activating myriad of genes as a response to various environmental stimuli. Kinetics becomes an important feature to reckon with in eukaryotic regulatory networks with many targets like the  $NF\kappa B$  system. In particular models based on the classical picture of genetic switches predict slow down regulation of  $NF\kappa B$  which can lead to wasteful over-expression of genes. A way to resolve this difficulty is to evolve faster ways of deactivating  $NF\kappa B$ . There is evidence from experiments and our simulations that this is done by an  $IkB$  induced process of stripping  $NF\kappa B$  off directly from its genetic sites instead of waiting for autonomous dissociation. The broadcasting mechanism proposed in this work solves the time scale problem inherent in the classical picture. Using combination of stochastic and deterministic models we show how such a mechanism results in efficient regulation of  $NF\kappa B$  network.

**M1.00282 Processing oscillatory signals by incoherent feedforward loops<sup>1</sup>**, CAROLYN ZHANG, FEILUN WU, RYAN TSOI, IGOR SHATS, LINGCHONG YOU, Duke University — From the timing of amoeba development to the maintenance of stem cell pluripotency, many biological signaling pathways exhibit the ability to differentiate between pulsatile and sustained signals in the regulation of downstream gene expression. While networks underlying this signal decoding are diverse, many are built around a common motif, the incoherent feedforward loop (IFFL), where an input simultaneously activates an output and an inhibitor of the output. With appropriate parameters, this motif can generate temporal adaptation, where the system is desensitized to a sustained input. This property serves as the foundation for distinguishing signals with varying temporal profiles. Here, we use quantitative modeling to examine another property of IFFLs, the ability to process oscillatory signals. Our results indicate that the system's ability to translate pulsatile dynamics is limited by two constraints. The kinetics of IFFL components dictate the input range for which the network can decode pulsatile dynamics. In addition, a match between the network parameters and signal characteristics is required for optimal "counting". We elucidate one potential mechanism by which information processing occurs in natural networks with implications in the design of synthetic gene circuits for this purpose.

<sup>1</sup>This work was partially supported by the National Science Foundation Graduate Research Fellowship (CZ).

**M1.00283 Shock wave irradiations avoiding fluid flow evoke intracellular  $\text{Ca}^{2+}$  signaling**, TORU TAKAHASHI, AKIRA TSUKAMOTO, SHIGERU TADA, National Defense Academy of Japan — Shock wave irradiation accelerates therapeutic effects including angiogenesis. One mechanism underlying those effects is cellular responses evoked by shock wave irradiation. Fluid flow is one of major physical phenomena induced by shock wave irradiation. Cellular responses evoked by fluid flow are similar to those evoked by shock wave irradiation. Thus, fluid flow could be responsible for cellular responses evoked by shock wave irradiation. However, it is obscure whether fluid flow is required for the cellular responses evoked by shock wave irradiation. In this study, intracellular  $\text{Ca}^{2+}$  signaling was observed in cells seeded in down-sized chambers. In the down-sized chambers, fluid flow was supposed to be suppressed because size of chambers (6 mm in diameter, 1 mm in thickness) was analogous to size of shock wave focus region (3mm in diameter). Dynamics of polystyrene microbeads suspended in the chambers were visualized with a CCD camera and analyzed with a particle image velocimetry (PIV) method to quantify fluid flow in the chamber. As a result, shock wave irradiation evoked intracellular  $\text{Ca}^{2+}$  signaling. However, fluid flow was not observed in the chamber due to shock wave irradiation. Thus, it was suggested that physical mechanics, not fluid flow, are further required for evoking intracellular  $\text{Ca}^{2+}$  signaling following to shock wave irradiation.

**M1.00284 Dynamics of phenotypic reversibility of bacterial cells with oscillating hydrostatic pressure**, SUDIP NEPAL, Univ of Arkansas-Fayetteville, PRADEEP KUMAR, Department of Physics, Univ of Arkansas-Fayetteville — Bacterial cells encounter and respond to physiochemical fluctuations. The response depends on the extent and type of the stresses applied. The response of bacterial cells to the fluctuating stress is relatively unknown. Here, we have studied the response of wild type *Escherichia coli* (*E. coli*) under fluctuating hydrostatic pressures ranging from 1 atm to 500 atm. High pressure acts as a stress to *E. coli* since these bacteria are adapted to grow optimally at atmospheric pressure. Cell division of *E. coli* is inhibited at high pressures resulting in increase in the length of the cells. Cell-length is reversible in nature and bacterial cells revert back to normal size on a time scale that is proportional to the strength and time of continuous pressure applied upon relaxing the high pressure condition. We have studied the dynamics of cellular reversibility of *E. coli* under the conditions in which continuous pressure is applied and subsequently relaxed over different time scales. We have quantified the dynamics of cellular reversibility with different relaxation times. Furthermore, we propose a model to describe the reversibility of the bacterial cell with the relaxation time. Our theoretical model fits well to the experimental data. We further

**M1.00285 Chiral pattern formation in compact microbial colonies**, KIRILL KOROLEV, ASHISH BINO GEORGE, Boston University — Chirality is ubiquitous in biology from single molecules to entire populations. Yet, we are still lacking a detailed understanding of how chiral patterns emerge from cell competition and growth, even in simple microbial colonies. Although many microbes grow as dense colonies with no apparent chirality, recent experiments with *Escherichia coli* have demonstrated that internal dynamics in such populations can be in fact chiral. We show that there is a unique way to extend the commonly-used reaction-diffusion models of colony growth to account for the emergent chirality. This new model connects microscopic and macroscopic chirality and explains the origin of logarithmic spirals separating different sub-populations in a colony. We also show that chirality is substantially enhanced by the cooperation among the cells at the expansion frontier. In heterogeneous populations composed of strains with different chiralities and growth rates, our model predicts a very rich set of possible dynamics. For example, different chiralities can result in either sharp boundaries between the strains or promote their intermixing depending on the preferred twisting directions of the strains.

**M1.00286 Adhesion of Mycobacterium smegmatis to Charged Surfaces and Diagnostics Implications.**<sup>1</sup> , DIANE GORSE, ALI DHINOJWALA, Univ of Akron, FRANCISCO MOORE, Univ of Akron, NSF — Pulmonary tuberculosis (PTB) causes more than 1 million deaths annually. Smear microscopy is a primary rapid detection tool in areas where 95 % of PTB cases occur. This technique, in which the sputum of a symptomatic patient is stained and examined using a light microscope for Mycobacterium tuberculosis (MTB) shows sensitivity between 20 and 60 %. Insufficient bacterial isolation during sample preparation may be a reason for low sensitivity. We are optimizing a system to capture bacteria on the basis of electrostatic interactions to more thoroughly isolate bacteria from suspension and facilitate more accurate detection. Silica supports coated with positively-charged polyelectrolyte, poly(diallyldimethylammonium chloride), captured approximately 4.1 times more Mycobacterium smegmatis, a model organism for MTB, than was captured on negatively-charged silica substrates. Future experimentation will employ branched polymer systems and seek to justify the use of colloidal stability theories to describe initial capture.

<sup>1</sup>Supported by University of Akron, Department of Polymer Science, Department of Biology; LORD Corporation

**M1.00287 Cell motility and antibiotic tolerance of bacterial swarms** , WENLONG ZUO<sup>1</sup>, Shenzhen Research Institute, The Chinese University of Hong Kong; Department of Physics, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong — Many bacteria species can move across moist surfaces in a coordinated manner known as swarming. It is reported that swarm cells show higher tolerance to a wide variety of antibiotics than planktonic cells. We used the model bacterium *E. coli* to study how motility affects the antibiotic tolerance of swarm cells. Our results provide new insights for the control of pathogenic invasion via regulating cell motility.

<sup>1</sup>Mailing address: Room 306 Science Centre North Block, The Chinese University of Hong Kong, Shatin, N.T. Hong Kong SAR. Phone: +852-3943-6354. Fax: +852-2603-5204. E-mail: zwlong@live.com

**M1.00288 The Effect of Graphene Oxide/Reduced Graphene Oxide Functionalized with Metal Nanoparticles on Dermal, Bacterial, and Cancerous/Non-Cancerous Epithelial Cells**<sup>1</sup> , ARTHUR CHEN, MIRIAM RAFAILOVICH, MARCIA SIMON, State Univ of NY- Stony Brook, REBECCA ISSEROFF, Lawrence Public High School, STEPHEN WALKER, State Univ of NY- Stony Brook, JAE HEE CHO, Boston University, JOHN JEROME, Suffolk University — Graphene and metal nanoparticles are permeating health products but their effects individually and combined on human skin are uncertain. This project studied the effect of graphene oxide (GO) and reduced graphene oxide (rGO) functionalized with Ag or Pt nanoparticles (Ag/PtNPs) on bacterial, dermal (DFBC's), and cancerous (SCC13's) and non-cancerous (DO33's) epidermal cells. GO was functionalized with AgNPs or PtNPs, forming metallized-GO; then reduced with NaBH<sub>4</sub>. FTIR and SEM confirmed the synthesis and composition. Confocal and SEM showed that Ag-rGO, depending on nanoparticle size, killed either *S. Aureus* or *K. Pneumoniae*, while Pt-rGO and rGO had no effect. Rhodamine staining revealed that Ag-rGO was very toxic to SCC13's, but only slightly toxic to DO33's. Pt-rGO and rGO had little effect on SCC13's and DO33's. At high concentrations all GO solutions inhibited cell growth but were not cytotoxic. Optical microscopy displayed that every GO/rGO solution adhered to DFBC's and influenced their direction of growth, making GO/rGO potentially applicable for wound healing.

<sup>1</sup>Garcia MRSEC Polymers at Engineered Interfaces

**M1.00289 The functional consequences of non-genetic diversity in cellular navigation**<sup>1</sup> , THIERRY EMONET, ADAM J WAITE, NICHOLAS W FRANKEL, YANN DUFOUR, JESSICA F JOHNSTON, Yale University — Substantial non-genetic diversity in complex behaviors, such as chemotaxis in *E. coli*, has been observed for decades, but the relevance of this diversity for the population is not well understood. Here, we use microfluidics to show that non-genetic diversity leads to significant structuring of the population in space and time, which confirms predictions made by our detailed mathematical model of chemotaxis. We then use genetic tools to show that altering the expression level of a single chemotaxis protein is sufficient to alter the distribution of swimming behaviors, which directly determines the performance of a population in a gradient of attractant, a result also predicted by our model.

<sup>1</sup>Supported by NIH 1R01GM106189, the James S McDonnell Foundation, and the Paul Allen foundation

**M1.00290 Allosteric Small-Molecule Inhibitors of the AKT Kinase** , D. S. DALAFAVE, The College of New Jersey — This research addresses computational design of small druglike molecules for possible anticancer applications. AKT and SGK are kinases that control important cellular functions. They are highly homologous, having similar activators and targets. Cancers with increased SGK activity may develop resistance to AKT-specific inhibitors. Our goal was to design new molecules that would bind both AKT and SGK, thus preventing the development of drug resistance. Most kinase inhibitors target the kinase ATP-binding site. However, the high similarity in this site among kinases makes it difficult to target specifically. Furthermore, mutations in this site can cause resistance to ATP-competitive kinase inhibitors. We used existing AKT inhibitors as initial templates to design molecules that could potentially bind the allosteric sites of both AKT and SGK. Molecules with no implicit toxicities and optimal drug-like properties were used for docking studies. Binding energies of the stable complexes that the designed molecules formed with AKT and SGK were calculated. Possible applications of the designed putative inhibitors against cancers with overexpressed AKT/SGK is discussed.

**M1.00291 Effects of Chemotherapy-Induced Alterations in Cell Mechanical Properties on Cancer Metastasis** , SRUTI PRATHIVADHI, ANDREW EKPENYONG, MICHAEL NICHOLS, CAROLYN TAYLOR, JIANHAO NING, Creighton University — Biological cells can modulate their mechanical properties to suit their functions and in response to changes in their environment. Thus, mechanical phenotyping of cells has been employed for tracking stem cell differentiation, bacterial infection, cell death, etc. Malignant transformation of cells also involves changes in mechanical properties. However, the extent to which mechanical properties of cancer cells contribute to metastasis is not well understood. Yet, more than 90% of all cancer deaths are directly related to metastasis. Transit of cells through the microcirculation is one of the key features of metastasis. We hypothesize that cancer treatment regimens do inadvertently alter cell mechanical properties in ways that might promote cancer metastasis. We use a microfluidic microcirculation mimetic (MMM) platform which mimics the capillary constrictions of the pulmonary and peripheral microcirculation to determine if *in-vivo*-like mechanical stimuli can evoke different responses from cells subjected to various cancer drugs. In particular, we show that cancer cells treated with chemotherapeutic drugs such as daunorubicin, become more deformable at short timescales (0.1 s) and transit faster through the device. Our results are first steps in evaluating the pro- or anti-metastatic effects of chemotherapeutic drugs based on their induced alterations in cell mechanical properties.

**M1.00292 Collective motion in Proteus mirabilis swarms** , XU HAORAN<sup>1</sup>, Shenzhen Research Institute, The Chinese University of Hong Kong; Department of Physics, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong — *Proteus mirabilis* is a Gram-negative, rod-shaped bacterium. It is widely distributed in soil and water, and it is well known for exhibiting swarming motility on nutrient agar surfaces. In our study, we focused on the collective motility of *P. mirabilis* and uncovered a range of interesting phenomena. Here we will present our efforts to understand these phenomena through experiments and simulation.

<sup>1</sup>Mailing address: Room 306 Science Centre North Block, The Chinese University of Hong Kong, Shatin, N.T. Hong Kong SAR. Phone: +852-3943-6354. Fax: +852-2603-5204. E-mail: xhrphx@gmail.com

**M1.00293 Swimming and transport of bacteria in time-periodic flows<sup>1</sup>** , REBECCA WINTER, ALISON PATTESON, DAVID GAGNON, PAULO ARRATIA, Univ of Pennsylvania — The transport of bacteria can be highly influenced by external flows in oceans, rivers, and intestinal tracts. This has implications in biological systems for the performance of major biological processes, such as biofilm formation. In this study, we experimentally investigate the aggregation and transport of swimming *Vibrio cholerae* bacteria in time-periodic flows. Bacteria are placed in a well-characterized flow, and bacterial concentrations are recorded for a range of Reynolds numbers (Re) that spans two orders of magnitude, from 0.1 to 10. It is generally found that bacteria deplete from regions of high deformation rate and accumulate near vortices. This phenomenon seems to be dictated by a combination of bacterial activity and background flow vorticity.

<sup>1</sup>R.W. supported by NSF-GRFP

**M1.00294 Emergence of collective motion in bacterial suspensions** , SONG LIU<sup>1</sup>, Shenzhen Research Institute, The Chinese University of Hong Kong; Department of Physics, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong — It is well known that bacterial suspensions will exhibit collective motion at high concentrations, in which both steric and hydrodynamic interactions play important roles. We aim to investigate whether steric and hydrodynamic interactions are of equal importance to the emergence of collective motion. Here we will present our efforts to experimentally tune the relative strength of these interactions in bacterial suspensions. Our preliminary results suggest that the transition to collective motion may depend on the interplay between steric and hydrodynamic interactions.

<sup>1</sup>Mailing address: Room 306 Science Centre North Block, The Chinese University of Hong Kong, Shatin, N.T. Hong Kong SAR. Phone: +852-3943-6354. Fax: +852-2603-5204. E-mail: songliuphy@gmail.com

**M1.00295 Effect of microemulsions on cell viability of human dermal fibroblasts** , JUYI LI, TATSIANA MIRONAVA, MARCIA SIMON, MIRIAM RAFILOVICH, NISSIM GARTI, State Univ of NY- Stony Brook — Microemulsions are optically clear, thermostable and isotropic mixture consisting of water, oil and surfactants. Their advantages of ease preparation, spontaneous formation, long-term stability and enhanced solubility of bioactive materials make them great potentials as vehicles in food and pharmaceutical applications. In this study, comparative in vitro cytotoxicity tests were performed to select a best formulation of microemulsion with the least toxicity for human dermal fibroblasts. Three different kinds of oils and six different kinds of surfactants were used to form microemulsions by different ratios. The effect of oil type and surfactant type as well as their proportions on cell proliferation and viability were tested.

**M1.00296 Experimental evolution of *E. coli*** , MENGSHI ZHANG<sup>1</sup>, Shenzhen Research Institute, The Chinese University of Hong Kong; Department of Physics, The Chinese University of Hong Kong, Shatin, N.T., Hong Kong — The evolution from unicellular to multicellular behavior is an essential step in the history of life. Our aim is to investigate the emergence of collective behavior in the model organism *Escherichia coli* (*E. coli*) and its selection advantages, such as better utilization of public goods. Our preliminary results suggest that the evolution of collective behavior may be a natural response to stressed conditions.

<sup>1</sup>Mailing address: Room 306 Science Centre North Block, The Chinese University of Hong Kong, Shatin, N.T. Hong Kong SAR. Phone: +852-3943-6354. Fax: +852-2603-5204. E-mail: mengshi0928@gmail.com

**M1.00297 Centrosome Positioning in 1D Cell Migration** , KATRINA ADLERZ, HELIM ARANDA-ESPINOZA, Univ of Maryland-College Park — During cell migration, the positioning of the centrosome and nucleus define a cell's polarity. For a cell migrating on a two-dimensional substrate the centrosome is positioned in front of the nucleus. Under one-dimensional confinement, however, the centrosome is positioned behind the nucleus in 60% of cells. It is known that the centrosome is positioned by CDC42 and dynein for cells moving on a 2D substrate in a wound-healing assay. It is currently unknown, however, if this is also true for cells moving under 1D confinement, where the centrosome position is often reversed. Therefore, centrosome positioning was studied in cells migrating under 1D confinement, which mimics cells migrating through 3D matrices. 3 to 5  $\mu\text{m}$  fibronectin lines were stamped onto a glass substrate and cells with fluorescently labeled nuclei and centrosomes migrated on the lines. Our results show that when a cell changes directions the centrosome position is maintained. That is, when the centrosome is between the nucleus and the cell's trailing edge and the cell changes direction, the centrosome will be translocated across the nucleus to the back of the cell again. A dynein inhibitor did have an influence on centrosome positioning in 1D migration and change of directions.

**M1.00298 Active microrheology reveals molecular-level variations in the viscoelastic properties of *Chaetopterus mucus*** , WILLIAM WEIGAND, Univ of San Diego, ASHLEY MESSMORE, University of California, San Diego, RAE ANDERSON, Univ of San Diego — The sea annelid, *Chaetopterus Variopedatus*, secretes a bioluminescent mucus that also exhibits complex viscoelastic properties. The constituents of the mucus are relatively unknown but it does play an important role in the development of the worms' parchment-like housing tubes. In order to determine how and why this mucus can exhibit material properties ranging from fluidity to rigidity we perform microrheology experiments. We determine the microscale viscoelastic properties by using optical tweezers to produce small oscillations in the mucus which allow us to determine both the linear storage and loss moduli ( $G'$ ,  $G''$ ) along with the viscosity of the fluid. By varying the size of the microspheres (2-10  $\mu\text{m}$ ) and oscillation amplitude (.5-10  $\mu\text{m}$ ) we are able to determine the dominant intrinsic length scales of the molecular mesh comprising the mucus. By varying the oscillation frequency (1-15Hz) we determine the crossover frequency at which  $G'$  surpasses  $G''$ , to quantify the longest relaxation time of the mesh network. Initial results show a strong dependence on bead size which indicate that the dominant entanglement lengthscale of the mucus mesh is  $\sim 5 \mu\text{m}$ . Microspheres of this size exhibit a wide variety of stress responses in different regions of the mucus demonstrating the substantial microscale heterogeneity of the mucus. We carry out measurements on a population of worms of varying size and age to determine mucus variability between worms.

**M1.00299 Regulation of muscle contraction by Drebrin-like protein 1 probed by atomic force microscopy.** , RENATA GARCES, EUGENIA BUTKEVICH, MITJA PLATEN, CHRISTOPH F. SCHMIDT, Third Institute of Physics - Biophysics, Georg August University, Göttingen, BIOPHYSICS TEAM — Sarcomeres are the fundamental contractile units of striated muscle cells. They are composed of a variety of structural and regulatory proteins functioning in a precisely orchestrated fashion to enable coordinated force generation in striated muscles. Recently, we have identified a *C. elegans* drebrin-like protein 1 (DBN-1) as a novel sarcomere component, which stabilizes actin filaments during muscle contraction. To further characterize the function of DBN-1 in muscle cells, we generated a new *dbn-1* loss-of-function allele. Absence of DBN-1 resulted in a unique worm movement phenotype, characterized by hyper-bending. It is not clear yet if DBN-1 acts to enhance or reduce the capacity for contraction. We present here an experimental mechanical study on *C. elegans* muscle mechanics. We measured the stiffness of the worm by indenting living *C. elegans* with a micron-sized sphere adhered to the cantilever of an atomic force microscope (AFM). Modeling the worm as a pressurized elastic shell allows us to monitor the axial tension in the muscle through the measured stiffness. We compared responses of wild-type and mutant *C. elegans* in which DBN-1 is not expressed..

**M1.00300 Quantifying Microtentacle Dynamics for Non-adherent Tumor Cells<sup>1</sup>**, ELEANOR ORY, DESU CHEN, University of Maryland, College Park, KRISTI CHAKRABARTI, STUART MARTIN, University of Maryland School of Medicine, WOLFGANG LOSERT, University of Maryland, College Park, UNIVERSITY OF MARYLAND, COLLEGE PARK COLLABORATION, UNIVERSITY OF MARYLAND SCHOOL OF MEDICINE COLLABORATION — In current cancer medicine, metastasis is still responsible for 90

<sup>1</sup>Era of Hope Scholar award from the Department of Defense

**M1.00301 Measuring shear force transmission across a biomimetic glycocalyx**, ISABEL BRAY, DYLAN YOUNG, JAN SCRIMGEOUR, Department of Physics, Clarkson University, Potsdam NY 13699 — Human blood vessels are lined with a low-density polymer brush known as the glycocalyx. This brush plays an active role in defining the mechanical and biochemical environment of the endothelial cell in the blood vessel wall. In addition, it is involved in the detection of mechanical stimuli, such as the shear stress from blood flowing in the vessel. In this work, we construct a biomimetic version of the glycocalyx on top of a soft deformable substrate in order to measure its ability to modulate the effects of shear stress at the endothelial cell surface. The soft substrate is stamped on to a glass substrate and then enclosed inside a microfluidic device that generates a controlled flow over the substrate. The hydrogel chemistry has been optimized so that it reliably stamps into a defined shape and has consistent mechanical properties. Fluorescent microbeads embedded in the gel allow measurement of the surface deformation, and subsequently, calculation of the shear force at the surface of the soft substrate. We investigate the effect of the major structural elements of the glycocalyx, hyaluronic acid and charged proteoglycans, on the magnitude of the shear force transmitted to the surface of the hydrogel.

**M1.00302 Micro-mechanical model for the tension-stabilized enzymatic degradation of collagen tissues**, THAO NGUYEN, Mechanical Engineering, Johns Hopkins University, JEFFERY RUBERTI, Department of Bioengineering, Northeastern University — We present a study of how the collagen fiber structure influences the enzymatic degradation of collagen tissues. Experiments of collagen fibrils and tissues show that mechanical tension can slow and halt enzymatic degradation. Tissue-level experiments also show that degradation rate is minimum at a stretch level coincident with the onset of strain-stiffening in the stress response. To understand these phenomena, we developed a micro-mechanical model of a fibrous collagen tissue undergoing enzymatic degradation. Collagen fibers are described as sinusoidal elastica beams, and the tissue is described as a distribution of fibers. We assumed that the degradation reaction is inhibited by the axial strain energy of the crimped collagen fibers. The degradation rate law was calibrated to experiments on isolated single fibrils from bovine sclera. The fiber crimp and properties were fit to uniaxial tension tests of tissue strips. The fibril-level kinetic and tissue-level structural parameters were used to predict tissue-level degradation-induced creep rate under a constant applied force. We showed that we could accurately predict the degradation-induced creep rate of the pericardium and cornea once we accounted for differences in the fiber crimp structure and properties.

**M1.00303 Mechanical model of kinesin moving on microtubule**, KIWING TO, Institute of Physics, Academia Sinica, YA-CHANG CHOU, YI-FENG HSIAO, KUAN-HUA CHEN, Department of Physics, National Tsing Hua University — Kinesins are biomolecules that serve as intercellular motors for carrying cellular cargos along microtubules. Although the mechanism of converting the chemical energy of ATP to mechanical work is not fully understood, the motion of a kinesin on a microtubule has been measured and two different mechanisms, namely the hand-over-hand and inchworm, has been proposed. The particular shape of kinesin and microtubules suggest a possible mechanism for force generation similar to Brownian ratchet. Using a bead chain connected to two heads that are attracted to a vibrated ratchet plate as a scaled up analog of the kinesin-microtubule system, we manage to simulate both handoverhand and inchworm motion [Chou, et. al., Physica A443, 66 (2015)]. In addition, we find that chain, which play the role of the stalk in a kinesin molecule, can also generate force by interacting with the ratchet plate [Chen, et. al. Phys. Rev. E87, 012711 (2013)].

**M1.00304 Food category consumption and obesity prevalence across countries: an application of Machine Learning method to big data analysis.**, JOCELYN DUNSTAN, Johns Hopkins Bloomberg Public Health School, SAEIDEH FALLAH-FINI, Cal Poly Pomona, CLAUDIA NAU, THOMAS GLASS, Johns Hopkins Bloomberg Public Health School, GLOBAL OBESITY PREVENTION CENTER TEAM — The applications of sophisticated mathematical and numerical tools in public health has been demonstrated to be useful in predicting the outcome of public intervention as well as to study, for example, the main causes of obesity without doing experiments with the population. In this project we aim to understand which kind of food consumed in different countries over time best defines the rate of obesity in those countries. The use of Machine Learning is particularly useful because we do not need to create a hypothesis and test it with the data, but instead we learn from the data to find the groups of food that best describe the prevalence of obesity.

**M1.00305 An analytically tractable model for community ecology with many species<sup>1</sup>**, BENJAMIN DICKENS, Department of Physics, Boston University, CHARLES FISHER, Bayesian Inference Group, Pfizer, Cambridge, MA, PANKAJ MEHTA, Department of Physics, Boston University, PANKAJ MEHTA BIOPHYSICS THEORY GROUP TEAM — A fundamental problem in community ecology is to understand how ecological processes such as selection, drift, and immigration yield observed patterns in species composition and diversity. Here, we present an analytically tractable, presence-absence (PA) model for community assembly and use it to ask how ecological traits such as the strength of competition, diversity in competition, and stochasticity affect species composition in a community. In our PA model, we treat species as stochastic binary variables that can either be present or absent in a community: species can immigrate into the community from a regional species pool and can go extinct due to competition and stochasticity. Despite its simplicity, the PA model reproduces the qualitative features of more complicated models of community assembly. In agreement with recent work on large, competitive Lotka-Volterra systems, the PA model exhibits distinct ecological behaviors organized around a special ("critical") point corresponding to Hubbell's neutral theory of biodiversity. Our results suggest that the concepts of "phases" and phase diagrams can provide a powerful framework for thinking about community ecology and that the PA model captures the essential ecological dynamics of community assembly.

<sup>1</sup>PM was supported by a Simons Investigator in the Mathematical Modeling of Living Systems and a Sloan Research Fellowship

**M1.00306 Speeding up evolution**, WOUTER HOFF, Oklahoma State University — Proteins and cells offer great opportunities for green chemistry and renewable energy. However, few of these possible applications have been put into practice because of details that turn out to be major barriers to cost-efficient implementation and that prove difficult to solve by genetic engineering. A better understanding of molecular evolution promises a novel approach to addressing these important challenges. While major advances have been made, major gaps remain in understanding the evolution of proteins. Different approaches to accelerating molecular evolution into targeted directions will be discussed, including recent progress on evolution in non-homogeneous environments.

**M1.00307 Population heterogeneity promotes a preference for blind cooperation**<sup>1</sup>, ALFONSO PEREZ-ESCUERO, JONATHAN FRIEDMAN, JEFF GORE, Massachusetts Institute of Technology — Game theory—and common sense—recommend to carefully weigh costs and benefits before deciding on a course of action. Yet we often disapprove of people who do so, even when their actual decision benefits us. For example, we prefer people who directly agree to do us a favor over those who agree only after securing enough information to ensure that the favor will not be too costly. Why should we care about how people make their decisions, rather than just focus on the decisions themselves? Hoffman et al. (2015) have shown that such aversion to information gathering may be beneficial when it is strong enough to increase the level of cooperation. Here we show that the same type of aversion arises in heterogeneous populations, but for a different reason: individuals who seek additional information may reveal themselves to be undesirable partners, since they are less likely to cooperate in the future when conditions change. Aversion to information gathering thus facilitates preferential interactions with blind cooperators, who are more favorable partners. Due to this new mechanism the prevalence of such aversion rapidly increases with population diversity, because partner discrimination is more useful in populations which harbor partners of a more varied quality.

<sup>1</sup>We gratefully acknowledge funding from the Paul G. Allen Family Foundation, EMBO and Human Frontier Science Program

**M1.00308 Complex sound stimuli representation by small neural groups in subcortical auditory structure**<sup>1</sup>, DOMINIKA LYZWA, Institute of Neuroscience, Newcastle University & Institute for Nonlinear Dynamics, University of Goettingen — The neural representation of complex natural sound stimuli in higher auditory structures is not yet well understood. Based on neurophysiological recordings from the mammalian auditory midbrain, neural responses to complex (natural and also artificial) sounds are investigated and mapped with respect to temporal and spectral neural tuning in the subcortical structure. The mapping includes spiking activity of single neurons and small neural clusters and local field potential activity. A neural model is presented which captures the mapping and also the similarity of responses across the auditory structure, and is used to predict responses to novel sound.

<sup>1</sup>Financial support by Bernstein Focus Neural Technology Goettingen, grant number 01GQ0811

**M1.00309 A phylogenetic study of the section moduli of the humerus in bipedal theropod dinosaurs.**, SCOTT LEE, ZACHARY RICHARDS, University of Toledo — The section modulus of a bone is a measure of its ability to resist bending torques. Carnivorous dinosaurs including Tyrannosauroidae and Allosauroidae had strong humeri, presumably to hold struggling prey during hunting. The herbivorous dinosaurs of Ornithomimosauria had weak arm bones. This is believed to reflect the fact that their arms were never subjected to large bending torques. The unusual dinosaurs of Therizinosauria had arms as strong as found in the carnivorous dinosaurs. This is consistent with the hypothesis that their manus suggests a digging lifestyle. Other groups including Oviraptorosauria, Troodontidae, Dromaeosauridae and Compsognathidae are also examined.

**M1.00310 Physics of the Brain: Interaction of the Optical-Fiber-Guided Multi-Ultraviolet-Photon Beams with the Epilepsy Topion, (the Seizure Onset Area)**<sup>1</sup>, V. ALEXANDER STEFAN, Institute for Advanced Physics Studies, Stefan University, La Jolla, California 92037 — A novel method for the possible prevention of epileptic seizures is proposed, based on the multi-ultraviolet-photon beam interaction<sup>2</sup> with the epilepsy topion, (nonlinear coupling of an ultra high frequency mode to the brain beta phonons). It is hypothesized that epilepsy is a chaotic-dynamics phenomenon: small electrical changes in the epilepsy-topion lead, (within the 10s of milliseconds), to the onset of chaos, (seizure—excessive electrical discharge), and subsequent cascading into adjacent areas.<sup>3</sup> The ultraviolet photons may control the imbalance of sodium and potassium ions and, consequently, may prove to be efficient in the prevention of epileptic seizures.

<sup>1</sup>Supported by Nikola Tesla Labs, Stefan University.

<sup>2</sup> V. Stefan, B. I. Cohen, C. Joshi, *Science*, 243, 4890, (Jan.27, 1989); Stefan et al., *Bull. APS* 32, No.9, 1713, (1987); Stefan, APS-March-2015, # P1.00099; V. Alexander Stefan, *Neurophysics, Stem Cell Physics, and Genomic Physics: Beat-Wave-Driven-Free Electron Laser Beam Interactions with the Living Matter*, (S-U-Press, La Jolla, Calif, 2012).

<sup>3</sup> H.P. Zaveri et al., Localization-related epilepsy exhibits significant connectivity away from the seizure-onset area, *Neuroreport*, 20(9), 891-5, Jun17, 2009.

**M1.00311 Asynchronous electrical activity in epileptic seizures**<sup>1</sup>, KATHERINE HOLMAN, Towson University, EUGENE LIM, Ohio Wesleyan University, STEPHEN GLISKE, WILLIAM STACEY, University of Michigan, CHRISTIAN FINK, Ohio Wesleyan University — High-frequency oscillations (HFOs) have been postulated to be potential biomarkers for focal epileptic seizures, with fast ripples (>250 Hz) as the most interesting candidate. The mechanisms underlying the generation of fast ripples, however, are not well understood. In this study, we draw upon results from previous computational studies on HFOs to develop a new mathematical model from first principles describing the generation of HFOs through asynchronous neuronal firing. Asynchrony in the model is obtained with the introduction of two parameters of heterogeneity: variability in the inter-spike interval (ISI) and jitter. The model predicts the generation of harmonic narrow-band oscillations if the heterogeneity-governing parameters do not differ from the predefined ISI by more than 20%. Comparisons against results from a separately constructed computational model verify the accuracy of the model in study. These results provide us with a rigorous framework in which we may investigate the mechanisms driving the generation of abnormal HFOs, and may serve as groundwork for future research in epileptogenesis.

<sup>1</sup>NSF Grant 1003992, Ohio Wesleyan University SSRP

**M1.00312 Columnar organization of orientation domains in V1**, JOSCHA LIEDTKE, FRED WOLF, Max Planck Institute for Dynamics and Self-Organization — In the primary visual cortex (V1) of primates and carnivores, the functional architecture of basic stimulus selectivities appears similar across cortical layers (Hubel & Wiesel, 1962) justifying the use of two-dimensional cortical models and disregarding organization in the third dimension. Here we show theoretically that already small deviations from an exact columnar organization lead to non-trivial three-dimensional functional structures. We extend two-dimensional random field models (Schnabel et al., 2007) to a three-dimensional cortex by keeping a typical scale in each layer and introducing a correlation length in the third, columnar dimension. We examine in detail the three-dimensional functional architecture for different cortical geometries with different columnar correlation lengths. We find that (i) topological defect lines are generally curved and (ii) for large cortical curvatures closed loops and reconnecting topological defect lines appear. This theory extends the class of random field models by introducing a columnar dimension and provides a systematic statistical assessment of the three-dimensional functional architecture of V1 (see also (Tanaka et al., 2011)).

**M1.00313 A Topological Perspective of Neural Network Structure**, ANN SIZEMORE, CHAD GIUSTI, University of Pennsylvania, MATTHEW CIESLAK, SCOTT GRAFTON, University of California Santa Barbara, DANIELLE BASSETT, University of Pennsylvania — The wiring patterns of white matter tracts between brain regions inform functional capabilities of the neural network. Indeed, densely connected and cyclically arranged cognitive systems may communicate and thus perform distinctly. However, previously employed graph theoretical statistics are local in nature and thus insensitive to such global structure. Here we present an investigation of the structural neural network in eight healthy individuals using persistent homology. An extension of homology to weighted networks, persistent homology records both circuits and cliques (all-to-all connected subgraphs) through a repetitive thresholding process, thus perceiving structural motifs. We report structural features found across patients and discuss brain regions responsible for these patterns, finally considering the implications of such motifs in relation to cognitive function.

**M1.00314 Automated Region of Interest Detection of Fluorescent Neurons for Optogenetic Stimulation**, JONATHAN MISHLER, DIETMAR PLENZ, Natl Inst of Mental Health - NIMH — With the emergence of optogenetics, light has been used to simultaneously stimulate and image neural clusters *in vivo* for the purpose of understanding neural dynamics. Spatial light modulators (SLMs) have become the choice method for the targeted stimulation of neural clusters, offering unprecedented spatio-temporal resolution. By first imaging, and subsequently selecting the desired neurons for stimulation, SLMs can reliably stimulate those regions of interest (ROIs). However, as the cluster size grows, manually selecting the neurons becomes cumbersome and inefficient. Automated ROI detectors for this purpose have been developed, but rely on neural fluorescent spiking for detection, requiring several thousand imaging frames. To overcome this limitation, we present an automated ROI detection algorithm utilizing neural geometry and stationary information from a few hundred imaging frames that can be adjusted for sensitivity.

**M1.00315 An in vivo analysis of facial muscle change treated with botulinum toxin type A using digital image speckle correlation**, YAN XU, SAMANTHA PALMACCIO PALMACCIO, DUC BUI, ALEXANDER DAGUM, MIRIAM RAFILOVICH, State Univ of NY- Stony Brook — Been famous for clinical use from early 1980s, the neuromuscular blocking agent Botulinum toxin type A (BTX-A), has been used to reduce wrinkles for a long time. Only little research has been done to quantify the change of muscle contraction before and after injection and most research paper depend on subjective evaluation from both patients and surgeons. In our research, Digital Image Speckle Correlation (DISC) was employed to study the mechanical properties of skin, contraction mode of muscles (injected) and reaction of neighbor muscle group (un-injected). At the same time, displacement patterns (vector maps) generated by DISC can predict injection locus for surgeons who normally handle it depending only on visual observation.

**M1.00316 Learning physical biology via modeling and simulation: A new course and textbook for science and engineering undergraduates**<sup>1</sup>, PHILIP NELSON, Univ Pennsylvania — To a large extent, undergraduate physical-science curricula remain firmly rooted in pencil-and-paper calculation, despite the fact that most research is done with computers. To a large extent, undergraduate *life-science* curricula remain firmly rooted in descriptive approaches, despite the fact that much current research involves quantitative modeling. Not only does our pedagogy not reflect current reality; it also creates a spurious barrier between the fields, reinforcing the narrow silos that prevent students from connecting them. I'll describe an intermediate-level course on "Physical Models of Living Systems." The prerequisite is first-year university physics and calculus. The course is a response to rapidly growing interest among undergraduates in a broad range of science and engineering majors. Students acquire several research skills that are often not addressed in traditional undergraduate courses: •Basic modeling skills; •Probabilistic modeling skills; •Data analysis methods; •Computer programming using a general-purpose platform like MATLAB or Python; •Pulling datasets from the Web for analysis; •Data visualization; •Dynamical systems, particularly feedback control.

<sup>1</sup>Partially supported by the NSF under Grants EF-0928048 and DMR-0832802.

**M1.00317 Light, Imaging, Vision: An interdisciplinary undergraduate course**<sup>1</sup>, PHILIP NELSON<sup>2</sup>, Univ Pennsylvania — The vertebrate eye is fantastically sensitive instrument, capable of registering the absorption of a single photon, and yet generating very low noise. Using eyes as a common thread helps motivate undergraduates to learn a lot of physics, both fundamental and applied to scientific imaging and neuroscience. I'll describe an undergraduate course, for students in several science and engineering majors, that takes students from the rudiments of probability theory to the quantum character of light, including modern experimental methods like fluorescence imaging and Frster resonance energy transfer. After a digression around color vision, we then see how the Feynman principle explains the apparently wavelike phenomena associated to light, including applications like diffraction, subdiffraction imaging, total internal reflection and TIRF microscopy. Then we see how scientists documented the single-quantum sensitivity of the eye seven decades earlier than 'ought' to have been possible, and finally close with the remarkable signaling cascade that delivers such outstanding performance. Course materials are available upon request.

<sup>1</sup>Partially supported by the NSF under Grants EF-0928048 and DMR-0832802.

<sup>2</sup>A second oral abstract is allowed if it's to Biophysics Education.

**M1.00318 A Comparative Study Environmental and Radiological Causes Of Cancer In River Nile State, Sudan**, EYAD HAMID, International University of Africa, HATIM KHAIR, King Mohamed ibn saud University — The causes of cancer in River Nile state are differ between environmental and radiological, this paper tried to make comparison between the two causes, to determine the real cause behind the large rising of cancer cases in this state, considering the daily habits for the patients and the possible contamination in the natural resources around them. The noticeable thing that most of cancer cases are might be due to the high concentration of nitrate pollutant detected in natural resources such as drinking water; also by looking to the radioactive elements we see there's high concentration of some radioactive elements specially the K-40 which found in Portulaca Oleracea.

**M1.00319 Dissociative Electron Attachment**, ESMERALDA ARREOLA, None, ESMERALDA ARREOLA COLLABORATION, LEIGH HARGREAVES COLLABORATION — Since the pioneering work of Boudiffa et al. [1], it has been understood that electrons, even with energies near or below the ionization threshold, are capable of initiating strand-breaks in human DNA. This discovery raised important questions for cancer treatments, since sub-ionizing electrons are known to be the most copiously produced secondary product of radiation therapy. But even to date these factors are largely excluded from dosimetry calculations. This lack of inclusion is, at least in part, certainly due to the dearth of fundamental data describing low-energy electron interactions with nucleotide molecules that form the basis of DNA. Understanding of how such slow electrons are able to damage DNA remains incomplete, but the strongly peaked nature of Boudiffa et al.'s data gives strong hints at resonantly driven collision processes. DNA damage is therefore most likely driven by "dissociative electron attachment" (DEA). DEA is a rather complicated process to model due to the coupling of electronic and nuclear degrees of freedom in the molecule. At the California State University Fullerton, we are currently commissioning a new spectrometer to study dissociation channels, reaction rates and orientation effects in DEA collisions between slow electrons and nucleotide molecules. At the meeting we will present design parameters and commissioning data for this new apparatus. -/abstract- [1] Boudiffa et al., Science, 8

**M1.00320 ENERGY RESEARCH AND APPLICATIONS** —

**M1.00321 Photocurrent Enhancement in the ICG Dye Sensitized ZnO Nanowire Device<sup>1</sup>**, GEN LONG, MICHAEL BEATTIE, HUIZHONG XU, MOSTAFA SADOQI, Department of Physics, St John's University — In this presentation, we report a systematic study of photocurrent in ICG dye sensitized ZnO nanowire/FTO devices. ZnO nanowire is grown by hydrothermal method, with length of ~200nm to 1  $\mu$ m and diameter of ~30 to 60nm. ICG dye is incorporated by immersing ZnO grown FTO substrate. Different concentrations, solvents of ICG dye, sizes of ZnO nanowires and annealing temperatures and atmosphere after immersion were studied. The synthesized nanostructures and devices were characterized by XRD, UV-VIS absorption, SEM, AFM, solar simulator, etc. And an enhancement in the photocurrent due to ICG is observed.

<sup>1</sup>The authors thank Center for Functional Nanomaterials of DOE for providing facilities access.

**M1.00322 DFT+U Modeling of Hole Polarons in Organic Lead Halide Perovskites**, ERIC WELCH, Texas State Univ-San Marcos, PAUL ERHART, Chalmers Institute of Technology, LUISA SCOLFARO, ALEX ZAKHIDOV, Texas State Univ-San Marcos — Due to the ever present drive towards improved efficiencies in solar cell technology, new and improved materials are emerging rapidly. Organic halide perovskites are a promising prospect, yet a fundamental understanding of the organic perovskite structure and electronic properties is missing. Particularly, explanations of certain physical phenomena, specifically a low recombination rate and high mobility of charge carriers still remain controversial. We theoretically investigate possible formation of hole polarons adopting methodology used for oxide perovskites. The perovskite studied here is the ABX<sub>3</sub> structure, with A being an organic cation, B lead and C a halogen; the combinations studied allow for A<sub>1-x</sub>A<sub>2,1-x</sub>BX<sub>1-x</sub>X<sub>2,3-x</sub> where the alloy convention is used to show mixtures of the organic cations and/or the halogens. Two organic cations, methylammonium and formamidinium, and three halogens, iodine, chlorine and bromine are studied. Electronic structures and polaron behavior is studied through first principle density functional theory (DFT) calculations using the Vienna Ab Initio Simulation Package (VASP). Local density approximation (LDA) pseudopotentials are used and a +U Hubbard correction of 8 eV is added; this method was shown to work with oxide perovskites. It is shown that a localized state is realized with the Hubbard correction in systems with an electron removed, residing in the band gap of each different structure. Thus, hole polarons are expected to be seen in these perovskites.

**M1.00323 Photovoltaic conversion via hot electron induced thermionic emission from quantum dots**, ANDREI SERGEEV, KIMBERLY SABLON, U.S. Army Research Laboratory, Adelphi, MD 20783, USA — Quantum dot (QD) nanomaterials provide numerous possibilities for nanoscale engineering of photoelectron processes for specific applications, such as lighting, sensing, and energy conversion. It has been found that QDs may increase the photovoltaic conversion efficiency due to enhanced coupling with electromagnetic radiation, multiple exciton generation, and two-step light absorption. The hot electron induced thermionic emission from QDs is a novel mechanism, which may be significantly enhanced due to optimization of QD parameters. In this two-step process the photoelectrons excited from the valence band to localized quantum dot states are extracted from QDs via thermionic emission, which may be initiated by thermal phonons, hot phonons, and hot electrons. Strong interaction between the localized quantum dot electrons and hot photoelectrons excited by high energy photons substantially increases the conversion efficiency due to use of energy of sub-bandgap photons and energy of hot photoelectrons, which otherwise would be lost in relaxation processes. Here we present the theoretical model of the conversion via thermionic emission from quantum dots, results of optimization of photoelectron processes, and experimental data, which evidence in favor of this mechanism.

**M1.00324 Strain-induced tuning of surface energetics, electron conductivity and reduction drive in spinel LiMn<sub>2</sub>O<sub>4</sub> cathodes<sup>1</sup>**, IVAN SCIVETTI, GILBERTO TEOBALDI, University of Liverpool — LiMn<sub>2</sub>O<sub>4</sub> (LMO) implementation in cathodes of rechargeable Li-ion batteries (LIBs) is hampered by the limited lifetime of the material and the stability of its interfaces, starting from the Solid Electrolyte Interphase [1,2]. Recent experiments [2] and Density Functional Theory (DFT) simulations [3] indicate that the formation and effectiveness of the SEI on LMO are related to the surface orientation. In this context, we analyse the role of geometrical strain for the relative energy, magnetic ordering and the reduction drive of several LMO surfaces. DFT simulations reveal LMO surfaces to be markedly sensitive to geometrical strain. Strain lower than 10% can lead to insulator-metal and ferromagnetic-antiferromagnetic transitions, alter the relative energy of LMO surfaces, and induce changes as large as 1.0 eV in the surface chemical potential, thence the reduction drive. Prompted by advances in the synthesis of metal-oxide core-shell nanostructures [4], the use of strained LMO coating to enhance SEI-formation is put forward as a potential nano-engineered strategy for longer lived SEI on LMO substrates.

1. JCPD 2012, 116, 9852-9861
2. J. Am. Chem. Soc. 2010, 132, 15268-15276
3. J. Phys. Chem. C 2015, 119, 21358-21368
4. ACS Nano 2012, 6, 5531.

<sup>1</sup>EU FP7 project SIRBATT (Ref. 608502, end date: August 2016)

**M1.00325 Defect physics vis-à-vis electrochemical performance in layered mixed-metal oxide cathode materials**, KHANG HOANG, North Dakota State University, MICHELLE JOHANNES, Naval Research Laboratory — Layered mixed-metal oxides with different compositions of (Ni,Co,Mn) [NCM] or (Ni,Co,Al) [NCA] have been used in commercial lithium-ion batteries. Yet their defect physics and chemistry is still not well understood, despite having important implications for the electrochemical performance. In this presentation, we report a hybrid density functional study of intrinsic point defects in the compositions LiNi<sub>1/3</sub>Co<sub>1/3</sub>Mn<sub>1/3</sub>O<sub>2</sub> (NCM<sub>1/3</sub>) and LiNi<sub>1/3</sub>Co<sub>1/3</sub>Al<sub>1/3</sub>O<sub>2</sub> (NCA<sub>1/3</sub>) which can also be regarded as model compounds for NCM and NCA. We will discuss defect landscapes in NCM<sub>1/3</sub> and NCA<sub>1/3</sub> under relevant synthesis conditions with a focus on the formation of metal antisite defects and its implications on the electrochemical properties and ultimately the design of NCM and NCA cathode materials.

**M1.00326 Modified Graphene Oxide for Long Cycle Sodium-Ion Batteries<sup>1</sup>**, MUHAMED SHAREEF, Kansas State University, HARRISON GUNN, Syracuse University, VICTORIA VOIGT, GURPREET SINGH, Kansas State University — Hummer's process was modified to produce gram levels of 2-dimensional nanosheets of graphene oxide (GO) with varying degree of exfoliation and chemical functionalization. This was achieved by varying the weight ratios and reaction times of oxidizing agents used in the process. Based on Raman and Fourier transform infra red spectroscopy we show that potassium permanganate (KMnO<sub>4</sub>) is the key oxidizing agent while sodium nitrate (NaNO<sub>3</sub>) and sulfuric acid (H<sub>2</sub>SO<sub>4</sub>) play minor role during the exfoliation of graphite. Tested as working electrode in sodium-ion half-cell, the GO nanosheets produced using this optimized approach showed high rate capability and exceptionally high energy density of ~500 mAh/g for up to at least 100 cycles, which is among the highest reported for sodium/graphite electrodes. The average Coulombic efficiency was approximately 99 %.

<sup>1</sup>NSF Grant No. 1454151

**M1.00327 Use of TiO<sub>2</sub> nano particles in Sulfur electrodes to enhance cyclability of Li-S batteries**<sup>1</sup>, RUCHIRA DHARMASENA, GAMINI SUMANASEKERA, Department of Physics- University of Louisville, JACEK JASINSKI, ARJUN THAPA, MAHENDRA SUNKARA, Conn center-University of Louisville — Herein we investigate a novel and facile technique to fabricate Sulfur cathode for Li-S batteries with better cyclability and higher stable gravimetric capacity of around 750 mAh/g over 50 cycles. In this study we have experimented the use of TiO<sub>2</sub> nano particles to prevent polysulfide dissolution into the electrolyte. Absorption and adsorption properties of TiO<sub>2</sub> nano particles are used to trap Lithium Polysulfides. Excellent electrical conductivity property of carbonized polyacrylonitrile (PAN) carbon fibers is effectively used in this technique to establish better electrical connection to Sulfur in the bulk electrode. The thermal annealing technique we use in this work introduces a facile way to load Sulfur into the electrode. Mechanical properties of the Sulfur electrode is improved using a relatively easy way to sustain expansion and contraction at stable coulombic capacity with almost 100 % efficiency. The mechanism of the said Sulfur electrode is discussed in detail using cyclic voltammetry and Impedance spectrum analysis.

<sup>1</sup>Funded by KY EPSCoR, project number T1 2014-2019

**M1.00328 Incorporation of Platinum and Gold Partially Reduced Graphene Oxide in Polymer Electrolyte Membrane Fuel Cells for Increased Carbon Monoxide Tolerance**<sup>1</sup>, LEE BLACKBURN, REBECCA ISSEROFF, MIRIAM RAFILOVICH, State Univ of NY- Stony Brook, JAYMO KANG, University of California, Berkeley, HONGFEI LI, MOLLY GENTLEMAN, State Univ of NY- Stony Brook, QIAO QIAO, Brookhaven National Laboratory — Polymer Electrolyte Membrane Fuel Cells (PEMFCs) can potentially provide “green” energy but the platinum catalyst’s susceptibility to carbon monoxide (CO) poisoning reduces output power. This project hypothesized that gold and platinum-partially reduced graphene oxide (Au/Pt-prGO) catalysts, incorporated into the electrodes and Nafion membrane of a PEMFC, will increase CO tolerance. Aliquots of graphene oxide (GO) were functionalized with platinum and/or gold nanoparticles. Partial reduction with NaBH<sub>4</sub> prevented precipitation. Raman Spectroscopy and HRTEM verified the chemical identity, structure, and presence of the materials. Setups were tested in a PEM fuel cell with a gas feed containing 1000 ppm of CO, and averaged an output power >200% over the control, with the most effective sample, Pt-prGO Electrode + Membrane, yielding an output power ~250% greater than the control. Additionally, each setup’s poisoned output power (P<sub>P</sub>) was compared to its highest possible output power (P<sub>M</sub>). AuPt-prGO Electrode + Membrane produced 100% of its highest possible output power when poisoned, displaying 100% resistance to all CO poisoning at the resistances tested.

<sup>1</sup>Garcia MRSEC

**M1.00329 Harvesting Energy from the Flow-Induced Flutter of a ‘Piezoleaf’**, ANDRE RUAS, SANTIAGO ORREGO, KYLE DORAN, AARON RIPS, KOUROSH SHOELE, SUNG HOON KANG, RAJAT MITTAL, Johns Hopkins University — The objective of our research is to examine energy harvesting from the flow-induced flutter of a small piezoelectric membrane, which we call a ‘Piezoleaf’. Piezoleaves are small, low-cost, low-maintenance devices capable of powering small portable electronics or wireless sensors in remote areas. It is well known that piezoelectric membranes subjected to time-varying strains generate electrical energy that can be harvested. In the current project, we have designed and constructed a new, low-speed wind-tunnel (1’x1’, cross-section) to analyze the flow-induced flutter and energy harvesting performance of a small (approximately 1”x2”) piezoleaf. One of the novel features of this research is that the membrane is fixed at its trailing-edge (i.e. an inverted flag) since this is expected to generate more energy than a regular flag configuration. Guided by numerical simulation, we are conducting tests of this configuration in our wind tunnel for various wind speeds (maximum speeds of about 10 m/s) to examine the effect of wind-speed on the flutter and energy harvesting. High-speed videography is also being used to examine the dynamics of the flag and results from this project will be presented.

**M1.00330 High Temperature Concentrated Solar Power Using Liquid Metal**, ASEGUN HENRY, Georgia Institute of Technology — One of the most attractive ways to try and reduce the cost of concentrated solar power (CSP) is to increase the system efficiency and the biggest loss in the system occurs in the conversion of heat to electricity via heat engine. Heat engines that utilize turbomachinery currently operate near their thermodynamic limitations and thus one of the only ways to improve heat engine efficiency is to increase the turbine inlet temperature. Significant effort is being devoted to the development of supercritical CO<sub>2</sub> heat engines, but the most efficient heat engines are combined cycles, which reach efficiencies as high as 60%. However, such heat engines require turbine inlet temperatures ~1300-1500C, which is far beyond what is currently feasible with the state of the art molten salt infrastructure. In working towards the development of a system that can operate in the 1300-1500C temperature range, the most significant challenges lie in the materials and forming functional and reliable components out of new materials. One of the most attractive options from a cost and heat transfer perspective is to use liquid metals, such as tin and aluminum-silicon alloys along with a ceramic based infrastructure. This talk will overview ongoing efforts in the Atomistic Simulation and Energy (ASE) research group at Georgia Tech to develop prototype components such as an efficient high temperature cavity receiver, pumps and valves that can make a liquid metal based CSP infrastructure realizable.

**M1.00331 Cadmium Telluride Solar Cells with PEDOT:PSS Back Contact**<sup>1</sup>, MICHAEL MOUNT, FERNANDA DUARTE, Seton Hall University, NABA PAUDEL, YANFA YAN, University of Toledo, WEINING WANG, Seton Hall University — Cadmium Telluride (CdTe) solar cell is one of the most promising thin film solar cells and its highest efficiency has reached 21%. To keep improving the efficiency of CdTe solar cells, a few issues need to be addressed, one of which is the back contact. The back contact of CdTe solar cells are mostly Cu-base, and the problem with Cu-based back contact is that Cu diffuses into the grain boundary and into the CdS/CdTe junction, causing degradation problem at high temperature and under illumination. To continue improving the efficiency of CdTe/CdS solar cells, a good ohmic back contact with high work function and long term stability is needed. In this work, we report our studies on the potential of conducting polymer being used as the back contact of CdTe/CdS solar cells. Conducting polymers are good candidates because they have high work functions and high conductivities, are easy to process, and cost less, meeting all the requirements of a good ohmic back contact for CdTe. In our studies, we used poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) with different conductivities and compared them with traditional Cu-based back contact. It was observed that the CdTe solar cell performance improves as the conductivity of the PEDOT:PSS increase, and the efficiency (9.1%) is approaching those with traditional Cu/Au back contact (12.5%).

<sup>1</sup>Cadmium Telluride Solar Cells with PEDOT:PSS Back Contact

**M1.00332 Interface Conductance Modal Analysis**, ASEGUN HENRY, Georgia Institute of Technology — A formalism termed the interface conductance modal analysis (ICMA) method will be presented, which allows for calculations of the modal contributions to thermal interface conductance within the context of molecular dynamics (MD) simulations, which inherently include anharmonicity to full order. The eigen modes of vibration are calculated from harmonic lattice dynamics (LD) calculations, however the generality of ICMA formalism also allows for incorporation of anharmonic LD results into the calculations. The formalism itself is based on a modal decomposition of the heat flow across an interface, which is then substituted into expressions for the conductance either based on equilibrium or nonequilibrium MD. Several example cases will be covered and the interesting insights that emerge from the ICMA analyses will be discussed in detail. The ICMA method enables more in-depth study of various effects such as temperature, anharmonicity, interdiffusion, roughness, imperfections, dislocations, stress, changes in crystal structure through a single unified model, as it can essentially treat any material or object where the atoms vibrate around equilibrium sites (e.g., ordered or disordered solids and molecules).

**M1.00333 Transport and thermoelectric properties of hot-pressed  $\text{SnSe}_2$** , NGUYEN VAN QUANG<sup>1</sup>, NGUYEN THI MINH HAI, DUONG ANH TUAN, DUONG VAN THIET, CHO SUNGLAE<sup>2</sup>, University of Ulsan, SONG JAE YONG, PARK HYUNMIN, Korea Research Institute of Standards and Science, JAE YONG SONG COLLABORATION, HYUN-MIN PARK COLLABORATION — Recently,  $\text{SnSe}$  has been reported as ultralow thermal conductivity material which make it become a very high thermoelectric figure of merit ZT material, up to 2.6 at 923 K. But, it is hard to use  $\text{SnSe}$  for applications in high temperature range because  $\text{SnSe}$  decomposes at 700 K. Therefore, searching for crystalline materials with high ZT value at lower temperature is still an attracted field of research.  $\text{SnSe}_2$  is also 2D material which is expected to have low lattice thermal conductivity. However, less is known about thermoelectric property of  $\text{SnSe}_2$ . Eutectic  $\text{SnSe}_2\text{-Bi}_2\text{Se}_3$  has been repoted as a promising low-temperature thermoelectric material with  $\text{ZT}=0.56$  at 593 K. Here, we prepared the polycrystalline  $\text{SnSe}_2$  using hot pressure method. At temperature range up to 573 K, it exhibited an anisotropic n-type charge carrier. Ultra low thermal conductivity is achieved along parallel direction, however, ZT value is still very low whose maximum was 0.045 at 573 K due to low electrical conductivity, and increased with temperature. Our work showed the possibility to enhance ZT of  $\text{SnSe}_2$  polycrystalline via n- and p-type doping experiments.

<sup>1</sup>Presenter

<sup>2</sup>corresponding author

**M1.00334 Correlation between dimensional crossover and thermoelectric performance in conducting polymer**, JUNHYEON JO, IN-SEON OH, MI-JIN JIN, JUNG-WOO YOO, Ulsan National Institute of Science and Technology (UNIST) — Conjugated polymers are emerging as attractive thermoelectric materials, resulting from low thermal conductivity, easy process and variable potentials for change. Recently, there are significant improvements of the Seebeck coefficient ( $S$ ) and electric conductivity ( $\sigma$ ) in the conjugated polymers by adding chemical additives to reform its ordinary disordered structure system. However, the relation between thermoelectricity and charge transport in the system is not well understood, which gives us a new challenge to improve thermoelectricity in the organic system. Here, we studied thermoelectric performance of dimethyl sulfoxide (DMSO) doped poly(3,4-ethylenedioxythiophene)-poly(styrenesulfonate) (PEDOT:PSS) with adding variable amounts of fluorosurfactant Zonyl. The charge transport in this disordered system was analyzed within variable range hopping (VRH), which showed the change of hopping dimensionality with further molecular dopants. The morphological change and its effect on charge transport and thermoelectric performance were further investigated through AFM, XPS, etc. As a result, we found the optimal condition for increasing both the Seebeck coefficient and electric conductivity, resulting in a significant improvement for the power factor ( $S^2\sigma$ ).

**M1.00335 ABSTRACT WITHDRAWN** —

**M1.00336 Structural And Magnetic Properties In Off-Stoichiometric  $\text{MnNiGe}$  Based Thin Film And Bulk Compounds**, ANIL ARYAL, ABDIEL QUETZ, SUDIP PANDEY, SIUC, USA, IGOR RODIONOV, VALERII PRUDNIKOV, Moscow State Univ,Russia, TAPAS SAMANTA, LSU, USA, ALEXANDER GRANOVSKY, Moscow State Univ,Russia, ANDREI SOKOLOV, UNL, USA, IGOR DUBENKO, SIUC,USA, SHANE STADLER, LSU, USA, NAUSHAD ALI, SIUC,USA — The crystal structure, magnetic properties and magnetocaloric effect in  $\text{NiMnGe}$  based thin film and bulk compounds are studied by room temperature XRD and magnetization measurements. The bulk compounds  $\text{Ni}_{0.895}\text{Cr}_{0.105}\text{MnGe}_{1.05}$  and  $\text{Ni}_{0.93}\text{Cr}_{0.07}\text{MnGe}_{1.05}$  were prepared by arc melting process. Thin film was obtained from  $\text{Ni}_{0.895}\text{Cr}_{0.105}\text{MnGe}_{1.05}$  target using Pulsed Laser Deposition technique on  $\text{MgO}$  substrate. Both bulk and thin film crystalizes into hexagonal structure. For bulk  $\text{Ni}_{0.895}\text{Cr}_{0.105}\text{MnGe}_{1.05}$  a first order magnetostructural transition from antiferromagnetic orthorhombic to ferromagnetic hexagonal structure was observed near transition temperature 134 K followed by the second order transition (SOT) from ferromagnetic to paramagnetic near Curie temperature  $T_c = 204$  K. In case of thin film only the presence of SOT was observed near  $T_c$ . For  $\text{Ni}_{0.93}\text{Cr}_{0.07}\text{MnGe}_{1.05}$ ,  $\Delta T = 0.65\text{K}$  near  $T_c = 209$  K for  $\Delta H = 1.8$  T was observed. This work was supported by the U.S. DOE Award No. DE-FG02-06ER46291 & DE-FG02-13ER46946. Authors at Moscow State Univ. acknowledge Russian Foundation for Basic Research (Grant No. 15-02-01976). A. Sokolov acknowledges support from NSF DMR-1310542 grant.

**M1.00337 Efficiency, Power and Period of a model quantum heat engine working in a finite time**<sup>1</sup>, MULUGETA BEKELE, Associate Professor of Physics, AAU, TOLASA A DIMA, Graduate student, MEKUANNENT ALEMYE, Lecturer: Debre Tabor University, WARGA CHEGENO, Lecturer: Wolkite University — We take a spin-half quantum particle undergoing Carnot type cyclic process in a finite time assisted by two heat reservoirs and an external magnetic field. We find that the power of the heat engine is maximum at a particular period of the cyclic process and efficiency at the maximum power is at least half of the Carnot efficiency. We further apply the Omega-criterion for a figure of merit representing a compromise between useful power and lost power determining the corresponding efficiency for the optimization criterion to be at least three fourth of the Carnot efficiency.

<sup>1</sup>The authors are thankful to the International Science programme, IPS, Uppsala, Sweden for their support to our research lab.

**M1.00338 Enhancing photovoltaic efficiency through radiative cooling of solar cells below ambient temperature.**, TAQIYYAH SAFI, JEREMY MUNDAY, University of Maryland, College Park — Sunlight heats up solar cells and the resulting elevated solar cell temperature adversely effects the photovoltaic efficiency and the reliability of the cell. Currently, a variety of active and passive cooling strategies are used to lower the operating temperature of the solar cell. Passive radiative cooling requires no energy input, and is ideal for solar cells; however, previously demonstrated devices still operate above the ambient, leading to a lower efficiency as compared to the ideal Shockley-Queisser limit, which is defined for a cell in contact with an ideal heat sink at ambient temperature (300 K). In this talk, we will describe the use of radiative cooling techniques to lower the cell temperature below the ambient temperature. We show that by combining specifically designed radiative cooling structures with solar cells, efficiencies higher than the limiting efficiency achievable at 300 K can be obtained for solar cells in both terrestrial and extraterrestrial environments. We show that these structures yield an efficiency 0.87% higher than a typical PV module at operating temperatures in a terrestrial application. We also demonstrate an efficiency advantage of 0.4-2.6% for cells in an extraterrestrial environment in near-earth orbit.

**M1.00339 Li-air, rechargeable, solid-state batteries using graphene and boron nitride aerogel matrices.**<sup>1</sup>, ONUR ERGEN, THANG THOAN PHAM, SALLY DEMAIO-TURNER, ALEX ZETTL, University of California at Berkeley — The recent explosion of research on Li-Air batteries has provided new insights into developing more efficient air cathodes. Graphene and boron nitride aerogel matrix is anticipated to be an ideal candidate to produce a high throughput air-breathing system. We developed a Li-Air battery model that accounts for efficient  $\text{O}_2$  throughput. These unique aerogel matrices exhibit the ability to orient the  $\text{O}_2$  passing through and keep out  $\text{H}_2\text{O}$ ,  $\text{CO}_2$ , and  $\text{N}_2$ . Thus, the solid-state cells demonstrate a long cycle life, thermal stability, and high rechargeable characteristics. These cells also show an explicit discharge capacity with a constant discharge current density of  $0.1\text{mA}/\text{cm}^2$ .

<sup>1</sup>Department of Physics, University of California at Berkeley, Ca 94720, USA 2Materials Sciences Division, Lawrence Berkeley National Laboratory, Ca, 94720, USA 3Kavli Energy Nanosciences Institute at the University of California, Berkeley, , Ca, 94720, US

NASA HBCU Renewable Energy and Technology Utilization Project (NHRETU) and 2. Center for the Study of Terrestrial and Extraterrestrial Atmospheres (CSTEA)).

**M1.00340 Experimental characterization of a small custom-built double-acting gamma-type stirling engine.**<sup>1</sup> , PETER INTSIFUL, Prairie View A & M University, Prairie View, TX, FRANCIS MENSAH, Virginia Union University, Richmond, VA, ARTHUR THORPE, Howard University, Washington, DC — This paper investigates characterization of a small custom-built double-acting gamma-type stirling engine. Stirling-cycle engine is a reciprocating energy conversion machine with working spaces operating under conditions of oscillating pressure and flow. These conditions may be due to compressibility as well as pressure and temperature fluctuations. In standard literature, research indicates that there is lack of basic physics to account for the transport phenomena that manifest themselves in the working spaces of reciprocating engines. Previous techniques involve governing equations: mass, momentum and energy. Some authors use engineering thermodynamics. None of these approaches addresses this particular engine. A technique for observing and analyzing the behavior of this engine via parametric spectral profiles has been developed, using laser beams. These profiles enabled the generation of pv-curves and other trajectories for investigating the thermos-physical and thermos-hydrodynamic phenomena that manifest in the exchangers. The engine's performance was examined. The results indicate that with current load of 35.78A, electric power of 0.505 kW was generated at a speed of 240 rpm and 29.50 percent efficiency was obtained.

<sup>1</sup>NASA grants to Howard University NASA/HBCU-NHRETU & CSTE

**M1.00341 Effects of pH on the characteristics of ZnS thin films grown by using the CBD method**<sup>1</sup> , HEEJIN AHN, DONGCHAN LEE, SUJUNG PARK, YOUNGHO UM, Univ of Ulsan — In CIGS-based thin film solar cells, a chemically deposited ZnS buffer layer with high resistivity is generally used between the absorber layer and transparent conducting oxide layer. In this work, we report a chemical process to prepare ZnS films by the CBD technique based on the typical bath deposition. The influences of ammonia (NH<sub>4</sub>OH) and Na<sub>2</sub>EDTA (Na<sub>2</sub>C<sub>10</sub>H<sub>16</sub>N<sub>2</sub>O<sub>8</sub>) as complexing agents on structural, morphological, and optical properties of ZnS thin films are investigated ranging pH concentration from 5 to 10. To investigate effects of pH on the characteristics of ZnS thin films, by using UV-visible transmittance, atomic force microscopy, and optical absorption were investigated. With changing the pH range, the ZnS thin films demonstrate high transmittance of 75~80% in the visible region, indicating the films are potentially useful in photovoltaic applications. The results will be presented in detail.

<sup>1</sup>This research was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education(2011-0024709)

**M1.00342 Silicon and phosphorus dual doped graphene as the promising metal-free catalysts for oxygen reduction reaction**<sup>1</sup> , ZHANSHENG LU, SHUO LI, ZONGXIAN YANG, Henan Normal University, RUQIAN WU, University of California Irvine — The pathways of oxygen reduction reaction (ORR) on the metal-free silicon and phosphorus dual doped graphene (Si-P-G) catalyst are systematically investigated based on the dispersion-corrected density functional theory (DFT-D) method. It is found that the Si-P-G can be stable at high temperature from the first-principles molecular dynamics simulation and the local region of dopants displays an important role in the adsorption and reduction of oxygen. Both of the four-electron O<sub>2</sub> direct dissociation and the two-electron OOH dissociation pathways are probable for ORR on the Si-P-G, while the latter pathway is mainly followed by the pathway of the OH hydrogenation into H<sub>2</sub>O. For the OOH dissociation pathway, the hydrogenation of O<sub>2</sub> to OOH is the rate-limiting step with a rather small barrier energy of 0.66 eV. The current results indicate that the Si-P-G is a novel metal-free catalyst for ORR, and which is comparable to that of the Pt catalyst.

<sup>1</sup>Work was supported by the National Science Foundation Center for Chemical Innovation on Chemistry at the Space-Time Limit (CaSTL) under Grant No. CHE-1414466, and the National Natural Science Foundation of China (Grant Nos. 51401078, and 11474086)

**M1.00343 Lattice-Boltzmann-based Simulations of Diffusiophoresis** , JOSHUA CASTIGLIEGO, JENNIFER KREFT PEARCE, Roger Williams University — We present results from a lattice-Boltzmann-based Brownian Dynamics simulation on diffusiophoresis and the separation of particles within the system. A gradient in viscosity that simulates a concentration gradient in a dissolved polymer allows us to separate various types of particles by their deformability. As seen in previous experiments, simulated particles that have a higher deformability react differently to the polymer matrix than those with a lower deformability. Therefore, the particles can be separated from each other. This simulation, in particular, was intended to model an oceanic system where the particles of interest were zooplankton, phytoplankton and microplastics. The separation of plankton from the microplastics was achieved.

**M1.00344 Electro-responsive supramolecular graphene oxide hydrogels for active bacteria adsorption and removal**<sup>1</sup> , BIN XUE, YI CAO, WEI WANG, Nanjing Univ — Bacteria are major contaminations in drinking water and healthcare products. Bacteria contamination may cause severe health problems, including food poisoning and diseases. Currently water sterilization and purification methods to remove contaminated bacteria are mainly based on the size-exclusion mechanism. In order to completely remove all bacteria in water, the pore sizes of the membranes or cartilages should be comparable to the size of bacteria, which inevitable leads to high cross-membrane water pressure and slow purification speed. Moreover, the membranes can easily get clogged. Therefore it is highly demanded to develop efficient methods and novel materials for water purification. Recently, Cui and coworker have introduced a bacteria inactivation method with high efficiency and fast purification speed based on a kind of complex materials made of silver nanofibers, carbon nanotubes and cotton, operating in an electric field. With the help of electric field, the bacteria can be efficiently kill when passing through the membrane even the pore sizes are larger than bacteria. Inspired by their work, here we report a proof-of-principle demonstration of bacteria removal using electro-responsive hydrogels.

<sup>1</sup>This work is funded by Six talent peaks project in Jiangsu Province, the National Natural Science Foundation of China (Nos. 11304156, 11334004, 31170813, 81421091 and 91127026), the 973 Program of China (No. 2012CB921801 and 2013CB834100), the Priority Ac

**M1.00345 From Compartmentalized to Agent-based Models of Epidemics**<sup>1</sup> , CHARLES MACAL, Argonne National Laboratory — Supporting decisions in the throes of an impending epidemic poses distinct technical challenges arising from the uncertainties in modeling disease propagation processes and the need for producing timely answers to policy questions. Compartmental models, because of their relative simplicity, produce timely information, but often do not include the level of fidelity of the information needed to answer specific policy questions. Highly granular agent-based simulations produce an extensive amount of information on all aspects of a simulated epidemic, yet complex models often cannot produce this information in a timely manner. We propose a two-phased approach to addressing the tradeoff between model complexity and the speed at which models can be used to answer to questions about an impending outbreak. In the first phase, in advance of an epidemic, ensembles of highly granular agent-based simulations are run over the entire parameter space, characterizing the space of possible model outcomes and uncertainties. Meta-models are derived that characterize model outcomes as dependent on uncertainties in disease parameters, data, and structural relationships. In the second phase, envisioned as during an epidemic, the meta-model is run in combination with compartmental models, which can be run very quickly. Model outcomes are compared as a basis for establishing uncertainties in model forecasts.

<sup>1</sup>This work is supported by the U.S. Department of Energy under contract number DE-AC02-06CH11357 and National Science Foundation (NSF) RAPID Award DEB-1516428.

**M1.00346 Analytical vacuum force, atmospheric pressure dispute**, HAN YONGQUAN, 15611860790 — Typically, the gap gas molecules is  $10^{-9}$  m, since the center speed of the tornado is over 100 m / sec, it divided by the speed of a tornado, the gap of the gas molecules becomes  $10^{-11}$  m. Equivalent to the gap when there is no tornado that the gas molecules allow radiation to pass through, equivalent to the gap is reduced gas molecules 100 times by a tornado. There is no change in the Earth's radiate, the Earth's radiation is reduced to one percent of the original intensity by the radiation through the tornado periphery into the center of the tornado. According to the APS Division of Nuclear Physics in APS -2013 Fall Meeting - Event - Gravitational radiation theory <http://meetings.aps.org/Meeting/DNP13/Session/FB.8>, which I published, the gravity will be reduced to the original gravity percentage one. Waterspout by the Earth's gravity to become the original one percent. Cause the external of the tornadoes atmospheric pressure is constant, the height waterspout should support column height atmospheric pressure is 100 times, that height waterspout may reach nearly kilometers.

**M1.00347 Observation of anomalous dielectric properties in low-dimensional spin 1/2  $\alpha$ - $\text{Cu}_2\text{V}_2\text{O}_7$  magnetic system**, YU-JEN CHEN, KAKARLA-DEVI CHANDRASEKHAR, KO-JUNG FAN, Department of Physics, National Sun Yat-Sen University, JIUNN-YUAN LIN, Institute of Physics, National Chiao Tung University, JENN-MIN LEE, JIN-MING CHEN, National Synchrotron Radiation Research Center, HUNG-DUEN YANG, Department of Physics, National Sun Yat-Sen University — Recently, low-dimensional magnetic systems have received much attention from both theoretical and experimental physics point of view due to their fascinating physical properties. In general,  $\text{Cu}_2\text{V}_2\text{O}_7$  can stabilize at least two sibling polymorphs named as  $\alpha$  and  $\beta$  phases. In  $\alpha$  phase,  $\text{Cu}_2\text{V}_2\text{O}_7$  crystallized in orthorhombic with  $Fdd2$  space groups. The complex magnetic exchange interaction between the Cu-O-Cu ion within the intra and interchain creates the Dzyaloshinskii-Moriya interaction that leads to weak ferromagnetism below the magnetic transition temperature  $T_N = 34$  K. In this study, we present the results of multiple dielectric anomalies observed in the low dimensional spin 1/2  $\alpha$ - $\text{Cu}_2\text{V}_2\text{O}_7$  magnetic system. The observed dielectric signatures can be ascribed to the complex magnetic interaction  $\alpha$ - $\text{Cu}_2\text{V}_2\text{O}_7$  system. Further, the chemical doping effect on the magnetic and multiferroic properties of  $\alpha$ - $\text{Cu}_2\text{V}_2\text{O}_7$  is underway.

**M1.00348 Quantum antiferromagnetic Heisenberg half-odd integer spin model as the entanglement Hamiltonian of the Affleck-Kennedy-Lieb-Tasaki valence bond solid states**, GUANG-MING ZHANG, Tsinghua University, Beijing — Applying a symmetric bulk bipartition to the one-dimensional Affleck-Kennedy-Lieb-Tasaki valence bond solid (VBS) states for the integer spin-S Haldane gapped phase, we can create an array of fractionalized spin-S/2 edge states with the super unit cell  $l$  in the reduced bulk system, and the topological properties encoded in the VBS wave functions can be revealed. The entanglement Hamiltonian (EH) with  $l = \text{even}$  corresponds to the quantum antiferromagnetic Heisenberg spin-S/2 model. For the even integer spins, the EH still describes the Haldane gapped phase. For the odd integer spins, however, the EH just corresponds to the quantum antiferromagnetic Heisenberg half-odd integer spin model with spinon excitations, characterizing the critical point separating the topological Haldane phase from the trivial gapped phase. Our results thus demonstrate that the topological bulk property not only determines its fractionalized edge states, but also the quantum criticality associated with the topological phase, where the elementary excitations are precisely those fractionalized edge degrees of freedom *confined* in the bulk of the topological phase.

**M1.00349 The flexibility of Daubechies wavelets for Linear Scaling DFT calculations**, LUIGI GENOVESE, STEPHAN MOHR, Commissariat l'nergie Atomique et aux nergies Alternatives, LAURA ELISABETH RATCLIFF, Argonne National Laboratory, DAMIEN CALISTE, THIERRY DEUTSCH, Commissariat l'nergie Atomique et aux nergies Alternatives, STEFAN GOEDECKER, Basel University — In recent works, we presented the linear scaling version of the BigDFT code [1] based on Daubechies wavelets, where a minimal set of localized support functions is optimized in situ. Our linear scaling approach is able to generate support functions for systems in various boundary conditions, like isolated, surface and periodic [2], and it is based on a algorithm which is universally applicable, requiring only moderate amount of computing resources. We will present how the flexibility of this approach is helpful in providing a basis set that is optimally tuned to the chemical environment surrounding each atom. In addition than providing a basis useful to project Kohn-Sham orbitals informations like atomic charges and partial density of states, it can also be reused as-is, i.e. without reoptimization, for charge-constrained DFT calculations within a fragment approach [3]. We demonstrate the interest of this approach to express highly precise and efficient calculations for preparing diabatic states and for the computational setup of systems in complex environments [4]. [1] J. Chem. Phys. 140, 204110 (2014) [2] Phys. Chem. Chem. Phys., 2015, DOI: 10.1039/C5C P00437C [3] J. Chem. Phys. 142, 23, 234105 (2015) [4] J.Chem. Theory Comput. 2015, 11, 2077

**M1.00350 Interdependent Lattice Networks in High Dimensions**, STEVEN LOWINGER, GABRIEL CWILICH, SERGEY BULDYREV, Yeshiva University — We study the mutual percolation of two interdependent lattice networks following the procedure outlined by Buldyrev *et al*<sup>1</sup>. We studied lattices of dimensions 2, 3, 4, 5 and 6. We imposed that the length of interdependent links connecting the nodes from one lattice to the other be less than a certain value,  $r$ . We find that for each dimension,  $D < 6$ , there is a value of  $r = r_I > 1$  such that for  $r \geq r_I$ , the cascading failures occur as a discontinuous first order transition, while for  $r < r_I$ , the system undergoes a continuous second order transition, as in the classical percolation theory.  $r_I$  decreases when the dimension of the lattice increases. For  $D = 6$ ,  $r_I = 1$ , which is the same as in random regular (RR) graphs with the same degree (coordination number) of nodes.  $D = 6$  is the upper critical dimension for classical percolation, the point at which the critical exponents of the lattice model become identical to those of RR graphs. We found that in all dimensions the maximal vulnerability of the networks, as a function of  $r$ , is achieved at a distance of  $r = r_{max} > r_I$ , but for  $r > r_{max}$  the vulnerability starts to decrease as  $r \rightarrow \infty$ . However, the decrease becomes less significant as the dimension increases and becomes negligible for  $D = 6$ . Results on how the parameters of the transition scale with the size of the system will be presented. [1] Catastrophic cascade of failures in interdependent networks, Buldyrev, Parshani, Paul, Stanley & Havlin, **Nature** 464, 1025-1028 (15 April 2010)

**M1.00351 Behavioral analysis of the escape response in larval zebrafish**, RUOPEI FENG, KIRAN GIRDHAR, YANN CHEMLA, MARTIN GRUEBELE, Univ of Illinois - Urbana — The behavior of larval zebrafish is of great interest because the limited number of locomotor neurons in larval zebrafish couples with its rich repertoire of movements as a vertebrate animal. Current research uses a priori-selected parameters to describe their swimming behavior while our lab has built a parameter-free model based on singular value decomposition analysis to characterize it. Our previous work has analyzed the free swimming of larval zebrafish and presented a different picture from the current classification of larval zebrafish locomotion. Now we are extending this work to the studies of their escape response to acoustic stimulus. Analysis has shown intrinsic difference in the locomotion between escape response and free swimming.

**M1.00352 Synchronization modulation of Na/K pumps on Xenopus oocytes**, PENGFEI LIANG, JASON MAST, WEI CHEN, Univ of South Florida — We developed a new technique named synchronization modulation to electrically synchronize and modulate the Na/K pump molecules by a specially designed oscillating electric field. This technique is based on the theory of energy-trap in quantum physics as well as the concept of electronic synchrotron accelerator. As a result, the Na-transporters are all entrapped into the positive half-cycle of the applied electric field and consequently, all of the K-transporters are entrapped into the negative half cycle of the field. To demonstrate the process of the pump synchronization and modulation, we use Xenopus oocytes as a platform and introduce two-electrode whole-cell voltage clamp in measurement of pump current. Practically, we first synchronize the pump molecules running at the same pace (rate and phase) by a specially designed oscillation electric field. Then, we carefully maintain the pump synchronization status and gradually change the field frequency (decrease and increase) to modulate the pump molecules to newer pumping rate. The result shows a separation of the inward K current from the outward Na current, and about 10 time increase of the total (inward plus outward) pump current from the net outward current from the random paced pump molecules. Also, the ratio of the modulated total pump current with synchronized total pump current is consistent with the ratio of their field frequencies.

**M1.00353 Kinetic inductance parametric up-converter**, ADITYA KHER, California Institute of Technology, PETER DAY, NASA Jet Propulsion Laboratory, BYEONG HO EOM, JONAS ZMUIDZINAS, California Institute of Technology, H. G. LEDUC, NASA Jet Propulsion Laboratory — We describe a novel class of devices based on the nonlinearity of the kinetic inductance of a superconducting thin film. By placing a current-dependent inductance in a microwave resonator, small currents can be measured through their effect on the resonator's frequency. By using a high-resistivity material for the film and nanowires as kinetic inductors, we can achieve a large coefficient of nonlinearity to improve device sensitivity. We demonstrate a current sensitivity of  $8 \text{ pA/Hz}^{1/2}$ , making this device useful for transition edge sensor readout and other cutting-edge applications. An advantage of these devices is their natural ability to be multiplexed in the frequency domain, enabling large detector arrays for TES-based instruments. A traveling-wave version of the device, consisting of a thin-film microwave transmission line, is also sensitive to small currents as they change the phase length of the line due to their effect on its inductance. We demonstrate a current sensitivity of  $5 \text{ pA/Hz}^{1/2}$  for this version of the device, making it also suitable for TES readout and other applications. It has the advantage of multi-GHz bandwidth and greater dynamic range, offering a different approach to the resonator version of the device.

**M1.00354 Atomistic study on the generation and gliding properties of pyramidal dislocations in magnesium**, HIDEO KABURAKI, MITSUHIRO ITAKURA, MASATAKE YAMAGUCHI, Japan Atomic Energy Agency — Plastic deformation of magnesium and its alloys is attracting great interest as one of the candidate materials for energy-conserving lightweight structural metals. The generation of non-basal pyramidal dislocations near the c-axis direction is the key to enhancing plasticity in these highly anisotropic hcp magnesium materials. However, the fundamental understanding of the generation and gliding properties of pyramidal dislocations is still not clear because of the large Burgers vector. Using the molecular dynamics method, we have successfully generated  $\langle c+a \rangle$  type I and II screw dislocations from the crack set in the perfect magnesium crystal by applying the shear stress. Visualization of these dislocations is important because the core structures are complex and largely extended. Comparing the results by first-principles calculations, we have found that the core of the type I screw dislocation is smoothly extended while that of the type II screw dislocation has a corrugated structure. We also found that both dislocations can easily cross-slip to other slip planes. In particular, it is observed that the core of the gliding pyramidal type I screw dislocation cross-slips to other slip planes. The detailed processes of cross-slip are elucidated in the presentation.

**M1.00355 Outdoor concert hall sound design: idea and possible solutions**, YANG-HANN KIM, JUNG-MIN LEE, Korea Adv Inst of Sci & Tech, WANJUNG KIM, HWAN KIM, NARU-EMS co. Ltd., JUNG-WOO CHOI, Korea Adv Inst of Sci & Tech, SEMYUNG WANG, Gwangju Inst of Sci & Tech — Sound design of outdoor concert halls needs to satisfy two contradictory objectives: good sound reproduction within the hall, as well as the minimization of external sound radiation. Outdoor concert hall usually has open space, therefore good sound for the listeners can be bad sound for its neighborhood. It would be a good attempt to have a virtual sound wall that can reflect all sound, therefore making a relatively quiet zone in the outside. This attempt can be possible if we could produce invisible but very high impedance mismatch around the hall, for a selected frequency band. This can be possible if we can generate an acoustically bright zone inside and a dark (quite) zone outside. Earlier work [Choi, J.-W. and Kim, Y.-H. (2002). J. Acoust. Soc. Am. 111, 1695–1700], at least, assures it is possible for a selected region and frequencies. Simulations show that it is possible for a two-dimensional case. Experimental verification has been also tried. The discrepancies have been explained in terms of the number of loudspeakers, their spatial distributions, spacing with regard to wavelength. The dependency of its performances with respect to the size of bright and dark zone scaled by wavelength of interest has also been explained.

**M1.00356 Multiscale modeling of nanostructured ZnO based devices for optoelectronic applications: Dynamically-coupled structural fields, charge, and thermal transport processes.**<sup>1</sup>, ABDULMUIN ABDULLAH, SAAD ALQAHTANI, MD REZAU KARIM NISHAT, SHAIKH AHMED, Southern Illinois University at Carbondale, SIU NANO-ELECTRONICS RESEARCH GROUP TEAM — Recently, hybrid ZnO nanostructures (such as ZnO deposited on ZnO-alloys, Si, GaN, polymer, conducting oxides, and organic compounds) have attracted much attention for their possible applications in optoelectronic devices (such as solar cells, light emitting and laser diodes), as well as in spintronics (such as spin-based memory, and logic). However, efficiency and performance of these hybrid ZnO devices strongly depend on an intricate interplay of complex, nonlinear, highly stochastic and dynamically-coupled structural fields, charge, and thermal transport processes at different length and time scales, which have not yet been fully assessed experimentally. In this work, we study the effects of these coupled processes on the electronic and optical emission properties in nanostructured ZnO devices. The multiscale computational framework employs the atomistic valence force-field molecular mechanics, models for linear and non-linear polarization, the 8-band  $sp^3s^*$  tight-binding models, and coupling to a TCAD toolkit to determine the terminal properties of the device. A series of numerical experiments are performed (by varying different nanoscale parameters such as size, geometry, crystal cut, composition, and electrostatics) that mainly aim to improve the efficiency of these devices.

<sup>1</sup>Supported by the U.S. National Science Foundation Grant No. 1102192

**M1.00357 ZnO nanowire-based CO sensor**, MON-SHU HO, Physics Department, National Chung Hsing University, WEI-HAO CHEN, Institute of Electronics Engineering, National Tsing Hua University, YU-LIN CHEN, Physics Department, National Chung Hsing University, MENG-FAN CHANG, Institute of Electronics Engineering, National Tsing Hua University — This study applied ZnO nanowires to the fabrication of a CO gas sensor operable at room temperature. Following the deposition of a seed layer by spin coating, an aqueous solution method was used to grow ZnO nanowires. This was followed by the self-assembly of an electrode array via dielectrophoresis prior to the fabrication of the CO sensing device. The material characteristics were analyzed using FE-SEM, EDS, GIXRD, FE-TEM, and the measurement of photoluminescence (PL). Our results identified the ZnO nanowires as a single crystalline wurtzite structure. Extending the growth period from 30 min to 360 min led to an increase in the length and diameter of the nanowires. After two hours, the ZnO presented a preferred crystal orientation of [002]. Sensor chips were assembled using 60 pairs of electrodes with gaps of  $2 \mu\text{m}$ , over which were laid nanowires to complete the sensing devices. The average sensing response was 48.37 s and the average recovery time was 65.61 s, with a sensing response magnitude of approximately 6.8% at room temperature.

**M1.00358 Neutron Imaging Studies of In Situ Growth of Neutron and Gamma Detector Materials**, NICHOLAS STRANGE, CHRISTOPHER CRAIN, FATEMA WAHIDA, ZACH STROUPE, J.Z. LARESE, University of Tennessee — The studies described here are aimed at addressing the critical need to develop dependable crystal growth techniques of solid-state materials used as radiation detectors for both national security and medical applications. We present our activities using pulsed neutron, radiographic imaging and simultaneous diffraction techniques to examine the synthesis of both CZT and CLYC with the goal of identifying the conditions that favor the production of defect free materials. Using a pulsed neutron beam and time of flight detection methods, we exploit the penetrating power and wavelength dependence of neutron absorption to perform measurements during crystal growth. Furthermore, solid boules can be examined either inside the furnace or free standing. The objective of these studies include the validation/improvement of the modeling studies of CLYC and CZT growth behavior, the development of new/improved furnace design, and the identification of optimum growth techniques that enable the production of large boules of defect free, single crystalline materials in a timely/cost effective manner. We provide our preliminary results that include the experiential setup at LANSCE and sample neutron radiographic and synchrotron based IR images of CZT flat solid plates.

**M1.00359 Investigation of Natural *Bombyx mori* Silk Fibroin Proteins Using INS**, CHRISTOPHER CRAIN, NICHOLAS STRANGE, J.Z. LARESE, Univ of Tennessee, Knoxville — The mechanical properties of many protein comprised biomaterials are a direct reflection of non-covalent (i.e. weak) interacting ions such as F-actin in muscles, tubulin in the cytoskeleton of cells, viral capsids, and silk. Porter and Vollrath underscored the two main factors that are critical for understanding the high mechanical strength of silks: the nanoscale semi-crystalline folding structure, which gives it exceptional toughness and strength, and the degree of hydration of the disordered fraction, which acts to modify these properties. Understanding and controlling these two principal factors are the key to the functionality of protein elastomers, and render silk an ideal model protein for (bio)material design. We will describe our investigation of electrospun silk of the *Bombyx mori* (silk worm), using Inelastic Neutron Scattering (INS). These techniques were used to investigate the microscopic dynamics of the dry and hydrated protein.

**M1.00360 Study of the nanosurface properties by analyzing its absorption and scattering cross-section.**, IRINA BARIAKHTAR, Boston College — The interest to study the nanoparticles absorbed on the dielectric or semiconductor substrate is caused by the multiple practical applications of these systems such as nanosensors, electronic devices and lately in PV elements for improving of their efficiency [1, 2]. The author suggests a method of examining the properties of the nanosurface with the absorbed nanoparticle by calculating the absorption and scattering of the electromagnetic field by such system based on construction of its effective electric susceptibility. It was built based on the Green's function approach [3]. The computer simulations show good correspondence with the theory. It was shown that this approach can be applied to investigate the optical absorption and scattering on the nanoparticles on the substrate to be used in PV engineering. 1. Schaad, D. M., Feng, B., Yu, E. Appl. Phys. Lett. 86 (6): 063106 (2005) 2. K. R. Catchpole and A. Polman, Opt. Express 16, 21793-21800 (2008) 3. I. Bariatkhar, Y. Demidenko, S. Kriuchenko, V. Lozovski, Surf. Sci. 323 (1995).

**M1.00361 Controlling Spin State of Magnetic Molecules by Oxygen Binding Studied Using Scanning Tunneling Microscopy**, SOON-HYEONG LEE, Korea University, YUN HEE CHANG, KAIST, HOWON KIM, KYUNG MIN KIM, Korea University, YONG-HYUN KIM, KAIST, SE-JONG KAHNG, Korea University — Binding and unbinding between molecular oxygen and metallo-porphyrin is a key process for oxygen delivery in respiration. It can be also used to control spin state of magnetic metallo-porphyrin molecules. Controlling and sensing spin states of magnetic molecules in such reactions at the single molecule level is essential for spintronic molecular device applications. Here, we demonstrate that spin states of metallo-porphyrin on surfaces can be controlled over by binding and unbinding of oxygen molecule, and be sensed using scanning tunneling microscopy and spectroscopy. Kondo localized state of metallo-porphyrin showed significant modification by the binding of oxygen molecule, implying that the spin state was changed. Our density functional theory calculation results explain the observations with the hybridization of unpaired spins in d and  $\pi^*$  orbitals of metallo-porphyrin and oxygen, respectively. Our study opens up ways to control molecular spin state and Kondo effect by means of molecular binding and unbinding reactions on surfaces.

**M1.00362 Spotting the Gel Point of Photopolymers by Examining NMR Relaxation**, JACK LEE, GRETCHEN HOFMEISTER, MARTHA-ELIZABETH BAYLOR, Carleton College — Spotting when a polymer goes from liquid to solid during polymerization is necessary when working with certain optically cured polymers used to fabricate optofluidic devices that contain both optical and microfluidic features. Through the use of nuclear magnetic resonance (NMR) it may be possible to determine when the transition from liquid to solid, called the gel point, occurs. In examining the proton longitudinal relaxation time for one species of monomers in our polymer mix, our data shows as the polymer cures the relaxation time increases. By examining this data we were able to extract a time to gel point that was within the margin of error of the theoretical gel point of our materials. Outlined here is evidence of why we think longitudinal relaxation is applicable to studying polymerization, and how we are using it to attempt to extract the gel point.

**M1.00363 Observation of Voltage Oscillations in VO<sub>2</sub> with Negative Differential Resistance**, DAE-JOON KANG, HYOUNG WOO YANG, GARAM BAE, Department of Physics, Sungkyunkwan University, Republic of Korea — Many strongly correlated electron systems exhibit complex nonlinear behaviors with electric fields. The origin of the electrical instabilities is closely related to a negative differential resistance (NDR). Here, we report electrical characteristics of two-terminal devices based on vanadium dioxide (VO<sub>2</sub>) thin films fabricated on c-cut sapphire substrates, exhibiting NDR behavior in their I-V characteristics that may work as a voltage oscillator of high efficiency. We show that the NDR behavior can be better understood in the context of metal-insulator phase transition. Furthermore, we found that the source voltage and frequency affect greatly the NDR behaviors, which is indicated by an evident shift of oscillation voltage from 10 V to 1 V. Based on the experimental results, with the source voltage and the frequency systematically varied, the mechanism of the oscillation was found to be the ascribed to an alternate occurrence of an electric-field-induced resistance switching in the MIT of VO<sub>2</sub>. We discuss herein, the origin and potential applications of NDR based devices in detail and investigated the voltage oscillation behaviors of VO<sub>2</sub> to elucidate the underlying physics of its metal insulator transition behavior.

**M1.00364 Cloisite 30B as Nanoclay Compatibilizer for Polysulfone/Polyimide Blend Films.**, ALI AMMAR, Akron Univ, AHMED ELZATAHRY, MARIAM AL-MAADEED, Qatar Univ, ABDULLAH ALLENIZI, King Saud Univ, KARIM ALAMGIR, Akron Univ — Polysulfone (PSF) and polyimide (PI) are used in many applications including membranes for gas separation and water purification. The phase separation issues limit the blend application of these polymers. We studied the effect of nanoclay and Cloisite 30B had on (PSF/PI) films. This was done in order to examine the compatibility effects of clay on phase separation behavior, mechanical strength, and structure properties. The addition of weight percentage of organoclay strongly compatibilized the blend phases for all compositions, decreasing the scale of blend phase separation by a factor of 5-10. Interestingly, the net phase separated domain area converged to the 50% blend composition in all cases. This is attributed to a high degree of exfoliation and degradation of nanoclay particles within the PSF/PI matrix as well as interfacial regions, independent of the blend composition. AFM confirmed these optically observed compatibilization effects by quantitative reduction of aspect ratio (width/height) of surface phase separated domains. The surface free energies of the films decreased by adding C30B. This has led us to conclude that there is a changing of surface topography, which conformed to the contact angle. PSF/PI films showed decreasing in thermal stability due to the surfactant modification of C30B.

**M1.00365 Electronic state modulation of iron selenide by intercalating copper**, KAYA KOBAYASHI, Y ITO, F NAGAI, S MATSUMOTO, T KAMBE, Y BENINO, T NAMBA, Okayama University — FeSe is one of the iron-based superconductors that have the simplest structure. Its superconducting properties are easily modulated by chemical and mechanical method, such as alkali metal intercalation and thinning down to monolayer. The synthesis of copper intercalation by melt method brought the structural change of the system in increasing the copper amount. To investigate the superconducting property of the system, we have synthesized copper intercalated FeSe single crystal. The decrease of superconducting transition temperature observed here is discussed in relation to its modulation on to electronic state of irons.

**M1.00366 Boson Sampling with Trapped Ions**, KATHERINE COLLINS, Univ of Maryland-College Park, KENNETH WRIGHT, CHRISTOPHER RICKERD, CHRISTOPHER MONROE, Univ of Maryland-College Park and Joint Quantum Institute — A classical computer is limited in its ability to solve certain types of problems. A quantum computer might be able to solve some of these problems more efficiently. Calculating the permanent of an  $N \times N$  matrix is an example of a problem that cannot be efficiently solved by a classical computer. Computing the permanent of an  $N \times N$  matrix can be related to the probability of finding a given occupation distribution for  $M$  bosonic modes populated with  $N$  identical bosons. This type of experiment is known as boson sampling. Classically, the computation time required to evaluate the permanent of an  $N \times N$  matrix scales on the order of  $2^N N^2$ .<sup>1</sup> A quantum device that is able to compute an  $N \times N$  permanent through boson sampling represents a physical device that can evaluate a problem not efficiently solvable by a classical system. Some experiments have already demonstrated boson sampling with photons for a small number of bosonic modes, but it is difficult to increase the number of bosons in such experiments. One way to demonstrate a larger-scale boson sampling problem is to use the phonon excitations of a trapped ion chain. We present our progress towards experimentally demonstrating boson sampling with trapped ions.

<sup>1</sup> C. Shen, Z. Zhang, and L.-M. Duan, Phys. Rev. Lett. 112, 050504, 2014

**M1.00367 Block Copolymer-Based Supramolecular Elastomers with High Extensibility and Large Stress Generation Capability**<sup>1</sup>, ATSUSHI NORO, MIKIHIRO HAYASHI, Nagoya University — We prepared block copolymer-based supramolecular elastomers with high extensibility and large stress generation capability. Reversible addition fragmentation chain transfer polymerizations were conducted under normal pressure and high pressure to synthesize several large molecular weight polystyrene-*b*-[poly(butyl acrylate)-*co*-polyacrylamide]-*b*-polystyrene (S-Ba-S) block copolymers. Tensile tests revealed that the largest S-Ba-S with middle block molecular weight of 3140k achieved a breaking elongation of over 2000% with a maximum tensile stress of 3.6 MPa and a toughness of 28 MJ/m<sup>3</sup> while the reference sample without any middle block hydrogen bonds, polystyrene-*b*-poly(butyl acrylate)-*b*-polystyrene with almost the same molecular weight, was merely viscous and not self-standing. Hence, incorporation of hydrogen bonds into a long soft middle block was found to be beneficial to attain high extensibility and large stress generation capability probably due to concerted combination of entropic changes and internal potential energy changes originating from the dissociation of multiple hydrogen bonds by elongation.

<sup>1</sup> This work was supported by JSPS KAKENHI Grant Numbers 13J02357, 24685035, 15K13785, and 23655213 for M.H. and A.N. A.N. also expresses his gratitude for Tanaka Rubber Science & Technology Award by Enokagaku-Shinko Foundation, Japan.

**M1.00368 Continued Growth on Graphene Edges**, ZHENG TANG LUO, Hong Kong Univ of Sci & Tech — Previously, we have shown that the large-size single crystal graphene can be obtained by suppressing the nucleation density during Chemical Vapor Deposition (CVD) growth. Here we demonstrate that the graphene single crystal can be amplified by a continued growth method. In this process, we used a mild oxidation step after the first-growth, which lead to the observed formation of oxides at the vicinity of graphene edges, which allows the graphene growth at seed edges due to reduced activation energy. Consequently, we successfully grown a secondary single-crystal graphene structures with the same lattice structure, orientation on the graphene edges. This amplification method would enable the production of graphene electronics with controlled properties.

**M1.00369 Nonlinear Transport and Noise Properties of Acoustic Phonons**.<sup>1</sup>, KAMIL WALCZAK, Pace University — We examine heat transport carried by acoustic phonons in molecular junctions composed of organic molecules coupled to two thermal baths of different temperatures. The phononic heat flux and its dynamical noise properties are analyzed within the scattering (Landauer) formalism with transmission probability function for acoustic phonons calculated within the method of atomistic Green's functions (AGF technique). The perturbative computational scheme is used to determine nonlinear corrections to phononic heat flux and its noise power spectral density with up to the second order terms with respect to temperature difference. Our results show the limited applicability of ballistic Fourier's law and fluctuation-dissipation theorem to heat transport in quantum systems. We also derive several noise-signal relations applicable to nanoscale heat flow carried by phonons, but valid for electrons as well. We also discuss the extension of the perturbative transport theory to higher order terms in order to address a huge variety of problems related to nonlinear thermal effects which may occur at nanoscale and at strongly non-equilibrium conditions with high-intensity heat fluxes.

<sup>1</sup>This work was supported by Pace University Start-up Grant.

**M1.00370 Spectroscopic study of some diatomic molecules via the proper quantization rule**, B. FALAYE, IPN, Mexico City, Mexico — Spectroscopic techniques are very essential tools in studying electronic structures, spectroscopic constants and energetic properties of diatomic molecules. These techniques are also required for parametrization of new method based on theoretical analysis and computational calculations. In this research, we apply the proper quantization rule in spectroscopic study of some diatomic molecules by solving the Schrödinger equation with two solvable quantum molecular systems-Tietz-Wei and shifted Deng-Fan potential models for their approximate nonrelativistic energy states via an appropriate approximation to the centrifugal term. We show that the energy levels can be determined from its ground state energy. The beauty and simplicity of the method applied in this study is that, it can be applied to any exactly as well as approximately solvable models. The validity and accuracy of the method is tested with previous techniques via numerical computation for H<sub>2</sub> and CO diatomic molecules. The result also include energy spectrum of 5 different electronic states of NO and 2 different electronic state of ICl.

**M1.00371 “Dual Society Ever Precedes through Trevor SWAN & Wassily Leontief”**<sup>1</sup>, WH-MAKSOED<sup>2</sup>, Prodi of Physics UI, Depok 16424- INDONESIA — “Dual Society” introduced by E.F. Schumacher are classified as non-stable society who easy to shakes by politics uncertainties.in Robert J. Barro & X. Sala-i-Martin: “**Convergence**” states: “ a key economic issue is whether poor countries or regions tend to grow faster than rich ones”.For growth models from Roy Forbes Herrod & Evsey Domar, three assumptions described by Eduardo Ley are?(U+2639)i). output is proportional to capital,(ii). Investment *ex ante* equals saving & (iii) saving proportional to output. Underlines Trevor SWAN, developing countries differ significantly among themselves. Economic growth models comprises Herrod-Domar growth model, Solow growth model & endogenous growth model.Further, for five stages of economic growth from Rostov of Leontief technology, ever retrieves the Jens Beckett:“**Institutional Isomorphism revisited: Convergence & Divergence in Institutional Change**” instead Frumkin's “**Institutional Isomorphism & Public Sector Organizations**”.

<sup>1</sup>Acknowledgment devotes to theLates HE. Mr. BrigadierGeneral-TNI[rtd].Prof. Ir. HANDOJO

<sup>2</sup>a Devotes to Robert J. Barro & Xavier Sala-i-Martin:“ECONOMIC GROWTH” whose design depict coincidences with Salvador Dali painting:”The Persistence of Memory”

**M1.00372 “the Human BRAIN & Fractal quantum mechanics”<sup>1</sup>**, GLORY ROSARY-OYONG, SE<sup>2</sup>, Kompas-TV, Jl. Palmerah Selatan 1, Jakarta 10270- INDONESIA — In mtDNA ever retrieved from Iman Tuassoly, *et.al*: **Multifractal analysis of chaos game representation images of mtDNA**. Enhances the price & value tales of HE. Prof. Dr-Ing. B.J. HABIBIE's N-219, in J. Bacteriology, Nov 1973 sought: “219 exist as separate plasmidDNA species in E.coli & Salmonella panama” related to “the brain 2 distinct molecular forms of the (Na,K)-ATPase..” & “neuron maintains different concentration of ions(charged atoms) thorough Rabi & Heisenberg Hamiltonian. Further, after “fractal space time are geometric analogue of relativistic quantum mechanics” [Ord], sought L.Marek Crnjac: “Chaotic fractals at the root of relativistic quantum physics” & from famous Nottale: “Scale relativity & fractal space-time:” Application to Quantum Physics, Cosmology & Chaotic systems”, 1995.

<sup>1</sup>acknowledgements to HE. Mr. H. TUK SETYOHADI, Jl. Sriwijaya Raya 3, South-Jakarta, INDONESIA

<sup>2</sup>Those were in search of fusion/fission if occurs as well as in 219 plasmidDNA instead in mtDNA

**M1.00373 “From Fundamental Motives to Rational Expectation Equilibrium[REE, hence-worth] of Indeterminacy”<sup>1</sup>**, WH- MAKSOED, SSI<sup>2</sup>, Prodi of Physics UI, Depok 16424- INDONESIA — For “Principle of Indeterminacy” from Heisenberg states: “one of the fundamental cornerstone of quantum mechanics is the Heisenberg uncertainty principle”. whereas canonically conjugate quantities can be determined simultaneously only with a characteristic indeterminacy [M. Arevalo Aguilar, *et.al*]. Accompanying Alfred North Whitehead conclusion in “The Aims of Education” that mathematical symbols are artificial before new meanings given, two kinds of fundamental motives: (i) expectation-expectation, (ii) expectation-certainty inherently occurs with determinacy properties of rational expectation equilibrium (REE, henceworth)- Guido Ascari & Tizano Ropele: “Trend inflation, Taylor principle & Indeterminacy”, Kiel Institute, June 2007. Further, relative price expression can be compare of their  $\alpha$  and  $(1 - \alpha)$  configurations in the expression of possible activity.

<sup>1</sup>Acknowledgment to Prof[asc]. Dr. Bobby Eka Gunara for “made a rank through physics” denotes...

<sup>2</sup>Devotes to Kompas-100 of Tony Skyrme's magnetic excitation of skyrmion coincides with “bipolar affective disorder current episode hypomanic” medical conclusions

**M1.00374 Can we judge an oxide by its cover? The case of the metal/oxide interface from first principles<sup>1</sup>**, MAYTAL CASPARY TOROKER, Department of Materials Science and Engineering — Metal/metal-oxide interfaces appear in a wide variety of disciplines including electronics, corrosion, electrochemistry, and catalysis. Specifically, covering a metal-oxide with a metal is often thought to enhance solar energy absorption and to improve photocatalytic activity. For example, the platinum/hematite (Pt/ $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>) interface has demonstrated improved functionality. In order to advance our understanding of how metal coverage over an oxide helps performance, we characterize the geometry and electronic structure of the Pt/ $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> interface. We investigate the interface using density functional theory +U, and find a stable crystallographic orientation relationship that agrees with experiment. Furthermore, there are significant changes in the electronic structure of  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> as a result of Pt coverage. We therefore suggest the concept of “judging” the electronic properties of an oxide only with its cover. Specifically, covering Fe<sub>2</sub>O<sub>3</sub> with Pt reduces carrier effective mass and creates a continuum of states in the band gap. The former could be beneficial for catalytic activity, while the latter may cause surface recombination. In order to circumvent this problem, we suggest putting metal coverage behind the oxide and far from the electrolyte in a photoelectrochemical device in order to quickly collect electron carriers and avoid recombination with vulnerable holes accumulating as a result of catalysis at the surface. Reference: O. Neufeld and M. Caspary Toroker, “Can we judge an oxide by its cover? The case of platinum over  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> from first principles”, Phys. Chem. Chem. Phys. 17, 24129 (2015).

<sup>1</sup>This research was supported by the Morantz Energy Research Fund, the Nancy and Stephen Grand Technion Energy Program, the I-CORE Program of the Planning and Budgeting Committee, and The Israel Science Foundation (Grant No. 152/11).

**M1.00375 Carbon nanotube transistor based high-frequency electronics**, MICHAEL SCHROTER, Technical University Dresden — At the nanoscale carbon nanotubes (CNTs) have higher carrier mobility and carrier velocity than most incumbent semiconductors. Thus CNT based field-effect transistors (FETs) are being considered as strong candidates for replacing existing MOSFETs in digital applications. In addition, the predicted high intrinsic transit frequency and the more recent finding of ways to achieve highly linear transfer characteristics have inspired investigations on analog high-frequency (HF) applications. High linearity is extremely valuable for an energy efficient usage of the frequency spectrum, particularly in mobile communications. Compared to digital applications, the much more relaxed constraints for CNT placement and lithography combined with already achieved operating frequencies of at least 10 GHz for fabricated devices make an early entry in the low GHz HF market more feasible than in large-scale digital circuits. Such a market entry would be extremely beneficial for funding the development of production CNTFET based process technology. This talk will provide an overview on the present status and feasibility of HF CNTFET technology will be given from an engineering point of view, including device modeling, experimental results, and existing roadblocks.

**M1.00376 Gate Opening Transition of Zeolitic Imidazolate Framework – 8 in Xenon adsorption and Carbon Monoxide Adsorption.**, DINUKA H GALLABA, ALDO D MIGONE, Department of Physics, Southern Illinois University, Carbondale IL 62901, KARIM SAPAG, JHONNY VILLAROEL, Universidad Nacional de San Luis, San Luis 5700, Argentina. — Zeolitic Imidazolate Framework – 8 (ZIF-8) is a porous metal-organic framework material that shows flexibility in adsorbing larger molecules. We have investigated Xe adsorption on ZIF-8 for temperatures in the range between 95K and 157.5 K and we are exploring CO adsorption between 80K and 110K. ZIF-8 is known to undergo a structural (“gate-opening”) transition when sorbent loading increases. We report on this gate-opening phenomenon for Xe and CO on ZIF-8. The gate-opening transition appears as a sub-step at higher loadings in the adsorption isotherm data. For Xe the sub-step disappeared for temperatures above 145 K. All isotherms below this temperature clearly show the extra step. Gate-opening occurs as a result of the re-orientation of the organic linkers in ZIF-8. This re-orientation increases the size of the apertures in the structure, consequently allowing more molecules or atoms to adsorb into the ZIF -8 (which produces the additional sub-step). The isosteric heat of adsorption as a function of loading, and, the energy associated with the structural transition were determined from the adsorption data. We also report on the kinetics of sorption for Xe on ZIF-8: there are two rates that dominate the sorption kinetics on ZIF-8. We report on the values of the rates as a function of sorbent loading.

**M1.00377 Majorana fermion mean field study of two-dimensional inequivalent bipartite kondo lattice**, SAYED ALI AKBAR GHORASHI, Department of physics and Texas center for superconductivity, University of Houston, RUI WANG, Texas center for superconductivity, university of Houston, CHIN-SEN TING, Department of physics and Texas center for superconductivity, University of Houston — We study the antiferromagnetic kondo lattice in a bipartite square lattice using Majorana fermion representation mean field theory. In different sublattice, we introduce different kondo coupling interaction between the local moment and the conduction electrons, and discuss the possible phases of ground state. It is shown that for weak coupling regime there is more competition between two sublattices local moment interactions. Next, we turn on an equal ferromagnetic Heisenberg interaction for both sublattices and we show possible competition and cooperation between these three interactions. Finally, to gain more physical insights we investigate static magnetic susceptibility for different ratios of couplings.

**M1.00378 A universal scaling law for the evolution of granular gases**, MATHIAS HUMMEL, JAMES CLEWETT, MARCO G. MAZZA, Max Planck Institute for Dynamics and Self-Organization — Dry, freely evolving granular materials in a dilute gaseous state coalesce into dense clusters only due to dissipative interactions. This clustering transition is important for a number of problems ranging from geophysics to cosmology. Here we show that the evolution of a dilute, freely cooling granular gas is determined in a universal way by the ratio of inertial flow and thermal velocities, that is, the Mach number. Theoretical calculations and direct numerical simulations of the granular Navier–Stokes equations show that irrespective of the coefficient of restitution, density or initial velocity distribution, the density fluctuations follow a universal quadratic dependence on the system's Mach number. We find that the clustering exhibits a scale-free dynamics but the clustered state becomes observable when the Mach number is approximately of  $O(1)$ . Our results provide a method to determine the age of a granular gas and predict the macroscopic appearance of clusters.

**M1.00379 Development, Selection, and Validation of Tumor Growth Models**, AMIR SHAHMORADI<sup>1</sup>, ERNESTO LIMA<sup>2</sup>, J. TINSLEY ODEN<sup>3</sup>, The University of Texas at Austin — In recent years, a multitude of different mathematical approaches have been taken to develop multiscale models of solid tumor growth. Prime successful examples include the lattice-based, agent-based (off-lattice), and phase-field approaches, or a hybrid of these models applied to multiple scales of tumor, from subcellular to tissue level. Of overriding importance is the predictive power of these models, particularly in the presence of uncertainties. This presentation describes our attempt at developing lattice-based, agent-based and phase-field models of tumor growth and assessing their predictive power through new adaptive algorithms for model selection and model validation embodied in the Occam Plausibility Algorithm (OPAL), that brings together model calibration, determination of sensitivities of outputs to parameter variances, and calculation of model plausibilities for model selection.

<sup>1</sup>Institute for Computational Engineering and Sciences

<sup>2</sup>Institute for Computational Engineering and Sciences

<sup>3</sup>Institute for Computational Engineering and Sciences

**M1.00380 Evidence for quantization and topological states in spin Hall conductivity of low-dimensional systems**, SEBASTIAN KUEFNER, LARS MATTHES, JUERGEN FURTHMUELLER, FRIEDHELM BECHSTEDT, FSU Jena — *Ab initio* relativistic band structure calculations are performed for the frequency-dependent spin Hall conductivity of two-dimensional atomically thin crystals and one-dimensional nanoribbons. We study the influence of topology, quantization and topological edge states. As model systems, fully halogenated germanene, Gel, and its zigzag nanoribbons are investigated. Gel represents a topological insulator due to strong spin-orbit interaction and, hence, band inversion. We demonstrate the quantization of the static spin Hall conductivity. It is hardly influenced by temperature variation but significantly by Fermi level shift. The frequency dependence of the conductivity is governed by the band-structure details. Topological edge states influence the conductivity mainly for vanishing frequencies.

**M1.00381 Ultrafast spectroscopy of exciton and exciton dynamics in mono and few layers of WS<sub>2</sub>**, SUDIKSHA KHADKA, SHROUQ ALEITHAN, MAX LIVSHITS, JEFFREY J. RACK, MARTIN KORDESCH, ERIC STINAFF, Ohio University — Single layer of Transitional metal dichalcogenides (MX<sub>2</sub>) are 2D semiconductors that have a direct band gap in visible spectrum and fill the gap in between 2D metallic and insulating materials. They have possible application in optoelectronic devices, photovoltaics and photodetection, molecular sensing, 'valleytronics', and flexible transparent electronics. Tungsten Disulphide (WS<sub>2</sub>), one of the member of MX<sub>2</sub> family, has a direct band gap of 2.2 eV and a large valley splitting of about 0.4 eV. Here, we present a detailed study of exciton states and their decay mechanisms in mono and few layer WS<sub>2</sub> using femto-second transient absorption spectroscopy. We report a new peak at 3.010.1 eV whose origin in k space is believed to be at or around K point and further investigation is under way. The exponential fitting of decay curve of the exciton A reveals three time components as 1.70.3 ps, 33.510 ps and 67015 ps, most likely corresponding to carrier-carrier scattering, carrier-phonon scattering, and radiative relaxation respectively.

**M1.00382 Enhanced  $T_C$  in granular and thin film Al-Al<sub>2</sub>O<sub>3</sub> nanostructures<sup>1</sup>**, J. S. HIGGINS, R. L. GREENE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland — It is known since the 1970s that the superconducting transition temperature of granular aluminum films can be as high as two to three times the transition temperature of bulk aluminum, depending on the grain size and how strongly the nanometer size grains are connected<sup>1,2</sup>. As the strength of the grain connectivity becomes increasingly weak, the enhanced  $T_C$  is suppressed. The mechanism behind this enhancement is still under debate. Recently, work on larger aluminum nanoparticles (18nm) embedded in an insulating Al<sub>2</sub>O<sub>3</sub> matrix showed an onset of the superconducting transition as high as three times that of bulk aluminum<sup>3</sup>. In this situation, the Al grains are electrically disconnected and in a regime far removed from that of the granular films. Here we compare the two situations through electronic and thermal measurements in order to help elucidate the mechanism behind the enhancements. <sup>1</sup>S. Pracht, *et al.*, arXiv:1508.04270v1 [cond-mat.supr-con] (2015). <sup>2</sup>G. Deutscher, *New Superconductors From Granular to High  $T_C$* , New Jersey: World Scientific, 2006, p. 72-74. <sup>3</sup>V. N. Smolyaninova, *et al.*, Sci. Rep. **5**, 15777 (2015).

<sup>1</sup>Funding by NSF DMR 1410665

**M1.00383 Substitution and “site-decoupled doping” in iron pnictides**, M. MERZ, P. SCHWEISS, P. NAGEL, M.-J. HUANG, A. PLOG, R. EDER, TH. WOLF, H. V. LÖHNESEN, S. SCHUPPLER, Karlsruhe Institute of Technology, Germany — The composition-dependent electronic structure of iron pnictides, in particular the question if and how charge carriers are introduced to the system upon substitution – by Sr or alkali metals, *AM*, for Ba; by transition metals, *TM*, for Fe; and/or by P for As – continues to provide surprises. Our ongoing systematic study of spatial structure and electronic states by x-ray diffraction and x-ray absorption, performed on a large number of compositions in the (Ba,Sr,*AM*)(Fe,*TM*)<sub>2</sub>(As,P)<sub>2</sub> family of compounds, shows, for instance, that valences are rarely as expected, that doping can be “effective” or “slow” depending on substituent, and that most doping effects are completely “site decoupled”, meaning that they occur *either* on the Fe site or on the As site but not on both simultaneously. Furthermore, the energy-level schemes derived from electronic and spatial structure differ from the present “standard” assumptions. In all, it appears that substitutional effects may be more crucial to magnetism and superconductivity in iron pnictides than direct doping effects.

**M1.00384 ABSTRACT WITHDRAWN —**

**M1.00385 STM imaging of vortex cores states in superconducting graphene**, YU JI, MAOZ OVADIA, Harvard University, JENNIFER HOFFMAN, University of British Columbia, GIL-HO LEE, PHILIP KIM COLLABORATION<sup>1</sup>, WENJING FANG COLLABORATION<sup>2</sup> — Graphene becomes superconducting via the proximity effect when it comes in good contact with a superconductor. In the presence of a magnetic field, superconducting vortices will form and will each contain Andreev bound states. If the normal electrons in the vortices have a Dirac dispersion and they are surface bound states, the zero modes of the Dirac dispersion are then Majorana fermions. We investigate the electronic properties of graphene on superconducting NbN and search for these vortex bound states using our home built low temperature scanning tunneling microscope.

<sup>1</sup>Harvard University

<sup>2</sup>MIT

**M1.00386 Singular manifestation of square-planar coordination of an iridate  $\text{Na}_4\text{IrO}_4$** <sup>1</sup>, SUDIPTA KANUNGO, BINGHAI YAN, PATRICK MERZ, CLAUDIA FELSER, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, MARTIN JANSEN, Max-Planck-Institut für Solid State Research, Stuttgart, Germany — Local environments and valence electron counts primarily determine the electronic states and physical properties of transition metal complexes. For example, square-planar surroundings found in transition oxometalates such as cuprates, nickelates are usually associated with the  $d^8$  or  $d^9$  electron configuration. In this work, we address an experimentally observed exotic square-planar mono-oxoanion  $[\text{IrO}_4]^{4-}$  in  $\text{Na}_4\text{IrO}_4$  with Ir(IV) in  $d^5$  ( $S=\frac{3}{2}$  state) configuration, using ab-initio calculations. On contrary, in its 3d counterpart,  $\text{Na}_4\text{CoO}_4$ , Co(IV) is in tetrahedral coordination with  $S=\frac{5}{2}$  high spin state. Our ab-initio calculations reveal that the on-site Coulomb interaction  $U$  is the essential factor for determining the stability of the local coordination as well as spin state. We find that due to weak Coulomb repulsion of Ir-5d electrons,  $\text{Na}_4\text{IrO}_4$  form in a square-planar coordination whereas for  $\text{Na}_4\text{CoO}_4$ , Co(IV) is in tetrahedral coordination, due to strong electron correlation at 3d Co site. Following the trend from 5d to 3d, we predict that the intermediate 4d material  $\text{Na}_4\text{RhO}_4$ , if synthesized, may favor tetrahedral coordination but with an  $S=\frac{1}{2}$  low spin state.

<sup>1</sup>Sudipta Kanungo, Binghai Yan, Patrick Merz, Claudia Felser and Martin Jansen. *Angew. Chem. Int. Ed.* 54, 5417 (2015).

**M1.00387 Local electronic structure and ferromagnetic interaction in  $\text{La}(\text{Co,Ni})\text{O}_3$** , MENG-JIE HUANG, PETER NAGEL, DIRK FUCHS, HILBERT VON LOEHNEISEN, MICHAEL MERZ, STEFAN SCHUPPLER, Karlsruhe Institute of Technology, Germany — Perovskite-related transition-metal oxides exhibit a wide range of properties from insulating to superconducting as well as many peculiar magnetic phases, and cobaltites, in particular, have been known for their proximity to spin-state transitions. How this changes with partial substitution by Ni is the topic of the present study. The local electronic structure and the ferromagnetic interaction in  $\text{La}(\text{Co}_{1-x}\text{Ni}_x)\text{O}_3$  has been studied by x-ray absorption (XAS) and x-ray magnetic circular dichroism (XMCD). XAS clearly indicates a mixed-valence state for both Co and Ni, with both valences changing systematically with Ni content,  $x$ . While the gradual spin-state transition of  $\text{Co}^{3+}$  from low-spin (LS) to high-spin (HS) is preserved for low  $x$  it is suppressed in the high Ni-content samples. Regarding the spin configuration of Ni we find it stabilized in a “mixed” spin state, unlike the purely LS state of Ni in  $\text{LaNiO}_3$ . XMCD identifies the element-specific contributions to the magnetic moment and interactions. In particular, we find that it must be the coexistence of the HS state in both  $\text{Co}^{3+}$  and  $\text{Ni}^{3+}$  that induces  $t_{2g}$ -based ferromagnetic interaction via the double-exchange mechanism.

**M1.00388 Tuning band gap of monolayer and bilayer  $\text{SnS}_2$  by strain effect and external electric field : A first principles calculations**<sup>1</sup>, ABEERA RAHMAN, YOUNG-HAN SHIN, University of Ulsan — Recently many efforts have been paid to two-dimensional layered metal dichalcogenides (LMDs). Among them  $\text{MoS}_2$  has become a prototype LMD, and recent studies show surprising and rich new physics emerging in other van der Waals materials such as layered  $\text{SnS}_2$  [1-4].  $\text{SnS}_2$  is a semiconducting earth-abundant material and Sn is a group IV element replacing the transition metal in  $\text{MoS}_2$ .  $\text{SnS}_2$  shows new possibilities in various potential applications. However, the knowledge on basic properties of layered  $\text{SnS}_2$  is still not well understood. In this study, we consider two types of structures; 1T with  $P\bar{3}m1$  (164) space group and 1H with  $P6_3/mmc$  (194) space group. Our first principles calculations show that the 1T structure for  $\text{SnS}_2$  is more stable than the 1H structure whereas latter is more stable for  $\text{MoS}_2$ . Moreover, in contrast to  $\text{MoS}_2$ ,  $\text{SnS}_2$  shows an indirect band gap both for 1T and 1H structures while 1T  $\text{MoS}_2$  is metallic and 1H has a direct band gap. We also study strain effect in the range of 0-10% on the band structure for monolayer and bilayer  $\text{SnS}_2$  (both for 1T and 1H structures). We find significant change in their band gaps. We also investigate the bilayer  $\text{SnS}_2$  with and without out-of-plane stress.

<sup>1</sup>This research was supported by Brain Korea 21 Plus Program and Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Science, ICT and future Planning (NRF-2014M3A7B4049367, NRF-2014R1A2A1A1105089).

**M1.00389 Manipulating individual defects in graphene/BN heterostructures: a first-principles study**, LEDE XIAN, ANGEL RUBIO, Univ of the Basque Country — Recent experiments have demonstrated the possibility of manipulating defects in insulating hexagonal boron nitride (hBN) within a graphene/hBN heterostructure using scanning tunneling microscopy, opening a new pathway of manipulating individual defects of insulators at the nanoscopic scale. With first principle calculations, we are able to simulate this process and elucidate the relevant physics in experiments. Moreover, we calculate the band level alignments between graphene and possible defects states in hBN. Thus, we identify different defects observed in experiments and provide important reference for future experiments and applications.

**M1.00390 CVD-based, photolithographically patterned, highly-sensitive graphene Hall element on hexagonal BN**, JOONGGYU KIM, Center for Integrated Nanostructure Physics, Institute for Basic Science, DOES, Sungkyunkwan University, MIN-KYU JOO, JI-HOON PARK, Center for Integrated Nanostructure Physics, Institute for Basic Science, Sungkyunkwan University, VAN LUAN NGUYEN, Center for Integrated Nanostructure Physics, Institute for Basic Science, DOES, Sungkyunkwan University, KI KANG KIM, Department of Energy and Materials Engineering, Dongguk University, YOUNG HEE LEE, DONGSEOK SUH, Center for Integrated Nanostructure Physics, Institute for Basic Science, DOES, Sungkyunkwan University — Graphene is known to have a high carrier mobility, and the carrier density can be minimized at the charge neutrality point (CNP). Because such features are suitable for Hall sensor measuring magnetic field, we examined the possibility of graphene Hall element (GHE) as a highly sensitive magnetic sensor. For the high-throughput production of GHE in the future, the material synthesized by a chemical-vapor-deposition (CVD) method and the fabrication processes based on photolithography were adopted to show its mass-production feasibility. Specifically, the CVD synthesized hexagonal BN (hBN) was tested as a protection layer of graphene from extrinsic doping driven by  $\text{SiO}_2$  substrate, which causes the shift of CNP. In addition, post annealing sequences were also included between each step, such as the hBN attachment on  $\text{SiO}_2$  and the graphene transfer on hBN/ $\text{SiO}_2$  substrate followed by the PMMA removal. From this work, we can get minimum magnetic resolution around 10 mG/Hz<sup>0.5</sup> at 300 Hz.

**M1.00391 Study of correlations from Ab-Initio Simulations of Liquid Water**<sup>1</sup>, ADRIAN SOTO, MARIVI FERNANDEZ-SERRA, Stony Brook University, DEYU LU, SHINJAE YOO, Brookhaven National Lab — An accurate understanding of the dynamics and the structure of  $\text{H}_2\text{O}$  molecules in the liquid phase is of extreme importance both from a fundamental and from a practical standpoint. Despite the successes of Molecular Dynamics (MD) with Density Functional Theory (DFT), liquid water remains an extremely difficult material to simulate accurately and efficiently because of fine balance between the covalent O-H bond, the hydrogen bond and the attractive van der Waals forces. Small errors in those produce dramatic changes in the macroscopic properties of the liquid or in its structural properties. Different density functionals produce answers that differ by as much as 35% in ambient conditions, with none producing quantitative results in agreement with experiment at different mass densities [*J. Chem Phys.* 139, 194502(2013)]. In order to understand these differences we perform an exhaustive scanning of the geometrical coordinates of MD simulations and study their statistical correlations with the simulation output quantities using advanced correlation analyses and machine learning techniques.

<sup>1</sup>This work was partially supported by DOE Award No. DE-FG02-09ER16052, by DOE Early Career Award No. DE-SC0003871, by BNL LDRD 16-039 project and BNL Contract No. DE-SC0012704.

**M1.00392 Improved methods for determining the secondary structure of proteins using FTIR spectroscopy** , DAVID NETO, Oklahoma State University — The determination of the secondary structure is vitally important in the study of proteins. An oft overlooked and underused method to probe the secondary structure of a protein is Fourier transform infrared (FTIR) spectroscopy. A great compliment to both X-ray and NMR techniques, the speed and relatively low cost of FTIR measurements provide a wealth of information about the structure of a protein. To enhance the accuracy of secondary structure calculations, improved methods in the fitting of absorbance spectra are needed. In this talk, we will explore the development of these methods and apply them to a few well studied proteins.

**Wednesday, March 16, 2016 10:45AM - 11:30AM —**

**Session N1 APS: Meet the Editors of APS Coffee Break** Exhibit Hall EF -

**10:45AM N1.00001 Meet the Editors of APS Reception —**

**Wednesday, March 16, 2016 12:00PM - 3:00PM —**

**Session N2 APS: Careers in Physics Workshop: Putting Your Science to Work** Hilton Baltimore Key Ballrooms 9/10 -

**12:00PM N2.00001 Careers in Physics Workshop: Putting Your Science to Work —**

**Wednesday, March 16, 2016 2:30PM - 5:30PM —**

**Session P1 APS: The Fred Kavli Special Symposium on Physics Frontiers** Exhibit Hall C - Sharon Glotzer, University of Michigan

**2:30PM P1.00001 New perspectives on quantum simulation with ultra-cold atoms** , ANA MARIA REY, University of Colorado, Boulder — Understanding the behavior of interacting electrons in solids or liquids is at the heart of modern quantum science and necessary for technological advances. However, the complexity of their interactions generally prevents us from coming up with an exact mathematical description of their behavior. Precisely engineered ultracold gases are emerging as a powerful tool for unraveling these challenging physical problems. In this talk, I will present recent ideas on using alkaline-earth atoms —currently the basis of the most precise atomic clock in the world— for the investigation of complex many-body phenomena and magnetism. I will also discuss a new research direction of using atomic clocks not only as precise time keepers but also as unique quantum laboratories for the investigation of new forms of matter with no known counterpart in nature.

**3:06PM P1.00002 Illuminating biology at the nanoscale with single-molecule and super-resolution fluorescence microscopy** , XIAOWEI ZHUANG, Harvard University — Dissecting the inner workings of a cell requires imaging methods with molecular specificity, molecular-scale resolution, and dynamic imaging capability such that molecular interactions inside the cell can be directly visualized. Fluorescence microscopy is a powerful imaging modality for investigating biological systems largely owing to its molecular specificity and dynamic imaging capability. However, the diffraction-limited resolution of light microscopy is substantially larger than molecular length scales in cells, making many sub-cellular structures difficult to resolve. We developed a super-resolution fluorescence microscopy method, stochastic optical reconstruction microscopy (STORM), which overcomes the diffraction limit by using photo-switchable fluorescent probes to temporally separate the spatially overlapping images of individual molecules. This approach has allowed multicolor and three-dimensional imaging of living cells with nanometer-scale resolution and enabled discoveries of novel sub-cellular structures. In this talk, I will present to concept and technological advances of STORM, as well as some of the recent biological discoveries enabled by STORM. I will also describe a new single-cell transcriptome imaging method multiplexed error-robust fluorescent in situ hybridization (MERFISH), which allows numerous RNA species to be imaged and quantified in single cells. This approach enables unique analyses based on copy numbers and spatial distributions of many RNA species within single cells, facilitating the delineation of gene regulatory networks and in situ identification of cell types.

**3:42PM P1.00003 Making New Particles One By One** , DAVID A. WEITZ, Dept. of Physics and SEAS, Harvard University, Cambridge MA — This talk will describe the use of microfluidic devices to create new structures with unusual properties and enormous potential for technological applications. The particles are formed using fluid drops as templates, and take advantage of the exquisite control afforded by the use of microfluidic devices to very simply create complex structures. These new structures facilitate the study of new properties of materials. It is also feasible to use these methods to very easily create nanoparticles of almost any material through a microfluidic spray drier. Remarkably, if these nanoparticles are small enough, they are amorphous, even if the material is otherwise always crystalline. For example, it is even feasible to produce amorphous nanoparticles of table salt (NaCl). The talk will also describe how it is feasible to produce large quantities of these materials, despite making the particles one at a time. This makes the particles valuable for both fundamental studies and for technological applications

**4:18PM P1.00004 Plasmons, hot electrons and nanoscale heat transfer** , NAOMI HALAS, Rice University — TBD

**4:54PM P1.00005 The Observation of Gravitational Waves from a Binary Black Hole Merger** , DUNCAN BROWN, Syracuse University — On September 14, 2015 the the two detectors of the Laser Interferometer Gravitational-Wave Observatory (LIGO) simultaneously observed gravitational waves from a binary black hole merger. The gravitational waves observed match the waveform predicted by general relativity for the inspiral and merger of a pair of black holes and the ringdown of the resulting single black hole. This is the first direct detection of gravitational waves and the first observation of a binary black hole merger. I will discuss the discovery of this event, the properties of the source, and the future of the new field of gravitational-wave astronomy.

**Wednesday, March 16, 2016 2:30PM - 5:18PM —**

**Session P5 GMAG DMP FIAP: Spins in Two Dimensions: Graphene, 2DEGs and Quantum Wells** 301 - Hanan Dery, University of Rochester

### **2:30PM P5.00001 Homoepitaxial graphene tunnel barriers for spin transport**, ADAM FRIEDMAN,

Naval Research Laboratory — Tunnel barriers are key elements for both charge-and spin-based electronics, offering devices with reduced power consumption and new paradigms for information processing. Such devices require mating dissimilar materials, raising issues of heteroepitaxy, interface stability, and electronic states that severely complicate fabrication and compromise performance. Graphene is the perfect tunnel barrier. It is an insulator out-of-plane, possesses a defect-free, linear habit, and is impervious to interdiffusion. Nonetheless, true tunneling between two stacked graphene layers is not possible in environmental conditions (magnetic field, temperature, etc.) usable for electronics applications. However, two stacked graphene layers can be decoupled using chemical functionalization. We demonstrate successful tunneling, charge, and spin transport with a fluorinated graphene tunnel barrier on a graphene channel. We show that while spin transport stops short of room temperature, spin polarization efficiency values are the highest of any graphene spin devices. We also demonstrate that hydrogenation of graphene can also be used to create a tunnel barrier. We begin with a four-layer stack of graphene and hydrogenate the top few layers to decouple them from the graphene transport channel beneath. We demonstrate successful tunneling by measuring non-linear IV curves and a weakly temperature dependent zero-bias resistance. We demonstrate lateral transport of spin currents in non-local spin-valve structures and determine spin lifetimes with the non-local Hanle effect to be commensurate with previous studies. The measured spin polarization efficiencies for hydrogenated graphene are higher than most oxide tunnel barriers on graphene, but not as high as with fluorinated graphene tunnel barriers. However, here we show that spin transport persists up to room temperature. Our results for the hydrogenated graphene tunnel barriers are compared with fluorinated tunnel barriers and we discuss the possibility that magnetic moments in the graphene tunnel barriers affect the spin transport of our devices.

### **3:06PM P5.00002 Tight-binding description of spin-orbit coupling in graphene due to adatoms<sup>1</sup>**

SUSANNE IRMER, DENIS KOCHAN, KLAUS ZOLLNER, MARTIN GMITRA, TOBIAS FRANK, JAROSLAV FABIAN, University of Regensburg — We present realistic effective tight-binding models for proximity spin-orbit coupling in graphene due to adatoms at top, bridge, and hollow positions. The models are built from symmetry arguments and fitted to ab initio calculations for a variety of adsorbants, such as H [1], F [2], Cu, and CH<sub>3</sub> [3]. For each of these adatoms we provide magnitudes for orbital couplings to the adsorbants, as well as the intrinsic Rashba, and pseudospin-inversion asymmetry (PIA) couplings. Our models can be used to study spin relaxation, spin Hall effect, and spin transport using quantum transport models. [1] M. Gmitra, D. Kochan, J. Fabian, Phys. Rev. Lett. 110, 246602 (2013). [2] S. Irmer, T. Frank, S. Putz, M. Gmitra, D. Kochan, J. Fabian, Phys. Rev. B 91, 115141 (2015). [3] K. Zollner, T. Frank, S. Irmer, M. Gmitra, D. Kochan, J. Fabian, arXiv:1507.02820

<sup>1</sup>This work was supported by the DFG SFB 689 and GRK 1570, and by the European Union Seventh Framework Programme under Grant Agreement No. 604391 Graphene Flagship.

### **3:18PM P5.00003 Spintronics with Graphene and van der Waals heterostructures**, SAROJ DASH,

M.VENKATA KAMALAKAR, ANDR DANKERT, Chalmers University of Technology, QUANTUM DEVICE PHYSICS LABORATORY TEAM — Two-dimensional (2D) atomic crystals provide a large class of materials proposed to be important for nanoelectronics and spintronic. Here we present two important advancements in graphene spintronics by employing 2D materials and heterostructures. Graphene is considered to be an ideal material for spin transport due to the high mobility and long spin lifetime of the carriers. We realized spin transport over a long distance of 16  $\mu$ m and spin lifetimes up to 1.2 ns in large area CVD graphene on SiO<sub>2</sub>/Si substrate at room temperature [1]. Subsequently, using the h-BN tunnel barrier/graphene van der Waals heterostructure; we observe an enhancement in the tunnel spin polarization [2], and a negative spin signal for thicker h-BN barriers. These findings open a platform for exploring novel spin functionalities in 2D crystal heterostructures and understanding the basic science that control their behavior. [1] M. V. Kamalakar et al., Long Distance Spin Communication in Chemical Vapor Deposited Graphene, Nature Communications 6, 6766 (2015). [2] M. V. Kamalakar et al., Enhanced Tunnel Spin Injection into Graphene using Hexagonal Boron Nitride; Scientific Reports 4, 61446 (2014).

### **3:30PM P5.00004 Proximity Anisotropic Magnetoresistance in Graphene**, JEONGSU LEE, JAROSLAV

FABIAN, Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — We theoretically investigate charge transport in graphene that is on a ferromagnetic-insulator substrate. The substrate induces spin polarization in graphene—ferromagnetic proximity effect—as demonstrated recently experimentally [1]. We show, using realistic models [2, 3], that the presence of spin-orbit coupling in proximity ferromagnetic graphene leads to anisotropic magnetoresistance whereby graphene's resistance changes with varying magnetic field orientation (both in and out of plane). We evaluate the magnitude as well as the angular dependence of this novel effect using conventional transport models [4] and propose specific experimental schemes to measure it. This work is supported by DFG SFB 689. References [1] Z. Wang, C. Tang, R. Sachs, Y. Barlas, and J. Shi, Phys. Rev. Lett. 114, 016603, (2015) [2] M. Gmitra, D. Kochan, and J. Fabian, Phys. Rev. Lett. 110, 246602 (2013). [3] M. Gmitra, S. Konschuh, C. Ertler, C. Ambrosch-Draxl, and J. Fabian, Phys. Rev. B 80, 235431, (2009) [4] S. Adam, E. H. Hwang, V. M. Galitski, and S. Das Sarma, Proc. Natl. Acad. Sci. U.S.A., 104, 18392, (2007)

### **3:42PM P5.00005 Stoner-like theory of Magnetism in Silicon MOSFETs<sup>1</sup>**, DENIS GOLOSOV, Bar-

Ilan University — We consider quasi-two-dimensional gas of electrons in a typical Si-MOSFET, assuming contact repulsive interaction between electrons. Magnetisation and susceptibility are evaluated within the mean-field approach. The finite thickness of inversion layer results in an interaction-induced electron wave function change, not found in both purely two-dimensional and three-dimensional (bulk) cases. Taking this self-consistent change into account leads to an increased susceptibility and ultimately to a ferromagnetic transition deep in the high-density metallic regime. We further find that in the paramagnetic state, magnetisation increases sublinearly with increasing in-plane magnetic field. In the opposite limit of low carrier densities, the effects of long-range interaction become important and can be included phenomenologically via bandwidth renormalisation. Our treatment then suggests that with decreasing density, the metal-insulator transition is preceded by a ferromagnetic instability. We discuss the validity of our mean-field scheme, and relate the results to the available experimental data.

<sup>1</sup>Supported by Israeli Absorption Ministry

### **3:54PM P5.00006 Rashba scattering in the dilute limit**, JOEL HUTCHINSON, JOSEPH MACIEJKO, University of

Alberta — In two-dimensional (2D) noncentrosymmetric crystals, the spin degeneracy of the electronic band structure may be lifted by Rashba spin-orbit coupling. The resulting spin-split dispersion is responsible for the spin Hall effect and has desirable applications to spintronics. This spin-split dispersion is described in terms of two distinct helicity bands, but below a threshold energy, electrons are confined to one of these. At the bottom of this lower band, the density of states exhibits a van Hove singularity. This is the relevant regime for a dilute spin-orbit coupled 2D electron gas, which has been shown to host a variety of exotic phases in the presence of electron-electron interactions. In this talk we investigate scattering of Rashba electrons off a circular potential barrier in this dilute limit, which is relevant both for impurity scattering in the noninteracting limit as well as for short-range two-particle scattering in the interacting problem. The S matrix and scattering cross section are determined, and it is found that scattering becomes effectively one-dimensional at the band bottom.

**4:06PM P5.00007 Edge spin accumulation in a two-dimensional electron gas with two subbands<sup>1</sup>**, ALEXANDER KHAETSKII, State Univ of NY - Buffalo, J. CARLOS EGUES, Instituto de Física de Sao Carlos, Brazil — We have studied the edge spin accumulation in 2D electron gas due to the intrinsic mechanism of spin-orbit interaction for the case of a two-subband structure. This study is strongly motivated by recent experiments [1] which observed the spin accumulation near the edges of a high mobility 2D electron system in a bilayer symmetric GaAs structure in contrast to zero effect in a single-layer configuration. Our theoretical explanation is based on the Rashba-like spin-orbit interaction which arises as a result of the coupling between two subband states of opposite parities in a symmetric quantum well [2]. Following the method developed in [3], we have calculated the edge spin density in a quasi-ballistic regime, and explained the experimental results, in particular, a large magnitude of the edge spin density. We showed that one can easily proceed from the regime of strong spin accumulation to the regime of weak one. It opens up a possibility to construct an interesting new spintronic device. [1]. F. Hernandez et al., Phys. Rev. B **88**, 161305(R) (2013). [2]. E. Bernardes et al., Phys. Rev. Lett. **99**, 076603 (2007). [3]. A. Khaetskii, Phys. Rev. B **89**, 195408 (2014).

<sup>1</sup>Supported by FAPESP (Brazil)

**4:18PM P5.00008 Dynamical spin injection into a two-dimensional electron gas in an Al-GaAs/GaAs structure**, KENRO OHTOMO, YUICHIRO ANDO, TERUYA SHINJO, Kyoto University, TETSUYA UEMURA, Hokkaido University, MASASHI SHIRAIISHI, Kyoto University — A two-dimensional electron system in a GaAs-based heterostructure is the attractive platform for spintronics since it has high mobility and spin-orbit interaction can be modulated by the gate voltage<sup>1</sup>. Thus, it is a possible platform to realize electric gate-controlled spin transistor<sup>2</sup>. However, room-temperature spin transport through GaAs-based heterostructure has yet to be shown. We report first spin transport through the quantum well at GaAs/AlGaAs interface at room temperature. We used spin pumping under ferromagnetic resonance to inject spins from the Ni<sub>80</sub>Fe<sub>20</sub> to the GaAs/AlGaAs quantum well. Generated spin current propagated through the 1  $\mu$ m channel and was detected using spin-charge conversion inverse spin Hall effect in the Pt electrode. In agreement with spin pumping theory, polarity of the spin transport signal was reversed together with magnetization of the Ni<sub>80</sub>Fe<sub>20</sub>. This first demonstration of spin transport through a quantum well at a semiconductor heterostructure interface at room temperature opens a way to realize Datta-Das spin-based transistor.

<sup>1</sup> J. Nitta, et al., PRL **78**, 1335 (1997).

<sup>2</sup> S. Datta and B. Das, Appl. Phys. Lett. **56**, 665 (1990).

**4:30PM P5.00009 Hole spin coherence in coupled GaAs/AlAs quantum wells<sup>1</sup>**, CHRISTIAN GRADL, MICHAEL KEMPF, JOHANNES HOLLER, DIETER SCHUH, DOMINIQUE BOUGEARD, CHRISTIAN SCHUELLER, TOBIAS KORN, University of Regensburg — Due to its p-like character, the valence band in GaAs-based heterostructures offers rich and complex spin-dependent phenomena. Especially for some low-symmetry growth directions, a strong anisotropy of the hole g factor with respect to the in-plane magnetic field direction is theoretically predicted. Therefore, we perform time-resolved Kerr rotation measurements on an undoped [113]-grown double quantum well (QW) structure to resolve the spin dynamics of hole ensembles at low temperatures. Our gated system consists of two QWs with different well widths, which we use for the spatial separation of the optically excited electron-hole pairs. Thus, we are able to create hole ensembles with spin lifetimes of several hundreds of picoseconds in the broader QW without any doping. This allows the observation of a strong hole g factor anisotropy by varying the magnetic field direction in the QW plane. The experimental g factor values are in very good agreement with theoretical predictions. Furthermore, we observe an unexpected additional non-precessing component in the Kerr signal for certain in-plane magnetic field directions. This might have its origin in a precession axis that is tilted relative to the magnetic field due to the crystal structure of this low-symmetry growth direction.

<sup>1</sup>Financial support by the DFG via SFB 689 is gratefully acknowledged

**4:42PM P5.00010 Investigation and direct mapping of the persistent spin helix in confined structures<sup>1</sup>**, MARKUS SCHWEMMER, MATTHIAS WEINGARTNER, ROLAND VÖLKL, MARTIN OLTSCHER, DIETER SCHUH, DOMINIQUE BOUGEARD, TOBIAS KORN, CHRISTIAN SCHÜLLER, University Regensburg — The spin-orbit field in GaAs-based quantum well (QW) structures typically consists of two different contributions: Dresselhaus and Rashba field. The geometry of the Dresselhaus field, which arises due to the bulk inversion asymmetry, is mostly determined by the growth direction of the quantum well. The Rashba field instead is caused by a structure inversion asymmetry, which can be controlled, e.g. by the modulation doping. For the specific case of a (001)-grown GaAs quantum well with equal strength of Dresselhaus and Rashba fields, the effective spin-orbit field is oriented along the in-plane [110] direction for all  $k$  values and the spin splitting for this direction vanishes. For optically injected spins, which are initially oriented perpendicular to the QW plane, a persistent spin helix (PSH) state forms. We use a femtosecond pulsed TiSa-Laser system combined with a magneto-optical Kerr effect microscope for time- and space-resolved mapping of the PSH. With this technique, we investigate the PSH behavior in confined structures, e.g., thin channels along the helix direction. Hence we find that lateral confinement increases the effective PSH lifetime drastically. In more complex structures, we observe that PSH formation is even stable under a forced direction change.

<sup>1</sup>Financial support by the DFG via SFB 689 and SPP 1285 is gratefully acknowledged.

**4:54PM P5.00011 Role of contact resistance in the effective spin relaxation rate in graphene spin valves<sup>1</sup>**, GORDON STECKLEIN, YOSKA ANUGRAH, JING LI, STEVEN J. KOESTER, PAUL CROWELL, University of Minnesota — Recent experiments (Maassen et al., PRB **86** 235408 (2012), Idzuchi et al., PRB **91** 241407(R) (2015)) have identified the role of finite contact resistances in determining the spin lifetime in graphene based on Hanle measurements of lateral spin valves. We have investigated this effect in spin valves fabricated using Co/AIOx tunnel barriers and graphene grown by chemical vapor deposition. By carrying out non-local spin valve and Hanle measurements over a wide range of gate voltages, we observe a variation in the spin signal that can be explained by the role of the contacts. Using the measured interface resistance, we quantify the degree of contact-induced spin sinking as the ratio of the contact resistance to the channel spin resistance and show that the variation in spin signal is explained by variation in this spin sinking parameter. By properly accounting for the effect of the contact resistance, we measure a spin lifetime that varies between 150-500 picoseconds.

<sup>1</sup>This work was supported by NSF ECCS-1124831, the NRI NEB program, and C-SPIN, a SRC STARNET center sponsored by MARCO and DARPA.

**5:06PM P5.00012 Boundary conditions for transition-metal dichalcogenide monolayers in the continuum model**, CSABA G. PÉTERFALVI, ANDOR KORMÁNYOS, GUIDO BURKARD, Department of Physics, University of Konstanz, D-78464 Konstanz, Germany — We derive the boundary conditions for MoS<sub>2</sub> and similar transition-metal dichalcogenide honeycomb (2H polytype) monolayers with the same type of  $k \cdot p$  Hamiltonian within the continuum model around the K points. [1] In an effective 2-band description, the electron-hole symmetry breaking quadratic terms are also taken into account. We model the effect of the edges with a linear edge constraint method that has been applied previously to graphene. Focusing mainly on zigzag edges, we find that different reconstruction geometries with different edge-atoms can generally be described with one scalar parameter varying between 0 and  $2\pi$ . We analyze the edge states and their dispersion relation in MoS<sub>2</sub> in particular, and we find good agreement with the results of previous density functional theory calculations for various edge types. [1] Cs. G. Péterfalvi, A. Kormányos, G. Burkard, arXiv:1509.00184 (2015).

## Wednesday, March 16, 2016 2:30PM - 5:30PM –

Session P6 GMAG DMP: Magnetic Complex Oxides I 302 - Gian Guzman-Verri, University of Costa Rica / Argonne National Lab

**2:30PM P6.00001 High antiferromagnetic transition temperature for a layered hexagonal compound:  $\text{SrRu}_2\text{O}_6$** <sup>1</sup>, JIAQIANG YAN, Oak Ridge National Laboratory and University of Tennessee — 4d or 5d transition metal oxides (TMOs) are less correlated and have a larger bandwidth than 3d TMOs. A high magnetic ordering temperature for 4d/5d TMOs is not expected. It was therefore a surprise when a perovskite,  $\text{SrTcO}_3$ , was reported to order magnetically around 1000 K. Unfortunately, the radioactive nature of Tc prevented further investigation of the underlying mechanism for the high magnetic ordering temperature. Here we report antiferromagnetic order of  $\text{SrRu}_2\text{O}_6$  at 565 K. Two features distinguish this compound from  $\text{SrTcO}_3$ : (1)  $\text{SrRu}_2\text{O}_6$  is not radioactive, which allows the study of the underlying physics by a large variety of techniques as well as the possible fine tuning of the magnetic ground state; and (2)  $\text{SrRu}_2\text{O}_6$  crystallizes into a quasi-two-dimensional structure with layers of edge-sharing  $\text{RuO}_6$  octahedra separated by nonmagnetic Sr layers. Our density functional calculations and Monte Carlo simulations suggest an origin of the reduced moment size and the high Neel temperature.

<sup>1</sup>Work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division and by the CEM and NSF MRSEC under Grant No. DMR-1420451.

**3:06PM P6.00002 Molecular orbitals vs. relativistic orbitals in  $t_{2g}$  honeycomb lattices:  $\text{SrRu}_2\text{O}_6$  as compared to  $\text{Na}_2\text{IrO}_3$ ,  $\text{RuCl}_3$ , and  $\text{Li}_2\text{RuO}_3$ .**<sup>1</sup>, IGOR MAZIN, Naval Research Laboratory, SERGEY STRELTISOV, Institute of Metal Physics, Ekaterinburg, Russia, KATERYNA FOYEVTSEVA, University of British Columbia, Canada —  $t_{2g}$  states on a honeycomb lattice tend to form non-dispersive localized states even if large intersite hopping is present. In the nonrelativistic case, these are molecular orbitals (MO) localized on metal hexagons, if the ligand-assisted nearest and next nearest neighbor hoppings,  $t'_1$  and  $t'_2$ , dominate, or dimers (DO), if the direct overlap,  $t_1$ , dominates. In the ultrarelativistic limit  $t_{2g}$  form effective relativistic orbitals (RO),  $j_{eff} = 3/2$ , which are atomically localized if  $t'_1$  is the dominant hopping. On the first glance, the three regimes are defined by the conditions  $t'_1 \gg t_1, \lambda$  or  $t_1 \gg t'_1, \lambda$  or  $\lambda \gg t_1, t'_1$ . In reality, the latter condition is never fulfilled, especially in ruthenates, yet not only  $\text{Na}_2\text{IrO}_3$ , but also  $\text{RuCl}_3$  appear to be in a regime dominated by RO, even though the residual effect of MO critically influences magnetic interactions, while  $\text{Li}_2\text{RuO}_3$ , not far removed from  $\text{RuCl}_3$  in the parameter space, is firmly in the DO regime. Most surprisingly,  $\text{SrRu}_2\text{O}_6$ , which is even closer to  $\text{RuCl}_3$ , happens to be fully in the MO regime, with negligible spin-orbit effects. In this talk, we will show that an additional, decisive factor is the doping level per site. The principal difference between  $\text{Na}_2\text{IrO}_3$  or  $\text{RuCl}_3$ ,  $\text{Li}_2\text{RuO}_3$ , and  $\text{SrRu}_2\text{O}_6$  is that the first two have one  $t_{2g}$  hole per site, the second one two holes, and the last three electrons. In particular, the total dominance of MO in the latter compound fully explains its unique and unexpected magnetic properties.

<sup>1</sup>This work was supported by ONR (IIM) and CRDF (IIM and SVS)

**3:18PM P6.00003 Magnetization reversal and negative volume thermal expansion in Fe doped  $\text{Ca}_2\text{RuO}_4$** <sup>1</sup>, T. F. QI, S. J. YUAN, Center for Advanced Materials, Department of Physics and Astronomy, University of Kentucky, Lexington, KY 40506, USA, F. YE, S. CHI, Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA, J. TERZIC, H. ZHANG, Center for Advanced Materials, Department of Physics and Astronomy, University of Kentucky, Lexington, KY 40506, USA, Z. ZHAO, Department of Geological and Environmental Sciences, Stanford University, Stanford, CA 94305, USA, X. LIU, Institute of Physics, Chinese Academy of Sciences, Beijing, 100190, China, S. PARKIN, Department of Chemistry, University of Kentucky, Lexington, KY 40506, USA, W. L. MAO, Department of Geological and Environmental Sciences, Stanford University, Stanford, CA 94305, USA, G. CAO, Center for Advanced Materials, Department of Physics and Astronomy, University of Kentucky, Lexington, KY 40506, USA — We report structural, magnetic, transport and thermal properties of single-crystal  $\text{Ca}_2\text{Ru}_{1-x}\text{Fe}_x\text{O}_4$  ( $0 \leq x \leq 0.2$ ) as functions of pressure, magnetic field and temperature. The central findings of this work are a pronounced magnetization reversal and a negative thermal expansion that are induced by Fe doping. Our results including neutron diffraction data suggest that the magnetization reversal is primarily a result of different temperature dependences of two antiparallel, competing Ru and Fe sublattices and that the negative thermal expansion is achieved via magnetic and metal-insulator transitions. We will present and discuss our results with comparison drawn with relevant systems.

<sup>1</sup>This work was supported by the NSF via Grant No. DMR-1265162

**3:30PM P6.00004 NMR study of new ruthenates with high magnetic ordering**, P.L. PAULOSE, TANMOY CHAKRABARTY, Tata Institute of Fundamental Research, Mumbai, India — The Ru based compounds,  $\text{Ca}_3\text{LiRuO}_6$  and  $\text{Ca}_3\text{NaRuO}_6$  show unusually high magnetic ordering temperature. Extended super exchange model is invoked to explain the magnetic behavior in the isostructural compound  $\text{Ca}_3\text{LiOsO}_6$ . We have carried out NMR investigation on these two Ru-based compounds.  $\text{Ca}_3\text{LiRuO}_6$  is a weak ferromagnet with a magnetic ordering temperature ( $T_C$ ) of 115 K which is explored by the temperature dependence of  $^7\text{Li}$  NMR line shift, line-width and spin-lattice relaxation rate ( $1/T_1$ ). Above  $T_C$ , a broad maximum is observed in the evolution of line-width of the spectra. We speculate that this feature might be attributed to some low-dimensional magnetic behavior. Contrastingly,  $\text{Ca}_3\text{NaRuO}_6$  with similar structure and local geometry of the  $\text{Ru}^{5+}$  ions is a conventional antiferromagnet with a transition temperature of 90 K. The temperature dependence of  $^{23}\text{Na}$  NMR line shift and  $1/T_1$  is studied across magnetic transition in  $\text{Ca}_3\text{NaRuO}_6$ . The temperature variation of line-width is found to be different compared to  $\text{Ca}_3\text{LiRuO}_6$ . In both these systems,  $1/T_1$  decreases significantly below ordering temperature, characteristic of many antiferromagnetic systems.

**3:42PM P6.00005 Spin-orbit dimers in double perovskites**, GEORGE JACKELI, University of Stuttgart and Max Planck Institute for Solid State Research, Stuttgart, Germany — In Mott insulators, unquenched orbital degrees of freedom often frustrate the magnetic interactions and lead to a plethora of interesting phases with unusual spin patterns or non-magnetic states without long-range order. Here, we present a theoretical study of interplay of spin and orbital degrees in double-perovskite compounds with  $d^1$  ions occupying the fcc sublattice. We show that the ground state of such a system is non-magnetic dimer pseudo-spin singlet with extensive orientational degeneracy of dimers. We discuss how the pseudo-spin state forming the singlet is altered upon increasing the strength of the relativistic spin-orbit coupling and show that the dimer 'gas' phase remains the ground state throughout. Our theoretical findings support and explain the experimentally observed non-magnetic amorphous valence bond state in  $\text{Ba}_2\text{YMoO}_6$  and in related compounds.

**4:18PM P6.00006 Doping an antiferromagnetic insulator : A route to an antiferromagnetic metallic phase**, PRIYA MAHADEVAN, SHISHIR PANDEY, S.N.Bose National Centre for Basic Sciences, D.D. SARMA, SSCU, Indian Institute of Science, Bangalore — Usually antiferromagnetism is accompanied by an insulating character of the ground state, while ferromagnetism is accompanied by metallicity. In the limit of half-filling, the Hubbard model yields an antiferromagnetic insulator as the ground state. From the Nagaoka theorem we expect ferromagnetism at any finite electron doping of this half filled state. Numerical studies on the other hand, have however shown, that at low doping concentrations one has a narrow region of an antiferromagnetic metallic phase. The question is whether this is realizable in real materials. Among the 3d transition metal oxides, this antiferromagnetic metallic phase has remained elusive as strong electron-phonon coupling results in a different phase diagram. The 5d transition metal oxides are therefore more suitable. In this work we solve a multiband Hubbard model relevant for a 5d transition metal oxide within a mean-field approach and show that the large bandwidth and the small intra-atomic Hund's exchange associated with this limit gives us a robust AFM-M ground state for 25% electron doping. The conclusions are supported by ab-initio electronic structure calculations for NaOsO<sub>3</sub>.

**4:30PM P6.00007 Excitations and enhanced coupling at the magnetic metal-insulator transition in NaOsO<sub>3</sub> and Cd<sub>2</sub>Os<sub>2</sub>O<sub>7</sub>**, S. CALDER, J. H. LEE, M. B. STONE, ORNL, J. G. VALE, C. DONNERER, UCL, N. A. BOGDANOV, IFW Dresden, J. LANG, APS, M. FEYGENSON, ORNL, X. LIU, CAS, M. H. UPTON, D. CASA, APS, M. D. LUMSDEN, Z. ZHAO, J.-Q. YAN, ORNL, Y.G. SHI, Y.S. SUN, Y. TSUJIMOTO, K. YAMAURA, NIMS, D. MANDRUS, University of Tennessee, S. NISHIMOTO, J. VD BRINK, IFW Dresden, J. P. HILL, BNL, D. F. MCMORROW, UCL, A. D. CHRISTIANSON, ORNL — 5d oxides provide new paradigms of cooperative interactions that drive novel emergent behavior. This is exemplified in the osmates NaOsO<sub>3</sub> and Cd<sub>2</sub>Os<sub>2</sub>O<sub>7</sub> that host MITs where magnetic order appears intimately entwined. However, unlike the iridates where spin-orbit coupling (SOC) behavior dominates, in the 5d<sup>3</sup> osmates an orbital singlet is expected and reduced effect of SOC. We measure the inelastic spectra with neutrons and RIXS. Our results uncover the 5d-manifold splitting to reveal a suppressed role of SOC in the creation of the electronic ground state but dominant behavior in the creation of the magnetic state. Moreover at the MIT in NaOsO<sub>3</sub> we find a giant spin-phonon coupling and in Cd<sub>2</sub>Os<sub>2</sub>O<sub>7</sub> a magnetic excitation corresponding to a superposition of multiple spin-flips.

**4:42PM P6.00008 Terahertz Spectroscopy of Osmate Double Perovskites<sup>1</sup>**, MATTHEW T. WARREN, Department of Physics, The Ohio State University. Columbus OH 43210, R. MORROW, Department of Chemistry, The Ohio State University. Columbus OH 43210, T. T. MAI, Department of Physics, The Ohio State University. Columbus OH 43210, J. XIONG, P. M. WOODWARD, Department of Chemistry, The Ohio State University. Columbus OH 43210, R. VALDÉS AGUILAR, Department of Physics, The Ohio State University. Columbus OH 43210 — Double perovskites containing 5d transition metal elements allow study of the interplay of spin-orbit coupling and electronic correlations due to the heavy nuclei and large electronic wavefunctions. Here we have studied polycrystalline Sr<sub>2</sub>MOsO<sub>6</sub> (M = Mg, Fe, Co; with Os electronic configuration of d<sup>2</sup>, d<sup>3</sup>, d<sup>2</sup>, respectively) with time-domain terahertz spectroscopy. Terahertz electrodynamics seem to be decoupled from observed magnetic and structural phase transitions in M=Mg, Co. A strong absorption is measured in M=Mg, Co around 1.5 THz, which softens with temperature, as expected for an optical phonon. The effectiveness of the variable-range hopping model and the origin of higher temperature conductivity are examined. Work at OSU supported by the NSF MRSEC Center for Emergent Materials under Grant DMR-1420451.

<sup>1</sup>Work supported by the Center for Emergent Materials: an NSF MRSEC under award DMR-1420451.

**4:54PM P6.00009 Numerical Implementation of a General Spinwave Model to Simulate Spin-wave Excitations Found in Inelastic Neutron Scattering Data**, D. CASAVANT, I. BRODSKY, G. J. MACDOUGALL, Dept. of Physics, Univ. of Illinois at Urbana-Champaign — Many important details regarding magnetism in a material can be inferred from the magnetic excitation spectrum, and in this context, general calculations of the classical spinwave spectrum are often necessary. Beyond the simplest of lattices, however, it is difficult to numerically determine the full spinwave spectrum, due primarily to the non-linearity of the problem. In this talk, I will present MATLAB code, developed over the last few years at the University of Illinois, that calculates the dispersions of spinwave excitations out of an arbitrarily defined ordered spin system. The calculation assumes a standard Heisenberg exchange Hamiltonian with the incorporation of a single-ion anisotropy term which can be varied site-by-site and can also simulate the application of an applied field. An overview of the calculation method and the structure of the code will be given, with emphasis on its general applicability. Extensions to the code enable the simulation of both single-crystal and powder-averaged neutron scattering intensity patterns. As a specific example, I will present the calculated neutron scattering spectrum for powders of CoV<sub>2</sub>O<sub>4</sub>, where good agreement between the simulated and experimental data suggests a self-consistent picture of the low-temperature magnetism.

**5:06PM P6.00010 Unusual behaviour of thermal conductivity in vanadium dioxide across the metal-insulator transition<sup>1</sup>**, KEDAR HIPPALGAONKAR, Institute of Materials Research and Engineering, SANGWOOK LEE, CHANGHYUN KO, University of California, Berkeley, FAN YANG, Lawrence Berkeley National Lab, JOONKI SUH, KAI LIU, KEVIN WANG, XIANG ZHANG, CHRIS DAMES, JUNQIAO WU, University of California, Berkeley — In an electrically conductive solid, the Wiedemann-Franz (WF) law requires the electronic contribution to thermal conductivity to be proportional to the product of electrical conductivity and absolute temperature, where the ratio is the Lorenz number, typically not much different from the Sommerfeld value  $L_0 = 2.44 \times 10^{-8}$  W-ohm-K<sup>-2</sup> at room temperature. The WF law reflects a basic property of metals where charge and heat are both carried by the same quasiparticles that both experience elastic scattering. At temperatures below the Debye temperature, the WF law has been experimentally shown to be robust in conventional conductors, with violations theoretically predicted or experimentally observed in strongly correlated electron systems or Luttinger liquids. However, the experimentally observed violations are at very low temperatures. Here we report breakdown of the WF law in a strongly correlated metal, in which the electronic thermal conductivity and L nearly vanish at temperatures above room temperature, where the electronic thermal conductivity amounts to only <~5% of the value expected from the WF law.

<sup>1</sup>Unusual behaviour of thermal conductivity in vanadium dioxide across the metal-insulator transition

**5:18PM P6.00011 Effects of Paramagnetism and Electron Correlations on the Electronic Structure of MnO: *Ab Initio* Study**, SANGMOON YOON, KYOUNGSUK JIN, Seoul Natl Univ, SEOUNG-HUN KANG, Kyung Hee Univ, KI TAE NAM, MIYOUNG KIM, Seoul Natl Univ, YOUNG-KYUN KWON, Kyung Hee Univ — Manganese oxide nanoparticles have attracted a lot of attentions as a promising candidate for next-generation catalyst. Therefore, understanding the electronic structure of manganese oxide in room temperature is highly required for the rational design of catalysts. We study the effects of paramagnetism and electron correlations on the electronic structure of MnO using *ab initio* density functional theory. Spin configurations of paramagnetism are postulated as the ensemble average of various spin disorders. Each initial disordered spin configuration is randomly generated with two constraints on magnetic local moments. We first investigate the influence of magnetic ordering on the electronic structure of MnO using noncollinear spin calculations and find that the magnetic disorders make valence band maximum more delocalized. Moreover, we examine the role of electron correlations in the electronic structure of paramagnetic MnO using DFT+U calculations. Strong electron correlations modify not only the size of band gap but also the magnitude of local moments as in the antiferromagnetic MnO. Besides, the initialized spin disorder remains almost unchanged as electron correlation gets stronger. Furthermore, our results obtained by considering both strong electron correlation and paramagnetism confirm experimentally-observed oxygen K edge X-ray emission spectra <sup>[1]</sup> reflecting the feature of valence bands. <sup>[1]</sup> E. Z. Kurmaev et al., Phys. Rev. B. **77**, 165127 (2008).

## Wednesday, March 16, 2016 2:30PM - 5:30PM –

Session P7 DMP FIAP: Dopants and Defects in Semiconductors: Oxides 303 - Michael Stavola, Lehigh University

**2:30PM P7.00001 Magnetic resonance studies of the Mg acceptor in thick free-standing and thin-film GaN<sup>1</sup>**, MARY ELLEN ZVANUT, University of Alabama at Birmingham — Mg, the only effective p-type dopant for the nitrides, substitutes for Ga and forms an acceptor with a defect level of about 0.16 eV. The magnetic resonance of such a center should be highly anisotropic, yet early work employing both optically detected magnetic resonance (ODMR) and electron paramagnetic resonance (EPR) spectroscopies revealed a defect with a nearly isotropic g-tensor. The results were attributed to crystal fields caused by compensation and/or strain typical of the heteroepitaxially grown films. The theory was supported by observation of the expected highly anisotropic ODMR signature in homoepitaxially grown films in which dislocation-induced non-uniform strain and compensation are reduced. The talk will review EPR measurements of thin films and describe new work which takes advantage of the recently available thick free-standing GaN:Mg substrates grown by hydride vapor phase epitaxy (HVPE) and high nitrogen pressure solution growth (HNPS). Interestingly, the films and HVPE substrates exhibit characteristically different types of EPR signals, and no EPR response could be induced in the HNPS substrates, with or without illumination. In the heteroepitaxial films, a curious angular dependent line-shape is observed in addition to the nearly isotropic g-tensor characteristic of the Mg-related acceptor. On the other hand, the free-standing HVPE crystals reveal a clear signature of a highly anisotropic shallow acceptor center. Comparison with SIMS measurements implies a direct relation to the Mg impurity, and frequency-dependent EPR studies demonstrate the influence of the anisotropic crystal fields. Overall, the measurements of the thick free-standing crystals show that the Mg acceptor is strongly affected by the local environment.

<sup>1</sup>The ODMR was performed by Evan Glaser, NRL and the free-standing Mg-doped HVPE crystals were grown by Jacob Leach, Kyma Tech. The work at UAB is supported by NSF Grant No. DMR-1308446.

**3:06PM P7.00002 Unusual electronic phase transition in hydrogenated TiO<sub>2</sub> thin layer**, CHUNLEI YUE, JIN HU, XUE LIU, ZHIQIANG MAO, JIANG WEI, Tulane University — Hydrogenated TiO<sub>2</sub> has been studied intensively in recently years for its effectiveness of engineering band gap by introducing the hydrogen doping level close to the conduction band edge. Consequently, significant improvement of solar absorption efficiency has been achieved and has been successfully showcased in the photovoltaic and photocatalytic applications. Although the room temperature optical enhancement is fascinating, the comprehensive electronic properties of such hydrogenated TiO<sub>2</sub> have hardly been investigated. Here we report our electric transport measurement of hydrogenated TiO<sub>2</sub> thin layer in the temperature range from 400K to 3.5K. We observed a stabilized metallic behavior of hydrogenated TiO<sub>2</sub>, which persists down to 50K, and then a surprising transition to an insulating phase between 50K and 20K. Furthermore, the insulating phase of hydrogenated TiO<sub>2</sub> shows a photocurrent response up to 4 orders magnitude. We interpret the possible mechanism as the transition of O-H vibrational modes, which leads to the freezing of electrons donated by the intercalated hydrogen.

**3:18PM P7.00003 Dynamics of H<sub>i</sub><sup>+</sup> in Indium Oxide<sup>1</sup>**, W. B. FOWLER, M. STAVOLA, YING QIN, P. WEISER, WEIKAI YIN, Lehigh University — Studies of IR absorption[1] under uniaxial stress[2] and diffusion[3] of H<sub>i</sub><sup>+</sup> as well as the dynamics of positively charged muonium[4] in In<sub>2</sub>O<sub>3</sub> provide an experimental framework to understand these processes in detail. While the bixbyite structure[5] of In<sub>2</sub>O<sub>3</sub> has overall cubic symmetry, its remarkable internal asymmetries lead to a number of candidate locations for H<sub>i</sub><sup>+</sup>. Furthermore, the unique topology of In<sub>2</sub>O<sub>3</sub> leads to constraints on possible H diffusion paths. We have used the CRYSTAL06 code[6] with a hybridized DFT Hamiltonian to determine equilibrium positions and vibrational frequencies for possible sites for H<sub>i</sub><sup>+</sup> and have analyzed candidate diffusion paths and processes for H<sub>i</sub><sup>+</sup> and Mu<sup>+</sup>. [1] W. Yin *et al.*, Phys. Rev. B **91**, 075208 (2015). [2] P. Weiser *et al.*, this meeting. [3] Ying Qin *et al.*, this meeting. [4] B. B. Baker *et al.*, AIP Conf. Proc. **1583**, 323 (2014). [5] M. Marezio, Acta Crystallogr. **20**, 723 (1966). [6] R. Dovesi *et al.*, *Crystal06 User's Manual* (University of Torino, Torino, 2006).

<sup>1</sup>Supported by NSF grant DMR-1160756.

**3:30PM P7.00004 Gd-Doped BaSnO<sub>3</sub> Thin Films: High Mobility in a Magnetically-Doped Transparent Conducting Oxide<sup>1</sup>**, URUSA ALAAN, Stanford University, PADRAIC SHAFER, ALPHA N'DIAYE, ELKE ARENHOLZ, Lawrence Berkeley National Laboratory, YURI SUZUKI, Stanford University — It has recently been shown that when the perovskite-structure BaSnO<sub>3</sub> (BSO) is doped with La<sub>Ba</sub><sup>'</sup>, the result is a transparent conducting oxide with room-temperature electron mobilities that are much higher than conventional ternary oxides. The ability to achieve high carrier mobilities in BSO is promising for future perovskite-structure devices. We have used pulsed laser deposition to grow epitaxial thin films of Ba<sub>0.96</sub>Gd<sub>0.04</sub>SnO<sub>3</sub> (Gd:BSO) and Ba<sub>0.96</sub>La<sub>0.04</sub>SnO<sub>3</sub> (La:BSO) on (001) SrTiO<sub>3</sub> and (001) MgO substrates. At 300 K, Gd:BSO films have  $\rho \sim 2$  m $\Omega$ ·cm,  $\mu_e \sim 28$  cm<sup>2</sup>/V·s and  $n \sim 1.0 \times 10^{20}$  cm<sup>-3</sup>. At the same temperature, La:BSO films have  $\rho \sim 0.4$  m $\Omega$ ·cm,  $\mu_e \sim 58$  cm<sup>2</sup>/V·s and  $n \sim 2.5 \times 10^{20}$  cm<sup>-3</sup>. While La:BSO is diamagnetic, Gd:BSO is paramagnetic with a clear magnetic response that saturates at  $\sim 7\mu_B/\text{Gd}^{3+}$ , and a negative ordinary magnetoresistance at low temperatures. Like La:BSO, Gd:BSO is transparent and colorless in the visible regime. Thus, we have shown that Gd is good dopant for BSO in order to achieve transparency and metallicity that is coincident with a magnetic response.

<sup>1</sup>We acknowledge support from the Army Research Office under grant W911NF-14-1-0611, the U.S. Department of Energy under Contract No. DE-AC02-05CH11231, and the National Science Foundation Graduate Research Fellowship Program.

**3:42PM P7.00005 Links in Superconducting, ferroelectric & antiferrodistortive instabilities in pristine & ion implanted SrTiO<sub>3</sub> by studying JT lattice distortions, Cubic-Tetragonal phase transition, incoherent lattice fluctuations & Phonons using RBS-Ion Channeling, XPS & Raman Scattering.**, KALYAN SASMAL, VIKTOR HADJIEV, QUARK CHEN, WEI-KAN CHU, Texas Center for Superconductivity & Dept of Physics, University of Houston, TX, USA — Perovskite SrTiO<sub>3</sub> is quantum paraelectric. Cubic-tetragonal phase transition at 105K, driven by condensation of zone corner phonon involving rotation of oxygen octahedra. Jahn-Teller centers allows dynamical charge transfer & polaron-bipolaron formation. Dynamical covalency elicit structural instability in layered superconductor approach ferroelectric. MeV He<sup>+</sup> RBS-Axial Ion Channeling, ultrafast real-space probe of sub-picometre atomic displacement is used to probe JT effect & incoherent lattice fluctuations as a function of temperature in ion implanted STO lattice. Critical channeling angle  $\psi_c$  & ratio of minima of Angular ICh-RBS spectral yield  $\chi_{\min}$  for Sr & Ti sub lattices determine lattice distortion. Cr & Fe impurities mostly distort Ti sublattice. Displacements of Ti<sup>4+</sup> are calculated. Similar values of  $\psi_{1/2}$  for Sr sublattice indicates no displacement of Sr. Actually Cr/Fe located in Ti positions. JT Cr<sup>4+</sup>, Cr<sup>5+</sup> & Fe<sup>4+</sup> impurity could induce Raman-active localized oxygen vibrational mode, which doesn't involve motion of nearest Fe or Ti ions. Displacive phase transition provides direct evidence of changes with temperature in thermal vibrational amplitude of lattice atoms across structural phase transition. Interplay of ferroelectric, antiferrodistortive distortions & superconducting order are discussed.

**3:54PM P7.00006 Collapse of electrons to a donor cluster in SrTiO<sub>3</sub>**, HAN FU, KONSTANTIN REICH, BORIS SHKLOVSKII, University of Minnesota — It is known that when a nucleus has charge  $Ze$  where  $Z > 137$ , electrons collapse onto the nucleus resulting in a net charge  $Z_n < Z$ . This effect is due to the relativistic dispersion law. Here a similar effect is found for a donor cluster in SrTiO<sub>3</sub> (STO), but with a different origin (see Phys. Rev. B 92, 035204 (2015)). At low temperatures, STO has an enormously large dielectric constant and the nonlinear dielectric response becomes dominant when the electric field is still small. This leads to the collapse of electrons into a charged spherical donor cluster with radius  $R$  when its total charge number  $Z$  exceeds a critical value  $Z_c \simeq R/a$  where  $a$  is the lattice constant. The net charge  $Z_n e$  grows with  $Z$  until  $Z$  exceeds  $Z^* \simeq (R/a)^{9/7}$ . After this point, the charge of the compact core  $Z_n$  remains  $\simeq Z^*$ , while the rest  $Z^*$  electrons form a sparse Thomas-Fermi electron atmosphere around it. We show that the thermal ionization of such two-scale atoms easily strips the outer atmosphere while the inner core remains preserved. We extend our results to the case of long cylindrical clusters. We discuss how our predictions can be tested by measuring conductivity of chain of discs of charge on the STO surface.

**4:06PM P7.00007 Point defects and band alignment in strontium cerate<sup>1</sup>**, MICHAEL SWIFT, CHRIS G. VAN DE WALLE, Univ of California - Santa Barbara — Strontium cerate (SrCeO<sub>3</sub>) is a well-known ionic conductor of both hydrogen and oxygen. In applications, it is frequently doped (for instance with yttrium or neodymium) to increase stability and promote diffusion. However, the microscopic effects of doping and native defects are not fully understood. Building on previous computational work in barium cerate (BaCeO<sub>3</sub>), we use density functional theory with a hybrid functional to study impurities, electronic structure, and band alignments in these systems. We establish trends that we expect to hold across the perovskite cerates. We also discuss the alignment of the thermodynamic charge-state transition levels of hydrogen, and applications to this class of materials.

<sup>1</sup>This work was supported by DOE.

**4:18PM P7.00008 Ferromagnetism in ZnO doped with alkaline elements**, YIREN WANG, JINGYUAN PIAO, GUOZHONG XIN, Univ of New South Wales, YUNHAO LU, Zhejiang University, ZHIMIN AO, University of Technology Sydney, NINA BAO, JUN DING, National University of Singapore, SEAN LI, JIABAO YI, Univ of New South Wales — We have observed room temperature ferromagnetism (RTFM) in ZnO doped with alkaline elements. Using first-principles calculations we found the magnetization in these systems is originated from the O2p hole states around Zn vacancies. Calculations indicate that the formation energy of Zn vacancies alone is rather high while further investigation indicates the formation can be much stabilized by the alkaline dopants in the form of defect complexes. By calculating the formation energy of concerned defects and complexes, we found the role of the dopants that under a certain doping concentration: Zn vacancy, substitutional and interstitial dopants can form a defect complex, which can lower formation energy, therefore stabilizing Zn vacancies. Moreover K dopants have shown unique functions on the ferromagnetism since the substitutional K can induce magnetic moments to the system by forming partial zinc vacancy via lattice distortion. Hence K doped ZnO can be magnetic at low doping concentrations. Experimentally, Li, Na doped ZnO films and K doped ZnO nanorods with different doping levels are synthesized, RTFM can be observed in all these systems. The magnetization is found to be greatly influenced by the doping concentrations. The experimental results have shown good consistence with our theoretical calculations. Our studies can inspire the defect induced ferromagnetism as a new route for the fabrication of new diluted magnetic semiconductors.

**4:30PM P7.00009 Oxygen vacancies in amorphous-Ta<sub>2</sub>O<sub>5</sub> from first-principles calculations<sup>1</sup>**, JIHANG LEE, EMMANOUIL KIOUPAKIS, Materials Science and Engineering, University of Michigan, WEI LU, Electrical Engineering and Computer Science, University of Michigan — Oxygen vacancies are thought to play a crucial role in the electrical and optical properties of tantalum pentoxide (Ta<sub>2</sub>O<sub>5</sub>) devices. Even though numerous experimental studies on oxygen vacancies in Ta<sub>2</sub>O<sub>5</sub> exist, experimentally detected defects are ambiguously identified due to the absence of an accurate and conclusive theoretical analysis. We investigate oxygen vacancies in amorphous Ta<sub>2</sub>O<sub>5</sub> with first-principles calculations based on hybrid density functional theory. The calculated thermodynamic and optical transition levels of stable oxygen vacancies are in good agreement with measured values from a variety of experimental methods, providing conclusive clues for the identification of the defect states observed in experiments. We determine the concentration of oxygen vacancies and their dominant oxidation state as a function of growth conditions. We analyze the characteristics of extra electrons introduced by donor-like oxygen vacancies, which include the formation of polarons. Our results provide insight into the fundamental properties of oxygen vacancies in Ta<sub>2</sub>O<sub>5</sub>, which is essential to controlling the properties of films and optimize the performance of devices.

<sup>1</sup>This research was supported by the AFOSR through MURI grant FA9550-12-1-0038 and the National Science Foundation CAREER award through Grant No. DMR-1254314. Computational resources were provided by the DOE NERSC facility.

**4:42PM P7.00010 Charge storage in oxygen deficient phases of TiO<sub>2</sub>: defect Physics without defects<sup>1</sup>**, A. C. M. PADILHA, Univ. Federal do ABC, Santo Andre, SP, Brazil, H. RAEBIGER, Yokohama Natl Univ., Yokohama, Japan, A. R. ROCHA, Univ. Est. Paulista, S SP, Brazil, G. M. DALPIAN, Univ. Federal do ABC, Santo Andre, Brazil — Defects in semiconductors can exhibit multiple charge states, which can be used for charge storage applications. Here we consider such charge storage in a series of oxygen deficient phases of TiO<sub>2</sub>, known as Magnli phases. These Ti<sub>n</sub>O<sub>2n-1</sub> Magnli phases present well-defined crystalline structures, i. e., their deviation from stoichiometry is accommodated by changes in space group as opposed to point defects. We show that these phases exhibit intermediate bands with the same electronic transitions akin to interstitial Ti defect levels in TiO<sub>2</sub>-rutile. Thus, the Magnli phases behave as if they contained a very large pseudo-defect density:  $\frac{1}{2}$  per formula unit Ti<sub>n</sub>O<sub>2n-1</sub>. Depending on the Fermi Energy the whole material will become charged. These crystals are natural charge storage materials with a storage capacity that rivals the best known supercapacitors.

<sup>1</sup>We thank financial support from FAPESP and CNPq.

**4:54PM P7.00011 Influence of the “second gap” on the optical absorption of transparent conducting oxides**, VIET-ANH HA, DAVID WAROQUIERS, GIAN-MARCO RIGNANESE, GEOFFROY HAUTIER, Institut de la matière condensée et des nanosciences (IMCN), Université catholique de Louvain, Louvain-la-Neuve 1348, Belgium — Transparent conducting oxides (TCOs) are critical to many technologies (e.g., thin-film solar cells, flat-panel displays or organic light-emitting diodes). TCOs are heavily doped (*n* or *p*-type) oxides that satisfy many design criteria such as high transparency to visible light (i.e., a band gap  $> 3$  eV), high concentration and mobility of carriers (leading to high conductivity), ... In such (highly doped) systems, optical transitions from the conduction band minimum to higher energy bands in *n*-type or from lower energy bands to the valence band maximum in *p*-type are possible and can degrade transparency. In fact, it has been claimed that a high energy ( $> 3$  eV) for any of these transitions made possible by doping, commonly referred as a high “second gap”, is a necessary design criterion for high performance TCOs. Here, we study the influence of this second gap on the transparency of doped TCOs by using *ab initio* calculations within the random phase approximation (RPA) for several well-known *p*-type and *n*-type TCOs. Our work highlights how the second gap affects the transparency of doped TCOs, shining light on more accurate design criteria for high performance TCOs.

**5:06PM P7.00012 Small polarons and point defects in  $\text{LaFeO}_3$** , ZHEN ZHU, HARTWIN PEELAERS, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — The proton-conductive perovskite-type  $\text{LaFeO}_3$  is a promising negative-electrode material for Ni/metal-hydride (Ni-MH) batteries. It has a discharge capacity up to  $530 \text{ mAhg}^{-1}$  at 333 K, which is significantly higher than commercialized  $\text{AB}_5$ -type alloys. To elucidate the underlying mechanism of this performance, we have investigated the structural and electronic properties of bulk  $\text{LaFeO}_3$ , as well as the effect of point defects, using hybrid density functional methods.  $\text{LaFeO}_3$  is antiferromagnetic in the ground state with a band gap of 3.54 eV. Small hole and electron polarons can form through self- or point-defect-assisted trapping. We find that La vacancies and Sr substitutional on La sites are shallow acceptors with the induced holes trapped as small polarons, while O and Fe vacancies are deep defect centers. Hydrogen interstitials behave like shallow donors, with the donor electrons localized on nearby iron sites as electron polarons. With a large trapping energy, these polarons can act as electron or hole traps and affect the electrical performance of  $\text{LaFeO}_3$  as the negative electrode for Ni-MH batteries. We acknowledge DOE for financial support.

**5:18PM P7.00013 Time-resolved photoluminescence of  $\text{SiO}_x$  encapsulated  $\text{Si}^1$** , SEREF KALEM, Tubitak-Bilgem, AMAL HANNAS, TOMAS STERMAN, VILLY SUNDSTRM, Lund Laser Center, University of Lund, Sweden — Silicon and its oxide  $\text{SiO}_x$  offer a number of exciting electrical and optical properties originating from defects and size reduction enabling engineering new electronic devices including resistive switching memories. Here we present the results of photoluminescence dynamics relevant to defects and quantum confinement effects. Time-resolved luminescence at room temperature exhibits an ultrafast decay component of less than 10 ps at around 480 nm and a slower component of around 60 ps as measured by streak camera. Red shift at the initial stages of the blue luminescence decay confirms the presence of a charge transfer to long lived states. Time-correlated single photon counting measurements revealed a life-time of about 5 ns for these states. The same quantum structures emit in near infrared close to optical communication wavelengths. Nature of the emission is described and modeling is provided for the luminescence dynamics. The electrical characteristics of metal-oxide-semiconductor devices were correlated with the optical and vibrational measurement results in order to have better insight into the switching mechanisms in such resistive devices as possible next generation RAM memory elements.

<sup>1</sup>"This work was supported by ENIAC Joint Undertaking and Laser-Lab Europe"

## Wednesday, March 16, 2016 2:30PM - 5:30PM – Session P8 DCMP DMP: Superconductivity: Proximity Effects and SN Junctions I 304 -

**2:30PM P8.00001 Anisotropic Suppression of Superconductivity on  $\text{Pb(111)}/\text{Mn}_5\text{Ge}_3/\text{Ge(111)}$** , HOWON KIM, Institute for Solid State Physics, The Univ. of Tokyo, YUKI NAGAI, CCSE, Japan Atomic Energy Agency, TAKEO KATO, YUKIO HASEGAWA, Institute for Solid State Physics, The Univ. of Tokyo — When a superconductor comes in a good contact to non-superconducting materials, the superconducting pair correlation and its breaking penetrate each other from the interface. In particular, superconductor/ferromagnet(S/F) interface has been of great interests because of emergence of exotic superconducting (inverse) proximity effect on both sides. In spite of extensive efforts for the S/F interfaces, the experimental approach was limited because of difficulties in fabricating the high quality interface and probing it in the nanometer scales. Here, we studied superconductivity of  $\text{Pb(111)}$  layers which are formed on the ferromagnetic  $\text{Mn}_5\text{Ge}_3$  island structures grown on a  $\text{Ge(111)}$  substrate at  $T \sim 0.5 \text{ K}$ . From our spatially-resolved local tunneling spectra over the top surface of  $\text{Pb(111)}$  on the ferromagnetic islands, we found that the superconducting property above the magnetic island was strongly suppressed and that the suppression was laterally spread from the strongly suppressed area in an anisotropic manner. By considering the scattering and propagating behaviors of the broken cooper pairs at the fermi surface of  $\text{Pb(111)}$ , we calculate the local density of states at the top of the  $\text{Pb(111)}$  layer above the  $\text{Mn}_5\text{Ge}_3$  island, and found that the anisotropic suppression of superconductivity mainly due to the anisotropic shape of the fermi surface of Pb. Possible origins of anisotropic suppression of superconductivity will be discussed.

**2:42PM P8.00002 Spin-triplet superconducting proximity effect in  $\text{SrRuO}_3/\text{Sr}_2\text{RuO}_4$  hybrids**, MUHAMMAD SHAHBAZ ANWAR, Kyoto University, SEUNGRAN LEE, Seoul National University, R ISHIGURO, Tokyo University of Science, Y SUGIMOTO, Kyoto University, Y TANO, Tokyo University of Science, S. J. KANG, Y.J. SHIN, Seoul National University, SHINGO YONEZAWA, Kyoto University, H TAKAYANAGI, Tokyo University of Science, TAE WON NOH, Seoul National University, YOSHITERU MAENO, Kyoto University, YOSHITERU MAENO TEAM, TAE WON NOH TEAM, TAKAYANAGI COLLABORATION — Spin-triplet superconducting correlations can be induced into a ferromagnet (FM) out of a spin-singlet superconductor (SSC) via magnetic inhomogeneity at the SSC/FM interface. In this case, however, the proximity effect is not readily controllable because spins are quenched. In contrast, superconducting spintronics can be realized by using spin-triplet superconductors (TSCs) and FM hybrids. Theoretically, it has been predicted that spin-triplet proximity effect can be controlled by the relative orientations between the magnetization in the FM and the Cooper pair spin in TSC. We fabricate  $\text{Au(600-nm)}/\text{SrRuO}_3(15\text{-nm})/\text{Sr}_2\text{RuO}_4$  junctions by growing epitaxial  $\text{SrRuO}_3$  FM thin films on  $\text{Sr}_2\text{RuO}_4$  TSC single crystals. Differential conductance vs voltage shows the conductance enhancements with superconducting transitions at three different characteristic voltages. These three features can naturally be interpreted as originating from the SC gaps in bulk  $\text{Sr}_2\text{RuO}_4$  as well as at two distinct interfaces ( $\text{Au}/\text{SrRuO}_3$  and  $\text{SrRuO}_3/\text{Sr}_2\text{RuO}_4$ ). The effect of applied magnetic field reveals that the proximity effect is robust against the loss of magnetic inhomogeneity.

**2:54PM P8.00003 Waiting times of entangled electrons in normal-superconducting junctions**, DENIS CHEVALLIER, Univ of Basel, MATHIAS ALBERT, Univ of Nice Sophia-Antipolis, INLN, PIERRE DEVILLARD, Centre de Physique Thorique, Marseille — We consider a normal-superconducting junction in order to investigate the effect of new physical ingredients on waiting times. First, we study the interplay between Andreev and specular scattering at the interface on the distribution of waiting times of electrons or holes separately. In that case the distribution is not altered dramatically compared to the case of a single quantum channel with a quantum point contact since the interface acts as an Andreev mirror for holes. We then consider a fully entangled state originating from splitting of Cooper pairs at the interface and demonstrate a significant enhancement of the probability to detect two consecutive electrons in a short time interval. Finally, we discuss the electronic waiting time distribution in the more realistic situation of partial entanglement.

**3:06PM P8.00004 Measurements of the superconducting proximity effect in  $\text{Pd}/\text{Al}$  NS bilayers at GHz frequencies.**, ANI NERSISYAN, RICCARDO MANENTI, MICHAEL PETERER, EINAR MAGNUSSON, GIOVANNA TANCREDI, ANDREW PATTERSON, PETER LEEK, University of Oxford, Oxford, UK — The superconducting proximity effect, well known since the 1960s, describes superconductivity in the case of a superconductor contacted to a normal metal, and is typically studied experimentally using transport techniques such as tunneling spectroscopy [1-4]. Here we will present studies of the superconducting proximity effect in thin film palladium/aluminum NS bilayers using microwave frequency lumped element LC resonators. Measurements of the resonance frequency and quality factor as a function of temperature and film thickness reveal properties of the NS bilayers such as the critical temperature and penetration depth. Our results should be useful for understanding losses in superconducting quantum circuits that incorporate thin normal layers, and, in the particular case of Pd, should aid in design of hybrid superconducting quantum devices incorporating carbon nanotubes with high contact transparency [5]. [1] C. J. Adkins and B. W. Kingston, Phys. Rev 177, 777 (1969). [2] J. R. Toplicar and D. K. Finnemore, Phys. Rev. B 16, 2072 (1977). [3] A. Kastalsky, et. al., Phys. Rev. Lett. 64, 958 (1990). [4] S. Guéron, et. al., Phys. Rev. Lett. 77, 3025 (1996). [5] Y. Chai, et. al., IEEE Transactions on Electron Devices, 59, 1 (2012).

**3:18PM P8.00005 Electrostatic effects in semiconductor-superconductor heterostructures.** , PIYAPONG SITTHISON, TUDOR STANESCU, West Virginia University — We study the effects of an interface-induced bias on the charge distribution, proximity-induced superconducting gap, and spin-orbit coupling strength in semiconductor-superconductor hybrid structures. The effective bias potential is generated by the work function difference across the interface. We show that the size of the induced superconducting gap (relative to the bulk gap) depends on the geometry of the structure and, in addition, is controlled by two effective parameters: the work function difference and the effective semiconductor-superconductor coupling. The interface-induced bias also breaks inversion symmetry, which leads to a nonzero value of the Rashba spin orbit coupling. We systematically study the dependence of the induced gap and Rashba coupling strength on the geometry of the structure (e.g., the diameter of the wire) and the relevant effective parameters (i.e. work function difference and semiconductor-superconductor coupling strength).

**3:30PM P8.00006 Differential Conductance in Semiconductor-Superconductor Hybrid Structures** , JOHN STENGER, TUDOR STANESCU, West Virginia University — We construct a theory for calculating the differential conductance in semiconductor-superconductor hybrid structures that accounts for both the current carried by quasiparticles in the bulk superconductor and the contributions due to proximity effects induced in the semiconductor. Starting with a Blonder-Tinkham-Klapwijk (BTK) type approach, we show that the superconductor degrees of freedom can be conveniently integrated out and replaced by an interface 'Green function' determined by the properties of the superconductor and the original outgoing-wave boundary conditions corresponding to quasiparticle propagation. We find that the features present in the differential conductance are associated with both semiconductor and bulk superconductor spectral features, with a relative strength that depends on the parameters of the structure. We systematically investigate the dependence of the differential conductance on the parameters of the system, including coupling strength, semiconductor band occupancy, and barrier transparency, and correlate our findings with recent experimental measurements on proximity-coupled semiconductor wires.

**3:42PM P8.00007 Super-Hard induced gap in InSb nanowires** , JUN CHEN, PENG YU, Univ of Pittsburgh, MORA HOCEVAR, CEA, Grenoble, France, SBASTIEN PLISSARD, DIANA CAR, ERIK BAKKERS, Eindhoven University of Technology, the Netherlands, SERGEY FROLOV, Univ of Pittsburgh — In recent years, Majorana bound states were observed experimentally in InSb nanowire-superconductor hybrid devices, which manifested themselves as a zero-bias conductance peak (ZBP). However, there was still significant conductance inside the superconducting gap, which would smear sub-gap features. Moreover, fermionic states inside the gap would also break topological protection. Therefore, a hard gap is required in search of more deterministic signatures of Majorana bound states, and building up Majorana qubits. We report the observation of a hard induced gap in an InSb Josephson junction with an optimized superconducting contact recipe. The gap is resolved in magnetic field up to 2 Tesla, and demonstrates a peculiar kinked field dependence. In addition, we observed rich sub-gap features: Andreev levels appeared close to pinch off regime, while multiple Andreev reflection appeared in open regime.

**3:54PM P8.00008 Proximity semiconducting nanowire junctions from Josephson to quantum dot regimes** , KAVEH GHARAVI, GREGORY HOLLOWAY, JONATHAN BAUGH, Institute for Quantum Computing, University of Waterloo — Experimental low-temperature transport results are presented on proximity-effect Josephson junctions made from low bandgap III-V semiconductor nanowires contacted with Nb. Two regimes are explored in terms of the Nb/nanowire interface transparency  $t$ . (i) High  $t$  allows a supercurrent to flow across the junction with magnitude  $I_c$ , which can be modulated using the voltage  $V_g$  on a global back gate or a local gate. Relatively high values are obtained for the figure-of-merit parameter  $I_c R_N / (e\Delta) \sim 0.5$ , and  $t \sim 0.75$ , where  $R_N$  is the normal state resistance and  $\Delta$  the superconducting gap of the Nb leads. With the application of an axial magnetic field,  $I_c$  decays but exhibits oscillations before being fully suppressed. The period and amplitude of the oscillations depend on  $V_g$ . Possible explanations for this behaviour are presented, including Josephson interference of the orbital subbands in the nanowire. (ii) Lower transparency correlates with a spontaneous quantum dot (QD) formed in the nanowire channel. Pairs of Andreev Bound States (ABS) appear at energies  $|E| < \Delta$ , with one pair unexpectedly pinned at  $E = 0$  for a wide range of  $V_g$ . A description of the QD-ABS system beyond the Anderson model is presented to explain the latter results.

**4:06PM P8.00009 Metal organic chemical vapor deposition of core-shell InAs-Al nanowires for proximity-induced superconductivity**<sup>1</sup> , T. R. HARTKE, J. STEHLIK, J. R. PETTA, Department of Physics, Princeton University — The zero-bias conductance peaks observed in proximitized InSb nanowires have been interpreted as evidence of Majorana fermions.<sup>2</sup> However, these observations are complicated by the presence of a non-zero conductance throughout the gap, which has been termed a “soft-gap.” The characteristics of the gap can be improved by using MBE to epitaxially grow a superconducting aluminum shell around an InAs core.<sup>3</sup> Here we use metal organic chemical vapor deposition (MOCVD) to grow high quality InAs nanowires on predefined Au catalyst sites. An aluminum shell is deposited immediately after the InAs growth is terminated. The resulting core-shell nanowires are structurally and electrically characterized.

<sup>1</sup>Supported by the Gordon and Betty Moore Foundation's EPIQS Initiative through Grant No. GBMF4535.

<sup>2</sup>V. Mourik *et al.*, Science **336**, 1003 (2012).

<sup>3</sup>W. Chang *et al.*, Nature Nanotech. **10**, 232 (2015).

**4:18PM P8.00010 Superconducting gap closing and Zero-bias peak in InSb nanowire** , PENG YU, JUN CHEN, Department of Physics and Astronomy, University of Pittsburgh, MORA HOCEVAR, CEA, Grenoble, France, SBASTIEN PLISSARD, DIANA CAR, ERIK BAKKERS, Eindhoven University of Technology, The Netherlands, SERGEY FROLOV, Department of Physics and Astronomy, University of Pittsburgh — In a 1D superconductor-nanowire-normal contact system, Majorana bound states are expected to appear after topological phase transition. Although there are many experiments reported possible zero-bias conductance peak from Majorana bound states, mapping out of the topological phase diagram is still missing. In our InSb nanowire hybrid devices, we observed possible superconducting gap closing and re-opening with magnetic field. These gap closings appear near conductance resonances which show some feature of 1D subband edges. Interestingly, zero-bias conductance peak appears inside the split regime of crossings at finite magnetic field. The magnetic field onset of the zero-bias peak can be tuned by gates underneath the superconductor, which may result from the changing of chemical potential.

**4:30PM P8.00011 Symmetry breaking in SNS junctions: edge transport and field asymmetries**<sup>1</sup> , HENRI SUOMINEN, FABRIZIO NICHELE, MORTEN KJAERGAARD, ASBJORN RASMUSSEN, JEROEN DANON, KARSTEN FLENSBERG, Center for Quantum Devices & Station Q Copenhagen, LEONID LEVITOV, Department of Physics, Massachusetts Institute of Technology, JAVAD SHABANI, Physics Department, City College of New York, CHRIS PALMSTROM, California NanoSystems Institute, University of California Santa Barbara, CHARLES MARCUS, Center for Quantum Devices & Station Q Copenhagen — We study magnetic diffraction patterns in a tunable superconductor-semiconductor-superconductor junction. By utilizing epitaxial growth of aluminum on InAs/InGaAs we obtain transparent junctions which display a conventional Fraunhofer pattern of the critical current as a function of applied perpendicular magnetic field,  $B_{\perp}$ . By studying the angular dependence of the critical current with applied magnetic fields in the plane of the junction we find a striking anisotropy. We attribute this effect to dephasing of Andreev states in the bulk of the junction, leading to SQUID like behavior when the magnetic field is applied parallel to current flow. Furthermore, in the presence of both in-plane and perpendicular fields, asymmetries in  $\pm B_{\perp}$  are observed. We suggest possible origins and discuss the role of spin-orbit and Zeeman physics together with a background disorder potential breaking spatial symmetries of the junction.

<sup>1</sup>Research supported by Microsoft Project Q, the Danish National Research Foundation and the NSF through the National Nanotechnology Infrastructure Network

**4:42PM P8.00012 Proximity induced Shiba states in an organic radical molecular junction<sup>1</sup>**, JOSHUA ISLAND, ROCCO GAUDENZI, ENRIQUE BURZURI, HERRE VAN DER ZANT, Delft Univ of Tech — Superconductors containing magnetic impurities lead to interesting phenomena derived from the interaction between Cooper pairing and Kondo screening. Here, we present measurements on proximity induced superconducting break-junctions hosting a magnetic impurity in the form of a neutral and stable, all organic radical molecule. Transport measurements reveal sub-gap excitations which are characteristic of a spin-induced, Yu-Shiba-Rusinov (Shiba) bound state due to the interaction of the radical's unpaired spin with a strongly coupled, proximity-induced superconductor. We show that by applying an external magnetic field to suppress the proximity induced superconductivity, a zero bias peak emerges signaling Kondo screening of the radical's unpaired spin coupled to normal leads. Our results show that Shiba states are a robust feature of the interaction between a magnetic impurity and a proximity induced superconducting junction.

<sup>1</sup>This work is supported by the Dutch Organization for Fundamental Research on Matter (NWO/OCW).

**4:54PM P8.00013 Observation of conductance doubling in an Andreev quantum point contact<sup>1</sup>**, M KJAERGAARD, F NICHELE, H SUOMINEN, Center for Quantum Devices & Station Q Copenhagen, M NOWAK, M WIMMER, A AKHMEROV, Kavli Institute for Nanoscience, TU Delft, J FOLK, Department of Physics and Astronomy, University of British Columbia, K FLENSBERG, Center for Quantum Devices & Station Q Copenhagen, J SHABANI, Physics Department, City College of New York, C PALMSTROM, California NanoSystems Institute, University of California Santa Barbara, C MARCUS, Center for Quantum Devices & Station Q Copenhagen — One route to study the non-Abelian nature of excitations in topological superconductors is to realise gateable two dimensional (2D) semiconducting systems, with spin-orbit coupling in proximity to an s-wave superconductor. Previous work on coupling 2D electron gases (2DEG) with superconductors has been hindered by a non-ideal interface and unstable gateability. We report measurements on a gateable 2DEG coupled to superconductors through a pristine interface, and use aluminum grown in situ epitaxially on an InGaAs/InAs electron gas. We demonstrate quantization in units of  $4e^2/h$  in a quantum point contact (QPC) in such hybrid systems. Operating the QPC as a tunnel probe, we observe a hard superconducting gap, overcoming the soft-gap problem in 2D superconductor/semiconductor systems. Our work paves way for a new and highly scalable system in which to pursue topological quantum information processing.

<sup>1</sup>Research supported by Microsoft Project Q and the Danish National Research Foundation

**5:06PM P8.00014 Origin of Mesoscopic Superconductivity at Cd<sub>3</sub>As<sub>2</sub> Point-Contacts**, LEENA AGGARWAL, ABHISHEK GOURAV SINHA, Indian Institute of Science Education and Research, Mohali (Punjab) India, GOHIL S. THAKUR, Indian Institute of Technology, New Delhi, India, ZEBA HAQUE, Indian Institute of Technology, New Delhi, ASHOK K. GANGULI, Indian Institute of Technology, New Delhi, Institute of Nano Science & Technology, Mohali, (Punjab) India, GOUTAM SHEET, Indian Institute of Science Education and Research, Mohali (Punjab) India — I will present our point-contact spectroscopy results on the nature and origin of superconductivity that is observed at the mesoscopic interfaces between the conventional metals and the 3-D Dirac semimetal Cd<sub>3</sub>As<sub>2</sub>. From our experiments with metallic tips of varying mechanical properties we show that the local superconducting phase does not emerge due to pressure. We show that quantum fluctuations may play a significant role in the emergence of such novel superconducting phase.

**5:18PM P8.00015 Two-dimensional epitaxial superconductor-semiconductor heterostructures: A platform for topological superconducting networks**, J. SHABANI, Physics Department, CCNY, M. KJAERGAARD, H. J. SUOMINEN, F. NICHELE, Center for Quantum Devices, Copenhagen, Y. KIM, UCSB, K. PAKROUSKI, Theoretical Physics, ETH Zurich, S. KRAEMER, UCSB, T. STANKEVIC, P. KROGSTROP, R. FEIDENHANS, Center for Quantum Devices, Copenhagen, R. M. LUTCHYN, C. NAYAK, Microsoft Research, Station Q, M. TROYER, Theoretical Physics, ETH Zurich, C. M. MARCUS, Center for Quantum Devices, Copenhagen, C. J. PALMSTROM, UCSB — Theory suggests that the interface between a one-dimensional semiconductor (Sm) with strong spin-orbit coupling and a superconductor (S) hosts Majorana modes with nontrivial topological properties. A key challenge in fabrication of such hybrid devices is forming highly transparent contacts between Sm and S. Recently, it has been shown that a near perfect interface and a highly transparent contact can be achieved using epitaxial growth of aluminum on InAs nanowires [1, 2]. In this work, we present the first two-dimensional epitaxial superconductor-semiconductor material system that can serve as a platform for topological superconductivity, and the search for quasiparticles such as Majorana zero modes that are predicted to obey non-abelian statistics. We show that our material system, Al-InAs, satisfies all the requirements necessary to reach into the topological superconducting regime by individual characterization of the semiconductor two dimensional electron system, superconductivity of Al and performance of S-Sm-S junctions [3].

## Wednesday, March 16, 2016 2:30PM - 5:30PM – Session P9 DCMP FIAP: Superlattices and Terahertz 305 -

**2:30PM P9.00001 Broadband Midwave Infrared InAs/GaSb Superlattice Light-Emitting Diodes**, RUSSELL RICKER, SYDNEY PROVENCE, University of Iowa, DENNIS NORTON, None, JOHN PRINEAS, THOMAS BOGGESE, University of Iowa — Broadband (3.0  $\mu\text{m}$  to 5.0  $\mu\text{m}$ ) emission is reported from InAs/GaSb superlattice light-emitting diodes grown via molecular beam epitaxy. Stacked active regions, each with a different emission wavelength, were connected with tunnel junctions, resulting in multiple emission wavelengths in a monolithic structure. Eight active regions provided eight overlapping emission spectra, simulating a broadband spectrum. Chips with mesas of sizes ranging from 24  $\mu\text{m}$   $\times$  24  $\mu\text{m}$  to 400  $\mu\text{m}$   $\times$  400  $\mu\text{m}$  were fabricated and wire bonded to a leadless chip carrier (LCC). The LCC was mounted in a liquid nitrogen cryostat. At low input currents, distinct peaks were observed at 3.3  $\mu\text{m}$ , 3.6  $\mu\text{m}$ , 3.9  $\mu\text{m}$ , 4.2  $\mu\text{m}$ , 4.5  $\mu\text{m}$ , 4.9  $\mu\text{m}$ , and 5.3  $\mu\text{m}$ . At high input currents a continuous spectrum was observed with a peak near 3.8  $\mu\text{m}$  and with a full-width at half-maximum of 1.42  $\mu\text{m}$ . In quasi-continuous operation at 77 K, radiances exceeding 0.35 W/cm<sup>2</sup>-sr in a Lambertian profile were achieved. Current dependent electroluminescent spectra measured at liquid nitrogen temperatures demonstrate the blending of the various colors from each stage into one smooth spectrum at high currents.

**2:42PM P9.00002 Long Minority Carrier Lifetimes in InAs/InAsSb Type-II Superlattices<sup>1</sup>**, YIGIT AYTAC, University of Iowa, BENJAMIN OLSON, JIM K KIM, ERIC A SHANER, SAMUEL HAWKINS, JOHN KLEM, Sandia National Laboratories, MICHAEL FLATT, THOMAS F BOGGESE, University of Iowa, UNIVERSITY OF IOWA COLLABORATION, SANDIA NATIONAL LABORATORIES COLLABORATION — Three unintentionally doped MWIR InAs/InAsSb type-II superlattices (T2SLs) were designed and grown to have 15 % Sb content in their alloy layers. The individual layer thicknesses of InAs and InAsSb are systematically altered in configurations of 174/218, 87/109, and 65/82 (Å/Å) while the total absorber thickness is nominally 4  $\mu\text{m}$  and the bandgap is approximately 5.2  $\mu\text{m}$  for all the samples. A time- and temperature- dependent differential-transmission technique was used to evaluate the carrier lifetime of each of the samples. Significantly long minority carrier (MC) lifetimes of ~14  $\mu\text{s}$  and ~19  $\mu\text{s}$  were obtained for the sample with 174 Å /218 Å InAs/InAsSb layer ratio at the temperatures of 77 K and 125 K, respectively. The defect energy levels of the InAs/InAsSb T2SLs reported here are determined to be ~300 25 meV relative to InAs valance band edge strained to GaSb. Additionally, the electron dominated Auger coefficients, C<sub>n</sub>, are obtained from the excess carrier density and temperature dependent recombination rate data. These coefficients are found to increase with decreasing individual layer thickness values from 3.4 to 29.9  $\times 10^{-27}$  cm<sup>6</sup>/s at 77 K.

<sup>1</sup>Administration under Contract No. DE-AC04-94AL85000. This research was funded by the U.S. Government.

**2:54PM P9.00003 Towards the design of high performance IR photonics: Optical analysis of textured gallium antimonide surfaces**, ELLA WASSWEILER, JOHN PRINEAS, FATIMA TOOR, University of Iowa — Gallium antimonide (GaSb) is used for fabrication of various optoelectronics devices, such as laser diodes, light emitting diodes, and photodetectors for the mid-infrared (MIR) wavelengths of  $3\text{ }\mu\text{m}$  to  $30\text{ }\mu\text{m}$ . Light extraction or collection efficiency of GaSb-based MIR devices can be significantly enhanced by surface texturing due to the density graded effect. However to the best of our knowledge no systematic study exists that analyzes the etch chemistries, surface textures and resultant reflectivity of GaSb surfaces. In this work we present the characterization of GaSb textures and how they correlate to reflectivity in the visible and MIR wavelengths. A parametric sweep of etch chemistries involving hydrofluoric acid (HF), hydrogen peroxide ( $\text{H}_2\text{O}_2$ ), and citric acid ( $\text{C}_4\text{H}_6\text{O}_6$ ) provide a variety of surface textures that correspond to low reflectivity in different wavelength regimes. The size of the surface features causes scattering in wavelengths of the same magnitude and as a result lower the reflectivity. In addition an analytical equation derived from our experimental data is presented that correlates reflectivity measurements to etch depth and wavelength, which can be used to design high performance IR photonic devices.

**3:06PM P9.00004 Bias activated dielectric response of excitons and excitonic Mott transition in quantum confined lasers structures.**, KANIKA BANSAL, AMIT BHUNIA, SHOUVIK DATTA, Department of Physics, IISER, Pune 411008, Maharashtra, India, MARZOOK S ALSHAMMARI, National Center of Nanotechnology, KACST, Riyadh 11442, Saudi Arabia, MOHAMED HENINI, School of Physics and Astronomy, University of Nottingham, Nottingham NG7 2RD, UK — In contrast to the widely reported optical techniques, there are hardly any investigations on corresponding electrical signatures of condensed matter physics of excitonic phenomena. We studied small signal steady state capacitance response in III-V materials based multi quantum well (AlGaInP) and MBE grown quantum dot (InGaAs) laser diodes to identify signatures of excitonic presence. Conductance activation by forward bias was probed using frequency dependent differential capacitance response ( $\text{d}C/\text{d}f$ ), which changes characteristically with the onset of light emission indicating the occurrence of negative activation energy. Our analysis shows that it is connected with a steady state population of exciton like bound states. Calculated average energy of this bound state matches well with the binding energy of weakly confined excitons in this type of structures. Further increase in charge injection decreases the differential capacitive response in AlGaInP based diodes, indicating a gradual Mott transition of excitonic states into electron hole plasma. This electrical description of excitonic Mott transition is fully supplemented by standard optical spectroscopic signatures of band gap renormalization and phase space filling effects.

**3:18PM P9.00005 Effective chiral description of an exciton-polariton superfluid in one and two dimensions**, MANAS KULKARNI, GERMAN KOLMAKOV, Department of Physics, New York City College of Technology, City University of New York — There has been remarkable experiments recently on capturing hydrodynamic features of exciton-polariton condensates in optical microcavities which have potential implications for quantum and optical computing and information technologies. We present an effective chiral description for such one and two dimensional systems. This description captures the fingerprints of hydrodynamics, namely, nonlinearity, dispersion and dissipation. The resulting chiral equation for the condensate perturbation wave dynamics is found to be of the generalized-KdV-type. We describe the phenomenon of polariton shock waves, solitons and defects in such systems. Our mapping is expected to have broad implications for other systems and can further help one in engineering a delicate balance between the pump and damping to produce stable optical signals propagating in polariton circuits.

**3:30PM P9.00006 Optical bandgap determination of ultrathin amorphous films and superlattices**, STYLIANOS SIONTAS, PEI LIU, Brown University, PAOLO LONGO, Gatan Inc., ALEXANDER ZASLAVSKY, DOMENICO PACIFICI, Brown University — Quantum size confinement effects determine the optical bandgap of ultrathin  $<5\text{ nm}$  amorphous films and superlattices. Although widely used, the standard experimental approach of combining normal-incidence reflectance and transmittance measurements with a single-pass absorption model may not always provide reliable results. By using ultra-thin amorphous germanium (a-Ge) layers down to  $d = 2\text{ nm}$  thickness as an experimental platform, we show that a multiple-reflection interference model is necessary to provide a more accurate extraction of the absorption coefficient. We also compare the two most frequently-used analytical models (Tauc and Cody) used to extract the optical bandgap from the measured absorption coefficient and clearly demonstrate that the Cody model provides a more reliable bandgap dependence on  $d$ . Finally, we apply our proposed method to experimentally determine the optical bandgap of a-Ge/SiO<sub>2</sub> superlattices with alternating layers of a Ge and SiO<sub>2</sub> ranging from 2 to 30 nm. Such superlattice structures enable additional control over the optical bandgap that may prove useful for the fabrication of high-efficiency photodetectors and solar cells in the optical and near-infrared spectral ranges.

**3:42PM P9.00007 Imaging the Electronic States of a Two-Dimensional Assembled Quasicrystal**, LAURA C. COLLINS, THOMAS G. WITTE, University of Notre Dame, ROCHELLE SILVERMAN, Virginia Tech, DAVID B. GREEN, KENJIRO K. GOMES, University of Notre Dame — The behavior of electrons in a periodic lattice is well understood, but how do electrons move in quasicrystals, which are ordered but aperiodic? We used scanning tunneling microscopy and atomic manipulation to assemble a quasicrystal based on the Penrose tiling and we carried out scanning tunneling spectroscopy to study its electronic properties. Carbon monoxide molecules were arranged on Cu(111) to form a potential landscape. This constrained the electrons in the two-dimensional surface states to move along the edges of a Penrose tiling. We measured the differential conductance maps to visualize the electronic density of states of the assembled quasicrystal. The statistical analysis of these maps has been used to characterize the localization of the electronic states.

**3:54PM P9.00008 Conductivity Dynamics of the Metal-to-Insulator Transition in Nickelate Superlattices.**, VERNER THORSMOLLE, JINGDI ZHANG, University of California San Diego, SRIMANTA MIDDEY, University of Arkansas, ELSA ABREU, Swiss Federal Institute of Technology Zurich, GUFENG ZHANG, University of California San Diego, JAK CHAKHALIAN, University of Arkansas, RICHARD AVERITT, University of California San Diego — Complexity in transition metal oxides can be understood as a delicate balance between competing interactions, which give rise to an energy landscape whose details are not easily discerned. An increasingly successful approach to tackle this problem is that of time resolved experiments, where the fundamental timescales of the system properties can be investigated through their response to appropriately chosen femtosecond photoexcitation. Ultrafast optical studies of the insulator-metal transition (IMT) in transition metal oxides are of particular interest in terms of dynamics and control. The perovskite nickelates (RE)NiO<sub>3</sub> have emerged as an important class of IMT materials, exhibiting rich phenomena across the rare earth (RE) series that includes La, Pr, Nd, Sm, Eu, Y, and Lu. Quite recently, the growth of nickelate superlattices (SL) has been achieved, offering a route to control the IMT. Here, we will present the results of optical-pump THz-probe investigations of the IMT dynamics in these novel heterostructures.

**4:06PM P9.00009 First-principles Study of Atomic Rearrangement in GeTe-Sb<sub>2</sub>Te<sub>3</sub> Superlattice**, YOUNG-SUN SONG, SEUNG-HOON JHI, Pohang Univ of Sci & Tech, CNPL TEAM — GeTe-Sb<sub>2</sub>Te<sub>3</sub> chalcogenide superlattices, known as interfacial phase change memories (iPCMs), have been claimed to outperform Ge-Sb-Te-based phase-change materials. Despite its great potential as next-generation non-volatile memory devices, we still lack clear knowledge of the phase change mechanism. According to a recent work, the phase change processes in iPCMs involve two-step atomic rearrangements of Ge-Te layers, but the detailed interatomic features still remain unresolved. In this work, we studied the nature of atomic layer rearrangements in iPCMs using first-principles calculations and the interatomic potential model. We used the climbing image nudged elastic band (CI-NEB) method to obtain the intermediate structures and energies during the rearrangement processes. Applying a simple interatomic potential model to in-between steps, we investigated the interatomic motion during the phase change process. We found that a few selected atomic pairs determine most the energy barrier and also the response to external pressures.

**4:18PM P9.00010 Experimental demonstration of Luneburg waveguides**, CHRISTOPHER JENSEN, WILLIAM ZIMMERMAN, DAVID LAHNEMAN, TODD ADAMS, THOMAS GRESOCK, KATHRYN ZANDER, VERA SMOLYANINOVA, Towson University, IGOR SMOLYANINOV, University of Maryland — Transformation optics (TO) gives rise to numerous unusual optical devices, such as novel metamaterial lenses and invisibility cloaks. However, it is very difficult to create metamaterials with low-loss broadband performance, especially in the visible frequency range. In our TO devices we use metal/dielectric waveguides to emulate metamaterial properties [1]. Here we report the first experimental realization of TO Luneburg waveguides [2]. The individual Luneburg lenses in the fabricated design are based on lithographically defined metal/dielectric waveguides. We have studied wavelength and polarization dependent performance of the waveguides. Adiabatic variations of the waveguide shape enable control of the effective refractive index experienced by the TM light propagating inside the waveguide. Our experimental designs appear to be broadband, which has been verified in the 480-633 nm range. These novel optical devices considerably extend our ability to control light on sub-micrometer scales. [1]. V.N. Smolyaninova, et al., Phys. Rev. B 87, 075406 (2013); [2]. V.N. Smolyaninova, et al., Photonics 2, 440 (2015). This research was supported by the NSF grant DMR-1104676.

**4:30PM P9.00011 Terahertz radiation-induced sub-cycle field electron emission across a split-gap dipole antenna**<sup>1</sup>, JINGDI ZHANG, Department of Physics, University of California, San Diego, XIAO GUANG ZHAO, KEBIN FAN, XIAONING WANG, Department of Mechanical Engineering, Boston University, GU-FENG ZHANG, Department of Physics, University of California, San Diego, KUN GENG, Department of Physics, Boston University, XIN ZHANG, Department of Mechanical Engineering, Boston University, RICHARD D. AVERITT, Department of Physics, University of California, San Diego — We use intense terahertz pulses to excite the resonant mode (0.6THz) of a micro-fabricated dipole antenna with a vacuum gap. The dipole antenna structure enhances the peak amplitude of the in-gap THz electric field by a factor of ~170. Above an in-gap E-field threshold amplitude of ~10 MVcm<sup>-1</sup>, THz-induced field electron emission is observed (TIFEE) as indicated by the field-induced electric current across the dipole antenna gap. Field emission occurs within a fraction of the driving THz period. Our analysis of the current (I) and incident electric field (E) is in agreement with a Millikan-Lauritsen analysis where log (I) exhibits a linear dependence on 1/E. Numerical estimates indicate that the electrons are accelerated to a value of approximately one tenth of the speed of light. (arXiv: 1508.04737)

<sup>1</sup>We acknowledge support from DOE-BES No. DE-FG02-09ER46643 and NSF No. ECCS-1309835

**4:42PM P9.00012 Fabrication of THz Sensor with Metamaterial Absorber**<sup>1</sup>, HUGO GONZALEZ, Naval Postgraduate School, FABIO ALVES, Alion Science and Technology, GAMANI KARUNASIRI, Naval Postgraduate School — The terahertz (THz) portion of the electromagnetic spectrum (0.1-10 THz) has not been fully utilized due to the lack of sensitive detectors. Real-time imaging in this spectral range has been demonstrated using uncooled infrared microbolometer cameras and external illumination provided by quantum cascade laser (QCL) based THz sources. However, the microbolometer pixels in the cameras have not been optimized to achieve high sensitivity in THz frequencies. Recently, we have developed a highly sensitive micromechanical THz sensor employing bi-material effect with an integrated metamaterial absorber tuned to the THz frequency of interest. The use of bi-material structures causes deflection on the sensor to as the absorbed THz radiation increases its temperature, which can be monitored optically by reflecting a light beam. This approach eliminates the integration of readout electronics needed in microbolometers. The absorption of THz by metamaterial can be tailored by controlling geometrical parameters. The sensors can be fabricated using conventional microelectronic materials and incorporated into pixels to form focal plane arrays (FPAs). In this presentation, characterization and readout of a THz sensor with integrated metamaterial structure will be described.

<sup>1</sup>Supported by DoD

**4:54PM P9.00013 Nonperiodic metallic gratings transparent for broadband terahertz waves**, REN-HAO FAN, XIAO-PING REN, RU-WEN PENG, Nanjing University, XIAN-RONG HUANG, Argonne National Laboratory, MU WANG, Nanjing University — Recently, we demonstrate both theoretically and experimentally that nonperiodic metallic gratings can become transparent for broadband terahertz waves. Quasiperiodic and disordered metallic gratings effectively weaken and even eliminate Wood's anomalies, which are the diffraction-related characters of periodic gratings. Consequently, both the transparency bandwidth and transmission efficiency are significantly increased due to the structural aperiodicity. Furthermore, we show that for a specific light source, for example, a line source, a corresponding nonperiodic transparent grating can be also designed. We expect that our findings can be applied for transparent conducting panels, perfect white-beam polarizers, antireflective conducting solar cells, and beyond. References: X. P. Ren, R. H. Fan, R. W. Peng, X. R. Huang, D. H. Xu, Y. Zhou, and Mu Wang, Physical Review B, 91, 045111 (2015); R. H. Fan, R. W. Peng, X. R. Huang, J. Li, Y. Liu, Q. Hu, Mu. Wang, and X. Zhang, Advanced Materials, 24, 1980 (2012); and X. R. Huang, R. W. Peng, and R. H. Fan. Physical Review Letters, 105, 243901 (2010).

**5:06PM P9.00014 Tuning the Polarization State of Light over a Broad Frequency Range with Metasurfaces**, MU WANG, SHANG-CHI JIANG, ZHENG-HAN WANG, XIANG XIONG, RU-WEN PENG, Nanjing University, NANJING UNIVERSITY TEAM — Controlling the polarization state, the transmission direction and the phase of light within a confined space is an important issue in optics. By integrating metallic metastructure and dielectric interlayer, it is possible to realize the dispersion-free broadband device on sub-wavelength scale, where the strong response of the metallic structures helps to decrease the device size while the dielectric interlayer helps to eliminate the dispersion simultaneously in both the amplitude and the phase difference of the reflected/transmitted light. As an examples to apply this concept, a broadband quarter-wave plate and a half-wave plate are experimentally demonstrated. By carefully selecting the structural parameters, the polarization state of light can be freely tuned across a broad frequency range, and all of the polarization states on the Poincaré sphere can be realized dispersion free. Some contents of this talk can be found in the following references: [1] S.-C. Jiang, et al., *High-efficiency generation of circularly polarized light via symmetry-induced anomalous reflection*, **Physical Review B** 91, 125421 (2015), [2] S.-C. Jiang, et al., *Controlling the Polarization State of Light with a Dispersion-Free Metastructure*, **Physical Review X** 4, 021026 (2014), [3] X. Xiong, et al., *Metallic stereostructured layer: an approach for broadband polarization state manipulation*, **Applied Physics Letters** 105, 201105 (2014).

**5:18PM P9.00015 Freely-tunable broadband polarization rotator for terahertz waves**<sup>1</sup>, RU-WEN PENG, REN-HAO FAN, YU ZHOU, SHANG-CHI JIANG, XIANG XIONG, Nanjing University, XIAN-RONG HUANG, Argonne National Laboratory, MU WANG, Nanjing University — It is known that commercially-available terahertz (THz) emitters usually generate linearly polarized waves only along certain directions, but in practice, a polarization rotator that is capable of rotating the polarization of THz waves to any direction is particularly desirable and it will have various important applications. In this work, we demonstrate a freely tunable polarization rotator for broadband THz waves using a three-rotating-layer metallic grating structure, which can conveniently rotate the polarization of a linearly polarized THz wave to any desired direction with nearly perfect conversion efficiency. The device performance has been experimentally demonstrated by both THz transmission spectra and direct imaging. The polarization rotation originates from multi wave interference in the three-layer grating structure based on the scattering-matrix analysis. We can expect that this active broadband polarization rotator has wide applications in analytical chemistry, biology, communication technology, imaging, etc.. Reference: R. H. Fan, Y. Zhou, X. P. Ren, R. W. Peng, S. C. Jiang, D. H. Xu, X. Xiong, X. R. Huang, and Mu Wang, Advanced Materials 27,1201(2015).

<sup>1</sup>Freely-tunable broadband polarization rotator for terahertz waves

## Wednesday, March 16, 2016 2:30PM - 5:30PM –

Session P11 DMP: Correlations and Superconductivity in Fe chalcogenides II 307 - Makariy Tanatar, Ames Laboratory

**2:30PM P11.00001 BCS-BEC crossover physics in FeSe bulk superconductor<sup>1</sup>**, TAKASADA SHIBAUCHI, Department of Advanced Materials Science, University of Tokyo — The physics of the crossover between weak-coupling Bardeen-Cooper-Schrieffer (BCS) and strong-coupling Bose-Einstein-condensate (BEC) limits gives a unified framework of quantum bound (superfluid) states of interacting fermions. This crossover has been studied in the ultracold atomic systems, but is extremely difficult to be realized for electrons in solids. Through the superfluid response, transport, thermoelectric response [1], and quantum oscillations [2], we demonstrate that the Fermi energy of the bulk superconductor FeSe is extremely small, with the ratio of the gap to Fermi energy is of the order of unity, which qualifies FeSe to be deep inside the BCS-BEC crossover regime. Thus FeSe appears to be a key material to solve the longstanding issue in the crossover physics; the presence of preformed Cooper pairs giving rise to a pseudogap above the superconducting transition temperature  $T_c$ . We report experimental signatures of preformed Cooper pairing well above  $T_c = 8.5$  K in clean single crystals of FeSe. Our torque magnetometry reveals distinct diamagnetic signal below  $T^* \sim 20$  K indicating that the superconducting fluctuations above the transition temperature are strongly enhanced from the standard Gaussian theory. The transport and thermoelectric coefficients also exhibit distinct anomalies at  $\sim T^*$ , signaling a possible pseudogap formation. The multiband nature with the electron-hole compensation in FeSe may highlight a fundamentally new aspect of the BCS-BEC crossover physics. [1] S. Kasahara *et al.*, PNAS 111, 16309 (2014). [2] T. Terashima *et al.*, Phys. Rev. B 90, 144517 (2014); M. D. Watson *et al.*, Phys. Rev. Lett. 115, 027006 (2015).

<sup>1</sup>In collaboration with S. Kasahara, T. Yamashita, Y. Matsuda (Kyoto), Y. Mizukami (Tokyo), T. Wolf, F. Hardy, C. Meingast, H. v. Löhneysen (KIT), M. D. Watson, A. I. Coldea (Oxford), T. Terashima (NIMS), W. Knafo (Toulouse), T. Hanaguri (Riken).

**3:06PM P11.00002 Enhanced superconductivity in heavily electron doped surface layer of FeSe bulk crystal**, J.J. SEO, B.Y. KIM, Physics department, Yonsei University, B.S. KIM, Department of Physics and Astronomy, Seoul National University, J.K. JEONG, Physics department, Yonsei University, J.M. OK, J.S. KIM, Department of Physics, Pohang University of Science and Technology, J.D. DENLINGER, Advanced Light Source, Lawrence Berkeley National Laboratory, C. KIM, Department of Physics and Astronomy, Seoul National University, Y.K. KIM, Advanced Light Source, Lawrence Berkeley National Laboratory — The recording setting superconducting transition temperature of as high as 100 K discovered in 1 monolayer FeSe grown on SrTiO<sub>3</sub> immediately brought attention to the mechanism for the dramatically enhanced  $T_c$  from its original value of 7 K. At present, the two most popular views for the enhanced  $T_c$  are interfacial effect and excess electron with enhanced correlation strength. The issue is controversial and there are evidences supporting each view. Here, we report the observation of 20 K superconductivity in the electron doped surface layer mimics all the key spectroscopic aspects of the electronic structure of 1ML FeSe on STO but with a smaller superconducting gap opening of 4 meV. Our results clearly show that excess electron doping with enhanced correlation strength alone cannot induce the maximum  $T_c$ , which strongly suggests a need for additional interfacial effect.

**3:18PM P11.00003 Low temperature scanning tunneling microscopy and spectroscopy investigation of FeSe<sub>1- $\delta$</sub>  and FeSe<sub>1-x</sub>S<sub>x</sub> single crystals<sup>1</sup>**, S. A. MOORE, Department of Physics, Temple University, Philadelphia, PA 19122, J. CURTIS, Department of Physics, Temple University, Philadelphia, PA 19122 ; Department of Physics, Drexel University, Philadelphia, PA 19104, M. ABDEL-HAFIEZ, Center for High Pressure Science and Technology Advanced Research, Shanghai, 201203, China, O. S. VOLKOVA, A. N. VASILIEV, Low Temperature Physics and Superconductivity Department, Physics Faculty, M.V. Lomonosov Moscow State University, Moscow 119991, Russia, D. A. CHAREEV, Institute of Experimental Mineralogy, Russian Academy of Sciences, 142432 Chernogolovka, Moscow District, Russia, G. KARAPETROV, Department of Physics, Drexel University, Philadelphia, PA 19104, M. IAVARONE, Department of Physics, Temple University, Philadelphia, PA 19122 — Due to its relatively simple crystallographic structure, investigations into FeSe<sub>1- $\delta$</sub>  have held the promise to provide an avenue towards a better understanding of the mechanism of superconductivity in the iron-pnictides/chalcogenides and the relationship between nematicity and superconducting state. Here, we present low-temperature scanning tunneling microscopy and spectroscopy investigations of high purity FeSe<sub>1- $\delta$</sub>  and sulfur substituted FeSe<sub>1-x</sub>S<sub>x</sub> single crystals. Vortex core anisotropy and vortex matter in these systems will be discussed.

<sup>1</sup>Work at Temple University was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-SC0004556.

**3:30PM P11.00004 Thermal conductivity of the iron-based superconductor FeSe : Nodeless gap with strong two-band character**, PATRICK BOURGEOIS-HOPE, SVEN BADOUX, NICOLAS DOIRON-LEYRAUD, LOUIS TAILLEFER, University of Sherbrooke, Sherbrooke, Canada, SHUN CHI, RUIXING LIANG, WALTER HARDY, DOUG BONN, University of British Columbia, Vancouver, Canada — The thermal conductivity  $\kappa$  of the iron-based superconductor FeSe was measured at temperatures down to 50 mK in magnetic fields up to 17 T. In zero magnetic field, the residual linear term in the  $T = 0$  limit,  $\kappa_0/T$ , is vanishingly small. Application of a magnetic field  $H$  causes no increase in  $\kappa_0/T$  initially. Those two facts show that there are no zero-energy quasiparticles that carry heat and therefore no nodes in the superconducting gap of FeSe. The full field dependence of  $\kappa_0/T$  has the classic shape of a two-band superconductor, such as MgB<sub>2</sub>. It rises initially with a characteristic field  $H^* \simeq H_{c2}/25$ , and then more slowly up to  $H_{c2} = 14$  T. We interpret this in terms of a small gap  $\Delta_A \simeq \Delta_0/5$  on some part of the Fermi surface, with a large gap  $\Delta_B = \Delta_0$  in the region that controls  $H_{c2}$ .

**3:42PM P11.00005 Pressure-dependent upper critical field of FeSe superconductor<sup>1</sup>**, UDHARA KALUARACHCHI, Iowa State University/ Ames LabLaboratory, VALENTIN TAUFOR, Iowa State University/ Ames Laboratory, ANNA BÖHMER, Ames Laboratory, MAKARIY TANATAR, SERGEY BUD'KO, Iowa State University/ Ames Laboratory, VLADIMIR KOGAN, Ames Laboratory, RUSLAN PROZOROV, PAUL CANFIELD, Iowa State University/ Ames Laboratory — In FeSe, the superconducting transition temperature  $T_c$  ( $\approx 9$  K at ambient pressure) has a complicated pressure dependence with a local maximum near  $p_1 \approx 0.8$  GPa and a local minimum at  $p_2 \approx 1.2$  GPa. In this work, we study the upper critical field,  $H_{c2,c}(T)$ , of FeSe using c-axis resistivity measurements under hydrostatic pressure up to 1.56 GPa with the magnetic field  $H \parallel c$ . Application of both current and magnetic field along the same axis reduces the flux flow motion and give sharper transition in applied fields. We observe a non-monotonic evolution of the slope of  $H_{c2,c}(T)|_{T_c}$  with pressure, with changes around  $p_1$  and  $p_2$ . We employ two-band orbital  $H_{c2,c}$  calculation to show that the data can be explained using the Fermi velocities extracted from the recent quantum oscillations study [1] over the whole pressure range. [1] Terashima *et al.* arXiv:1510.01840v1 [cond-mat.supr-con] (2015)

<sup>1</sup>This work is supported by the US DOE, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

**3:54PM P11.00006 Microwave Conductivity Spectroscopy for Fe(Se,Te) Thin Films<sup>1</sup>**, FUYUKI NABESHIMA, KOSUKE NAGASAWA, DAISUKE ASAMI, YUICHI SAWADA, YOSHINORI IMAI, ATSUTAKA MAEDA, University of Tokyo — Iron chalcogenide superconductors Fe(Se,Te) have very small  $\epsilon_F$  and are considered to be in the BCS-BEC crossover regime[1]. Since Ginzburg number,  $G_i = (k_B T_c / \epsilon_F)^4$ , which is the relative temperature width of the superconducting fluctuation region, is large for materials in the BCS-BEC crossover regime, large superconducting fluctuations are expected in Fe(Se,Te). In order to investigate superconducting fluctuations in these materials we have performed microwave conductivity spectroscopy on Fe(Se,Te) thin films. Superfluid density of an Fe(Se,Te) film with  $T_c^{zero}=17$  K[2] took finite values above 25 K. This temperature is much higher than  $T_c$  estimated by the dc measurement, suggesting strong superconducting fluctuations in Fe(Se,Te). A dynamic scaling analysis of complex fluctuation conductivity revealed that the superconducting fluctuations of Fe(Se,Te) exhibit a 2-dimensional behavior, while BKT transition was not observed. We will also report on the thickness dependence and the Te content dependence of the superconducting fluctuation. [1] Y. Lubashevsky *et al.*, Nat. Phys. **8** (2012) 309. [2] Y. Imai *et al.*, PNAS **112** (2015) 1937.

<sup>1</sup>Partially supported by the Japan Society for the Promotion of Science (JSPS) Research Fellowship for Young Scientists and by JSPS KAKENHI Grant Numbers 15K17697.

**4:06PM P11.00007 Superconductivity and spin excitations in orbitally ordered FeSe<sup>1</sup>**, ANDREAS KREISEL, Niels Bohr Institute, Denmark, SHANTANU MUKHERJEE, Niels Bohr Institute, Denmark; State University of New York at Binghamton, USA, P. J. HIRSCHFELD, University of Florida, USA, B.M. ANDERSEN, Niels Bohr Institute, Denmark — We provide a band-structure with low-energy properties consistent with recent photoemission and quantum oscillations measurements on the Fe-based superconductor FeSe[1], including a mean-field like orbital ordering in the  $d_{xz}/d_{yz}$  channel, and show that this model also accounts for the temperature dependence of the measured Knight shift and the spin-relaxation rate[2]. An RPA calculation of the dynamical spin susceptibility yields spin excitations which are peaked at wave vector  $(\pi, 0)$  in the 1-Fe Brillouin zone, with a broad maximum at energies of order a few meV. Furthermore, the superconducting gap structure obtained from spin fluctuation theory exhibits nodes on the electron pockets, consistent with the 'V'-shaped density of states measured by tunneling spectroscopy on this material. The redistribution of spectral weight in the superconducting state creates a  $(\pi, 0)$  "neutron resonance" as seen in recent experiments[3]. Comparing to various experimental results, we give predictions for further studies. [1] S. Mukherjee, *et al.*, PRL **115**, 026402 (2015); A. Kresse, *et al.*, arXiv:1506.03593 [2] S.-H. Baek, *et al.*, Nat. Mater. **14**, 210 (2015); A.E. Böhmer, *et al.*, PRL **114**, 027001 (2015) [3] M.C. Rahn, *et al.*, PRB **91**, 180501 (2015); Q. Wang, *et al.*, arXiv:1502.07544

<sup>1</sup>A.K. and B.M.A. acknowledge financial support from a Lundbeckfond fellowship (Grant No. A9318). P.J.H. was partially supported by the Department of Energy under Grant No. DE-FG02-05ER46236.

**4:18PM P11.00008 Intercallation of  $\text{Li}_{1-x}\text{Fe}_x\text{O}_2$  in the superconducting FeSe**, DESPINA LOUCA, JUNJIE YANG, University of Virginia — The intercalation of  $\text{LiFeO}_2$  in the tetragonal lattice of the 8 K superconductor  $\text{Fe}_{1-y}\text{Se}$  leads to a great enhancement of the superconducting transition temperature,  $T_C \sim 43$  K, and to an antiferromagnetic transition at 8.5 K. While the  $\text{LiFeO}_2$  layer acts as a charge reservoir, its  $\text{Fe}^{3+}$  ion ( $3d^5$ ) is magnetic creating a magnetic buffer layer. Most recently, we developed a new synthesis method to control the Fe concentration in the intercalating layer as well as the filling ratio of the  $\text{Li}_{1-x}\text{Fe}_x\text{O}_2 : \text{FeSe}$  layers. Neutron scattering measurements were carried out on powder samples of  $(\text{Li}_{1-x}\text{Fe}_x\text{O}_2)_y\text{FeSe}$ . With the intercalation, no crystal structural transition from the  $P4/nmm$  symmetry occurs but the  $c$ -axis lattice constant expands substantially, evidence of the intercalation. At the same time, the tetrahedral FeSe layers remain intact with no compression or expansion and free of vacancies. Moreover, the intercalation along the  $c$ -axis although not uniform leads to a reduction in  $T_C$  when the ratio of  $\text{Li}_{1-x}\text{Fe}_x\text{O}_2 : \text{FeSe}$  layers is about 1 to 3. Our results also indicate that the amount of Fe in the  $\text{Li}_{1-x}\text{Fe}_x\text{O}_2$  layer has a direct correlation to the transition temperature as well.

**4:30PM P11.00009 The Dual Role of Fe Dopants in Enhancing Stability and Charge Transfer in  $(\text{Li}_{0.8}\text{Fe}_{0.2})\text{OHFeSe}$  Superconductors**, WEI CHEN, Harvard University; University of Science and Technology of China, CHANGGAN ZENG, University of Science and Technology of China, EFTHIMIOS KAXIRAS, Harvard University, ZHENYU ZHANG, University of Science and Technology of China — The recently discovered  $(\text{Li}_{0.8}\text{Fe}_{0.2})\text{OHFeSe}$  superconductor provides a new platform for exploiting the microscopic mechanisms of high- $T_C$  superconductivity in FeSe-derived systems. Using density functional theory calculations, we first show that substitution of Li by Fe not only significantly strengthens the attraction between the  $(\text{Li}_{0.8}\text{Fe}_{0.2})\text{OH}$  spacing layers and the FeSe superconducting layers along the  $c$  axis, but also minimizes the lattice mismatch between the two in the  $ab$  plane, both favorable for stabilizing the overall structure. Next we explore the electron injection into FeSe from the spacing layers, and unambiguously identify the  $\text{Fe}_{0.2}$  components to be the origin of the dramatically enhanced interlayer charge transfer. We further reveal that the system strongly favors collinear antiferromagnetic ordering in the FeSe layers, but the spacing layers can be either antiferromagnetic or ferromagnetic depending on the  $\text{Fe}_{0.2}$  spatial distribution. Based on these insights, we predict  $(\text{Li}_{0.8}\text{Co}_{0.2})\text{OHFeSe}$  to be structurally stable with even larger electron injection and potentially higher  $T_C$ .

**4:42PM P11.00010 Superconductivity in binary FeS single crystals**, DANIEL CAMPBELL, CHRIS ECKBERG, SHANTA SAHA, CHRIS BORG, XIUQUAN ZHOU, EFRAIN RODRIGUEZ, JOHNPierre PAGLIONE, Univ of Maryland-College Park — FeS is the third recently discovered member of the superconducting binary iron-chalcogenide series that includes the well-known FeSe and  $\text{FeSe}_{1-x}\text{Te}_x$  members. Grown via hydrothermal techniques, single crystals of FeS have been characterized using transport, thermodynamic and magnetic techniques. We will review experimental results and compare with the unconventional superconducting properties of the selenide and telluride counterparts.

**4:54PM P11.00011 High-pressure NMR Study of Magnetism and Superconductivity on FeSe Single Crystals**, WEIQIANG YU, PENGSHUAI WANG, WENHUA SONG, SHANSHAN SUN, YI CUI, TIANRUN LI, PING ZHOU, HECHANG LEI, Department of Physics, Renmin University of China, Beijing 100872, China — Bulk FeSe has a structure transition at  $T \sim 91$  K and a superconducting transition at  $T \sim 9.3$  K, but no magnetic ordering at the ambient pressure. With increasing pressure, the structure transition is suppressed, whereas a magnetic ordering emerges. This is in contrast to most iron arsenides, where the structure transition is usually accompanied by a stripe magnetic ordering. Here we report our high-pressure NMR study on high-quality FeSe single crystals. The spin fluctuations and the magnetic ordering observed by our measurements give fresh information for understanding the interplay among the structure transition, the superconductivity and the magnetism in bulk FeSe materials.

**5:06PM P11.00012 Cs vacancy ordering and properties of phase separated  $\text{Cs}_x\text{Fe}_{2-y}\text{Se}_2$ <sup>1</sup>**, OMAR CHMAISSEM, K.M. TADDEI, Physics - Northern Illinois University and Materials Science Division - Argonne National Lab, IL, S. ROSENKRANZ, R. OSBORN, H. CLAUS, M. STURZA, D.Y. CHUNG, Materials Science Division - ANL, M.G. KANATZIDIS, Chemistry, Northwestern University, IL, H.B. CAO, Quantum Condensed Matter Division, ORNL, TN — Iron-based selenides are among the most complex and least understood superconductors. At high temperature, a '122'-type structure with random iron vacancies undergoes a complex iron vacancy ordering scheme below  $\sim 500\text{K}$  causing the material to phase separate into  $\text{A}_2\text{Fe}_4\text{Se}_5$ , known as the 245 phase, and a minority A-site deficient and fully iron stoichiometric  $\text{A}_x\text{Fe}_2\text{Se}_2$  phase (122). At slightly lower temperatures, the material undergoes another transition with the Fe spins of the main '245' phase ordering into an exotic checkerboard-type magnetic structure with a large magnetic moment. The minority 122 phase is reported to either remain nonmagnetic or to become magnetic below  $\sim 200\text{K}$ . At temperatures below  $\sim 30\text{K}$ , the magnetic material becomes superconducting and the two states appear to coexist. I will present and discuss our recent synthesis and characterization of high quality  $\text{Cs}_x\text{Fe}_{2-y}\text{Se}_2$  single crystals and bulk samples with various Tc's that form a relatively large superconducting dome. I will discuss our findings of a previously unseen three dimensional cesium vacancy ordering in the low temperature 122 phase in addition to hosting superconductivity.

<sup>1</sup>At ANL, work supported by the US DOE Office of Science, MS&ED.

**5:18PM P11.00013 Effects of inversion symmetry breaking in monolayer FeSe**, JOSEPH O'HALLORAN, MINGXING CHEN, DANIEL AGTERBERG, MICHAEL WEINERT, Univ of Wisconsin, Milwaukee — In this talk, we will discuss the role of broken inversion symmetry due to a substrate on the electronic and magnetic correlated states of monolayer iron selenide (FeSe). We use the group theoretic method of invariants with first principles density functional theory (DFT) calculations to investigate differences between bulk and single layer superconducting and magnetic orders. We show that a spin vortex crystal phase is stabilized, and that two-gap superconductivity is stabilized (though the gaps may be of similar magnitude).

## Wednesday, March 16, 2016 2:30PM - 5:30PM –

Session P12 DPOLY DCOMP FIAP: Bridging Time and Length Scales in Polymers and Soft Materials: Computational Pathways to Accelerate the Lab to Fab Transition - Industry Day 308 - Mark Stevens, Sandia National Laboratories

**2:30PM P12.00001 Spanning From Atoms to Micrometers in Simulations of Contact, Adhesion and Friction<sup>1</sup>**, MARK ROBBINS, Johns Hopkins University — Improved understanding of the forces between realistic solid surfaces is needed to optimize adhesion and friction. Modeling these forces is challenging because they arise from interactions between atoms separated by less than a nanometer, but the number and spatial distribution of these contacting atoms depends on surface roughness and deformation on micrometer and larger scales. There are also strong scale effects in the role of elastic deformations along the surface. The talk will first describe a seamless Greens function (GF) method that allows a full treatment of elastic deformations and atomic contact for micrometer scale surfaces and multibody potentials. Next applications of the method to calculations of the contact area, contact stiffness, adhesion and friction for a range of geometries and interactions will be described. The results can be captured with simple analytic expressions and explain why most contacting surfaces do not adhere. Theoretical and experimental studies of single nanometer-scale asperities show that the frictional shear stress depends strongly on whether surfaces are commensurate. A large constant stress is obtained for identical, aligned crystalline surfaces, but the stress averages to zero in the more common case of incommensurate surfaces. The resulting ultralow friction is called superlubricity and is found in experiments and simulations of small contacts. Our simulations reveal dramatic changes in this behavior because different parts of the surface are able to advance independently as the contact radius increases towards micrometer scales. The friction between identical surfaces drops with increasing radius and then saturates at a low value. The force between incommensurate surfaces saturates at a similar value that can be related to the Peierls stress for dislocation motion at the interface. Studies of multiasperity contacts also show that incoherent motion along the interface can lead to pronounced changes in the macroscopic friction.

<sup>1</sup>This material is based on work supported by National Science Foundation Grant DMR-1411144.

**3:06PM P12.00002 Accelerating materials discovery through the development of polymer databases**, DEBRA AUDUS, Materials Science and Engineering Division, National Institute of Standards and Technology — Efficient materials discovery can be greatly aided by access to databases that tabulate material property measurements and that allow for the exploration of material-property relationships. Such databases are less prevalent for polymers than other materials such as metals, in part due to the variety of structures associated with a single polymer identifier. For example, polyethylene could be branched or linear; it could also have a narrow or broad molecular weight distribution. I will discuss initial efforts towards generating a polymer property database in collaboration with Prof. Juan de Pablo and colleagues at the University of Chicago. Specifically, we focused on tabulating the Flory-Huggins chi parameter, describing the miscibility of polymer blends, using a course-based approach coupled with specialty software. In the context of a class setting, the undergraduate students learned about the field of polymer physics and used the software to identify chi parameters and related quantities, such as the method of measurement, from previously identified articles from literature. Both successes and challenges of this approach are measured through metrics of the resulting database and feedback from the students.

**3:42PM P12.00003 Complex Suspension Rheology Using High Performance Computing**, DAVID HEINE, Corning, Incorporated — In processing advanced ceramic materials, the properties of the final product depend on the process conditions and the interactions between the materials at the scale of the individual particles. Along with general bulk properties, more subtle properties including particle orientation, segregation, and pore structure must be established during processing to achieve the desired functionality. Accomplishing this requires a thorough understanding of the mesoscale interactions and how they influence the macroscale behavior. We conduct a series of large scale simulations of highly filled polymer-nanoparticle composites as analogs of ceramic pastes and reveal how the ceramic particle and binder properties determine the structure and rheology of the bulk material. As with real ceramic pastes, particle shape and size distribution along with composition determine the shear modulus, extent of segregation, and degree of particle alignment. These factors are influenced by the binder through the rheology of the binder phase and the interaction between binder and particles. This talk presents the results of this study of polymer-nanoparticle composites along with a brief overview of research and development at Corning showing the similarities and differences between research in industry and academia.

#### **4:18PM P12.00004 Conduction and Narrow Escape in Dense, Disordered, Particulate-based Heterogeneous Materials**

JEREMY LECHMAN, Sandia National Laboratories — For optimal and reliable performance, many technological devices rely on complex, disordered heterogeneous or composite materials and their associated manufacturing processes. Examples include many powder and particulate-based materials found in phytotechnic devices for car airbags, electrodes in energy storage devices, and various advanced composite materials. Due to their technological importance and complex structure, these materials have been the subject of much research in a number of fields. Moreover, the advent of new manufacturing techniques based on powder bed and particulate process routes, the potential of functional nano-structured materials, and the additional recognition of persistent shortcomings in predicting reliable performance of high consequence applications; leading to ballooning costs of fielding and maintaining advanced technologies, should motivate renewed efforts in understanding, predicting and controlling these materials' fabrication and behavior. Our particular effort seeks to understand the link between the top-down control presented in specific non-equilibrium processes routes (i.e., manufacturing processes) and the variability and uncertainty of the end product performance. Our ultimate aim is to quantify the variability inherent in these constrained dynamical or random processes and to use it to optimize and predict resulting material properties/performance and to inform component design with precise margins. In fact, this raises a set of deep and broad-ranging issues that have been recognized and as touching the core of a major research challenge at Sandia National Laboratories. In this talk, we will give an overview of recent efforts to address aspects of this vision. In particular the case of conductive properties of packed particulate materials will be highlighted. Combining a number of existing approaches we will discuss new insights and potential directions for further development toward the stated goal. Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corporation, a Lockheed-Martin Company, for the U. S. Department of Energy's National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

#### **4:54PM P12.00005 Coarse-graining to the meso and continuum scales with molecular-dynamics-like models**

STEVE PLIMPTON, Sandia National Laboratories — Many engineering-scale problems that industry or the national labs try to address with particle-based simulations occur at length and time scales well beyond the most optimistic hopes of traditional coarse-graining methods for molecular dynamics (MD), which typically start at the atomic scale and build upward. However classical MD can be viewed as an engine for simulating particles at literally any length or time scale, depending on the models used for individual particles and their interactions. To illustrate I'll highlight several coarse-grained (CG) materials models, some of which are likely familiar to molecular-scale modelers, but others probably not. These include models for water droplet freezing on surfaces, dissipative particle dynamics (DPD) models of explosives where particles have internal state, CG models of nano or colloidal particles in solution, models for aspherical particles, Peridynamics models for fracture, and models of granular materials at the scale of industrial processing. All of these can be implemented as MD-style models for either soft or hard materials; in fact they are all part of our LAMMPS MD package, added either by our group or contributed by collaborators. Unlike most all-atom MD simulations, CG simulations at these scales often involve highly non-uniform particle densities. So I'll also discuss a load-balancing method we've implemented for these kinds of models, which can improve parallel efficiencies. From the physics point-of-view, these models may be viewed as non-traditional or ad hoc. But because they are MD-style simulations, there's an opportunity for physicists to add statistical mechanics rigor to individual models. Or, in keeping with a theme of this session, to devise methods that more accurately bridge models from one scale to the next.

### **Wednesday, March 16, 2016 2:30PM - 5:30PM –**

#### **Session P13 DMP: Mechanical Properties of 2D materials 309 -**

#### **2:30PM P13.00001 IUPAP Award: Ion transport in 2D materials**

WENZHONG BAO, Fudan University — Intercalation in 2D materials drastically influences both physical and chemical properties, which leads to a new degree of freedom for fundamental studies and expands the potential applications of 2D materials. In this talk, I will discuss our work in the past two years related to ion intercalation of 2D materials, including insertion of Li and Na ions in graphene and MoS<sub>2</sub>. We focused on both fundamental mechanism and potential application, e.g. we measured in-situ optical transmittance spectra and electrical transport properties of few-layer graphene (FLG) nanostructures upon electrochemical lithiation/delithiation. By observing a simultaneous increase of both optical transmittance and DC conductivity, strikingly different from other materials, we proposed its application as a next generation transparent electrode.

#### **3:06PM P13.00002 Tuning frictions between graphene layers via Li ion intercalation<sup>1</sup>**

AIJIANG LU, Donghua University, JIAYU WAN, TENG LI, LIANGBING HU, Univ of Maryland-College Park, UNIVERSITY OF MARYLAND, COLLEGE PARK TEAM — Graphite intercalated with Li ions are widely studied and applied in Li ion batteries. It was revealed in experiments that, the Li ion intercalation leads to a phase transition of the graphite with about 10% volume expansion. The increased interlayer distance should contribute to decrease the frictions between the graphene layers, but the Li ion intercalation would take an opposite effect. In order to show the total effect of the Li ion intercalation, we studied the frictions between graphene layers with and without lithiation, based on density functional theory (DFT). In a sandwich-like model, slipping of the middle sheet of the graphene was simulated. Displacements between layers were fixed and the other parts were relaxed, thus the energies were recorded to estimate the energy barriers accordingly. We found that the frictions between the graphene layers with the Li ion intercalation are higher than those without intercalation. The energy barrier appears correlated with the concentration of the intercalated ions. As the atomic ratio between lithium and carbon increases from 0 (no intercalation) to 1:6, the energy barriers increase from 0.01 eV/atom to 0.05 eV/atom or so. Such an interesting result indicates that, just via ion intercalation, we can effectively tune the friction between graphene layers.

<sup>1</sup>Tuning frictions between graphene layers via Li ion intercalation

#### **3:18PM P13.00003 Lithium Intercalation of Single-Layer Graphene / Boron Nitride Heterostructures**

SHU YANG FRANK ZHAO, Harvard University, GISELLE A. ELBAZ, Columbia University, CYNDIA YU, D. KWABENA BEDIAKO, Harvard University, YINSHENG GUO, Columbia University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, LOUIS BRUS, XAVIER ROY, Columbia University, PHILIP KIM, Harvard University — Graphene intercalate compounds form a new generation of graphene derivative systems where novel physical phenomena such as superconductivity and magnetism may emerge. Experimental realization of intercalated few-layer graphenes have been limited by harsh intercalation processes, often incompatible with mesoscopic device fabrication techniques. Using electrochemical methods, we demonstrate lithium intercalation of single and few-layer graphene encapsulated in hexagonal boron nitride (BN), where the BN simultaneously serves as a scaffold for the lithium atoms as well as protects the graphene from parasitic chemical reactions in the electrolyte. In addition, we developed techniques to monitor intercalation electronically. By performing in-situ Raman spectroscopy, we confirmed that the intercalated single layer graphene/BN heterostructure reached a Fermi energy in excess of 1.16eV, and corresponding Hall measurements showed a density in excess of  $7 \times 10^{13} \text{cm}^{-2}$ .

#### **3:30PM P13.00004 Slipping and friction at the interface between two-dimensional materials**

VIJAYASHREE PARSII SREENIVAS, RYAN NICHOLL, Vanderbilt University, KIRILL BOLOTIN, Vanderbilt University, Freie Universitt — Friction at the macroscopic scale is primarily due to the surface roughness while at the atomic scale it is governed by commensurability and environmental conditions. Here, we investigate slipping and friction at the interface between two dissimilar two-dimensional materials, such as graphene and monolayer molybdenum disulfide. Such a system provides a powerful platform to study frictional forces at the atomic scale as chemical nature of the interface and commensurability between the layers can be varied with ease. To carry out such a study, a monolayer of e.g. graphene is exfoliated onto a flexible substrate material – polypropylene – and clamped down by evaporating titanium to avoid slippage. A monolayer of e.g. MoS<sub>2</sub> is then transferred on top of graphene and the entire stack is strained using a four point bending apparatus. By measuring strain vs. bending via Raman spectroscopy, we detect slippage at graphene/MoS<sub>2</sub> interface and characterize frictional forces as a function of interface parameters.

### 3:42PM P13.00005 ABSTRACT WITHDRAWN —

**3:54PM P13.00006 Bilayer Graphene Electromechanical Systems**, ALEXANDRE CHAMPAGNE, Concordia University and Universit de Sherbrooke, MATTHEW STORMS, SERAP YIGEN, Concordia University, BERTRAND REULET, Universit de Sherbrooke — Bilayer graphene is an outstanding electromechanical system, and its electronic and mechanical properties, as well as their coupling, are widely tunable. To the best of our knowledge, simultaneous charge transport and mechanical spectroscopy (via RF mixing) has not been realized in bilayer graphene. We present data showing clear electromechanical resonances in three suspended bilayer devices whose length range from 1 to 2 microns. We first describe the low-temperature current annealing of the devices which is crucial to achieve the transconductance,  $I - V_G$ , necessary to implement a RF mixing detection method. We describe our RF mixing circuit and data. We measure clear mechanical resonances ranging in frequency from 50 to 140 MHz. We show that we can smoothly tune the resonance frequencies of our bilayer resonators with mechanical strain applied via a backgate voltage. We measure quality factors up to 4000. We briefly discuss the effects of the RF driving power on the dispersion of the mechanical resonance. We aim to use these high quality mechanical resonance as a mechanical sensor of the bilayer quantum Hall phase transitions. We show initial data of a bilayer mechanical resonance as a function of magnetic field and quantum Hall phase transitions.

**4:06PM P13.00007 Electro-vibronic Coupling Effects on "Intrinsic Friction" in Transition Metal Dichalcogenides<sup>1</sup>**, ANTONIO CAMMARATA, Czech Technical University in Prague, TOMAS POLCAR, Czech Technical University in Prague and University of Southampton — One of the main difficulties in understanding and predicting frictional response is the intrinsic complexity of highly non-equilibrium processes in any tribological contact, which include breaking and formation of multiple interatomic bonds between surfaces in relative motion. To understand the physical nature of the microscopic mechanism of friction and design new tribologic materials, we conducted a systematic quantum mechanic investigation at the atomic scale on prototypical Van der Waals MX<sub>2</sub> (M=Mo, W; X=S, Se, Te) Transition Metal Dichalcogenides under variable load. We combined the structural and dynamic information from group theoretical analysis and phonon band structure calculations with the characterisation of the electronic features using non-standard methods like orbital polarization and the recently formulated bond covalency and cophonicity analyses. We formulated guidelines on how to engineer macroscopic friction at nanoscale, and finally applied them to design a new Ti-doped MoS<sub>2</sub> phase. The formulated protocol can be promptly used for the design of new materials with diverse applications beyond tribology.

<sup>1</sup>This work has been done with the support of projects CZ.1.07/2.3.00/30.0034, CZ.1.05/1.1.00/02.0070 and LM2011033.

**4:18PM P13.00008 The positive piezoconductive effect in graphene**, KANG XU, Nanjing University, KE WANG, University of Science and Technology of China, WEI ZHAO, ERFU LIU, Nanjing University, WENZHONG BAO, MICHAEL S. FUHRER, University of Maryland, YAFEI REN, ZHENHUA QIAO, University of Science and Technology of China, BAIGENG WANG, DINGYU XING, FENG MIAO, Nanjing University — As the thinnest conductive and elastic material, graphene is expected to play a crucial role in post-Moore era. Besides applications on electronic devices, graphene has shown great potential for nano-electromechanical systems. While interlayer interactions play a key role in modifying the electronic structures of layered materials, no attention has been given to their impact on electromechanical properties. Here we report the positive piezoconductive effect observed in suspended bi- and multi-layer graphene. The effect is highly layer number dependent and shows the most pronounced response for tri-layer graphene. The effect, and its dependence on the layer number, can be understood as resulting from the strain-induced competition between interlayer coupling and intralayer transport, as confirmed by the numerical calculations based on the non-equilibrium Green's function method. Our results enrich the understanding of graphene and point to layer number as a powerful tool for tuning the electromechanical properties of graphene for future applications.

### 4:30PM P13.00009 ABSTRACT WITHDRAWN —

**4:42PM P13.00010 Mechanical Properties and Failure Mechanisms in Polycrystalline Graphene**, JOSEPH GONZALEZ, University of South Florida, ROMAIN PERRIOT, Los Alamos National Laboratory, IVAN OLEYNIK, University of South Florida — Large-scale growth of graphene using chemical vapor deposition produces polycrystalline material containing grain boundaries. Recent experiments demonstrate that polycrystalline graphene is nearly as strong as pristine. In this work, the mechanical properties of bi-crystal and polycrystalline graphene samples are investigated by simulating nano-indentation of a circular membrane using classical molecular dynamics and a novel Screened Environment Dependent Reactive Bond Order (SED-REBO) potential. The failure mechanisms and crack propagation in graphene samples containing grain boundaries are also discussed.

**4:54PM P13.00011 Highly Stretchable MoS<sub>2</sub> and Phosphorene Kirigami**, DAVID CAMPBELL, PAUL HANAKATA, HAROLD PARK, Boston University — Several recent works have shown how nanomesh and kirigami patterning can be used to increase the ductility of monolayer graphene and thin film electrodes, suggesting that this approach should be useful for other 2D materials. We have studied the effects of kirigami patterning on the mechanical properties of MoS<sub>2</sub> and phosphorene "monolayers," using classical molecular dynamics simulations. We have explored several different kirigami structures, focusing on two simple non-dimensional parameters found to be relevant in our previous study of graphene [1]. These parameters are related to the density of cuts and to the ratio of the overlapping cut length to the nanoribbon length. We found that these membranes, despite not having the single atomic layer planar structure of graphene, show a significantly enhanced ductility that can be understood in terms of the two geometric parameters. For instance, fracture strains of MoS<sub>2</sub> kirigami can be enhanced by a factor of six relative to pristine MoS<sub>2</sub> nanoribbons. Our findings suggest that the kirigami cuts are the key to changing the morphology of 2D membranes to allow out of plane deflection and to prevent early failure. [1] Zenan Qi, David K. Campbell, and Harold S. Park, Phys. Rev. B 90, 245437 (2014).

**5:06PM P13.00012 Modulated Nanoindentation (MoNI) – a novel characterization tool of two-dimensional materials and nanotubes<sup>1</sup>**, YANG GAO, CUNY Advanced Science Research Center, SUENNE KIM, Hanyang University, SI ZHOU, Georgia Institute of Technology, HSIANG-CHIH CHIU, National Taiwan Normal University, DANIEL NELIAS, Universit de Lyon, CNRS, INSA-Lyon, LaMCoS, CLAIRE BERGER, Institut Nel, Universit Grenoble Alpes-CNRS, WALT DE HEER, Georgia Institute of Technology, LAURA POLLONI, ROMAN SORDAN, L-NESS, Politecnico di Milano, CHRISTIAN KLINKE, University of Hamburg, ANGELO BONGIORNO, College of Staten Island, CUNY, ELISA RIEDO, CUNY Advanced Science Research Center — We report on a novel Atomic Force Microscopy (AFM) based technique with sub-angstrom vertical resolution – Modulated Nanoindentation (MoNI). MoNI has been applied to measure the radial elasticity of multi-walled nanotubes. Recently the interlayer coupling of two-dimensional materials (such as graphene and MoS<sub>2</sub>) characterized by strong in-plane bonds and weak interlayer interactions has been studied by MoNI combined with semi-analytical methods (SAM) and DFT calculations. The out-of-plane stiffness of varied 2D materials and its dependence on number of layers and intercalated water has been investigated in different environmental conditions. This non-destructive technique provides a new path to study the interlayer elastic coupling and the Van der Waals forces in few-layer-thick 2D materials, offering the possibility to understand how interlayer coupling is related to the electronic, phononic, and thermal properties of 2D materials.

<sup>1</sup>Y. Gao et al., Nature Materials 14, 714-720 (2015)

**5:18PM P13.00013 Coherent Generation of Photo-Thermo-Acoustic Wave from Graphene Sheets<sup>1</sup>**, YICHAO TIAN, Institute of Physics, CAS, HE TIAN, Tsinghua University, YANLING WU, LEILEI ZHU, Institute of Physics, CAS, LUQI TAO, Tsinghua University, WEI ZHANG, Institute of Physics, CAS, YI SHU, DAN XIE, YI YANG, Tsinghua University, ZHIYI WEI, XINGHUA LU, Institute of Physics, CAS, TIAN-LING REN, Tsinghua University, CHIH-KANG SHIH, Department of Physics, Texas University at Austin, JIMIN ZHAO, Institute of Physics, CAS — Many remarkable properties of graphene are derived from its large energy window for Dirac-like electronic states and have been explored for applications in electronics and photonics. In addition, strong electron-phonon interaction in graphene has led to efficient photo-thermo energy conversions, which has been harnessed for energy applications. By combining the wavelength independent absorption property and the efficient photo-thermo energy conversion, here we report a new type of applications in sound wave generation underlined by a photo-thermo-acoustic energy conversion mechanism. Most significantly, by utilizing ultrafast optical pulses, we demonstrate the ability to control the phase of sound waves generated by the photo-thermal-acoustic process. Our finding paves the way for new types of applications for graphene, such as remote non-contact speakers, optical-switching acoustic devices, etc.

<sup>1</sup>National Basic Research Program of China MOST (2012CB821402), External Cooperation Program of Chinese Academy of Sciences (GJHZ1403), and National Natural Science Foundation of China (11274372)

**Wednesday, March 16, 2016 2:30PM - 5:30PM –**  
**Session P14 FIP DCOMP: International Cooperative Efforts for Electronic Structure Methods**  
310 - Aldo Romero, West Virginia University

**2:30PM P14.00001 The European Theoretical Spectroscopy Facility: an illustration for the power of collective research**, LUCIA REINING, CNRS-Ecole Polytechnique — As researchers and citizens, we should contribute to facing the grand challenges of our epoch. It is important to work on problems such as climate change or limited resources. However, maybe the biggest challenge is to find ways to unite our forces and develop models of collaborative problem solving. This is mandatory to deal with complex problems, and it can boost efficiency in any case. Code development is just one example where a constructive and well-organized collaboration can take us much further than individual attempts. On the background of this general idea, we will analyze the impact of the European Theoretical Spectroscopy Facility (ETSF, [www.etsf.eu](http://www.etsf.eu)) on the day-to-day research of its members, on the theoretical and computational tools that are produced, and on a wider field of theoretical or experimental research. We will see that much can be learnt from this attempt to consider ideas in competition, with people in collaboration.

**3:06PM P14.00002 The ABINIT software project**, GIAN-MARCO RIGNANESE, Univ Catholique de Louvain — The ABINIT software project aims at providing the total energy, charge density and electronic structure of systems made of electrons and nuclei (molecules and periodic solids) thanks to a first-principle approach. The ground state properties are calculated in the framework of the Density-Functional Theory (DFT). The excited states properties are computed within the Many-Body Perturbation Theory (MBPT). Finally, the response properties are obtained from Density-Functional Perturbation Theory (DFPT). The ABINIT software project was started in 1997 as an open software project, without a definite goal, developed using several software engineering techniques to allow international collaboration of many different groups. The first publicly available version of ABINIT was released in December 2000 under the GNU GPL. The software has already been described in various articles [1-4]. The last stable version of the package (7.10.4) has now a 70 MBytes size, consisting in nearly 1400 files written in F90 (830000 lines) and including documentation, tutorials and more than one thousand tests. The code is developed by an always opened community (around fifty people) and it is used by more than a thousand individuals worldwide.

#### References

1. X. Gonze *et al.*, *Comp. Mat. Sci.* **25**, 478492 (2002).
2. X. Gonze *et al.*, *Z. Kristallogr.* **220**, 558562 (2005).
3. X. Gonze *et al.*, *Comput. Phys. Commun.* **180**, 2582-2615 (2009).
4. X. Gonze *et al.*, in preparation (2015).

**3:42PM P14.00003 The Road to Interoperable Simulation Software: Examples Using the Qbox Code<sup>1</sup>**, FRANCOIS GYGI, University of California Davis — The diversity of available simulation software implementing various methods—from atomistic classical molecular dynamics to quantum many-body perturbation theory—makes it highly desirable to couple these codes in a seamless fashion. We discuss the approach taken with the Qbox code to couple first-principles molecular dynamics with advanced sampling algorithms and with GW electronic structure calculations.  
<http://qboxcode.org>  
<http://www.quantum-simulation.org>

<sup>1</sup>Supported by DOE Office of Basic Energy Sciences

**4:18PM P14.00004 The CECAM Electronic Structure Library: community-driven development of software libraries for electronic structure simulations**, MICAEL OLIVEIRA, Universite de Liege — The CECAM Electronic Structure Library (ESL) is a community-driven effort to segregate shared pieces of software as libraries that could be contributed and used by the community. Besides allowing to share the burden of developing and maintaining complex pieces of software, these can also become a target for re-coding by software engineers as hardware evolves, ensuring that electronic structure codes remain at the forefront of HPC trends. In a series of workshops hosted at the CECAM HQ in Lausanne, the tools and infrastructure for the project were prepared, and the first contributions were included and made available online (<http://esl.cecam.org>). In this talk I will present the different aspects and aims of the ESL and how these can be useful for the electronic structure community.

**4:54PM P14.00005 The Yambo code: a comprehensive tool to perform ab-initio simulations of equilibrium and out-of-equilibrium properties<sup>1</sup>**, ANDREA MARINI, Istituto di Struttura della Materia of the National Research Council — Density functional theory and many-body perturbation theory methods (such as GW and Bethe-Salpeter equation) are standard approaches to the equilibrium ground and excited state properties of condensed matter systems, surfaces, molecules and other several kind of materials. At the same time ultra-fast optical spectroscopy is becoming a widely used and powerful tool for the observation of the out-of-equilibrium dynamical processes. In this case the theoretical tools (such as the Baym-Kadanoff equation) are well known but, only recently, have been merged with the ab-Initio approach. And, for this reason, highly parallel and efficient codes are lacking. Nevertheless, the combination of these two areas of research represents, for the ab-initio community, a challenging perspective as it requires the development of advanced theoretical, methodological and numerical tools. Yambo is a popular community software implementing the above methods using plane-waves and pseudo-potentials. Yambo is available to the community as open-source software, and oriented to high-performance computing. The Yambo project aims at making the simulation of these equilibrium and out-of-equilibrium complex processes available to a wide community of users. Indeed the code is used, in practice, in many countries and well beyond the European borders. Yambo is a member of the suite of codes of the MAX European Center of Excellence (Materials design at the exascale). It is also used by the user facilities of the European Spectroscopy Facility and of the NFFA European Center (nanoscience foundries & fine analysis). In this talk I will discuss some recent numerical and methodological developments that have been implemented in Yambo towards to exploitation of next generation HPC supercomputers. In particular, I will present the hybrid MPI+OpenMP parallelization and the specific case of the response function calculation. I will also discuss the future plans of the Yambo project and its potential use as tool for science dissemination, also in third world countries.

<sup>1</sup>ETSF, MAX European Center of Excellence and NFFA European Center

**Wednesday, March 16, 2016 2:30PM - 5:30PM –**

**Session P15 DMP: 2D Materials: Preparation and Characterization** 314 - Huili Xing, Cornell University

**2:30PM P15.00001 Electronic Transport Properties of New 2-D Materials GeH and NaSn<sub>2</sub>As<sub>2</sub><sup>1</sup>**, BIN HE, Department of Mechanical Engineering, the Ohio State University, Columbus, Ohio USA 43210, NICHOLAS CULTRARA, MAXX ARGUILLA, JOSHUA GOLDBERGER, Department of Chemistry and Biochemistry, the Ohio State University, Columbus, OH 43210, JOSEPH HEREMANS, Department of Mechanical Engineering, the Ohio State University, Columbus, Ohio USA 43210 — 2-D materials potentially have superior thermoelectric properties compared to traditional 3-D materials due to their layered structure. Here we present electrical and thermoelectric transport properties of 2 types of 2-D materials, GeH and NaSn<sub>2</sub>As<sub>2</sub>. GeH is a graphane analog which is prepared using chemical exfoliation of CaGe<sub>2</sub> crystals. Intrinsic GeH is proven to be a highly resistive material at room temperature. Resistance and Seebeck coefficient of Ga doped GeH are measured in a cryostat with a gating voltage varying from -100V to 100V. NaSn<sub>2</sub>As<sub>2</sub> is another 2-D system, with Na atom embedded between nearly-2D Sn-As layers. Unlike GeH, NaSn<sub>2</sub>As<sub>2</sub> is a metal based of Hall measurements, with p-type behavior, and with van der Pauw resistances on the order of 5mΩ/square. Thermoelectric transport properties of NaSn<sub>2</sub>As<sub>2</sub> will be reported.

<sup>1</sup>This work is support by the NSF EFRI-2DARE project EFRI-1433467

**2:42PM P15.00002 Microwave Assisted 2D Materials Exfoliation**, YANBIN WANG, Univ of Maryland — Two-dimensional materials have emerged as extremely important materials with applications ranging from energy and environmental science to electronics and biology. Here we report our discovery of a universal, ultrafast, green, solvo-thermal technology for producing excellent-quality, few-layered nanosheets in liquid phase from well-known 2D materials such as such hexagonal boron nitride (h-BN), graphite, and MoS<sub>2</sub>. We start by mixing the uniform bulk-layered material with a common organic solvent that matches its surface energy to reduce the van der Waals attractive interactions between the layers; next, the solutions are heated in a commercial microwave oven to overcome the energy barrier between bulk and few-layers states. We discovered the minutes-long rapid exfoliation process is highly temperature dependent, which requires precise thermal management to obtain high-quality inks. We hypothesize a possible mechanism of this proposed solvo-thermal process; our theory confirms the basis of this novel technique for exfoliation of high-quality, layered 2D materials by using an as yet unknown role of the solvent.

**2:54PM P15.00003 A *first principles* investigation of point defects in monolayer, few-layer, and bulk WS<sub>2</sub><sup>1</sup>**, WUN-FAN LI, CHANGMING FANG, MARJOLEIN DIJKSTRA, MARIJN A. VAN HUIS, Soft Condensed Matter, Debye Institute for Nanomaterials Science, Utrecht University, SOFT CONDENSED MATTER TEAM — We present the results of a systematic study of physics of point defects in 2D WS<sub>2</sub> materials conducted by means of density functional theory. First, we investigate the physics of point defects in monolayer (ML) WS<sub>2</sub>. Second, we examine the impact of point defects on the physical properties of multi-layer defective WS<sub>2</sub> as a function of slab thickness. The studied point defects are: monovacancies, interstitials and anti-sites, and the considered physical properties include local geometry, defect formation energy, electronic structure and magnetism. Van der Waals interaction, spin-polarization and spin-orbit coupling effects are also incorporated in the calculations to ensure accurate results. In a ML WS<sub>2</sub>, we predict that I<sub>S</sub> is the most favorable defect inside WS<sub>2</sub> having a low formation energy of 1.21 eV. W<sub>S</sub> and WS<sub>2</sub> anti-sites result in a total magnetic moment of 2 μ<sub>B</sub>. By studying ML, few-layer (up to 4 layers), and bulk WS<sub>2</sub> slabs we find that, all point defects cause only localized perturbation, thus have little influence on the thickness-dependent evolution of the physical properties. The depth-dependence of the defect formation energy is also found: V<sub>S</sub> prefers to stay on the surface, while V<sub>W</sub> prefers the slab center.

<sup>1</sup>This work is supported by the Dutch Science Foundation NWO, VIDI Grant (Grant Nr. 723.012.006).

**3:06PM P15.00004 Towards the Intrinsic Limit in As-Exfoliated MoS<sub>2</sub>**, ERIN SUTTON, EDWARD GEORGE, EMILY WHAPHAM, KENNETH BURCH, Boston College, BURCH GROUP TEAM — In recent years, two-dimensional transition metal dichalcogenide (TMDC) semiconductors have been intensively studied as exciting non-zero band gap analogs to graphene. For example, molybdenum disulfide (MoS<sub>2</sub>), a TMDC, is a van der Waals material which can be thinned down to single atomic layers less than a nanometer thick via micro-mechanical cleavage. In this regime, quantum confinement effects give rise to properties not seen in the bulk crystal. The attractive properties of ultrathin MoS<sub>2</sub> have inspired myriad applications, including spin- and valley-tronics, and LED and photo-detecting devices. As the performance of these devices is optimized, a method of modulating these properties is strongly desired. Through exfoliating MoS<sub>2</sub> on various substrates in an inert glovebox environment, we have produced as-exfoliated MoS<sub>2</sub> doped at the intrinsic level. We study the changes in the MoS<sub>2</sub> via Raman and photoluminescence spectra and see shifts in excitonic behavior. The ability to create intrinsic MoS<sub>2</sub> without the need for chemical doping or gating has exciting implications for optical studies of the material in addition to device applications such as photovoltaic, photocatalytic, and LED devices.

**3:18PM P15.00005 ABSTRACT WITHDRAWN –**

**3:30PM P15.00006 Preparation and Electronic Characterization of Substrate-Scale MoS<sub>2</sub> Single-Layer Films**, JOSEPH MARTINEZ, MICHAEL GOMEZ, MIKE VALENTIN, EDWIN PRECIADO, VELVETH KLEE, ARIANA NGUYEN, ADAM BERGES, DANIEL LU, MIGUEL ISARRARAZ, LUDWIG BARTELS, University of California Riverside — Using a novel high vacuum chemical vapor deposition process we synthesize substrate scale (2x2 cm) homogeneous monolayer MoS<sub>2</sub> films. Our process involves exposure of a hot Mo filament to organic chalcogen precursors that volatilize MoS<sub>x</sub> species which then precipitate on a thermally-controlled substrate. The resultant films are photoluminescent at 1.87 eV as expected for monolayer material; their Raman modes are indistinguishable from exfoliated material. Metal contact formation to these films was investigated under UHV conditions utilizing X-Ray Photoelectron Spectroscopy. These measurements permit us to follow the formation of a Schottky Barrier with increasing metal film thickness on the Angstrom scale. We utilize core level spectroscopy to indicate the evolution of the MoS<sub>2</sub> valence band under metal deposition. Our measurements provide direct indication on the charge transfer direction at metal contacts and the ensuing band-bending in two-terminal devices.

**3:42PM P15.00007 Synthesis and electronic structure of single-layer TaS<sub>2</sub>**, CHARLOTTE SANDERS, ARLETTE SOHANFO NGANKEU, MACIEJ DENDZIK, MARCO BIANCHI, PHILIP HOFMANN, Aarhus University — Bulk TaS<sub>2</sub> is an intriguing material that exhibits charge density wave phases, Mott physics, and superconductivity; however, little work has been done on single-layer (SL) TaS<sub>2</sub>. Progress in this area demands a method for controllably fabricating high-quality, uniform samples with low defect densities. We have succeeded in epitaxially growing SL TaS<sub>2</sub>, using the Au(111) substrate. The monolayer exhibits a well-defined orientation with respect to the substrate, a strong preference toward forming triangular islands, and a moire superstructure. Furthermore, long deposition times lead to smooth layer-by-layer growth of TaS<sub>2</sub>. In this talk, I will present band structure measurements acquired by angle-resolved photoemission spectroscopy (ARPES) on TaS<sub>2</sub>/Au samples fabricated in situ at the SGM3 end station of the ASTRID2 synchrotron facility in Denmark. Scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED) elucidate the material's structural properties and interaction with the substrate.

**3:54PM P15.00008 Observation of Interlayer Phonons in Transition Metal Dichalcogenide Heterostructures**, RUI HE, ZHIPENG YE, CHAO JI, CASIE MEANS-SHIVELY, HEIDI ANDERSON, TIM KIDD, University of Northern Iowa, KUANG-CHANG CHIU, CHENG-TSE CHOU, JENN-MING WU, YI-HSIEN LEE, National Tsing Hua Univ, Taiwan, TROND ANDERSEN, MIT, CHUN HUNG LUI, UC Riverside — Interlayer phonon modes in transition metal dichalcogenide (TMD) heterostructures are observed for the first time. We measured the low-frequency Raman response of MoS<sub>2</sub>/WSe<sub>2</sub> and MoSe<sub>2</sub>/MoS<sub>2</sub> heterobilayers. We discovered a distinct Raman mode (30 - 35 cm<sup>-1</sup>) that cannot be found in any individual monolayers. By comparing with Raman spectra of Bernal bilayer (2L) MoS<sub>2</sub>, 2L MoSe<sub>2</sub> and 2L WSe<sub>2</sub>, we identified the new Raman mode as the layer breathing vibration arising from the vertical displacement of the two TMD layers. The layer breathing mode (LBM) only emerges in bilayer regions with atomically close layer-layer proximity and clean interface. In addition, the LBM frequency exhibits noticeable dependence on the rotational angle between the two TMD layers, which implies a change of interlayer separation and interlayer coupling strength with the layer stacking.

**4:06PM P15.00009 Distinct Reconstruction Patterns and Spin-Resolved Electronic States along the Zigzag Edges of Transition Metal Dichalcogenides<sup>1</sup>**, PING CUI, JIN-HO CHOI, WEI CHEN, JIANG ZENG, University of Science and Technology of China, CHENDONG ZHANG, CHIH-KANG SHIH, University of Texas at Austin, ZHENYU LI, ZHENYU ZHANG, University of Science and Technology of China — Two-dimensional transition metal dichalcogenides are a new class of materials exhibiting various intriguing physical, chemical, and mechanical properties. Integration of such materials for potential device applications will necessarily encounter creation of different boundaries. Using first-principles approaches, here we investigate the structural, electronic, and magnetic properties along two inequivalent M- or X-terminated zigzag edges of MX<sub>2</sub> (M=Mo, W; X=S, Se). Along the M-terminated edges, we discover a previously unrecognized but energetically strongly preferred (2x1) reconstruction pattern, which is universal for all the MX<sub>2</sub>, characterized by place exchanges of the outmost X and M edge atoms. In contrast, the X-terminated edges undergo a more moderate (2x1) or (3x1) reconstruction for MoX<sub>2</sub> or WX<sub>2</sub>, respectively. We further use the prototypical examples of zigzag MoX<sub>2</sub> nanoribbons to demonstrate that the M- and X-terminated edges possess distinctly different electronic and magnetic properties, which can be exploited for a broad range of spintronic and catalytic applications

<sup>1</sup>Supported by NNSF of China, MOST, and USNSF.

**4:18PM P15.00010 Low-frequency Raman modes as fingerprints of layer stacking configurations of transition metal dichalcogenides<sup>1</sup>**, LIANGBO LIANG, ALEXANDER PURETZKY, BOBBY SUMPTER, Oak Ridge National Lab, VINCENT MEUNIER, Rensselaer Polytechnic Institute, DAVID GEOHEGAN, Oak Ridge National Lab, DAVID B. GEOHEGAN TEAM, VINCENT MEUNIER TEAM — The tunable optoelectronic properties of stacked two-dimensional (2D) crystal monolayers are determined by their stacking orientation, order, and atomic registry. Atomic-resolution Z-contrast scanning transmission electron microscopy (AR-Z-STEM) can be used to determine the exact atomic registration between different layers in few-layer 2D stacks; however, fast and relatively inexpensive optical characterization techniques are essential for rapid development of the field. Using two- and three-layer MoSe<sub>2</sub> and WSe<sub>2</sub> crystals synthesized by chemical vapor deposition, we show that the generally unexplored low-frequency (LF) Raman modes (~50 cm<sup>-1</sup>) that originate from interlayer vibrations can serve as fingerprints to characterize not only the number of layers, but also their stacking configurations [Puretzky and Liang et al, ACS Nano 2015, 9, 6333]. First-principles Raman calculations and group theory analysis corroborate the experimental assignments determined by AR-Z-STEM and show that the calculated LF mode fingerprints are related to the 2D crystal symmetries. Our combined experimental/theoretical work demonstrates the LF Raman modes potentially more effective than HF Raman modes to probe the layer stacking and interlayer interaction for 2D materials.

<sup>1</sup>The authors acknowledge support from Eugene P. Wigner Fellowship at the Oak Ridge National Laboratory and the Center for Nanophase Materials Sciences, a DOE Office of Science User Facility.

**4:30PM P15.00011 Excitons and exciton-phonon interactions in 2D MoS<sub>2</sub>, WS<sub>2</sub> and WSe<sub>2</sub> studied by resonance Raman spectroscopy**, MARCOS PIMENTA, ELENA DEL CORRO, BRUNO CARVALHO, LEANDRO MALARD, JULIANA ALVES, CRISTIANO FANTINI, Departamento de Física, Universidade Federal de Minas Gerais, HUMBERTO TERRONES, Rensselaer Polytechnic Institute, Department of Physics, ANA LAURA ELIAS, MAURICIO TERRONES, Department of Physics and Materials Science and Engineering, Penn-State University — The 2D materials exhibit a very strong exciton binding energy, and the exciton-phonon coupling plays an important role in their optical properties. Resonance Raman spectroscopy (RRS) is a very useful tool to provide information about excitons and their couplings with phonons. We will present in this work a RRS study of different samples of 2D transition metal dichalcogenides (MoS<sub>2</sub>, WS<sub>2</sub> and WSe<sub>2</sub>) with one, two and three layers (1L, 2L, 3L) and bulk samples, using more than 30 different laser excitation lines covering the visible range. We have observed that all Raman features are enhanced by resonances with excitonic transitions. From the laser energy dependence of the Raman excitation profile (REP) we obtained the energies of the excitonic states and their dependence with the number of atomic layers. In the case of MoS<sub>2</sub>, we observed that the electron-phonon coupling is symmetry dependent, and our results provide experimental evidence of the C exciton recently predicted theoretically. The RRS results WSe<sub>2</sub> show that the Raman modes are enhanced by the excited excitonic states and we will present the dependence of the excited states energies on the number of layers.

**4:42PM P15.00012 Giant blue shifted photoluminescence peak from the edges of CVD grown monolayer MoS<sub>2</sub>**, ALEXANDER YORE, WENDY CRUMRINE, San Francisco State Univ, KIRBY SMITHE, ERIC POP, Stanford University, BIN WANG, University of Oklahoma, AKM NEWAZ, San Francisco State Univ — To probe the electronic and optical properties of direct band-gap monolayer transition metal dichalcogenides, such as band structure and excitons, micro-photoluminescence spectroscopy has become an attractive and standard tool. Here, we present our experimental work on spatial scanning of photoluminescence of monolayer MoS<sub>2</sub> grown by chemical vapor deposition (CVD) using an ultrasmall blue laser (wavelength 405 nm) beam spot with beam diameter as small as  $\sim 200$  nm. We have observed a giant blue shift, as large as  $\sim 40$  nm or  $\sim 100$  meV, of the A-excitonic peak in the photoluminescence spectra from the edges when compared to luminescence from the inside. This giant blue shift may result from the following: (i) compressive strain at the edges; (ii) the enhanced dielectric screening caused by the increased electron density at the metallic Mo-edges; and (iii) chemical impurities.

**4:54PM P15.00013 High Resolution X-ray investigation of few-layer Molybdenum Disulfide (MoS<sub>2</sub>) Based Heterostructures**, HASSANA SAMASSEKOU, RICHARD PETERSON, SAIKAT TALAPATRA, DIPANJAN MAZUMDAR, Southern Illinois University-Carbondale — Due to its favorable band gap, few-layer MoS<sub>2</sub> can play an important role in optoelectronics and magneto-optics applications. Device applications necessitate a heterostructure combination of MoS<sub>2</sub> with other compatible materials. Here we report the growth and characterization of structural properties of few-layer MoS<sub>2</sub> based prototypes on Si substrates deposited by means of magnetron sputtering. A number of heterostructure combinations such as MoS<sub>2</sub>/BN, MoS<sub>2</sub>/SiO<sub>2</sub> shall be analyzed using high resolution X-ray reflectivity, scattering and diffraction methods. Our preliminary work already indicates that MoS<sub>2</sub> deposited on BN is quite favorable for optoelectronic applications [1]. But substantial work remains in order to obtain abrupt interfaces and atomic-level control. High resolution X-ray analysis can provide the essential understanding into the various structural aspects (crystal structure, interface roughness, density thickness) which could be valuable for developing a diversity of optoelectronic applications using MoS<sub>2</sub> or other *transition metal dichalcogenides*. Ref 1: Wasala, Samassekou, et al. (under review).

**5:06PM P15.00014 Anisotropic Dielectric Breakdown of Hexagonal Boron Nitride Film<sup>1</sup>**, YOSHI-AKI HATTORI, The University of Tokyo, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, KOSUKE NAGASHIO, The University of Tokyo and PRESTO-JST — Hexagonal boron nitride (h-BN) is considered as ideal substrate for 2D material devices. However, the reliability of insulating properties of h-BN itself has not been clarified yet. In this study, the anisotropic dielectric breakdown of h-BN is studied. We have found that the dielectric breakdown in *c* axis direction using a conductive atomic force microscope proceeded in the layer-by-layer manner. The obtained dielectric field strength was  $\sim 12$  MV/cm, which is comparable to the conventional SiO<sub>2</sub>. On the other hand, to estimate the dielectric field strength in a direction perpendicular to *c* axis, voltage is applied to a relatively thick h-BN (10-60 nm) through Cr/Au electrodes fabricated on the h-BN. We realized that the absorbed water on h-BN significantly affect the *IV* characters and the breakdown voltage. After the adsorbed water was removed by the heating in vacuum, the dielectric field strength was determined to be  $\sim 3$  MV/cm, which is the same order as that in *c* axis direction. This value could be increased when we consider the effect of electric field concentration around the metal electrode. Although the large difference in dielectric field strength for two directions was initially expected due to the highly-anisotropic layered structure with the van der Waals bonding, it was not the case because the sp<sup>2</sup> bonding should be broken for dielectric breakdown regardless of its direction.

<sup>1</sup>This research was supported by Grants-in-Aid for Scientific Research on Innovative Areas and for Research Activity Start-up by MEXT, Japan.

**5:18PM P15.00015 The effective bending rigidity of a fluctuating ribbon<sup>1</sup>**, DUANDUAN WAN, MARK BOWICK, Department of Physics, Syracuse University — We study the vibration of a two-dimensional ribbon using molecular dynamics. We find the effective bending rigidity tends to a constant which can be orders of magnitude larger than the bare bending rigidity in the limit that the bare bending rigidity goes to zero, consistent with theoretical expectations. Experimental realizations include graphene, molybdenum disulfide and some doped membranes.

<sup>1</sup>We thank NSF DMREF 7454419 for support.

## Wednesday, March 16, 2016 2:30PM - 5:30PM –

Session P16 DMP: 2D Devices: Black Phosphorous, III-IV, and IV-VI Materials 315 - Jewook Park, ORNL

**2:30PM P16.00001 Twisted Phosphorene Nanoribbons**, WOOSUN JANG, KISUNG KANG, ALOYSIUS SOON, Department of Materials Science and Engineering, Yonsei University — Many different forms of structural deformations have been employed to alter the electronic structure of various two-dimensional (2D) nanomaterials in various optoelectronic devices [1]. Given the recent interest in the new class of 2D nanomaterials – phosphorene, it is important to understand how the anisotropic strain-dependent electronic properties of low-dimensional phosphorene may be exploited for technological gain. Here, using first-principles density-functional theory, we investigate the mechanical stability of twisted one-dimensional phosphorene nanoribbons (PNR) by measuring its critical twist angle ( $\theta_c$ ) and shear modulus as a function of the applied mechanical torque [2-4]. We find a strong anisotropic behaviour in PNRs with different edge terminations and directions, and report the direct consequence of this applied mechanical stress on its corresponding electronic (and optical) properties. [1] E. S. Reich, *Nature*, **506**, 19 (2014); [2] C. D. Reddy *et al.*, *Appl. Phys. Lett.* **94**, 101904 (2009); [3] E. M. Diniz, *Appl. Phys. Lett.* **104**, 083119 (2014); [4] V. Sorkin and Y. Zhang, *Nanotechnology*, **26**, 235707 (2015)

**2:42PM P16.00002 Ground state degeneracy, energy barriers, and molecular dynamics evidence for two-dimensional disorder in black phosphorus and monochalcogenide monolayers at finite temperature**, MEHRSHAD MEHBOUDI, SALVADOR BARRAZA-LOPEZ, ALEX M. DORIO, University of Arkansas, WENJUAN ZHU, AREND VAN DER ZANDE, University of Illinois, HUGH O. H. CHURCHILL, University of Arkansas, ALEJANDRO A. PACHECO-SANJUAN, Universidad del Norte, EDMUND O. HARRISS, PRADEEP KUMAR, University of Arkansas — Mono-layers of black phosphorus and other two dimensional materials such as mono-layers of SiSe, GeS, GeSe, GeTe, SnS, SnSe, and SnTe with a similar crystalline structure have a four-fold degenerate ground state that leads to two-dimensional disorder at finite temperature. Disorder happens when neighboring atoms gently re-accommodate bonds beyond a critical temperature. In this talk, the effect of atomic numbers on the transition temperature will be discussed. In addition Car-Parinello molecular dynamics calculations at temperatures 30, 300 and 1000 K were performed on supercells containing more than five hundred atoms and the results from these calculations confirm the transition onto a two-dimensional disordered structure past the critical temperature, which is close to room temperature for many of these compounds. References: M. Mehboudi, A.M. Dorio, W. Zhu, A. van der Zande, H.O.H. Churchill, A.A. Pacheco Sanjuan, E.O.H. Harris, P. Kumar, and S. Barraza-Lopez. arXiv:1510.09153.

**2:54PM P16.00003 Remarkably low-energy one-dimensional fault line defects in single-layered phosphorene**, ALOYSIUS SOON, WOOSUN JANG, KISUNG KANG, Department of Materials Science and Engineering, Yonsei University — Systematic engineering of atomic-scale low-dimensional defects in two-dimensional nanomaterials is a promising way to modulate the electronic properties of these nanomaterials. Defects at interfaces such as grain boundaries and line defects can often be detrimental to technologically important nanodevice operations and thus a fundamental understanding of how such one-dimensional defects may have an influence on its physio-chemical properties is pivotal to optimizing their device performance. In this study [1], using density-functional theory, we investigate the temperature-dependent energetics and electronic structure of a single-layered phosphorene with various fault line defects. We have generated different line defect models based on a fault method, rather than the conventional rotation method. This has allowed us to study and identify new low-energy line defects, and we show how these low-energy line defects could well modulate the electronic band gap energies of single-layered two-dimensional phosphorene – offering a range of metallic to semiconducting properties in these newly proposed low-energy line defects in phosphorene. [1] A. Soon et al. *Nanoscale*, DOI 10.1039/C5NR05605E (2015)

**3:06PM P16.00004 Black phosphorus edges: a polarized Raman study<sup>1</sup>**, H RIBEIRO, Mackgraphe-Mackenzie University, C VILLEGAS, IFT-UNESP, D BAHAMON, Mackgraphe-Mackenzie University, A CASTRO NETO, CA2DM and GRC, National University of Singapore, E DE SOUZA, Mackgraphe-Mackenzie University, A ROCHA, IFT-UNESP, M PIMENTA, Departamento de Física, UFMG, C DE MATOS, Mackgraphe-Mackenzie University — Black phosphorus (BP) has been recently exfoliated down to few-layer thicknesses revealing numerous interesting features such as a tunable direct bandgap. Ever since, demonstrations of BP electronic devices have bloomed, as well as studies of the electric, optical, mechanical and thermal properties of its bulk and few-layer forms. However, the edges of BP crystals have, so far, been poorly characterized, even though the terminations of layered crystals are known to possess a range of interesting properties. In this work, the edges of exfoliated BP flakes are characterized by polarized confocal Raman spectroscopy. We will present experimental Raman spectra at zigzag and armchair edges, as well as density functional theory calculations that explain the peculiarities of the experimental data.

<sup>1</sup>FAPESP, INCT/Nanocarbono, Fapemig, CNPq, MackPesquisa, Grid-Unesp, CENAPAD-SP, and NRF

**3:18PM P16.00005 Tight-binding model study of topological properties in few-layer black phosphorus<sup>1</sup>**, HYEONJIN DOH, HYOUNG JOON CHOI, Yonsei Univ — We study the simplest tight-binding model describing the band structures of mono- and bilayer phosphorus. The band structures are analyzed for various tight-binding parameters, and the gap-closing conditions are found where the system turns into a Dirac semi-metal. We show the tight-binding model Hamiltonian can be reduced to Dirac Hamiltonian and investigate its topological properties. The doping, electric field and pressure effects on topological properties of black phosphorus are discussed and these analyses suggest directions the the control of the energy gap in these system.

<sup>1</sup>This work was supported by NRF of Korea (Grant No. 2011-0018306) and KISTI supercomputing center (Project No. KSC-2015-C3-039).

**3:30PM P16.00006 N-type doping of black phosphorus by using benzyl viologen.**, DEWU YUE, DAEYEONG LEE, JUNGJIN RYU, MIN SUP CHOI, HYE JIN NAM, DUK-YOUNG JUNG, WON JONG YOO, Sungkyunkwan Univ, NDPL COLLABORATION — Black phosphorus (BP) meets several critical material requirements for the development of future nanoelectronic applications, but the realization of n-type semiconductor behavior form it has remained elusive. Here, we report the ambipolar characteristics of few-layer BP, induced using an novel technique: chemical doping with benzyl viologen (BV), which serves as a surface charge transfer donor for BP flakes. The n-doped BP devices exhibit excellent electron mobility up to  $\sim 83 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$  from 2-terminal measurement at 300K, thereby demonstrating n-type behavior. On the basis of ambipolar BP devices, we also comprehensively analyzes temperature and BP thickness dependence of ambipolar devices, in which we found the degenerate doping limit below around 150K and highest electron transport performance in  $\sim 10 \text{ nm}$  BP flakes at 300K. As a proof of concept, ultrafast BP photodetectors were fabricated with a very high photoresponsivity of  $\sim 10^4 \text{ mA/W}$  over the UV, visible, and IR spectral ranges. Furthermore, we fabricated a homogeneous BP based inverter through BV doping and h-BN capping that offers a feasible approach to fabricating a key building block of future 2D logic semiconductors.

**3:42PM P16.00007 Oxidation of black phosphorus from the side**, MARIO BORUNDA, Oklahoma State University, SALVADOR BARRAZA, University of Arkansas — Two-dimensional black phosphorus, a recently discovered two-dimensional semiconductor material, has promising properties of interest in physics and materials science. We have performed density functional theory calculations at the early stages of the oxidation process from its side, and contrasted these results with oxidation processes happening at the top exposed surface.

**3:54PM P16.00008 Intrinsic Defects, Fluctuations of the Local Shape, and the Photo-Oxidation of Black Phosphorus**, KAINEN UTT, SALVADOR BARRAZA-LOPEZ, Univ of Arkansas-Fayetteville, ALEJANDRO PACHECO SANJUAN, Universidad del Norte, PABLO RIVERO, MERSHAD MEHBOUDI, EDMUND HARRISS, Univ of Arkansas-Fayetteville, MARIO BORUNDA, Oklahoma State University — The rapid degradation of black phosphorus (BP) under ambient condition is a well-known, but poorly understood phenomenon that represents a significant challenge to the feasibility of BP-based devices. Nearly 60 years after its discovery, BP has experienced a resurgence in popularity among the condensed matter community due to its recently demonstrated promise as a tunable two-dimensional semi-conductor. Despite this resurgence in popularity, the oxidation pathways have yet to be explored in great detail. A full characterization of the material's shape and of its electronic properties at the early stages of the oxidation process is presented and provides fundamental insights into the degradation dynamics of this novel layered material. Reference: K. L. Utt, P. Rivero, M. Mehboudi, E. O. Harriss, M. F. Borunda, A. A. Pacheco SanJuan, and S. Barraza-Lopez, *ACS Cent. Sci.* 1, 320 (2015)

**4:06PM P16.00009 Humidity Effects and Anisotropic Etching During Exfoliated Black Phosphorus Degradation**, ALEXANDRE FAVRON, PATRICIA MORAILLE, ETIENNE GAUFRES, TYCHO ROORDA, PIERRE L. LEVESQUE, RICHARD LEONELLI, RICHARD MARTEL, Universite de Montreal — Black phosphorus, a lamellar structure similar to graphene, is a high mobility semiconductor having a tunable optical band gap from 0.3 eV up to  $\sim 2 \text{ eV}$  with decreasing layer thickness. Our previous study has highlighted a fast photo-oxidation in ambient conditions when black phosphorus is exfoliated as thin layers. The kinetics of this degradation is also enhanced by quantum confinement effects and faster for the thinnest layers, which represents an important hurdle to prepare few layers. Here we further investigate the role of water in the process by following the reaction kinetics in different humidity using fast AFM imaging. We report on important changes of wettability of thin layers at room temperature depending on the degradation stages and layer thickness. For a given level of humidity at equilibrium, we observe the formation of water droplets. Those droplets form preferentially on defects sites and cracks and then grow on the thicker parts of the flake to finally accumulate on to the thinnest regions. This sequence of water droplet growth faster from thick to thin layers is interpreted as being due to a lowering of surface tension with decreasing layer thickness. In a second study, the oxidation kinetics of layers completely immersed in water reveal an anisotropic oxidation process with preferential etching in specific orientations of the crystal. This study will be discussed in the context of a reactivity of black phosphorus that appears both anisotropic and thickness-dependent.

**4:18PM P16.00010 First-principle study of the energy barrier and diffusivity of a Li atom on phosphorene**, CONGYAN ZHANG, MING YU, Univ of Louisville — The energy landscape of a Li atom adsorbed on the phosphorene was studied using the first principle method. Four types of preferential adsorption positions were found: three of them are located along the zigzag direction with the adsorption energy of -2.0~-1.9 eV/atom, forming potential valleys along zigzag direction. The other type is located on the top of the puckered bridge with the adsorption energy of -1.4 eV/atom, forming small isolated shallow basins between the potential valleys. Based on this energy landscape, we calculated energy barriers along various diffusion paths. The lowest energy barrier is along the zigzag direction in the valley (0.09 eV). The highest energy barrier is along the armchair direction through the top of P atoms (1.01 eV). While the energy barrier on the top of the bridge along the zigzag direction and along the armchair direction through the P-P bonds are 0.20 eV and 0.79 eV, respectively. Estimated diffusivity along the zigzag direction in the valley is almost  $10^{16}$  fast than that along the armchair direction through the top of P atoms, indicating the anisotropic diffusion.

**4:30PM P16.00011 Large Ultraviolet Photoresponsivity of Few-layer Black Phosphorus<sup>1</sup>**, JING WU, GAVIN KOK WAI KOON, DU XIANG, ANTONIO H. CASTRO NETO, BARBAROS OZYILMAZ, Natl Univ of Singapore, CENTRE OF ADVANCED 2D MATERIALS TEAM — Black phosphorus has recently gained much attention in the scientific community. Black phosphorus can be seen as a crystal generated by periodic repetition of tetraphosphorus ( $P_4$ ) molecules. It is known that tetraphosphorus  $P_4$  can be transformed temporarily to diphosphorus  $P_2$  upon ultraviolet (UV) irradiation. Thus, it is expected that the  $P_4$  structured black phosphorus also has strong interaction with light especially in the UV range. Here we report on the optoelectronic characteristics of few-layer black phosphorus field effect transistors (FETs) ranging from the UV to the near infrared (NIR). We demonstrate that black phosphorus is an excellent ultraviolet (UV) photodetector with a specific detectivity  $\sim 3 \times 10^{13}$  Jones. We report also an exceptional photo responsivity of  $10^7$  times higher than previously reported values for black phosphorus visible light photodetectors. We attribute such a colossal UV photo responsivity to the resonant-interband transition between two specially nested valence and conduction bands. These nested bands provide an unusually high density of states for high-efficient UV absorption due to their singularity nature.

<sup>1</sup>Large Ultraviolet Photoresponsivity of Few-layer Black Phosphorus

**4:42PM P16.00012 Few-layer III-VI and IV-VI 2D semiconductor transistors**, SUKRIT SUCHARITAKUL, Case Western Reserve University, MEI LIU, Shandong Normal University, RAJESH KUMAR, RAMAN SANKAR, FANG C. CHOU, YIT-TSONG CHEN, National Taiwan University, XUAN GAO, Case Western Reserve University — Since the discovery of atomically thin graphene, a large variety of exfoliable 2D materials have been thoroughly explored for their exotic transport behavior and promises in technological breakthroughs. While most attention on 2D materials beyond graphene is focused on transition metal-dichalcogenides, relatively less attention is paid to layered III-VI and IV-VI semiconductors such as InSe, SnSe etc which bear stronger potential as 2D materials with high electron mobility or thermoelectric figure of merit. We will discuss our recent work on few-layer InSe 2D field effect transistors which exhibit carrier mobility approaching  $1000 \text{ cm}^2/\text{Vs}$  and ON-OFF ratio exceeding  $10^7$  at room temperature. In addition, the fabrication and device performance of transistors made of mechanically exfoliated multilayer IV-VI semiconductor SnSe and  $\text{SnSe}_2$  will be discussed. **References** [1] Sucharitakul. S. *et al. Nano Lett.* **15**, 3815–3819 (2015).

**4:54PM P16.00013 Puckering Inversion in Monolayer Group IV Monochalcogenides SnS and GeSe Through Strain Engineering**, PAUL HANAKATA, Boston University, ALEXANDRA CARVALHO, National University of Singapore, DAVID CAMPBELL, HAROLD PARK, Boston University — We use first principles calculations to study the electronic and mechanical properties of the monolayer group IV monochalcogenides SnS and GeSe under uniaxial stress in the armchair or zigzag direction. We find that monolayer SnS and GeSe can sustain tensile stresses up to 3.5 GPa and 7 GPa, respectively. Applying uniaxial stress in the zigzag direction results in a structural phase transition to a rocksalt-like structure for both GeSe and SnS and followed by an inversion in the puckering structure. This puckering inversion results in a change of the band structure, in particular the valley configuration. Our findings show the potential applications of SnS and GeSe monolayer for phase-change memory and valley-based electronic devices.

**5:06PM P16.00014 ABSTRACT WITHDRAWN —**

**5:18PM P16.00015 Field Effect Transistors Using Atomically Thin Layers of Copper Indium Selenide ( $\text{CuInSe}$ )<sup>1</sup>**, PRASANNA PATIL, SUJOY GHOSH, MILINDA WASALA, Southern Illinois University Carbondale, SIDONG LEI, ROBERT VAJTAI, PULICKEL AJAYAN, Rice University, SAIKAT TALAPATRA, Southern Illinois University Carbondale — We will report fabrication of field-effect transistors (FETs) using few-layers of Copper Indium Selenide ( $\text{CuInSe}$ ) flakes exfoliated from crystals grown using chemical vapor transport technique. Our transport measurements indicate n-type FET with electron mobility  $\approx 3 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  at room temperature when Silicon dioxide ( $\text{SiO}_2$ ) is used as a back gate. Mobility can be further increased significantly when ionic liquid 1-Butyl-3-methylimidazolium hexafluorophosphate ( $\text{BMIM-PF}_6$ ) is used as top gate. Similarly subthreshold swing can be further improved from 103 V/dec to 0.55 V/dec by using ionic liquid as a top gate. We also found ON/OFF ratio of  $\approx 10^2$  for both top and back gate. Comparison between ionic liquid top gate and  $\text{SiO}_2$  back gate will be presented and discussed.

<sup>1</sup>This work is supported by the U.S. Army Research Office through a MURI grant W911NF-11-1-0362.

**Wednesday, March 16, 2016 2:30PM - 5:18PM —**

**Session P17 DMP: 2D Materials: Assembly and Characterization** 316 - Ching-Tzu Chen, IBM

**2:30PM P17.00001 Towards Lego Snapping; Integration of Carbon Nanotubes and Few-Layer Graphene**, MOHSEN NASSERI, MATHIAS BOLAND, M. JAVAD FARROKHI, DOUGLAS STRACHAN, University of Kentucky — Integration of semiconducting, conducting, and insulating nanomaterials into precisely aligned complicated systems is one of the main challenges to the ultimate size scaling of electronic devices, which is a key goal in nanoscience and nanotechnology. This integration could be made more effective through controlled alignment of the crystallographic lattices of the nanoscale components. Of the vast number of materials of atomically-thin materials, two of the  $sp^2$  bonded carbon structures, graphene and carbon nanotubes, are ideal candidates for this type of application since they are built from the same backbone carbon lattice. Here we report carbon nanotube and graphene hybrid nanostructures fabricated through their catalytic synthesis and etching. The growth formations we have investigated through various high-resolution microscopy techniques provide evidence of lego-snapped interfaces between nanotubes and graphene into device-relevant orientations. We will finish with a discussion of the various size and energy regimes relevant to these lego-snapped interfaces and their implications on developing these integrated formations.

**2:42PM P17.00002 Two-dimensional square structures of CuO and Cu<sub>2</sub>O monolayer.**<sup>1</sup>, YUYANG ZHANG, Vanderbilt Univ; Oak Ridge National Lab, KUIBO YIN, YILONG ZHOU, LITAO SUN, Southeast University, MATTHEW F. CHISHOLM, Oak Ridge National Lab, SOKRATES T. PANTELIDES, Vanderbilt Univ; Oak Ridge National Lab, WU ZHOU, Oak Ridge National Lab — Among 2D crystals, monolayer (ML) oxides are interesting because of the coupling of quantum confinement to other degrees of freedom that are present in bulk materials. However, as most oxides are not layered structures, fabrication of 2D oxides has been limited. Current studies focus on either two-to-three atomic layers thick materials, such as the exfoliated perovskites, or supported films that are bonded to the substrate. Unsupported single-atom-thick oxides have not been reported. Here we report the fabrication of single-atom-thick copper oxide ML. Quantum mechanical calculations indicate that free-standing copper oxide MLs are stable wide-bandgap semiconductors with a variable chemical stoichiometry ranging from CuO to Cu<sub>2</sub>O at similar lattice constants. The stoichiometry variation changes the bandgap from indirect for CuO ML to direct for Cu<sub>2</sub>O ML, suggesting that the electronic and optical properties of ML copper oxides can be tuned by the oxygen content.

<sup>1</sup>This work was supported by the DOE grant DE-FG02-09ER46554 and by the DOE BES DMSE.

**2:54PM P17.00003 Oxidation-derived two-dimensional MoO<sub>3</sub>/MoS<sub>2</sub> heterostructures**, TAEG YEOUNG KO, Department of Chemistry, Kyung Hee University, AREUM JEONG, Department of Applied Chemistry, Kyung Hee University, SUNMIN RYU<sup>1</sup>, Department of Chemistry, Division of Advanced Materials Science, Pohang University of Science and Technology — In order to explore the efficient formation of MoO<sub>3</sub>/MoS<sub>2</sub> heterostructures, we systematically investigated the course of surface oxidation of mechanically exfoliated single and few-layer MoS<sub>2</sub> induced by oxygen plasma treatment using photoluminescence (PL) and Raman spectroscopy, atomic force microscopy (AFM) and X-ray photoelectron spectroscopy (XPS). Raman and PL spectra served as sensitive indicators for defects generated by the plasma oxidation, showing Raman peak broadening and drastically reduced intensities for both Raman peaks and PL bands. XPS detected Mo<sup>6+</sup> as the major Mo species in the oxidized samples, confirming the conversion of MoS<sub>2</sub> into amorphous MoO<sub>3</sub>. The AFM studies also revealed that the thickness of MoS<sub>2</sub> layers more than doubles when oxidized and that the vertical reaction from the top dominates with a negligible contribution from the lateral attack when combined with the Raman measurements. Our results show that the oxygen plasma treatment can be successfully used in generating atomically thin MoO<sub>3</sub> or two-dimensional MoO<sub>3</sub>/MoS<sub>2</sub> heterostructures that may be useful for future electronic and optoelectronic application.

<sup>1</sup>Corresponding author

**3:06PM P17.00004 Microscopic theory of two-dimensional spatially-indirect-exciton condensates and exciton-polariton condensates**<sup>1</sup>, FEI XUE, FENG CHENG WU, ALLAN MACDONALD, Univ of Texas, Austin — BEC of excitons and polaritons have drawn attention in recent years because of the demonstration of their ability to host macroscopic quantum phenomena and because of their promise for applications. We study the case of a system containing two TMD monolayers that are separated and surrounded by h-BN. Under appropriate conditions this system is expected to support a spatially indirect thermal equilibrium exciton condensate. We combine a microscopic mean-field calculation and a weakly interacting boson model to explore the bilayer exciton condensates phase diagram. By varying the layer separation and exciton density, we find a phase transition occurs between states containing one and two condensate flavors. We also use a microscopic time-dependent mean-field theory to address condensate collective mode spectra and quantum fluctuations. Next we study the case of exciton-polariton formed by strong coupling between quantum well excitons and confined photon modes when the system is placed in a vertical microcavity. We build a microscopic mean-field theory starting from electrons and holes, and account for their coupling to coherent light field. We compare our model with the normal weakly interacting boson model that starts from weakly interacting excitons that are coupled to photons.

<sup>1</sup>This work was supported by the SRC and NIST under the Nanoelectronic Research Initiative (NRI) and SWAN, by the Welch Foundation under Grant No. F1473, and by the ARO Grant No. 26-3508-81.

**3:18PM P17.00005 Preparation and Characterization of Large Area Monolayer Films of Pt Nanoparticles**<sup>1</sup>, BRIAN KELLY, Department of Physics and Astronomy, University of Delaware, RONALD CICHOCKI, JIE REN, Department of Chemistry and Biochemistry, University of Delaware, ROBERT SCHMIDT, Department of Physics and Astronomy, University of Delaware, KLAUS THEOPOLD, Department of Chemistry and Biochemistry, University of Delaware, KARL UNRUH, Department of Physics and Astronomy, University of Delaware — Highly uniform monolayer thick coatings of Pt nanoparticles with areas as large as 20 cm<sup>2</sup> have been prepared by first self-assembling the desired Pt film at the interface between two immiscible liquids and then transferring the film to a glass substrate. The controlled addition of ethyl alcohol to a phase separated mixture of an aqueous colloidal solution of Pt nanoparticles and hexane allowed both monolayer and multilayer films to be prepared. Optical microscopy and UV-vis spectrophotometry measurements have been used to verify the large scale uniformity of the coatings while transmission electron and atomic force microscopy measurements confirmed that single and multilayer films can be prepared.

<sup>1</sup>This material is based upon work supported by the National Science Foundation under Grant No. 1410076

**3:30PM P17.00006 The 2D Selfassembly of Benzimidazole and its Co-crystallization.**, PAULO COSTA, JACOB TEETER, DONNA KUNKEL, ALEXANDER SINITSKII, AXEL ENDERS, University of Nebraska-Lincoln — Benzimidazoles (BI) are organic molecules that form ferroelectric crystals. Key to their ferroelectric behavior are the switchable N···HN type bonds and how they couple to the electron system of the molecules. We attempted to crystallize BI on various metal surfaces and studied them using STM. We observed that on Au and Ag, BI joins into zipper chains characteristic of its bulk structure that can pack into a continuous 2D layer. Because the dipole of BI lies in the direction of its switchable hydrogen bond, these zippers should in principle have reversible polarizations that point along the direction they run. BI's crystallization is reminiscent to how croconic acid (CA) crystallizes in 2D using O···HO bonding, suggesting that these molecules may be able to co-crystallize through OH···N bonds. This would present the opportunity to modify BI's properties, such as the energy needed to switch a hydrogen from a donor to acceptor site. When co-deposited, CA and BI successfully combine into a co-crystal formed by building blocks consisting of 2 CA and 2 BI molecules. These findings demonstrate the usefulness of using STM as a preliminary check to verify if two molecules are compatible with each other without having to attempt crystallization with multiple solvents and mixing methods.

**3:42PM P17.00007 Correlating Structural and Electronic Degrees of Freedom in 2D Transition Metal Dichalcogenides**, I-CHENG TUNG, Z. ZHANG, Advanced Photon Source, Argonne National Laboratory, K. L. SEYLER, A. M. JONES, Department of Physics, University of Washington, G. CLARK, Department of Materials Science and Engineering, University of Washington, D. XIAO, Department of Physics, Carnegie Mellon University, N. LAANAIT, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, X. XU, Department of Physics, University of Washington, H. WEN, Advanced Photon Source, Argonne National Laboratory — We have conducted a microscopic study of the interplay between structural and electronic degrees of freedom in two-dimensional (2D) transition metal dichalcogenide (TMD) monolayers, multilayers and heterostructures. Using the recently developed full field x-ray reflection interface microscopy with the photoluminescence microscopic probe capability at the Advanced Photon Source, we demonstrated the x-ray reflection imaging of a monolayer 2D material for the first time. The structural variation across an exfoliated WSe<sub>2</sub> monolayer is quantified by interlayer spacing relative to the crystal substrate and the smoothness of the layer. This structural information is correlated with the electronic properties of TMDs characterized by the *in-situ* photoluminescence measurements. This work is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-SC0012509. The use of Advanced Photon Source is supported by U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-06CH11357.

**3:54PM P17.00008 Symmetry protected topological phases in a multi-band 2D electron gas.** , PETR STEPANOV, YAFIS BARLAS, CHUN NING LAU, Univ of California - Riverside, DMITRY SMIRNOV, National High Magnetic Field Lab, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science — Recently the observation of symmetry protected topological phases was reported in monolayer and bilayer graphenes in the  $\nu = 0$  quantum Hall state. Ground state in a multi-band Dirac systems such as ABA-trilayer graphene shows more complex phases than their mono- and bilayer counterparts. Tight-binding Hamiltonian in the absence of out-of-plane displacement field along with the mirror symmetry about the middle layer leads to a presence of non-interacting two bands. Relative shift of bands in the Landau Level energy spectrum map exhibits the existence of conductive counterpropagating phases with values  $\sigma_{xx} = 2\alpha e^2/h$  where  $\alpha$  is the spin-degeneracy. In addition, out-of-plane displacement field plays a crucial role in mixing those bands leading to broken symmetries and polarizing charge carriers in only bottom or top layer. We will present our most recent studies on quantum Hall phase diagram of  $\nu = 0$  in ABA-trilayers.

**4:06PM P17.00009 Thermoelectronic emission from monolayer graphene with temperature dependent work functions** , DILIP DE<sup>1</sup>, OLUKUNLE OLAWOLE, Covenant University — For the first time we have derived an equation for the temperature (T) dependent work function (W(T)) that will be important for modeling thermoelectronic current density (J) and energy distribution of emitted electrons specially, from nano-materials. The equation containing terms up to fifth power of T gives a modified Richardson-Dushman (MRDE) equation that fits excellently well the experimental data of J vs T for suspended graphene. It provides a unique technique for accurate determination of  $W_0$ , Fermi energy,  $E_{F0}$  at 0 K and surface density of charge carriers,  $n_s$  of graphene. The corresponding values obtained for suspended graphene are:  $W_0 = 4.42 + 0.01$  eV,  $E_{F0} = 0.166 + 0.002$  eV;  $n_s = 2.34 \times 10^{12} \text{ cm}^{-2}$ . The model gives -ve thermal expansion coefficient of graphene ( $-8 \times 10^{-6} \text{ /K}$ ) which has been experimentally confirmed. The equations are expected to hold for carbon nanotubes.

<sup>1</sup>Please send us acceptance notice early so that we can apply for sponsorship from our University in time.

**4:18PM P17.00010 Effect of dopant distribution on thermal conductivity of  $C_{(1-x)}N_x$**  , YANG ZHOU, Fudan Univ — The thermal conductivities of nanoscale nitrogen doped graphene ( $C_{(1-x)}N_x$ ) with various nitrogen ratio and distribution is studied by performing nonequilibrium molecular dynamics. The thermal conductivity of randomly doped  $C_{(1-x)}N_x$  is found much smaller than that of the regular alloy when the dopant ratios are the same. Meanwhile, thermal conductivity of random alloys is dopant ratio sensitive while that of regular alloy is not. Interestingly, localization mode analysis indicates that the inequality of atoms under translation and inversion is responsible for the change of the thermal conductivity and a linear relationship between them is found. The results may provide a general guidance for phonon manipulation and thermal engineering in alloys.

**4:30PM P17.00011 Doping and Thermal Conductivity Studies of  $CrSiTe_3$**  , AMANDA HAGLUND, Dept. of Materials Science and Engineering, Univ of Tennessee, JIAQIANG YAN, Univ of Tennessee; Oak Ridge National Laboratory, VEERLE KEPPENS, Dept. of Materials Science and Engineering, Univ of Tennessee, DAVID MANDRUS, Univ of Tennessee; Oak Ridge National Laboratory —  $CrSiTe_3$  is a layered material with a 2-dimensional crystal structure, and has recently become of more interest due to the possibility of using its ferromagnetic and semiconducting properties for spintronics applications. To further investigate the properties of  $CrSiTe_3$ , we doped it with various transition elements on the Cr site in an attempt to tune and control the magnetism, as well as study changes in the thermal conductivity. We synthesized pure  $CrSiTe_3$  and doped samples through flux growth, producing plate-like bulk crystals. Crystal quality was checked by x-ray diffraction and energy dispersive spectroscopy, and then thermal conductivity and magnetization measurements were obtained on the doped materials to compare variations from the pristine  $CrSiTe_3$ .

**4:42PM P17.00012 Electronic and Mechanical Properties of Graphene-Germanium Interfaces Grown by Chemical Vapor Deposition** , BRIAN KIRALY, Northwestern University , ROBERT JACOBBERGER, University of Wisconsin-Madison, ANDREW MANNIX, GAVIN CAMPBELL, MICHAEL BEDZYK, Northwestern University, MICHAEL ARNOLD, University of Wisconsin-Madison, MARK HERSAM, Northwestern University, NATHAN GUISSINGER, Argonne National Laboratory — Epitaxial graphene grown directly on semiconducting Ge wafers holds potential for fundamental science and electronics applications. However, since the initial demonstration, little work has been done on the structural and electronic properties of this system. To gain insight into the interface between graphene and Ge, we performed ultra-high vacuum scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) along with Raman and X-ray photoelectron spectroscopy experiments to probe the atomic structure and chemistry at the interface. STS confirms stronger interfacial interaction on Ge(110), consistent with models of epitaxial growth. Raman spectroscopy shows that strain is highly prevalent after growth. Furthermore, the native strain modifies the atomic structure of the Germanium, inducing new and metastable Ge surface reconstructions following annealing. These reconstructions, in turn, modify both the electronic and mechanical properties of the graphene. Finally, graphene/Ge(001) represents the extremely strained case. Here graphene forces restructuring of the Ge surface into [107] facets. From this work, we see that the interaction between graphene and Ge is both dependent on the substrate crystallographic orientation and tunable.

**4:54PM P17.00013 Optical activity and circular dichroism of plasmonic nanorod assemblies<sup>1</sup>** , LAROUSSE KHOSRAVI KHORASHAD, Department of Physics and Astronomy, Ohio University, Athens, Ohio 45701, USA, NA LIU, Max Planck Institute for Intelligent Systems, Heisenbergstrasse 3, D-70569 Stuttgart, Germany, ALEXANDER O. GOVOROV, Department of Physics and Astronomy, Ohio University, Athens, Ohio 45701, USA — Plasmonic circular dichroism (CD) has offered an efficient spectroscopy method for the electronic, chemical, and structural properties of different types of light active molecules in the subwavelength regime. Among the different chiral geometries of metal nanoparticles utilized by the plasmonic CD spectroscopy, gold nanorods (AuNRs) have shown strong CD signals in the visible frequency range. In this work, we theoretically study the CD signals of AuNR arrangements in order to mimic structures and chemical bonds of chiral biomolecules. In particular, our twisted three-AuNR geometries resemble a molecular structure of tartaric acid. This molecule played an important role in the discovery of chemical chirality. In our study, we show that the strength of CD signals changes dramatically by tuning the interparticle distances and angles. Since the CD signals are typically weak, we develop reliable computational approaches to calculate the plasmonic CD. Manipulating interparticle distances, size, and molecular bond angles result in full control over peak positions, handedness, and positive and negative bands which are observed in the CD spectra.

<sup>1</sup>This work has been supported under the grant from Volkswagen Foundation. We also acknowledge the financial support of Condensed Matter and Surface Science program of Ohio University.

**5:06PM P17.00014 Strong superchiral field in hot spots and its interaction with chiral molecules.<sup>1</sup>** , YINENG LIU, Xiamen University — We have found that strong superchiral fields created by surface plasmon resonance exist in hot spots of nonchiral plasmonic structure, which showed a chiral density greater than that of circularly polarized light by hundreds of times. We have demonstrated a direct correlation between the chirality of the local field and the circular dichroism (CD) response at the plasmon resonance bands induced by chiral molecules in the hot spots. Our results reveal that the wavelength-dependent superchiral fields in the hot spots can play a crucial role in the determination of the plasmonic CD effect. This finding is in contrast to the currently accepted physical model in which the electromagnetic field intensity in hot spots is a key factor to determine the peak intensity of the plasmonic CD spectrum. Some related experimental phenomena have been explained by using our theoretical analysis.

<sup>1</sup>The work was supported by the China National Natural Science Foundation (Grant No. 11504306).

## Wednesday, March 16, 2016 2:30PM - 5:30PM –

Session P18 GMAG DMP FIAP: Spin-Dynamics in Patterned Films and Devices 317 - Volker Sluka, New York University

**2:30PM P18.00001 Electrically driven magnetization dynamics in yttrium iron garnet<sup>1</sup>**, MATTHIAS BENJAMIN JUNGFLAISCH<sup>2</sup>, Argonne National Laboratory — Creation and manipulation of magnetization states by spin-orbital torques are important for novel spintronics applications. Magnetic insulators were mostly ignored for this particular purpose, despite their low Gilbert damping, which makes them outstanding materials for magnonic applications and investigation of nonlinear spin-wave phenomena. Here, we demonstrate the propagation of spin-wave modes in micro-structured yttrium iron garnet ( $\text{Y}_3\text{Fe}_5\text{O}_{12}$ , YIG) stripes. Spin waves propagating along the long side of the stripe are detected by means of spatially-resolved Brillouin light scattering (BLS) microscopy. The propagation distance of spin waves is determined in the linear regime, where an exponential decay of 10  $\mu\text{m}$  is observed<sup>3</sup>. We also explored the possibility of driving magnetization dynamics with spin Hall effects (SHE) in bilayers of YIG/Pt microstructures. For this purpose we adopted a spin-transfer torque ferromagnetic resonance (ST-FMR) approach. Here a *rf* charge current is passed through the Pt layer, which generates a spin-transfer torque at the interface from an oscillating spin current via the SHE. This gives rise to a resonant excitation of the magnetization dynamics. In all metallic systems the magnetization dynamics is detected via the homodyne anisotropic magnetoresistance of the ferromagnetic layer. However, since there is no charge flowing through ferromagnetic insulators there is no anisotropic magnetoresistance. Instead, we show that for the case of YIG/Pt the spin Hall magnetoresistance can be used. Our measured voltage spectra can be well fitted to an analytical model evidencing that the ST-FMR concept can be extended to insulating systems<sup>4</sup>. Furthermore, we employ spatially-resolved BLS spectroscopy to map the ST-FMR driven spin dynamics. We observe the formation of a strong, self-localized spin-wave intensity in the center of the sample<sup>5</sup>. This spin-wave 'bullet' is created due to nonlinear cross coupling of eigenmodes existing in the magnetic system, which is confirmed by micromagnetic simulations.

<sup>1</sup>The work at Argonne was supported by the U.S. Department of Energy, Office of Science, Materials Science and Engineering Division.

<sup>2</sup>This work was in collaboration with: W. Zhang, J. Sklenar, W. Jiang, J. Ding, H. Chang, F. Y. Fradin, S. M. Wu, J. E. Pearson, A. Bhattacharya, J. B. Ketterson, V. Novosad, M. Wu, and A. Hoffmann.

<sup>3</sup>M. B. Jungfleisch *et al.*, J. Appl. Phys. **117**, 17D128 (2015).

<sup>4</sup>J. Sklenar *et al.*, Phys. Rev. B, *in press*, arXiv:1505.07791 [cond-mat.mes-hall] (2015).

<sup>5</sup>M. B. Jungfleisch *et al.*, arXiv:1505.07791 [cond-mat.meshall] (2015).

**3:06PM P18.00002 Spin Hall Control of Magnetization in a Perpendicularly-Magnetized Magnetic Insulator**, CHI-FENG PAI, ANDY QUINDEAU, ASTERA TANG, MEHMET ONBASLI, MAXWELL MANN, LUCAS CARETTA, CAROLINE ROSS, GEOFFREY BEACH, Massachusetts Institute of Technology — Spin Hall effect (SHE)-induced spin-orbit torque (SOT) has been shown to be an efficient mechanism to control the magnetization in magnetic heterostructures. Although numerous works have demonstrated the efficacy of SOT in manipulating the magnetization of ferromagnetic metals (FM), SOT-controlled switching of ferromagnetic insulators (FMI) has not yet been observed. In this work we show that spin Hall currents in Pt and Ta can generate SOTs strong enough to control the magnetization direction in an adjacent thulium iron garnet FMI film with perpendicular magnetic anisotropy. We find that dc current in the heavy metal (HM) generates an out-of-plane effective field in the FMI consistent with an antidamping torque whose magnitude is comparable to that observed in all-metallic systems. Spin Hall magnetoresistance (SMR) measurements reveal a large spin-mixing conductance, which implies considerable spin transparency at the metal/insulator interface and explains the observed strong current-induced torque. Our results show that charge currents flowing in a HM can be used to both control and detect the magnetization direction in a FMI electrically.

**3:18PM P18.00003 Spin transfer torque switching in MTJ arrays with nanoengineered uniaxial anisotropy<sup>1</sup>**, ILYAS A. H. FARHAT, Khalifa University, AMS Dept. and KSRC, Abu Dhabi, UAE, E. GALE, University of Bath, UK, M. ABI JAOUDE, A. F. ISAKOVIC, Khalifa University, AMS Dept. and KSRC, Abu Dhabi, UAE — Enhancing Magnetic Tunnel Junction (MTJ) energy efficiency is the key to embed it in low power applications. We report a detailed study on the behavior of the analytical expression of switching current density as a function of geometrical and magnetic parameters, for both I-MTJs and P-MTJs. Our study shows that the current model requires some modifications to improve the match between the model and the experiment. We also show under which criteria a scaled-down of MTJ devices can help in reduction of current density. We then used the device model of MTJ to study the power performance of MTJ device, proposing a roadmap to lower switching power of the device. Comparisons between ours and data for similar devices in literature, combined with the above analysis, suggests the need for qualitatively different model, and for this purpose, we explored the variations of the effective energy density model [1], which may explain the device behavior better. [1] T. Taniguchi *et al.*, Phys. Rev. B **87**, 054406 (2013).

<sup>1</sup>Work supported by Mubadala-SRC 2012-VJ-2335. A part of the work done at Cornell CNF/CCMR, with special thanks to C. Alpha. A part of the work done at BNL-CFN, supported by DOE.

**3:30PM P18.00004 Vortex Gyrotropic Motion in patterned Ferromagnetic Dots<sup>1</sup>**, JUNJIA DING, PAVEL LAPA, TRUPTI CHAIR, CHRYSIAN POSADA, AXEL HOFFMANN, VALENTINE NOVOSAD, Argonne Natl Lab — A vortex state consists of a large region of in-plane curling magnetization and a small core region with out-of-plane magnetization. The gyrotropic oscillation frequency of the vortex core is known to be weakly dependent to the core position (which is adjustable by changing the applied field) and can only be efficiently tuned by changing the dimension of the dots. Here, we demonstrated that the vortex gyrotropic frequency can be stepwise tuned by introducing a vortex barrier to a regular ferromagnetic dot. Systematical investigations of the dynamic response of the engineered dots have been performed as a function of the outer dot diameter, barrier diameter and the barrier profile using both microwave absorption spectroscopy and micromagnetic simulation. We found that the vortex frequency is mostly dependent on the outer diameter of the dot when the core is outside the barrier, while it is more rely on the dimension of the barrier when the core is inside the barrier. This approach certainly gives several additional freedoms to adjust the vortex gyrotropic frequency and opens extra perspectives for spintronic applications.

<sup>1</sup>This work at Argonne was supported by the U.S. Department of Energy, Office of Science, Materials Science and Engineering Division

**3:42PM P18.00005 Dynamics of spin valves investigated using Magneto-Optical Kerr Effect Spectroscopy<sup>1</sup>**, CHRISTOPHER STEVENS, JAGANNATH PAUL, PRASENJIT DEY, Univ of South Florida, CASEY MILLER, Rochester Institute of Technology, STEPHEN MCGILL, National High Magnetic Field Lab, FSU, DENIS KARAIKAJ, Univ of South Florida — Through an all-optical approach, we are investigating the spin dynamics in different spin torque based structures. Using pump-probe Time-Resolved Magneto-Optical Kerr Effect (TR-MOKE) spectroscopy, we are able to monitor the ultrafast magnon propagation on a sub-picosecond timescale as well as the longer lived oscillations and demagnetization. This represents a recent efforts to realize magnon induced spin torque using an all optical method.

<sup>1</sup>This research at USF is supported by the National Science Foundation, Division of Electrical, Communications and Cyber Systems under grant number: 1231929. The work was done in part at the NHMFL, Tallahassee, FSU under grants: DMR-1229217, DMR-1157490

**3:54PM P18.00006 The shot noise like feature of the magnetic 1/f noise in CoFeB/MgO/CoFeB magnetic tunnel junctions.** , LIANG LIU, JIASSEN NIU, HUIQIANG GUO, JIAN WEI, International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China and Collaborative Innovation Center of Quantum, D. L. LI, J. F. FENG, X. F. HAN, Beijing National Laboratory of Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, X.-G. ZHANG, Center for Nanophase Materials Sciences, and Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6493, J. M. D. COEY, CRANN and School of Physics, Trinity College, Dublin 2, Ireland — The magnetic field dependent 1/f noise in magnetic multilayers and magnetic tunnel junctions (MTJs) is conventionally considered as resistance fluctuations ( $S_R$ ), for which an applied current ( $I$ ) is merely used to convert  $S_R$  to measurable voltage fluctuations ( $S_V = I^2 S_R$ ). From  $S_R$  and magnetoresistance, magnetization fluctuations can be inferred obeying the fluctuation-dissipation relation (FDR), thus comes the name magnetoresistive noise. However, we find that 1/f noise in CoFeB/MgO/CoFeB MTJs is better described by  $S_I/I$ , instead of  $S_V/I^2$ , particularly near the magnetic reversal fields of the reference layer and the free layer, the latter of which has not been previously investigated in detail. More surprisingly, the bias dependence resembles that of shot noise. These findings call for further investigation on FDR for magnetic noise in MTJs, especially in the far from equilibrium state with high bias and possible contribution from collective magnon excitations.

**4:06PM P18.00007 Coherent spin-transfer precession switching in orthogonal spin-torque devices** , COLM RYAN, GRAHAM ROWLANDS, BBN Technology - Massachusetts, DANIELE PINNA, LI YE, LAURA REHM, VOLKER SLUKA, ANDY KENT, Department of Physics, New York University, New York, NY 10003, USA, THOMAS OHKI, BBN Technology - Massachusetts — We present experimental results in concert with macrospin simulations of the switching characteristics of orthogonal spin-transfer devices incorporating an out-of-plane magnetized polarizing layer and an in-plane magnetized spin valve device at cryogenic temperatures. Switching at 3.4K between parallel and anti-parallel spin-valve states is investigated for current pulses with varying durations from 0.1 to 1.4ns to observe the averaged response of the time dependent dynamics of the spin-transfer induced precession of the magnetization. We demonstrate high speed switching at short pulse lengths, down to 100ps, and also observe ensemble decoherence effects with longer pulses. The results show that even at cryogenic temperatures finite temperature noise is still important in the dynamics of precessional switching.

**4:18PM P18.00008 Effects of spin relaxation on trap-assisted tunneling through ferromagnetic metal-oxide-semiconductor structures** , VIKTOR SVERDLOV, SIEGFRIED SELBERHERR, Institute for Microelectronics, TU Wien — A signal measured within a three-terminal setup at room temperature [1,2] is attributed to the spin injection from a ferromagnetic electrode into n-silicon; however, its amplitude is orders of magnitude larger than predicted by theory [3]. The reasons for this discrepancy are heavily debated [3-6], with trap-assisted resonant tunneling [4] and spin-dependent magnetoresistance gaining recognition. However, effects of spin relaxation important at room temperature were not considered in [4]. To elucidate the role of spin relaxation and coherence, corresponding Lindblad terms are added to the equation for the density matrix evolution of spin on a trap coupled to ferromagnetic contacts. Fast spin relaxation suppresses the magnetoresistance modulation. Interestingly, strong decoherence at fixed spin lifetime results in a more pronounced magnetoresistance modulation and in a narrower magnetoresistance linewidth as a function of the perpendicular magnetic field. 1.S.P.Dash *et al.*, Nature **462**,491 (2009). 2.C.Li *et al.*, Nature Commun.**2**, 245 (2011). 3.R.Jansen, Nature Mater.**11**, 400 (2012). 4.Y.Song and H.Dery, PRL **113**, 047205 (2014). 5.A.Spiesser *et al.*, PRB **90**, 205213 (2014). 6.K.-R.Jeon *et al.*, PRB **91**, 155305 (2015).

**4:30PM P18.00009 Thermally reliable clocked non-volatile spin wave logic device** , SOURAV DUTTA, Georgia Inst of Tech, DMITRI NIKONOV, SASIKANTH MANIPATRUNI, IAN YOUNG, Components Research, Intel Corporation, Hillsboro, AZAD NAEEMI, Georgia Inst of Tech — The possibility of utilizing spin waves for information transmission and computation has been an area of active research due to the unique ability to manipulate the amplitude and phase of the spin waves for building complex logic circuits. Here, we present a comprehensive scheme for building a thermally reliable clocked non-volatile spin wave logic device [1,2] (SWLD) by introducing a charge-to-spin converter that translates information from electrical domain to spin domain, exploiting the magneto-electric effect for spin wave transmission, detection and non-volatile memory, utilizing the phase of the spin wave as information token, ensuring phase-dependent deterministic switching of the magnetoelectric spin wave detector in the presence of thermal noise via compensation of demagnetization and a novel clocking scheme that ensures sequential transmission of information in a cascaded SWLD and non-reciprocity. [1] S. Dutta *et al.*, Non-volatile clocked spin wave interconnect for beyond-cmos nanomagnet pipelines, Scientific Reports **5** (2015). [2] S. Dutta *et al.*, Phase-dependent deterministic switching of magnetoelectric spin wave detector in the presence of thermal noise via compensation of demagnetization , Applied Physics Letters (accepted 2015).

**4:42PM P18.00010 Magnetotransport properties of Co<sub>90</sub>Fe<sub>10</sub>/Cu/Ni<sub>80</sub>Fe<sub>20</sub> pseudo-spin-valve with out-of-plane tilted magnetic field** , LINQIANG LUO, NAM DAO, SALINPORN KITTIWATANAKUL, STUART WOLF, JIWEI LU, Univ of Virginia, UVA NANOSTAR TEAM — The giant magnetoresistance (GMR) effect of a pseudo spin valve made of Co<sub>90</sub>Fe<sub>10</sub>/Cu/Ni<sub>80</sub>Fe<sub>20</sub> has been investigated, with a magnetic field applied perpendicularly tilted to the sample plane. Without using a pinning layer, the magnetic separation of the free and fixed layers is uniquely achieved by utilizing perpendicular fields due to different anisotropy energies between Ni<sub>80</sub>Fe<sub>20</sub> and Co<sub>90</sub>Fe<sub>10</sub>. The magneto-transport measurements are carried out by Van der Pauw method in current-in-plane geometry at room temperature. By tilting the magnetic field at different angles from out-of-plane, the GMR plateau's width can be tuned. A plateau width of about 2000 Oe is observed at tilted angle 0.5°, which opens a significantly larger window for high-resistance states comparing with a plateau width of 10 Oe for in-plane fields. With the out-of-plane tilted fields, the orientation of the magnetic moments can be tuned continuously out of the sample plane, and the relative orientation between Ni<sub>80</sub>Fe<sub>20</sub> and Co<sub>90</sub>Fe<sub>10</sub> can also be tuned by the tilted angle, enabling us to precisely control the sample's states for current-induced spin dynamics study that is very difficult in the case of in-plane applied magnetic fields.

## 4:54PM P18.00011 Spin-torque ferromagnetic resonance in arbitrarily magnetized thin films ,

JOSEPH SKLENAR<sup>1</sup>, Physics and Astronomy, Northwestern University, Evanston, IL. Materials Science Division, Argonne National Laboratory, Argonne, IL. — The spin Hall effect (SHE) in non-magnetic metals can be used to generate spin-transfer-torque (STT), subsequently inducing ferromagnetic resonance (FMR) in magnetic thin films; this experimental method is termed spin-torque ferromagnetic resonance (ST-FMR). Most ST-FMR experiments that are reported have an applied magnetic field in the plane of the sample and the research focuses on material combinations that have large and efficient STT. The most common way ST-FMR signals are detected is through an anisotropic magnetoresistance (AMR) rectification process. In this work we will present ST-FMR results in thin films where the magnetization has both an in-plane and out-of-plane component. The arbitrary magnetization direction is achieved by tipping the applied magnetic field out of the sample plane. We find that when the material system is a permalloy/Pt bilayer, ST-FMR signals are not mirror-symmetric upon magnetic field reversal<sup>2</sup>. This is because the combination of both a STT from the bulk SHE and the Oersted field-like torque from the device do not drive the dynamics in the same manner when the field is reversed. We interpret our results in the Py/Pt experiment by extending an already established ST-FMR lineshape model to describe the general case of arbitrarily magnetized films. We compare and contrast our Py/Pt experiment with another system we measured, a Py/MoS<sub>2</sub> bilayer. For the Py/MoS<sub>2</sub> system, in-plane experiments suggest that a large STT is present and are comparable to what is observed for the more traditional Py/Pt system<sup>3</sup>. On the other hand, the out-of-plane experiment for the Py/MoS<sub>2</sub> system is qualitatively very different from Py/Pt. Our results suggest that ST-FMR experiments for arbitrarily magnetized magnetic films are useful in characterizing STT generated from interface rather than bulk effects. Work at Northwestern was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Science and Engineering Division under grant number DE-SC0014424. Work at Argonne was supported by the U.S. Department of Energy, OS, Materials Science and Engineering Division. Lithography was carried out at the Center for Nanoscale Materials, which is supported by DOE, OS-BES under Contract No. DE-AC02-06CH11357.

<sup>1</sup>This work is in collaboration with: W. Zhang, M. B. Jungfleisch, W. Jiang, H. Saglam, S. Grudichak, J. E. Pearson, J. B. Ketterson, and A. Hoffmann.

<sup>2</sup>J. Sklenar *et al*, Submitted

<sup>3</sup>W. Zhang, J. Sklenar *et al*, Submitted

## Wednesday, March 16, 2016 2:30PM - 5:30PM – Session P19 GMAG DMP FIAP: Magnetic Materials 318 - Daniel Gopman, NIST

### 2:30PM P19.00001 Observation of Temperature Chaos in Mesoscopic Spin Glasses<sup>1</sup> , SAMARESH

GUCHHAIT, Laboratory for Physical Sciences, College Park, MD 20740 and Department of Physics, University of Maryland, College Park, MD 20742 — Temperature Chaos (TC) results from a change in temperature for spin glasses (SG), polymers, and other glassy materials. When the temperature is changed, TC means that the new state has no memory of the preparation of the initial state. TC was predicted long ago [PRL 48, 767 (1982)]. However, “An experimental measurement of TC is still missing” [EPL 103, 67003 (2013)]. One reason for this is the question of length scale. In the thermodynamic limit, even an infinitesimal temperature change,  $\Delta T$ , will create a chaotic condition. However, by working at the mesoscale, one can establish a length scale sufficiently small to exhibit reversible behavior before crossing over to chaotic behavior as the temperature change increases. Observation of TC is possible because, on reasonable laboratory time scales, the SG correlation length can grow to the size of the thickness of the film,  $L$ . The lower critical dimension for a SG is  $\sim 2.5$ , so that the thin film SG crosses over to a glass temperature  $T_g = 0$ . However, there remains quasi-equilibrium SG states with length scales  $< L$ . After crossover, a small  $\Delta T$  will generate a TC coherence length which, if greater than  $L$ , will leave the system in a reversible state. However, when  $\Delta T$  is sufficiently large, such that the TC coherence length is less than  $L$ , and chaos will ensue. I will discuss our recent results of temperature cycling on 15.5 nm SG films of amorphous Ge:Mn. By use of end of aging and temperature cycling, both the reversible region and the chaotic region are observed. Remarkably, the transition from a reversible to chaotic behavior is abrupt, and not smooth as a function of  $\Delta T$ . This is in contrast to previous work using polycrystalline materials where the distribution of length scales smoothed out the transition to chaos. Using the calculated TC critical exponent, the range of  $\Delta T$  for reversible behavior is calculated and is in very good agreement with the measured range.

<sup>1</sup>This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering under Award DE-SC0013599.

### 3:06PM P19.00002 An Investigation of the Spin Glass Properties of the Solid Solution

$\text{CuAl}_{2-2x}\text{Ga}_{2x}\text{O}_4$  , THOMAS BULLARD, UES Inc, JACILYNN BRANT, National Research Council/TheAir Force Research Laboratory, CHARLES EBBING, The University of Dayton Research Institute, NEIL DILLEY, J. HAMILTON, Quantum Design, TIMOTHY HAUGAN, The Air Force Research Laboratory — The complete anti-ferromagnetic oxide spinel solid solution between end members  $\text{CuAl}_2\text{O}_4$  and  $\text{CuGa}_2\text{O}_4$  has been synthesized. The crystallographic and magnetic properties are examined as Ga is replaced with iso-valent Al. Crystallographic results show the solid solution obeys Vegard's law, and the cation distribution among the tetrahedral and octahedral sites matches well with prior results. The evolution of the magnetic susceptibility is examined as a function of temperature and doping percentage. Evidence is presented that indicates that the majority of the solution displays paramagnetic behaviour at high temperatures and spin glass behaviour below 3K. Specifically, a freezing temperature in the AC susceptibility, irreversibility in the DC magnetization, and relaxation dynamics in the presence of a changing applied field are observed.

### 3:18PM P19.00003 Nonlinear scaling variable at the lower critical dimension: Scaling in the 2D random field Ising model<sup>1</sup> , LORIEN HAYDEN, JAMES SETHNA, Cornell Univ —

We systematically analyze the nonlinear invariant scaling variables at bifurcations in the renormalization-group flow, and apply our methods to the two-dimensional random-field Ising model (RFIM). At critical points, the universal scaling functions are usually written in terms of homogeneous invariant combinations of variables, like  $Lt^\nu$  in the finite-size scaling form for the magnetization  $M(T|L) \sim t^{-\beta} M(Lt^\nu)$ , where  $t \propto T_c - T$ . The renormalization-group flow for the RFIM has a pitchfork bifurcation in two dimensions, where the correlation length has been argued to diverge exponentially,  $\xi \propto \exp^{1/2At^2}$ , leading to the invariant scaling combination  $L/\xi \sim L/\exp^{1/2At^2}$ . Our analysis, inspired by normal-form theory, suggests that this exponential divergence can take a richer, more general scaling form at a generic pitchfork bifurcation. We explore possible consequences for simulations.

<sup>1</sup>This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. DGE-1144153.

**3:30PM P19.00004 Response to a field of the  $D = 3$  Ising spin glass with Janus and JanusII dedicated computers<sup>1</sup>**, BEATRIZ SEOANE, LPT, Ecole Normale Supérieure, JANUS COLLABORATION COLLABORATION<sup>2</sup> — Using the Janus dedicated computer, and its new generation JanusII, we study the linear response to a field of the Edwards-Anderson model for times that cover twelve orders of magnitude. The fluctuation-dissipation relations are investigated for several values of  $t_w$ . We observe that the violations of the fluctuation-dissipation theorem can be directly related to the  $P(q)$  measured in equilibrium at finite sizes, although a simple statics-dynamics dictionary  $L \leftrightarrow \xi(t_w)$  is not enough to account for the behavior at large times. We show that the equivalence can be easily restored by taking into account the growth of  $\xi(t + t_w)$ . Interestingly, experimental measurements of the spin glass correlation length rely precisely on the response of a spin glass to a field, although a direct relation between the measured object and the real  $\xi$  has never been established. In this work, we mimic the experimental protocol with Janus data, which lets us relate the experimental  $\xi$  with the length extracted from the spatial correlation function. These results allow us for the first time to make a quantitative comparison between experiments and simulations, finding a surprising good agreement with measurements in superspin glasses.

<sup>1</sup>This project has received funding from the European Unions Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 654971, the ERC grant CRIPHERASY (no. 247328) and from the MINECO (Spain) (no. FIS2012-35719-C02)

<sup>2</sup>First results of the new machine JanusII

**3:42PM P19.00005 Extremely large magnetoresistance and magnetic logic by coupling semiconductor nonlinear transport effect and anomalous Hall Effect.**, XIAOZHONG ZHANG, ZHAOCHU LUO, Tsinghua University — Size limitation of silicon FET hinders the further scaling down of silicon based CPU. To solve this problem, spin based magnetic logic devices were proposed but almost all of them could not be realized experimentally except for NOT logic operation. A magnetic field controlled reconfigurable semiconductor logic using InSb was reported. However, InSb is very expensive and not compatible with the silicon technology. Based on our Si based magnetoresistance (MR) device [1], we developed a Si based reconfigurable magnetic logic device [2], which could do all four Boolean logic operations including AND, OR, NOR and NAND. By coupling nonlinear transport effect of semiconductor and anomalous Hall effect of magnetic material, we propose a PMA material based MR device with a remarkable non local MR of >20000 % at ~1 mT. Based on this MR device, we further developed a PMA material based magnetic logic device which could do all four Boolean logic operations. This makes it possible that magnetic material does both memory and logic. This may result in a memory-logic integrated system leading to a non von Neumann computer. [1] CH Wan, et al, Nature **477**, 304, (2011). [2] ZC Luo et al. Adv. Funct. Mater. **25**, 158, (2015).

**3:54PM P19.00006 Effects of transverse fields on spin-valve sensor magnetic field measurements**, ALEX JEFFERS, University of Maryland, ANTONIO OROZCO, Neocera, Beltsville, MD, ALFRED CAWTHORNE, Trevecca Nazarene University, Nashville, TN, CHRISTOPHER ROWLETT, STEVE GARRAHAN, Neocera, Beltsville, MD, FREDERICK WELLSTOOD, University of Maryland, College Park, MD — Spin-valve sensors have become a popular magnetic sensor, used in many applications such as magnetic imaging or hard drive heads. Spin-valves are designed to measure only one component of the magnetic field. This component is determined by the composition of the spin-valve layers, the manufacturing conditions, shape anisotropy, and other design decisions. We took magnetic images of L-shaped samples in order to determine if magnetic fields transverse to the direction of measurement affect spin-valve sensors. Specifically, we used a 2 m by 4 m Cu-Mn-Ir spin-valve sensor to take image of chips with “L-shaped” currents. We find that transverse fields can significantly affect the measurement direction of spin-valve sensors.

**4:06PM P19.00007 Effect of tantalum on magnetocrystalline anisotropy and tunneling magnetoresistance in MgO/CoFeB junction from ab-initio calculations**, ROMAN CHEPULSKYY, DMYTRO APALKOV, New Memory Technology, Samsung Semiconductor RD Center, Samsung Electronics — Using ab-initio calculations, we demonstrate that boron is energetically attracted toward interface between MgO and CoFeB in MgO/CoFeB junction. We show that both magnetocrystalline anisotropy (MCA) and tunneling magnetoresistance (TMR) decrease when boron is present at the interface. However, when tantalum is used as seeding or capping layer (Ta/CoFeB/MgO), the segregation profile of boron changes. Namely, the most energetically preferable position of boron is inside and near tantalum rather than at MgO/CoFeB interface. Such change of boron segregation profile results in boron diffusion from MgO/CoFeB interface toward tantalum at annealing. The diffusion of boron toward tantalum may explain the experimentally observed effect of tantalum on increase of both MCA and TMR in MgO/CoFeB junction

**4:18PM P19.00008 Growth and properties of High-quality metal/ yttrium iron garnet/metal sandwich structures<sup>1</sup>**, MOHAMMED ALDOSARY, JUNXUE LI, CHI TANG, YADONG XU, JING SHI, University of California — Sandwiched structures of magnetic insulators (e.g. yttrium iron garnet or YIG) between two normal metals are potentially useful for spintronics. In this work, we report our approach of growing a single crystalline YIG thin film on a Pt or Cu thin layer using the combination of sputtering and PLD. First, either 5 nm of Pt or Cu is deposited on (110)-oriented gadolinium gallium garnet (GGG) substrate using sputtering and then YIG is grown by PLD at intermediate temperatures followed by rapid thermal annealing at higher temperatures. Surprisingly, YIG films show a well-defined single-crystal reflection high energy electron diffraction (RHEED) pattern, despite that they are grown on polycrystalline Pt or Cu. TEM images show flat, clean and sharp interfaces between YIG/metals and metals/GGG. The magnetic properties show in-plane magnetic anisotropy. However, when thicker metallic layers (20 nm) or amorphous (metals/SiO<sub>2</sub>) substrate are used, only YIG polycrystalline phase is observed. We will show that by properly controlling the growth conditions the metal/YIG/ metal structures are not only of high structural quality, but also have desired properties for spin current transport.

<sup>1</sup>This work was supported as part of the SHINES, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award SC0012670.

**4:30PM P19.00009 Switching behavior of Nb/Exchange spring magnet/Nb Josephson Junctions fabricated by Nanosphere Lithography**, JIYEONG GU, GILBERT ARIAS, SAMUEL HEDGES, Dept. of Physics and Astronomy, California State University, Long Beach — Superconductor(S)/ferromagnet(F)/superconductor Josephson junction was fabricated by nanosphere lithography method. Samarium-Cobalt (SmCo)/Permalloy(Py) exchange spring magnet system was used to generate an inhomogeneous magnetic structure in Niobium(Nb)-based Josephson junctions. We introduced nanosphere lithography in our device fabrication in order to decrease the lateral size of junctions and improve the quality of our devices. A bigger size junctions (tens of microns) were fabricated by optical photolithography using a mask.\* Materials were deposited through DC magnetron sputtering. Base structure of devices was patterned through photolithography. Modulations of the critical current and IV-curve characteristics of the junction were used to search for direct evidence of the odd-triplet component. In addition, to investigate the switching behavior of S/F/S junction for memory application junction critical current was measured as a function of magnetic field and the angle between an easy axis of ferromagnetic layer and the external magnetic field by rotating the sample under magnetic field. Magnetic switching behavior of the ferromagnetic layers in our junction was also characterized based on this observation. \* Junction fabrication in this research by an optical photolithography using a mask was conducted at the Center for Nanophase Materials Sciences at Oak Ridge National Laboratory (CNMS User Project CNMS2014-257).

#### 4:42PM P19.00010 How to move domain walls in an antiferromagnet<sup>1</sup>, SE KWON KIM, Univ of California

- Los Angeles — Domain walls (DWs) in an easy-axis antiferromagnet can be driven by several stimuli: a charge current (in conducting antiferromagnets), a magnon current, and a temperature gradient. In this talk, we discuss the dynamics of a DW induced by two latter external perturbations, which are applicable in both metallic and insulating antiferromagnets. First of all, we study the Brownian dynamics of a DW subjected to a temperature gradient [1]. To this end, we derive the Langevin equation for the DW's center of mass with the aid of the fluctuation-dissipation theorem. A DW behaves as a classical massive particle immersed in a viscous medium. By considering a thermodynamic ensemble of DWs, we obtain the Fokker-Planck equation, from which we extract the average drift velocity of a DW. We briefly address other mechanisms of thermally driven DW motion. Secondly, we analyze the dynamics of a DW driven by circularly polarized magnons [2]. Magnons passing through a DW reverse their spin upon transmission, thereby transferring two quanta of angular momentum to the DW and causing it to precess. A precessing DW partially reflects magnons back to the source. The reflection of magnons creates a previously identified reactive force [3]. We point out a second mechanism of propulsion of the DW, which we term redshift: magnons passing through a precessing DW reduce their linear momentum and transfer the decrease to the DW. We solve the equations of motion for magnons in the background of a uniformly precessing DW with the aid of supersymmetric quantum mechanics and compute the net force and torque applied by magnons to the DW. The theory agrees well with micromagnetic simulations.

[1] S. K. Kim, O. Tchernyshyov, and Y. Tserkovnyak, Phys. Rev. B **92**, 020402(R) (2015)

[2] S. K. Kim, Y. Tserkovnyak, and O. Tchernyshyov, Phys. Rev. B **90**, 104406(E) (2014)

[3] E. G. Tveten, A. Qaiumzadeh, and A. Brataas, Phys. Rev. Lett. **112**, 147204 (2014)

<sup>1</sup>This work has been supported in part by the ARO, the U.S. DOE-BES, and the U.S. NSF grants.

c Research (Grants No.15H05854, No.26107505, and No.26400308) from the Ministry of Education, Culture, Sports, Sci-

#### 5:18PM P19.00011 Spin correlations and spin-wave exci-

YASUFUMI ARAKI, Institute for Materials Research, Tohoku University; Frontier Research Institute for Material Science, Tohoku University; NOMURA, Institute for Materials Research, Tohoku University — We study correlations among spin correlations and spin-wave excitations in semimetals. Effective field theory for localized magnetic moments is derived by integrating out the spin correlation in the spatial direction parallel to local magnetization is more rigid than that in the nature of the Dirac Hamiltonian. Such an anisotropy becomes stronger for Fermi level close to the Dirac point by spin-orbit coupling. One can expect topologically nontrivial spin textures under this anisotropy, such as around an axis, as well as a uniform ferromagnetic order. We further investigate the characteristics of spin-wave dispersion also shows a spatial anisotropy, which is less dispersed in the direction transverse to the magnetization. The dispersion anisotropy can be traced back to the rigidity and flexibility of spin correlations discussed

ence and Technology (MEXT), Japan.

## Wednesday, March 16, 2016 2:30PM - 5:30PM –

Session P20 DCOMP: Quantum Many-Body Systems and Methods III 319 - Herbert Fotso

#### 2:30PM P20.00001 QMC calculations of the dynamical local field factor of the 2D electron gas

, NATALIA MATVEEVA, MARKUS HOLZMANN, LPMCM, UMR 5493 of CNRS, Universite Grenoble Alpes, F-38100 Grenoble, France, DAVID CEPERLEY, Department of Physics, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA — We develop a new quantum Monte Carlo method to calculate imaginary time correlation functions for fermions in continuous space in order to access spectral functions. Linear response in imaginary time is obtained based on the variational expression of the thermal density matrix. The exact dynamics is recovered in the non-interacting limit. We apply our new method to the electron gas in two dimensions in the high and low density region and calculate the density fluctuations including many-body correlations in the density matrix. The dynamic structure factor can be accessed by analytic continuation. Our results provides accurate estimation of the dynamical local field factor which quantifies corrections to the RPA approximation.

#### 2:42PM P20.00002 Ab Initio Thermodynamic Results for the Degenerate Electron Gas at Finite Temperatures

, TIM SCHOOF, TOBIAS DORNHEIM, SIMON GROTH, Kiel University, JAN VORBERGER, Helmholtz-Zentrum Dresden-Rossendorf, MICHAEL BONITZ, Kiel University — Recent advances in warm dense matter physics, e.g. laser compressed matter, lead to an increasing interest in the description of correlated, degenerate electrons at finite temperatures. The uniform electron gas (UEG) is of key relevance for the understanding of such systems. Accurate thermodynamic data for the UEG are essential for the development of the finite-temperature density functional theory (FT-DFT). Based on first principles, the Configuration PIMC approach (CPIMC) allows for the exact computation of thermodynamic properties of strongly degenerate fermionic many-body systems in the highly degenerate regime [1]. We present CPIMC exchange-correlation energies for the UEG [2] and compare our results with previous restricted path integral Monte Carlo (RPIMC) [3] and recently published permutation-blocking PIMC (PB-PIMC) [4] data. We show that the complementary sign problem of the CPIMC and PB-PIMC methods allows for results with an unprecedented accuracy in a wide range of temperatures and densities.

[1] Contrib. Plasma Phys. **51**, 687 (2011).

[2] Phys. Rev. Lett. **115**, 130402 (2015).

[3] Phys. Rev. Lett. **110**, 146405 (2013).

[4] arXiv:1508.03221 (2015).

#### 2:54PM P20.00003 Identification of polaronic defects in wide band gap semiconductors via diffusion Monte Carlo

, JAEHYUNG YU, ELIF ERTEKIN, Univ of Illinois - Urbana — Polaronic defects are important to understanding a wide variety of properties in semiconductors; for instance they are closely coupled to electron phonon interactions and can greatly affect carrier concentrations and mobilities. The formation of a polaronic defect in a semiconductor is an interesting phenomenon because it incorporates a trade off between electron localization and structural relaxation. Because of its small energy scale and the localized nature of polaronic defect levels, accurately describing polaronic defects in semiconductors requires high accuracy first principle calculation methods. We demonstrate the use of the fixed node diffusion Monte Carlo (DMC) method to the identification of polaronic nitrogen defects in the wide band gap semiconductor zinc oxide. Using DMC, we can demonstrate that nitrogen defects in ZnO are subject to a symmetry-breaking Jahn-Teller distortion, which deepens the defect level in the band gap. Our DMC results for defect transition levels and optical transitions are in good agreement with recent experiments. Our results demonstrates that highly accurate treatment of electron correlation can improve prediction of defect properties in challenging semiconductor materials.

**3:06PM P20.00004 Diffusion Monte Carlo study of the metal-insulator transition in stretched graphene<sup>1</sup>**, LI CHEN, LUCAS K. WAGNER, University of Illinois at Urbana Champaign — At low energies and equilibrium geometries, graphene is well-described by a single-band Hubbard model[1], with  $U/t$  1.4, which is well within the semimetal regime. One would expect that under tensile stress,  $U/t$  should increase and a transition from semimetal to Mott insulator should occur. However, the bonding  $\sigma$  electrons are also affected by the stretching and may affect the applicability of the single-band model. At the same time, the critical region near the metal-insulator transition is a highly multi-determinantal ground state which is a challenging case for fixed node diffusion Monte Carlo simulations. We address progress on both these points by assessing a number of wave functions for the critical region around the transition and assessing the validity of the single-band Hubbard model using the method of Ref 1. [1]. Changlani, Zheng, and Wagner, J. Chem. Phys. 143, 102814 (2015).

<sup>1</sup>This work was supported by NSF DMR 1206242.

**3:18PM P20.00005 Time-dependent many-variable variational Monte Carlo method for nonequilibrium strongly correlated electron systems**, KOTA IDO, TAKAHIRO OHGOE, MASATOSHI IMADA, Univ. of Tokyo — Strongly correlated electron systems driven out of equilibrium have attracted much attention because of potential routes to realizing intriguing phenomena that are not attainable in the equilibrium. To treat such systems, we propose a time-dependent trial wave function with many variational parameters for the time-dependent variational Monte Carlo (t-VMC) method [1]. As the trial state, we adopt the generalized pair-product wave function with correlation factors and quantum-number projections. This trial wave function has been proven to accurately describe ground states of strongly correlated electron systems [2]. To show the accuracy and efficiency of our trial wave function in nonequilibrium states as well, we present our benchmarks for relaxation dynamics during and after interaction quench protocols of the Hubbard models both at and away from half-filling. We find that our trial wave function well reproduces the exact results for the time evolution of physical quantities such as momentum distribution and superconducting correlations. We discuss how the accuracy depends on the level of trial wave functions. [1] K. Ido, T. Ohgoe, and M. Imada, arXiv: 1507.00274. [2] D. Tahara and M. Imada, J. Phys. Soc. Jpn. 77,114701(2008).

**3:30PM P20.00006 ABSTRACT WITHDRAWN —**

**3:42PM P20.00007 Stochastic Approximation of Dynamical Exponent at Quantum Critical Point**, HIDEMARO SUWA, Department of Physics, The University of Tokyo, SHINYA YASUDA, Department of Applied Physics, The University of Tokyo, SYNGE TODO, Department of Physics, The University of Tokyo — We have developed a unified finite-size scaling method for quantum phase transitions that requires no prior knowledge of the dynamical exponent  $z$ . During a quantum Monte Carlo simulation, the temperature is automatically tuned by the Robbins-Monro stochastic approximation method, being proportional to the lowest gap of the finite-size system. The dynamical exponent is estimated in a straightforward way from the system-size dependence of the temperature. As a demonstration of our novel method, the two-dimensional  $S = 1/2$  quantum  $XY$  model, or equivalently the hard-core boson system, in uniform and staggered magnetic fields is investigated in the combination of the world-line quantum Monte Carlo worm algorithm. In the absence of a uniform magnetic field, we obtain the fully consistent result with the Lorentz invariance at the quantum critical point,  $z = 1$ . Under a finite uniform magnetic field, on the other hand, the dynamical exponent becomes two, and the mean-field universality with effective dimension  $(2+2)$  governs the quantum phase transition. We will discuss also the system with random magnetic fields, or the dirty boson system, bearing a non-trivial dynamical exponent.

Reference: S. Yasuda, H. Suwa, and S. Todo *Phys. Rev. B* **92**, 104411 (2015); arXiv:1506.04837

**3:54PM P20.00008 Auxiliary-field based trial wave functions in quantum Monte Carlo simulations<sup>1</sup>**, CHIA-CHEN CHANG, Univ of California - Davis, BRENDA RUBENSTEIN, MIGUEL MORALES, Lawrence Livermore National Laboratory — We propose a simple scheme for generating correlated multi-determinant trial wave functions for quantum Monte Carlo algorithms. The method is based on the Hubbard-Stratonovich transformation which decouples a two-body Jastrow-type correlator into one-body projectors coupled to auxiliary fields. We apply the technique to generate stochastic representations of the Gutzwiller wave function, and present benchmark results for the ground state energy of the Hubbard model in one dimension. Extensions of the proposed scheme to chemical systems will also be discussed.

<sup>1</sup>This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344, 15-ERD-013

**4:06PM P20.00009 Diffusion Quantum Monte Carlo predictions for bulk  $\text{MnNiO}_3$ <sup>1</sup>**, CHANDRIMA MITRA, JARON KROGEL, FERNANDO A. REBOREDO, Oak Ridge National Laboratory —  $\text{MnNiO}_3$  is a strongly correlated transition metal oxide that has recently been investigated theoretically for its potential application as an oxygen-evolution photo-catalyst. However, there is no experimental report on critical quantities like its band gap or its bulk modulus. Recent theoretical predictions with standard functionals, such as PBE+U and HSE show large discrepancies in the band-gaps (about 1.23 eV), depending on the nature of the functional used. Hence, there is clearly a need for an accurate quantitative prediction of the band-gap in order to decide its usefulness as a photo-catalyst. In this work, we present Diffusion Quantum Monte Carlo (DMC) study of the bulk properties of  $\text{MnNiO}_3$ . This includes the quasiparticle band gap for the two spin channels, the equilibrium lattice parameter and the bulk modulus. The DMC approach has already been shown to achieve excellent agreement with experimental results for other oxides such as  $\text{ZnO}$ ,  $\text{NiO}$  and  $\text{Fe}_2\text{O}_3$ . To our knowledge,  $\text{MnNiO}_3$  is the first case where this theory is applied before experiments are done.

<sup>1</sup>This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division

**4:18PM P20.00010 Fragmented Molecular Orbital with Diffusion Monte Carlo for large molecular systems**, ANOUAR BENALI, SPENCER R. PRUITT, Argonne National Laboratory - USA, DMITRI G. FEDOROV, National Institute of Advanced Industrial Science and Technology (AIST) - Japan — Performing accurate quantum mechanics (QM) calculations on larger and larger systems, while maintaining a high level of accuracy is an ongoing effort in many ab initio fields. Many different attempts have been made to develop highly scalable and accurate methods. The fragment molecular orbital (FMO) method is an ab initio method capable of taking advantage of modern supercomputers, such as the Blue Gene Q system Mira at the Argonne National Laboratory Leadership Computing Facility (ALCF). FMO is based on dividing molecules into fragments and performing ab initio calculations on fragments, their dimers and, optionally, trimers. This decomposition makes it possible to perform QM calculations of real size biological molecules. In contrast to many other fragment-based methods, the effect of the environment is rigorously accounted for by computing the electrostatic potential (ESP) due to remaining fragments that are not explicitly included in a given monomer, dimer, or trimer calculation. The use of highly accurate levels of theory, such as Diffusion Monte Carlo (DMC-QMC), in conjunction with FMO allows for the goal of highly scalable and accurate all electron calculations demonstrated in this study, on a variety of relevant systems ( $\text{H}_2\text{O}$ )[3-6] and protein using GAMESS and QMCPACK.

**4:30PM P20.00011 Improved measurement scheme of the self energy in the worm-sampled hybridization-expansion quantum Monte Carlo**, MANCHEON HAN, CHOONG-KI LEE, HYOUNG JOON CHOI, Department of Physics, IPAP, and Center for Computational Studies of Advanced Electronic Material Properties, Yonsei University — Hybridization-expansion continuous-time quantum Monte Carlo (CT-HYB) is a popular approach in real material researches because it allows to deal with non-density-density-type interaction. In the conventional CT-HYB, we measure Green's function and find the self energy from the Dyson equation. Because one needs to compute the inverse of the statistical data in this approach, obtained self energy is very sensitive to statistical noise. For that reason, the measurement is not reliable except for low frequencies. Such an error can be suppressed by measuring a special type of higher-order correlation function and is implemented for density-density-type interaction [1]. With the help of the recently reported worm-sampling measurement [2], we developed an improved self energy measurement scheme which can be applied to any type of interactions. As an illustration, we calculated the self energy for the 3-orbital Hubbard-Kanamori-type Hamiltonian with our newly developed method. This work was supported by NRF of Korea (Grant No. 2011-0018306) and KISTI supercomputing center (Project No. KSC-2015-C3-039). [1] H. Hafermann et al., Phys. Rev. B, 85, 205106 (2012) [2] P. Gunacker et al., Phys. Rev. B, 92, 155102 (2015)

**4:42PM P20.00012 Reducing memory demands of splined orbitals in diffusion Monte Carlo calculations**<sup>1</sup>, JARON KROGEL, FERNANDO REBORDO, Oak Ridge National Lab — Quantum Monte Carlo calculations of defect properties of transition metal oxides have become feasible in recent years due to increases in computing power. As the system size has grown, availability of on-node memory has become a limiting factor. The main growth in memory demand stems from the B-spline representation of the single particle orbitals, especially for heavier elements such as transition metals where semi-core states are present. Despite the associated memory costs, splines are computationally efficient. In this work, we explore alternatives to reduce the memory usage of splined orbitals without significantly affecting numerical fidelity or computational efficiency. For the example case of bulk MnO we have currently achieved a memory savings of 50% while only increasing the overall computational cost of the simulation by 15%.

<sup>1</sup>This work is supported by the Materials Sciences & Engineering Division of the Office of Basic Energy Sciences, U.S. Department of Energy (DOE).

**4:54PM P20.00013 Quantum Monte Carlo Computations of the (Mg<sub>1-x</sub>Fe<sub>x</sub>)SiO<sub>3</sub> Perovskite to Post-perovskite Phase Boundary**<sup>1</sup>, YANGZHENG LIN, Extreme Materials Initiative, Geophysical Lab, Carnegie Institution, R.E. COHEN, EMI, Geophysical Lab, Carnegie Inst; Dept. für Geo- und Umweltwissenschaften, Ludwig-Maximilians-Universität, ANDREA FLORIS, Dept Physics, King's College, LUKE SHULENBURGER, Sandia National Labs, KEVIN P. DRIVER, Dept Earth & Planet Sci, Univ of California, Berkeley — We have computed total energies of FeSiO<sub>3</sub> and MgSiO<sub>3</sub><sup>[1]</sup> perovskite and post-perovskite using diffusion Monte Carlo with the qmcpack GPU code. In conjunction with DFT+U computations for intermediate compositions (Mg<sub>1-x</sub>Fe<sub>x</sub>)SiO<sub>3</sub> and phonons computed using density functional perturbation theory (DFPT) with the pwscf code, we have derived the chemical potentials of perovskite (Pv) and post-perovskite (PPv) (Mg<sub>1-x</sub>Fe<sub>x</sub>)SiO<sub>3</sub> and computed the binary phase diagram versus P, T, and X using a non-ideal solid solution model. The finite temperature effects were considered within quasi-harmonic approximation (QHA). Our results show that ferrous iron stabilizes PPv and lowers the Pv-PPv transition pressure, which is consistent with previous theoretical and some experimental studies. We will discuss the correlation between the Earth's D layer and the Pv to PPv phase boundary. Computations were performed on XSEDE machines, and on the Oak Ridge Leadership Computing Facility (OLCF) machine Titan under project CPH103geo of INCITE program. [1] Lin et al., Phys. Rev. B 90(18), 184103 (2014)

<sup>1</sup>E-mail: rcohen@carnegiescience.edu; This work is supported by NSF.

**5:06PM P20.00014 Fixed-phase vs fixed-node quantum Monte Carlo with local and nonlocal interactions**, LUBOS MITAS, CODY MELTON, North Carolina State Univ — We study several systems that can be formulated in the fixed-phase and/or fixed-node framework in quantum Monte Carlo calculations. In particular, we try to understand the differences between the biases caused by these approximations that result from using complex vs real trial wave functions. One system is a model that enables us to construct systematically the same type of nodal errors in both real and complex formalism. The errors are comparably similar whenever trial functions are correspondingly accurate. Another aspect of the fixed-phase vs fixed-node approximations is studied for systems with nonlocal operators such as with pseudopotentials and/or spin-orbit effects. We specify how to obtain variational formulation for complex wave functions and nonlocal operators in a manner analogous to the fixed-node calculations with T-moves algorithm. In particular, we show that the fixed-phase/fixed-node is the primary condition for proving that the upper bound property holds.

**5:18PM P20.00015 ABSTRACT MOVED TO C45.014 —**

**Wednesday, March 16, 2016 2:30PM - 5:30PM —**

**Session P21 GSCCM DCOMP DMP/DCP: Materials in Extremes: Energetic Materials and Reactive Chemistry** 320 - Gerrit Sutherland, Army Research Laboratory

**2:30PM P21.00001 Moving beyond feasibility in ultrafast shock chemistry experiments**<sup>1</sup>, MICHAEL ARMSTRONG, JAMES LEWICKI, JONATHAN CROWHURST, JOSEPH ZAUG, HARRY RADOUSKY, ELISSAIOS STAVROU, APRIL SAWVEL, Lawrence Livermore National Laboratory — Although ultrafast hydrodynamic methods to investigate the chemistry of shocked materials on ps to ns time scales are generally mature, questions about the interpretation of such experiments remain. Most ultrafast experiments employ shock etalon methods whose interpretation depends on assumptions about the index of refraction of the shocked state. Further, although signatures for chemistry in longer time scale time-of-flight (ToF) experiments are well understood, ultrafast chemistry experiments have not typically employed ToF methods. The use of ToF methods in ultrafast experiments would enable a more straightforward connection to longer time scale data, and would generally provide more information than shock etalon methods. Finally, ultrafast experiments have not been performed over time scales greater than a few hundred of picoseconds, significantly limiting the scope of experiments to observe shocked chemistry under typical conditions at larger length scales. Here we address all of these issues by presenting data from shocked polymers obtained using both ToF and shock etalon methods, using a 1 ns pump and observation window. We compare the results of these two methods to reconcile data from these different methods and strengthen the interpretation of both types of experiment.

<sup>1</sup>Prepared by LLNL under Contract DE-AC52-07NA27344.

**2:42PM P21.00002 High-temperature thermal degradation of polyethylene from reactive molecular dynamics**, J. MATTHEW D. LANE, NATHAN W. MOORE, Sandia Natl Labs — Thermal degradation of polyethylene is studied under extremely high-rate temperature ramp rates from  $10^{14}$  to  $10^{10}$  K/s in isochoric, condensed phases. The molecular evolution and macroscopic state variables are extracted as a function of density from reactive molecular dynamics simulations using the ReaxFF potential. These results are used to parameterize a kinetic rate model for the dissociation and coalescence of hydrocarbons as a function of temperature, temperature ramp rate, and density. The results are contrasted to first-order random-scission macrokinetic models often assumed for pyrolysis of linear polyethylene under ambient conditions. Sandia National Laboratories is a multi program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energys National Nuclear Security Administration under contract DE-AC04- 94AL85000.

**2:54PM P21.00003 Using Force-Matched Potentials To Improve the Accuracy of Density Functional Tight Binding for Reactive Conditions**, NIR GOLDMAN, Lawrence Livermore National Laboratory — In this work, we show that force matching can be used to determine accurate density functional tight binding (DFTB) models for reactive materials under extreme conditions. Determination of chemical reactivity in high-pressure experiments is an unsolved problem that can span timescales orders of magnitude longer than what can be achieved with standard quantum simulation approaches, such as Kohn-Sham Density Functional Theory. DFTB holds promise as a semi-empirical quantum simulation method that yields a high degree of computational efficiency while potentially retaining the accuracy of these higher order methods. Here, we show that force matching can be used to determine accurate repulsive energies for DFTB for chemical reactivity in condensed phases. Our new models yield improved predictions for physical properties of molten liquid carbon, as well as small molecule production in phenolic polymer combustion. Our approach is general and can be implemented as a way to extend quantum simulations to several orders of magnitude longer timescales than previously possible, allowing for direct comparison with experiments.

**3:06PM P21.00004 High-Velocity Collisions of Nanoparticles**, DONALD JOHNSON, WILLIAM MATTSON, Army Research Laboratory — Nanoparticles (NPs) are interesting materials with exciting applications due to their large surface-to-volume ratio and functionalizable surfaces. The large surface area and potentially high surface tension might result in unique materials behavior when subject to shock loading. Using density functional theory, we have simulated high-velocity NP collisions producing high-pressure, high-temperature, and extreme shock conditions. NPs composed of diamond-C, cubic-BN, and diamond-Si were considered with particle sizes up to 3.5 nm diameter. Some simulations involved NPs that were destabilized by incorporating internal strain. Normal, spherical NPs were carved out of bulk crystals and structurally optimized while the NPs with internal strain were constructed as a dense core (compressive strain) encompassed by a thin shell (tensile strain). Both on-axis and off-axis collisions were simulated at various speeds. Collision dynamics, shock propagation, and fragmentation will be presented and analyzed. The effect of material properties, internal strain, and collision velocity on the final temperature of the fragments will be discussed.

**3:18PM P21.00005 Non-equilibrium Reaction Kinetics in Molecular Solids**, MITCHELL WOOD, ALEJANDRO STRACHAN, Materials Engineering, Purdue University — We explore the possibility of non-statistical chemical reactions in condense-phase energetic materials via reactive molecular dynamics (MD) simulations. We characterize the response of three unique high energy density molecular crystals to different types of insults: electric fields of various frequencies ( $100\text{-}4000\text{cm}^{-1}$ ) and strengths and direct heating at various rates. We find that non-equilibrium states can be created for short timescales when energy input targets specific vibrations through the electric fields, and that equilibration eventually occurs even while the insults remain present. Interestingly, for strong fields these relaxation timescales are comparable to those of the initial chemical decomposition of the molecules. Details of how this vibrational energy localization affects the preferred uni- or multi-molecular reactions are discussed. These results provide insight into non-equilibrium or coherent initiation of chemistry in the condensed phase that would of interest in fields ranging from catalysis to explosives.

**3:30PM P21.00006 Detonation Propagation in Slabs and Axisymmetric Rate Sticks<sup>1</sup>**, CHRISTOPHER ROMICK, None, TARIQ ASLAM, Los Alamos National Laboratory — Insensitive high explosives (IHE) have many benefits; however, these IHEs exhibit longer reaction zones than more conventional high explosives (HE). This makes IHEs less ideal explosives and more susceptible to edge effects as well as other performance degradation issues. Thus, there is a resulting reduction in the detonation speed within the explosive. Many HE computational models, e. g. WSD, SURF, CREST, have shock-dependent reaction rates. This dependency places a high value on having an accurate shock speed. In the common practice of shock-capturing, there is ambiguity in the shock-state due to smoothing of the shock-front. Moreover, obtaining an accurate shock speed with shock-capturing becomes prohibitively computationally expensive in multiple dimensions. The use of shock-fitting removes the ambiguity of the shock-state as it is one of the boundaries. As such, the required resolution for a given error in the detonation speed is less than with shock-capturing. This allows for further insight into performance degradation. A two-dimensional shock-fitting scheme has been developed for unconfined slabs and rate sticks of HE. The HE modeling is accomplished by Euler equations utilizing several models with single-step irreversible kinetics in slab and rate stick geometries.

<sup>1</sup>Department of Energy - LANL

**3:42PM P21.00007 Laser-shocked energetic materials with metal additives: evaluation of detonation performance**, JENNIFER GOTTFRIED, ERIC BUKOWSKI, US Army Rsch Lab - Aberdeen — A focused, nanosecond-pulsed laser with sufficient energy to exceed the breakdown threshold of a material generates a laser-induced plasma with high peak temperatures, pressures, and shock velocities. Depending on the laser parameters and material properties, nanograms to micrograms of material is ablated, atomized, ionized and excited in the laser-induced plasma. The subsequent shock wave expansion into the air above the sample has been monitored using high-speed schlieren imaging in a recently developed technique, laser-induced air shock from energetic materials (LASEM) [1]. The estimated detonation velocities using LASEM agree well with published experimental values. A comparison of the measured shock velocities for various energetic materials including RDX, DNTF, and LLM-172 doped with Al or B to the detonation velocities predicted by CHEETAH for inert or active metal participation demonstrates that LASEM has potential for predicting the early time participation of metal additives in detonation events. The LASEM results show that reducing the amount of hydrogen present in B formulations increases the resulting detonation velocities. [1] J.L. Gottfried, Propellants Explos. Pyrotech. 40, 674 (2015).

**3:54PM P21.00008 The Equation of State of PBX 9502**, TARIQ ASLAM, Los Alamos Natl Lab — Reactive flow modeling of high explosives (HEs) requires accurate equation of states (EOS) for both the HE's reactants and products. The Wescott-Stewart-Davis "wide-ranging EOS" model will be examined. A procedure for calibrating both the reactants and products for this EOS will be presented. Several thermodynamic pathways will be explored for the plastic bonded HE PBX 9502. These include: isothermal compression, isentropic compression, single and multiple shock compression, isobaric thermal expansion, adiabatic expansion of the products and the overdriven detonation state. Data from several different experimental techniques are employed to constrain model parameters. Validation tests of the model EOS will also be presented.

**4:06PM P21.00009 Measuring HOMO/LUMO gap of explosive film at air interface using ESFG: model for explosive at void surface**, DARCIE FARROW, IAN KOHL, SEAN KEARNEY, STEPHEN RUPPER, LAURA MARTIN, KATHY ALAM, ROBERT KNEPPER, JEFFERY KAY, Sandia Natl Labs — Vibrational broadband sum frequency generation has enabled measurements of heat transfer/disorder under shock compression on monolayer length scales (Carter, JPCA, 2008). At Sandia, we are extending this approach to examine shock-induced changes in the electronic structure of secondary explosives at surfaces using electronic sum frequency generation (ESFG)(Yamaguchi, JCP, 2008). Theoretical studies suggest explosives at voids and grain boundaries may have different reactivity than bulk material based on shifts in the bandgap at defects (Kuklja, Appl. Phys. A 2003). We seek to measure these electronic shifts for the first time using a thin film explosive samples as a model for the void surface. We will report electronic sum frequency data from vapour deposited thin film explosive compared to UV/Vis data of the bulk film at ambient pressures and discuss application of ESFG technique to samples under shock compression.

**4:18PM P21.00010 Shock wave propagation in semi-crystalline polyethylene: An atomic-scale investigation**, ROBERT M. ELDER, U.S. Army Research Laboratory, THOMAS C. O'CONNOR, Johns Hopkins University, Physics and Astronomy, IN-CHUL YEH, TANYA L. CHANTAWANSRI, TIMOTHY W. SIRK, U.S. Army Research Laboratory, MARK O. ROBBINS, Johns Hopkins University, Physics and Astronomy, JAN W. ANDZELM, U.S. Army Research Laboratory — Highly oriented polyethylene (PE) fibers are used in protection applications, therefore elucidation of their response under high strain-rate impact events is vital. Although PE fibers can have high crystallinity (>95%), they also contain defects such as amorphous domains. Using molecular dynamics simulations, we investigate shock propagation through crystalline, amorphous, and semi-crystalline PE. We generate compressive shock waves of varying strength, quantify their dynamics, and characterize their effect on material properties at the atomic scale. In the semi-crystalline PE model, the differing density and molecular order of amorphous PE and crystalline PE result in differing shock impedances, which causes reflection and refraction of shock waves at interfaces between the phases. We quantify the properties (e.g. pressure, velocity) of the reflected and refracted waves, which differ from those of the incident wave, and compare with results from impedance matching. We also examine the reflection, absorption, and transmission of energy at the crystalline-amorphous interface. Depending on shock strength, amorphous defects can dissipate shock energy, which attenuates the shock and leads to effects such as localized heating.

**4:30PM P21.00011 Hierarchical Multiscale Framework for Materials Modeling: Advances in Scale-Bridging Applied to a Taylor Anvil Impact Test of RDX**, BRIAN BARNES, KENNETH LEITER, RICHARD BECKER, JAROSLAW KNAP, JOHN BRENNAN, US Army Research Laboratory — As part of a multiscale modeling effort, we present progress on a challenge in continuum-scale modeling: the direct incorporation of complex molecular-level processes in the constitutive evaluation. In this initial phase of the research we use a concurrent scale-bridging approach, with a hierarchical multiscale framework running in parallel to couple a particle-based model (the "lower scale") computing the equation of state (EOS) to the constitutive response in a finite-element multi-physics simulation (the "upper scale"). The lower scale simulations of 1,3,5-trinitroperhydro-1,3,5-triazine (RDX) use a force-matched coarse-grain model and dissipative particle dynamics methods, and the upper scale simulation is of a Taylor anvil impact experiment. Results emphasize use of adaptive sampling (via dynamic kriging) that accelerates time to solution, and its comparison to fully "on the fly" runs. Work towards inclusion of a fully reactive EOS is also discussed.

**4:42PM P21.00012 Instantaneous Point Explosion in Incompressible Fluid-like Media**, MICHAEL GRINFELD, STEVEN SEGLETES, The US Army Research Laboratory — The problem of point explosion is one of the most famous and extensively developed in in the sense of corresponding physics, mechanics, and applied mathematics. There are many reasons for that based on its practical importance and theoretical beauty. We refer interested readers to the publications of Sedov, Taylor, Landau and Lifshitz, and Lavrent'ev and Shabat. In the paper, we discuss this classical program from the standpoint of terminal ballistics and present our novel results relating to the special situation when the media can be treated as an "effective" incompressible liquid. Sedov, L.I., Similarity and Dimensional Methods in Mechanics, CRC Press, 1993. Taylor, J., Explosion. II. The Atomic Explosion of 1945. Proc. Roy. Soc. London, A201, 1065, 1950, p. 175. Landau, L.D. and Lifshitz, E.M., Fluid Mechanics, Pergamon Press, 1959. Zeldovich Ya. B. and Raizer, Yu.P., Physics of Shock Waves and High-Temperature Hydrodynamic Phenomena, Dover, New York, 2002. Lavrent'ev, M.A. and Shabat, B.V., Hydrodynamic Phenomena and Their Mathematical Models. Hauka, 1973 (in Russian).

**4:54PM P21.00013 Impacts on Dissipative Sonic Vacuum<sup>1</sup>**, YICHAO XU, VITALI NESTERENKO, Univ of California - San Diego — We investigate the propagating compression bell shape stress waves generated by the strikers with different masses impacting the sonic vacuum — the discrete dissipative strongly nonlinear metamaterial with zero long wave sound speed. The metamaterial is composed of alternating steel disks and Nitrile O-rings. Being a solid material, it has exceptionally low speed of the investigated stress waves in the range of 50 – 74 m/s, which is a few times smaller than the speed of sound or shock waves in air generated by blast. The shape of propagating stress waves was dramatically changed by the viscous dissipation. It prevented the incoming pulses from splitting into trains of solitary waves, a phenomenon characteristic of the non-dissipative strongly nonlinear discrete systems when the striker mass is larger than the cell mass. Both high-speed camera images and numerical simulations demonstrate the unusual rattling behavior of the top disk between the striker and the rest of the system. The linear momentum and energy from the striker were completely transferred to the metamaterial. This strongly nonlinear dissipative metamaterial can be designed for the optimal attenuation of dynamic loads generated by impact or contact explosion.

<sup>1</sup> Author 1 wants to acknowledge the support provided by UCSD.

**5:06PM P21.00014 High-Pressure High-Temperature Phase Diagram of the Organic Crystal Paracetamol<sup>1</sup>**, SPENCER SMITH, JEFFREY MONTGOMERY, YOGESH VOHRA, Univ of Alabama - Birmingham — High-pressure high-temperature (HPHT) Raman spectroscopy studies have been performed on the organic crystal paracetamol in a diamond anvil cell utilizing boron-doped diamond as heating anvil. The HPHT data obtained from boron-doped diamond heater is cross-checked with data obtained using a standard block heater diamond anvil cell. Isobaric measurements were conducted at pressures up to 8.5 GPa and temperature up to 520 K in a number of different experiments. Solid state phase transitions from monoclinic Form I → orthorhombic Form II were observed at various pressures and temperatures as well as transitions from Form II → unknown Form IV. The melting temperature for paracetamol was observed to increase with increasing pressures to 8.5 GPa. Our previous angle dispersive x-ray diffraction studies at the Advanced Photon Source has confirmed the existence of two unknown crystal structures Form IV and Form V of paracetamol at high pressure and ambient temperature. The phase transformation from Form II to Form IV occurs at ~8.5 GPa and from Form IV to Form V occurs at ~11 GPa at ambient temperature. Our new data is combined with the previous ambient temperature high-pressure Raman and X-ray diffraction data to create the first HPHT phase diagram of paracetamol.

<sup>1</sup> DOE-NNSA Carnegie DOE Alliance Center (CDAC) under grant number DE-NA0002006

**5:18PM P21.00015 Modeling the mechanical behavior of ceramic and heterophase structures manufactured using selective laser sintering and spark plasma sintering**, VLADIMIR A. SKRIPNYAK, EVGENIYA G. SKRIPNYAK, VLADIMIR V. SKRIPNYAK, IRINA K. VAGANOVA, National Research Tomsk State University — A model for predicting mechanical properties of ultra-high temperature ceramics and composites manufactured by selective laser sintering (SLS) and spark plasma sintering (SPS) under shock loading is presented. The model takes into account the porous structure, the specific volume and average sizes of phases, and the temperature of sintering. Residual stresses in ceramic composites reinforced with particles of refractory borides, carbides and nitrides after SLS or SPS were calculated. It is shown that the spall strength of diboride-zirconium matrix composites can be increased by the decreasing of porosity and the introduction of inclusions of specially selected refractory strengthening phases.

**Wednesday, March 16, 2016 2:30PM - 5:42PM –**  
**Session P22 DCOMP: General Theory/Computational Physics 321 - Daniel Finkenstadt**

**2:30PM P22.00001 First Principles Computation of G-Factors in Bi and Bi<sub>2</sub>Se<sub>3</sub>**, ZHIDA SONG, SIMIN NIE, XI DI, ZHONG FANG, Chinese Academy of Sci (CAS), T03 TEAM — In this talk, we propose a first principles computation method for g-factor tensor, which not only gives comparable results with experiments but also establishes a clear physical picture of Zeeman effect in materials. In our method, the Hilbert space of the electronic states is treated as a direct product of "inner" space and "orbital" space, which are spanned by Bloch wave-functions and envelope functions respectively. Correspondingly, vector-potential is divided into a periodic part acting only in inner space and a non-periodic part acting only in orbital space. With the above framework we define the g-factors as coupling coefficients between inner space and magnetic field. By the method we developed, we have further computed the g-factors of bismuth and Bi<sub>2</sub>Se<sub>3</sub> and get satisfactory results, which are in good agreement with the experimental data.

**2:42PM P22.00002 Adaptively truncated Hilbert spaces for Hamiltonian-based impurity solvers<sup>1</sup>**, ARA GO, ANDREW MILLIS, Columbia Univ — We investigate truncations of the exponentially large Hilbert space in the exact diagonalization (ED) as an impurity solver for the dynamical mean-field theory (DMFT). A key issue is to maintain the high degree of numerical accuracy required in the construction of Greens functions. We test various truncation schemes with similar number of Slater determinants in both Hilbert spaces for the ground state and a particle- or a hole-excited state, and show that the excited states play an important role in accurate computation as well as the ground state. Appropriate truncation for both spaces enables us to compute the accurate self-energy of the impurity Hamiltonian with up to eight correlated orbitals hybridized with a sufficient number of bath orbitals to obtain converged solutions of the self-consistent equation in the DMFT, which is not solvable by the original ED. Application to spin-orbit coupled multi-orbital models and the one-dimensional Hubbard model and comparison to results from exact diagonalization and the configuration interaction based impurity solvers demonstrate the power of the method.

<sup>1</sup>This work was supported by the US Department of Energy under Grants No. DE-FG02-04ER46169 and DE-SC0006613.

**2:54PM P22.00003 Equilibration properties of a disordered interacting open quantum system**, EVERT VAN NIEUWENBURG, SEBASTIAN HUBER, ETH - Hoenggerberg — The central question in the field of many body localization is if a closed interacting quantum system effectively thermalizes in the presence of disorder. However, any experimental test necessarily involves the opening of the ideally closed quantum system. Both from a fundamental point of view as well as for concrete experimental investigations of many body localization phenomena, a solid understanding of the effect of an attached bath is of significant importance. We study the equilibration properties of disordered interacting open quantum systems. On the one hand we consider the equilibration of such a many body localized system by coupling baths to the ends of a 1D spin chain. We find non-monotonous behaviour of the slowest relaxation time towards equilibrium. On the other hand, we take the bath itself to be a disordered interacting open quantum system and investigate the dephasing of a single qubit coupled to it. The model for the bath has a many body localization transition, affecting the dephasing of the single qubit.

**3:06PM P22.00004 ABSTRACT WITHDRAWN –**

**3:18PM P22.00005 Accurate, efficient, and scalable parallel simulation of mesoscale electrostatic/magnetostatic problems accelerated by a fast multipole method.<sup>1</sup>**, XIKAI JIANG, Argonne National Laboratory, DMITRY KARPEEV, JIYUAN LI, JUAN DE PABLO, University of Chicago, JUAN HERNANDEZ-ORTIZ, National University of Colombia, OLLE HEINONEN, Argonne National Laboratory — Boundary integrals arise in many electrostatic and magnetostatic problems. In computational modeling of these problems, although the integral is performed only on the boundary of a domain, its direct evaluation needs  $O(N^2)$  operations, where  $N$  is number of unknowns on the boundary. The  $O(N^2)$  scaling impedes a wider usage of the boundary integral method in scientific and engineering communities. We have developed a parallel computational approach that utilize the Fast Multipole Method to evaluate the boundary integral in  $O(N)$  operations. To demonstrate the accuracy, efficiency, and scalability of our approach, we consider two test cases. In the first case, we solve a boundary value problem for a ferroelectric/ferromagnetic volume in free space using a hybrid finite element-boundary integral method. In the second case, we solve an electrostatic problem involving the polarization of dielectric objects in free space using the boundary element method. The results from test cases show that our parallel approach can enable highly efficient and accurate simulations of mesoscale electrostatic/magnetostatic problems.

<sup>1</sup>Computing resources was provided by Blues, a high-performance cluster operated by the Laboratory Computing Resource Center at Argonne National Laboratory. Work at Argonne was supported by U. S. DOE, Office of Science under Contract No. DE-AC02-06CH11357.

**3:30PM P22.00006 Computational algorithms dealing with the classical and statistical mechanics of celestial scale polymers in space elevator technology**, STEVEN KNUDSEN, LEONARDO GOLUBOVIC, West Virginia University — Prospects to build Space Elevator (SE) systems have become realistic with ultra-strong materials such as carbon nano-tubes and diamond nano-threads. At cosmic length-scales, space elevators can be modeled as polymer like floppy strings of tethered mass beads. A new venue in SE science has emerged with the introduction of the Rotating Space Elevator (RSE) concept [1,2] supported by novel algorithms discussed in this presentation. An RSE is a loopy string reaching into outer space. Unlike the classical geostationary SE concepts of Tsiolkovsky, Artsutanov, and Pearson, our RSE exhibits an internal rotation. Thanks to this, objects sliding along the RSE loop spontaneously oscillate between two turning points, one of which is close to the Earth whereas the other one is in outer space. The RSE concept thus solves a major problem in SE technology which is how to supply energy to the climbers moving along space elevator strings. The investigation of the classical and statistical mechanics of a floppy string interacting with objects sliding along it required development of subtle computational algorithms described in this presentation. [1] L. Golubovic and S. Knudsen, Europhys. Lett. 86, 34001 (2009); [2] S. Knudsen and L. Golubovic, Eur. Phys. J. Plus 129, 242 (2014).

**3:42PM P22.00007 Convex Lower Bounds for Free Energy Minimization** , JONATHAN MOUSSA, Sandia National Laboratories — We construct lower bounds on free energy with convex relaxations from the nonlinear minimization over probabilities to linear programs over expectation values. Finite-temperature expectation values are further resolved into distributions over energy. A superset of valid expectation values is delineated by an incomplete set of linear constraints. Free energy bounds can be improved systematically by adding constraints, which also increases their computational cost. We compute several free energy bounds of increasing accuracy for the triangular-lattice Ising model to assess the utility of this method. This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

**3:54PM P22.00008 Stabilized quasi-Newton optimization of noisy potential energy surfaces** , BASTIAN SCHAEFER, Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland, S. ALIREZA GHASEMI, Institute for Advanced Studies in Basic Sciences, P.O. Box 45195-1159, IR-Zanjan, Iran, SHANTANU ROY, STEFAN GOEDECKER, Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland, GOEDECKER GROUP TEAM — Optimizations of atomic positions belong to the most frequently performed tasks in electronic structure calculations. Many simulations like global minimum searches or the identification of chemical reaction pathways can require the computation of hundreds or thousands of minimizations or saddle points. To automatize these tasks, optimization algorithms must not only be efficient but also very reliable. Unfortunately, computational noise in forces and energies is inherent to electronic structure codes. This computational noise poses a severe problem to the stability of efficient optimization methods like the limited-memory BroydenFletcherGoldfarbShanno algorithm. In this talk a recently published technique that allows to obtain significant curvature information of noisy potential energy surfaces is presented. This technique was used to construct both, a stabilized quasi-Newton minimization method and a stabilized quasi-Newton saddle finding approach. With the help of benchmarks both the minimizer and the saddle finding approach were demonstrated to be superior to comparable existing methods.

**4:06PM P22.00009 Phonon softening and mechanical failure of graphene under tensile strain** , JEONGWOON HWANG, JISOON IHM, Seoul Natl Univ, KYUNG-SUK KIM, MOON-HYUN CHA, Brown Univ — Phonon softening of graphene under tensile strain is investigated based on ab initio density functional theory calculations. From calculated phonon band structures, we show that the Kohn anomaly point shifts from a high symmetry  $K$  point to a lower symmetry one as a consequence of the Dirac point shift in the electronic band structure. We demonstrate that, over a wide range of tensile strain directions, the strain-induced enhancement of phonon softening can give rise to phonon instabilities resulting in a mechanical failure of graphene at lower strains. It is shown that there are two types of instabilities associated with phonons near  $K$  and  $\Gamma$  points, respectively, which induce symmetry-breaking structural distortions, and both of them lead to mechanical failure prior to the elastic failure commonly expected when the structural symmetry is retained.

**4:18PM P22.00010 Adjoint based data assimilation for phase field model using second order information of a posterior distribution** , SHIN-ICHI ITO, HIROMICHI NAGAO, The University of Tokyo, AKINORI YAMANAKA, Tokyo University of Agriculture and Technology, YUHKI TSUKADA, TOSHIYUKI KOYAMA, Nagoya University, JUNYA INOUE, The University of Tokyo — Phase field (PF) method, which phenomenologically describes dynamics of microstructure evolutions during solidification and phase transformation, has progressed in the fields of hydromechanics and materials engineering. How to determine, based on observation data, an initial state and model parameters involved in a PF model is one of important issues since previous estimation methods require too much computational cost. We propose data assimilation (DA), which enables us to estimate the parameters and states by integrating the PF model and observation data on the basis of the Bayesian statistics. The adjoint method implemented on DA not only finds an optimum solution by maximizing a posterior distribution but also evaluates the uncertainty in the estimations by utilizing the second order information of the posterior distribution. We carried out an estimation test using synthetic data generated by the two-dimensional Kobayashi's PF model. The proposed method is confirmed to reproduce the true initial state and model parameters we assume in advance, and simultaneously estimate their uncertainties due to quality and quantity of the data. This result indicates that the proposed method is capable of suggesting the experimental design to achieve the required accuracy.

**4:30PM P22.00011 Quantum Monte Carlo study of 4d vs 5d atomic and molecular systems.** , MICHAEL BENNETT, North Carolina State University, ADEM KULAHLIOGLU, Melikshah University, CODY MELTON, LUBOS MITAS, North Carolina State University — We investigate the electronic properties of Mo and W atomic and molecular systems by quantum Monte Carlo (QMC) methods. One area of interest in these systems are the systematic changes in the fixed-node errors from 4d to 5d elements and corresponding changes in the correlation effects. We find that similarly to first and second-row systems the fixed-node biases grow with increasing degree of charge localization for similarly complex wave functions and bonding patterns. The second area of interest is the impact of relativistic effects on the electronic structure, in particular, to which extent they affect the bonding properties. We use scalar-relativistic energy-consistent pseudopotentials with averaged spin-orbit effects and we contrast these calculations with the explicit inclusion of the spin-orbit in the two-component framework.

**4:42PM P22.00012 Information geometry with correlated data: Bayesian explorations of cosmological predictions for the microwave background radiation<sup>1</sup>** , KATHERINE QUINN, FRANCESCO DE BERNARDIS, MICHAEL NIEMACK, JAMES SETHNA, Cornell Univ — We developed a new, generalized fitting algorithm for multiparameter models which incorporates varying and correlated errors. This was combined with geometrical methods of sampling to explore model prediction space, notably to plot geodesics and determine the size and edges of the model manifold. We illustrate this using the microwave background spectra for all possible universes, as described by the standard  $\Lambda$ -cold dark matter ( $\Lambda$ -CDM) cosmological model. In this case, the predicted data are fluctuations and highly correlated with varying errors, resulting in a manifold with a varying metric (as the natural metric to use is given by the Fisher information matrix). Furthermore, the model manifold shares the hyperribbon structure seen in other models, with the edges forming a strongly distorted image of a hypercube. Practical applications of such an analysis include optimizing experimental instrumentation designed to test more detailed cosmological theories.

<sup>1</sup>Funding supported in part by NSERC

**4:54PM P22.00013 Recasting the 3D Wigner-Liouville equation with spectral components of the force** , MAARTEN VAN DE PUT, BART SORE, WIM MAGNUS, Univ of Antwerp, imec — The phasespace approach to many-body quantum mechanics, by means of the Wigner-function is interesting through its connection to classical mechanics. Time-evolution of any statistical distribution of states under influence of a (time-dependent) Hamiltonian is obtained through use of the Wigner-Liouville equation. The standard form of this equation contains two 3D integrals, over the entire phase space. As a result, this form emphasizes the non-locality of the interaction of the potential, but lacks simplicity and ease of understanding. Furthermore, the integrals make numerical solution of the Wigner-Liouville equation challenging. We present an alternative form to the Wigner-Liouville equation based on the force rather than the potential, in alignment with the classical Boltzmann equation. Decomposition of the force in its spectral components yields a simpler form of the Wigner-Liouville equation. This new form has only one 3D integral over the spectral force components, and is local in position, simplifying both interpretation and numerical implementation. Because of its use of the force, it straightforwardly reduces to the Boltzmann equation under classical conditions.

**5:06PM P22.00014 Exciton condensation in one dimension<sup>1</sup>** , DAVID ABERGEL, ADRIAN KANTIAN, NORDITA — We show the existence of a stable bilayer exciton condensate in one dimension, which demonstrates both true long-range order and non-negligible pairing amplitude. The condensate is stabilized by a finite inter-wire tunneling between two parallel quasi-1D wires, which we propose as the system in which to realize the condensate. Combining numerical DMRG, mean-field approaches, and bosonization to go beyond perturbation theory, we analyze experiments which will demonstrate the off-diagonal long-range order and verify the associated non-negligible pairing amplitude of the exciton condensate.

<sup>1</sup>DSLA acknowledges support from ERC grant DM-321031

**5:18PM P22.00015 Rotationally invariant ensembles of integrable matrices<sup>1</sup>** , JASEN SCARAMAZZA, EMIL YUZHASHYAN, Department of Physics and Astronomy, Rutgers University, SRIRAM SHASTRY, Physics Department, University of California, Santa Cruz — We construct ensembles of *random integrable matrices* with any prescribed number of nontrivial integrals and formulate *integrable matrix theory* (IMT) – a counterpart of random matrix theory (RMT) for quantum integrable models. A type- $M$  family of integrable matrices consists of exactly  $N - M$  independent commuting  $N \times N$  matrices linear in a real parameter. We first develop a rotationally invariant parameterization of such matrices, previously only constructed in a preferred basis. For example, an arbitrary choice of a vector and two commuting Hermitian matrices defines a type-1 family and vice-versa. Higher types similarly involve a random vector and two matrices. The basis-independent formulation allows us to derive the joint probability density for integrable matrices, in a manner similar to the construction of Gaussian ensembles in the RMT.

<sup>1</sup>This work was supported in part by the David and Lucille Packard Foundation. The work at UCSC was supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES) under Award FG02-06ER46319.

**5:30PM P22.00016 Matrix Elements for Hylleraas CI** , FRANK E. HARRIS, University of Florida — The limitation to at most a single interelectron distance in individual configurations of a Hylleraas-type multiconfiguration wave function restricts significantly the types of integrals occurring in matrix elements for energy calculations, but even then if the formulation is not handled efficiently the angular parts of these integrals escalate to create expressions of great complexity. This presentation reviews ways in which the angular-momentum calculus can be employed to systematize and simplify the matrix element formulas, particularly those for the kinetic-energy matrix elements.

**Wednesday, March 16, 2016 2:30PM - 5:30PM –**  
**Session P23 DMP DCOMP: Computational Materials Discovery and Design - Defects and Interfaces** 322 - Vladan Stevanovic, Colorado School of Mines

**2:30PM P23.00001 Computational design of inorganic-organic hybrid materials energy storage and conversion** , ALEXIE KOLPAK, Massachusetts Inst of Tech-MIT — Hybrid inorganic-organic materials are of interest for the design of new functional materials that combine the advantages of both organic and inorganic components to optimize properties and/or obtain new physical phenomena. In this talk, I will discuss our recent work using first-principles density functional theory to design nanostructured hybrid materials for energy storage and conversion applications. In particular, I will discuss the electronic, optical, thermal, and mechanical properties of a class of nanostructured hybrid materials based on layered transition metal phosphates, showing that these materials offer a highly tunable platform for the design of efficient, flexible photovoltaics and thermoelectrics. In addition to optimizing individual properties, I will also discuss exciting possibilities for using this platform for the design of materials with strong coupling between functionalities.

**3:06PM P23.00002 Theoretical and Experimental Studies of Designed Molecular Interfaces for Improved Thermal Conductivity<sup>1</sup>** , ALEX KERR, KIERAN MULLEN, Homer L. Dodge Dept. of Physics and Astronomy, DANIEL GLATZHOFFER, MATTHEW HOUCK, Department of Chemistry and Biochemistry, University of Oklahoma, PAUL HUANG, School of Chemical, Biological & Materials Engineering, University of Oklahoma — Certain molecular structures such as carbon nanotubes (CNTs) can potentially improve the thermal conductivity of composite materials. However, their thermal boundary resistance is an obstacle to their effective implementation as a medium for heat flow. We are concerned with overcoming this Kapitza resistance with the aid of chemical functional groups. These functional groups will, in principal, eliminate phonon mismatch between our structures and their matrix. The result will maximize the transmission of thermal vibrations to and from their surrounding medium. We develop a method to predict the thermal properties of our functionalized materials through the calculation of vibrational normal modes and Green's functions. We show how the configuration of attached functional groups affect the samples' thermal conductivity ( $\kappa$ ) and attempt to find the arrangement in which  $\kappa$  is maximized. We will make explicit comparisons with thermal conductivity experiments done on nanocomposites of functionalized and pristine CNTs. We will discuss how the bonds connecting the functional groups to the CNT affects  $\kappa$ . We compare these results to measurements on our particular synthesized materials and discuss how to better optimize their design.

<sup>1</sup>This work was supported by supported by NSF grant DMR-1310407.

**3:18PM P23.00003 Modifying the Optoelectronic Properties of Rubrene by Strain<sup>1</sup>** , SAHAR SHARIFZADEH, Department of Electrical and Computer Engineering, Boston University, ASHWIN RAMASUBRAMANIAM, Department of Mechanical & Industrial Engineering, University of Massachusetts Amherst — Rubrene crystals are promising organic electronic and optoelectronic materials due to their high charge carrier mobility. Recent studies have shown that the electronic properties of rubrene films can be tuned by substrate-induced strain, suggesting a new route towards the design of more efficient devices. Here, we present a first-principles density functional theory and many-body perturbation theory analysis of strain-induced changes to the mechanical, electronic, and optical properties of rubrene crystals. With an applied strain that is consistent with experiment, we predict changes of hole mobilities in excellent agreement with electrical conductivity measurements. Furthermore, we predict that the optical absorption and nature of low-energy excitons within the crystal can be tuned by an applied strain as low as 1%.

<sup>1</sup>This work utilized resources at the Center for Nanoscale Materials, supported by the U.S. Department of Energy under Contract No. DE-AC02-06CH11357.

**3:30PM P23.00004 First-principles studies of the electric-field effect on the band structure of trilayer graphenes<sup>1</sup>**, YUN-PENG WANG, XIANG-GUO LI, HAI-PING CHENG, University of Florida — Electric-field effects on the electronic structure of trilayer graphene are investigated using the density functional theory in the generalized gradient approximation. Two different stacking orders, namely Bernal and rhombohedral, of trilayer graphene are considered. Our calculations reproduce the experimentally data on band gap opening in Bernal stacking and band overlap in rhombohedral trilayer graphene. In addition, we studied effects of charge doping using dual gate configurations. The size of band gap opening in Bernal trilayer graphene can be tuned by charge doping, and charge doping also causes an electron-hole asymmetry in the density of states. Furthermore, hole-doping can reopen a band gap in the band overlapping region of rhombohedral trilayer graphene induced by electric fields, which contributes to an extra peak in the optical conductivity spectra.

<sup>1</sup>This work is supported by DOE DE-FG02-02ER45995

**3:42PM P23.00005 Design of transparent conductors and periodic two-dimensional electron gases without doping**, XIUWEN ZHANG, LIJUN ZHANG, ALEX ZUNGER, Renewable and Sustainable Energy Institute, University of Colorado, Boulder, Colorado, JOHN PERKINS, National Renewable Energy Laboratory, Golden, Colorado, MATERIALS BY DESIGN TEAM, JOHN D. PERKINS COLLABORATION — The functionality of transparency plus conductivity plays an important role in renewable energy and information technologies, including applications such as solar cells, touch-screen sensors, and flat panel display. However, materials with such seemingly contraindicated properties are difficult to come by. The traditional strategy for designing bulk transparent conductors (TCs) starts from a wide-gap insulator and finds ways to make it conductive by extensive doping. We propose a different strategy [1] for TC design—starting with a metallic conductor and designing transparency by control of intrinsic interband transitions and intraband plasmonic frequency. We identified specific design principles for prototypical intrinsic TC classes and searched computationally for materials that satisfy them. The electron gases in the 3D intrinsic TCs demonstrate intriguing properties, such as periodic 2D electron gas regions with very high carrier density. We will discuss a more extended search of these functionalities, in parallel with stability and growability calculations. [1] X. Zhang, L. Zhang, J. D. Perkins, and A. Zunger, Phys. Rev. Lett. 115, 176602 (2015). Supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Grant No. DEFG02-13ER46959.

**3:54PM P23.00006 Role of  $sp^3$  Defect in Ordered Nanoporous Carbon**, ENSHI XU, ANGELA LUEKING, VINCENT CRESPI, PAUL LAMMERT, Pennsylvania State Univ, KATHLEEN MALESKI, Washington College — Schwarzite is considered an ideal model for nanoporous carbon and is energetically more stable than fullerene. However, carbon don't form well-ordered Schwarzite-type nanoporous material possibly due to kinetic arrests under pyrolytic conditions. We computationally discovered a new thermodynamically stable local defect in carbon  $sp^2$  networks: an  $sp^3$  carbon defect, which inspires new solutions to the problem. The defect is most stable in nanoporous carbon (i.e., networks with negative curvatures, known as Schwarzites) and its topological merit, carrying negative curvature, results in the design of new model structures of nanoporous materials (periodic, negatively-curved networks), and provides a handle of the negative curvature carrier in nanoporous carbon, and we propose a kinetics-dominated synthetic route to novel nanoporous carbon with long range order by controlling the  $sp^3$  defect through  $sp^3$  carbon atom injection or Si atom substitution, with the aid of first principle molecular dynamics simulation. Calculations also suggest the defect can be observed by Raman.

**4:06PM P23.00007 Computational Discovery of a Novel Semiconductor: A Vacancy-Ordered  $Fe_{1.5}TiSb$  Heusler Phase**, VINAY ISHWAR HEGDE, Northwestern University, NARIMAN NAGHIBOLASHRAFI, SAHAR KESHAVARZ, KAMARAM MUNIRA, WILLIAM BUTLER, PATRICK LECLAIR, The University of Alabama, CHRIS WOLVERTON, Northwestern University — Many full- and half-Heusler phase compounds are half-metallic ferromagnets, and are attractive for spintronic applications due to their relatively high Curie temperatures. However, while it is known that defects such as vacancies (on the X site of an  $X_2YZ$  Heusler phase) can lead to a loss of half-metallic character, their effect on the stability and order of these compounds has not been adequately explored. To address this shortcoming, we perform a binary cluster expansion (CE) of Fe and vacancies on the Fe sublattice of the  $Fe_xVac_{2-x}TiSb$  Heusler compound. From our CE, we computationally predict the stability of a novel semiconductor phase with an interesting new structure type:  $R\bar{3}m$  spacegroup with composition  $Fe_{1.5}TiSb$ , i.e., between the full- and half-Heusler compositions. By comparing the electronic structure of all the competing structures at  $x = 1.5$ , we find that the gap opened in the minority-spin channel due to vacancies strongly correlates with the stability of the structure. We study the effect of vacancies on the structural order in  $Fe_{1.5}TiSb$  by generating special quasi-random structures (SQSs) as approximations to the true disordered state, and find that the material undergoes an order-disorder transition at elevated temperatures of  $\sim 1450$  K.

**4:18PM P23.00008 Doping and defects by design:  $Ga_2O_3$ <sup>1</sup>**, STEPHAN LANY, NREL — Density functional supercell calculations are widely employed to describe the defect physics in semiconductors and insulators. Due to a variety of challenges such as finite size effects for charged defects and the band gap error of DFT, results were often controversial in the past. With developments over the past decade, defect theory should hopefully be truly predictive, and be able to guide experimental efforts. The present work on n-type doping in  $Ga_2O_3$  compares different potential doping routes via anion-site doping with F, and cation site doping with group IV elements (C, Si, Ge, Sn). The study addresses dopant solubility, electrical activity, and compensation by native defects, including non-equilibrium effects due to supersaturated dopant concentrations and the mechanism of dopant-defect pair formation.

<sup>1</sup>supported by DOE-SC-BES as part of an Energy Frontier Research Center

**4:30PM P23.00009 Understanding the Impact of Point Defects on the Optoelectronic Properties of Gallium Nitride from First-Principles<sup>1</sup>**, KIRK LEWIS, MASAHICO MATSUBARA, ENRICO BELLOTTI, SAHAR SHARIFZADEH, Department of Electrical and Computer Engineering, Boston University — Gallium nitride (GaN) and related alloys form a class of wide bandgap semiconductors that have broad applications as components in optoelectronic devices; in particular, power electronics and blue and ultraviolet optical devices. Nitride films grow with high defect densities, and understanding the relationship between structural defects and optoelectronic function will be central to the design of new high-performance materials. Here, we take a first-principles density functional theory (DFT) and many-body perturbation theory (MBPT) approach to quantify the influence of defects on the electronic and optical properties of GaN. We predict, as expected, that introduction of a N or Ga vacancy results in several energetically favorable charged states within bulk GaN; these energetically favorable defects result in a significant modification of the quasiparticle and excitonic properties of GaN. We will discuss the implications of defect-induced-states for the electron transport and absorption properties of GaN.

<sup>1</sup>This work was partially supported by the Army Research Office (ARO) within the Collaborative Research Alliance (CRA-MSME).

**4:42PM P23.00010 Prediction of direct band gap silicon superlattices with dipole-allowed optical transition<sup>1</sup>**, SUNGHYUN KIM, Department of physics, KAIST, Daejeon, Republic of Korea, YOUNG JUN OH, Department of Materials Science and Engineering, University of Texas at Dallas, Richardson, TX 75080, USA, IN-HO LEE, Korea Research Institute of Standards and Science, Daejeon, Korea, JOOYOUNG LEE, Center for In Silico Protein Science, School of Computational Science, Korea Institute for Advanced Study, Seoul, Korea, K. J. CHANG, Department of physics, KAIST, Daejeon, Republic of Korea — While cubic diamond silicon (c-Si) is an important element in electronic devices, it has poor optical properties owing to its indirect gap nature, thereby limiting its applications to optoelectronic devices. Here, we report Si superlattice structures which are computationally designed to possess direct band gaps and excellent optical properties. The computational approach adopts density functional calculations and conformational space annealing for global optimization. The Si superlattices, which consist of alternating stacks of Si(111) layers and a defective layer with Seiwatz chains, have either direct or quasi-direct band gaps depending on the details of attacking layers. The photovoltaic efficiencies are calculated by solving Bethe-Salpeter equation together with quasiparticle G0W0 calculations. The strong direct optical transition is attributed to the overlap of the valence and conduction band edge states in the interface region. Our Si superlattices exhibit high thermal stability, with the energies lower by an order of magnitude than those of the previously reported Si allotropes. We discuss a possible route to the synthesis of the superlattices through wafer bonding.

<sup>1</sup>This work is supported by Samsung Science and Technology Foundation under Grant No. SSTF-BA1401-08.

**4:54PM P23.00011 From facets to facets: how does work function vary over a gold nanocluster?**, LINGYUAN GAO, JAIME SOUTO, JAMES CHELIKOWSKY, ALEX DEMKOV, Univ of Texas, Austin — Owing to their potential applications in catalysis, gold nanoclusters are a focus of intense research. The work function  $\Phi$ , which can be measured using photoemission spectroscopy is a key parameter used to characterize the catalytic performance of the cluster.  $\Phi$  is determined by the difference between the electrostatic potential just outside the metal surface and the Fermi energy of the cluster. We use a relativistic version of the real space first-principles code PARSEC to compute the work function of gold nanoclusters with dimensions on the order of a nanometer, which is similar in size to those used in experiment. We illustrate how the work function depends on the surface orientation of the nanocluster facets and compare our results with available experimental data. We acknowledge supports from SciDAC program, Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Sciences grant DE-SC0008877 for work on algorithms. Two of us (JRC and JS-C) acknowledge support for the work on nanostructures from grant from the U.S. Department of Energy: DE-FG02-06ER46286.

**5:06PM P23.00012 Gap engineering using Hellmann-Feynmann forces: method and applications<sup>1</sup>**, KIRAN PRASAI, Ohio University, PARTHAPRATIM BIAWAS, The University of Southern Mississippi, D. A. DRABOLD, Ohio University — Materials with optimized band gap are needed in many specialized applications. In this talk, we demonstrate that Hellmann-Feynman forces associated with the gap states can be used to find atomic coordinates that yield desired electronic density of states. Using tight-binding models, we show that this approach may be used to arrive at electronically designed models of amorphous silicon and carbon. We provide a simple recipe to include *a priori* electronic information in the formation of computer models of materials, and prove that this information may have profound structural consequences. We'll briefly discuss implementation of the method in *ab-initio* molecular dynamics simulations and highlight the latest feats of the method ranging from modeling amorphous semi-conducting materials to understanding the structure and properties of memory materials.

<sup>1</sup>K. Prasai, P. Biswas, and D. A. Drabold, Scientific reports, 5 (2015)

**5:18PM P23.00013 Bayesian cluster expansion with lattice parameter dependence for studying surface alloys**, LE NIU, TIM MUELLER, Johns Hopkins University, Department of Materials Science & Engineering — The Bayesian cluster expansion approach has proven to be an efficient method for predicting the structure and properties of materials with substitutional disorder. It is particularly effective for low-symmetry systems such as nanoparticles and surfaces. However for surfaces of solid solutions, the lattice parameter of the surface, and hence the interactions among near-surface atoms, varies with the composition of the underlying bulk material. We demonstrate that surfaces under a variety of strains can be used to train a single cluster expansion that predicts properties as a function of atomic order and surface strain. We have applied this method to study Ni-Pt alloys with up to a monolayer of adsorbed oxygen, an important class of catalysts for the oxygen reduction reaction. Through Monte Carlo simulations, we are able to determine how the structure and properties of these surfaces vary as a function of temperature, composition, chemical potential, and surface strain, enabling both the identification of thermodynamically stable surface structures and the rational design of Pt-Ni surfaces with high catalytic activity.

## Wednesday, March 16, 2016 2:30PM - 5:30PM –

Session P24 DMP: Many-Body Perturbation Theory for Electronic Excitations: Electronic Structure 323 - Noa Marom, Tulane University

**2:30PM P24.00001 Electronic structure from relativistic quasiparticle self-consistent GW calculations<sup>1</sup>**, STEFAN BLÜGEL, Peter Grünberg Institut and Institut for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — Most theoretical studies of topological insulators (TIs) are based on tight-binding descriptions and density functional theory (DFT). But recently, many-body calculations within the GW approximation attract much attention in the study of these materials. We present an implementation of the quasiparticle self-consistent (QS) GW method where the spin-orbit coupling (SOC) is fully taken into account in each iteration rather than added a posteriori. Within the all-electron FLAPW formalism, we show DFT, one-shot GW, and QSGW calculations for several, well-known TIs. We present a comparison of the calculations to photoemission spectroscopy and show that the GW corrected bands agree much better with experiment. For example, we show that Bi<sub>2</sub>Se<sub>3</sub> [1,2] is a direct gap semiconductor, in contrast to what was believed for many years by interpreting experimental results on the basis of DFT and that small strains in Bi can lead to a semimetal-to-semiconductor or trivial-to-topological transitions [3]. Quasiparticle calculations for low-dimensional systems are still very demanding. In order to study the topological surface states with an approach based on GW, we use Wannier functions to construct a Hamiltonian that reproduces the many-body band structure of the bulk, and that is used to construct a slab Hamiltonian. With this approach, we discuss the effect of quasiparticle corrections on the surface states of TIs and on the interaction between bulk and surface states. [1] I. Aguilera *et al.*, PRB **88**, 045206 (2013), *ibid.*, PRB **88**, 165136 (2013). [2] M. Michiardi *et al.*, PRB **90**, 075105 (2014). [3] I. Aguilera *et al.*, PRB **91**, 125129 (2015).

<sup>1</sup>Work was funded by the Virtual Institute for Topological Insulators of the Helmholtz Association and carried out in collaboration with Irene Aguilera, Gustav Bihlmayer, and Christoph Friedrich.

**3:06PM P24.00002 Quasiparticle electronic structure of  $\text{Bi}_2\text{Se}_3$  via the sc-COHSEX+GW approach<sup>1</sup>**, BRADFORD A. BARKER, University of California-Berkeley and Lawrence Berkeley National Laboratory, JACK DESLIPPE, Lawrence Berkeley National Laboratory, OLEG YAZYEV, University of California-Berkeley and Ecole Polytechnique Federale de Lausanne (EPFL), STEVEN G. LOUIE, University of California-Berkeley and Lawrence Berkeley National Laboratory — We present ab initio calculations of the quasiparticle electronic band structure of three-dimensional topological insulator material  $\text{Bi}_2\text{Se}_3$  using the full spinor GW approach. The mean-field is initially computed at the DFT level in the local density approximation (LDA) using fully-relativistic pseudopotentials. We then improve the mean-field electronic structure by solving Dyson's equation in the static COHSEX approximation, self-consistently updating the eigenvalues, eigenvectors, and dielectric screening. After a few iterations, we then perform a GW calculation to determine the quasiparticle energies. We compare our calculated results to experimental values of the band gaps and effective masses.

<sup>1</sup>This work was supported by NSF grant No. DMR15-1508412 and U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at LBNLs NERSC facility and the NSF through XSEDE resources at NICS.

**3:18PM P24.00003 Ubiquitous electron-plasmon coupling in doped semiconductors**, FABIO CARUSO, FELICIANO GIUSTINO, Department of Materials, University of Oxford — The interplay between electrons and bosonic excitations [as, e.g., phonons, collective charge-density fluctuations (plasmons), and magnons] is pervasive in matter and underlies an extremely broad spectrum of physical phenomena, as, for instance, current dissipation, superconductivity, hot-carrier thermalisation, and band structure replicas [1]. At variance with phonons, however, questions pertaining the strength of electron-plasmon coupling in solids are still awaiting further investigations. We developed and implemented a first-principles theory of electron-plasmon coupling based on many-body perturbation theory. Our first-principles calculations reveal that electron-plasmon coupling alters ubiquitously the dynamical and optical properties of semiconductors at high doping concentrations. This behaviour stems from the emergence of low-energy extrinsic plasmons which may couple electronic states in the vicinity of the Fermi energy. [1] F. Caruso, H. Lambert, and F. Giustino, *Phys. Rev. Lett.* **114**, 146404 (2015).

**3:30PM P24.00004 Quasiparticle excitations of adsorbates on doped graphene**, JOHANNES LISCHNER, Imperial College London, SEBASTIAN WICKENBURG, DILLON WONG, CHRISTOPH KARRASCH, YANG WANG, JIONG LU, ARASH A. OMRANI, VICTOR BRAR, HSIN-ZON TSAI, QIONG WU, UC Berkeley, FABIANO CORSETTI, ARASH MOSTOFI, Imperial College London, ROLAND K. KAWAKAMI, UC Riverside, Ohio State University, JOEL MOORE, ALEX ZETTL, STEVEN G. LOUIE, MIKE CROMMIE, UC Berkeley — Adsorbed atoms and molecules can modify the electronic structure of graphene, but in turn it is also possible to control the properties of adsorbates via the graphene substrate. In my talk, I will discuss the electronic structure of F4-TCNQ molecules on doped graphene and present a first-principles based theory of quasiparticle excitations that captures the interplay of doping-dependent image charge interactions between substrate and adsorbate and electron-electron interaction effects on the molecule. The resulting doping-dependent quasiparticle energies will be compared to experimental scanning tunnelling spectra. Finally, I will also discuss the effects of charged adsorbates on the electronic structure of doped graphene.

**3:42PM P24.00005 First Principles Charge Transfer Excitations in Curved Aromatic Materials**, LAURA ZOPPI, University of Zurich, LAYLA MARTIN SAMOS, University of Nova Gorica, KIM K. BALDRIDGE, University of Zurich — Understanding excitation properties and charge transport phenomena of curved  $\pi$ -conjugated materials is critical for a rational utilization of buckybowls as electrically active materials in solid-state devices. In this respect, the class of materials based on the smallest bowl-shaped fullerene fragment, corannulene,  $\text{C}_{20}\text{H}_{10}$ , offers a unique possibility for building up scaffolds with a tunable spectrum of structural and electronic properties.[1] Here, GW-BSE based approaches are applied to investigation and prediction of charge transfer excitations of  $\text{C}_{20}\text{H}_{10}$  materials systems at functional interfaces, [1-3] with a special emphasis on design aspects of materials relevant in the experimental domain. Theoretical predictions together with experimental findings illustrate the possibility of integrating corannulene electronic functions in molecular devices. [1] L. Zoppi, L. Martin-Samos, K. K. Baldrige, *Acc. Chem. Res.*, **47**, 3310–3320 (2014) [2] L. Zoppi, L. Martin-Samos, K. K. Baldrige, *J. Am. Chem. Soc.* **133**, 14002-14009 (2011) [3] L. Zoppi, L. Martin Samos, K. K. Baldrige, *Phys. Chem. Chem. Phys.* **17**, 6114-6121 (2015)

**3:54PM P24.00006 Electronic and optical excitations in building blocks of the metal organic framework MOF-5<sup>1</sup>**, BIN SHI, University of Illinois at Chicago, LINDA HUNG, TANER YILDIRIM, National Institute of Standards and Technology, SERDAR OGUT, University of Illinois at Chicago — Metal organic frameworks (MOFs) are a relatively new class of materials which are made of metal-oxide clusters linked by organic bridging ligands. In recent years, MOFs have received considerable attention due to their widely tunable structural, chemical and physical properties. We investigate one of the well characterized MOFs, MOF-5, whose framework consists of tetrahedral  $[\text{Zn}_4\text{O}]^{6+}$  units linked by rigid arylcarboxylate ligands. We use many-body perturbation (GW+BSE) and time-dependent DFT methods in real space to examine the electronic and optical excitations in the building blocks of MOF-5, such as  $\text{Zn}_4\text{O}(\text{COOH})_6$ , basic zinc acetate  $[\text{Zn}_4\text{O}(\text{CH}_3\text{COO})_6]$ , and tetranuclear zinc benzoate  $[\text{Zn}_4\text{O}(\text{C}_6\text{H}_5\text{COO})_6]$ . The calculated spectra are compared with available experimental measurements and existing calculations to shed light on the controversy regarding the nature (metal-ligand versus ligand-ligand) of low-energy electronic and optical excitations in MOF-5.

<sup>1</sup>Supported by DOE Grant No. DE-SC0001853

**4:06PM P24.00007 Energy level alignment at hybridized organic-metal interfaces from a GW projection approach<sup>1</sup>**, YIFENG CHEN, Department of Physics and Centre for Advanced 2D Materials, National University of Singapore, ISAAC TAMBLYN, Department of Physics, University of Ontario Institute of Technology, Canada, SU YING QUEK, Department of Physics and Centre for Advanced 2D Materials, National University of Singapore — Energy level alignments at organic-metal interfaces are of profound importance in numerous (opto)electronic applications. Standard density functional theory (DFT) calculations generally give incorrect energy level alignments and missing long-range polarization effects. Previous efforts to address this problem using the many-electron GW method have focused on physisorbed systems where hybridization effects are insignificant. Here, we use state-of-the-art GW methods to predict the level alignment at the amine-Au interface, where molecular levels do hybridize with metallic states. This non-trivial hybridization implies that DFT result is a poor approximation to the quasiparticle states. However, we find that the self-energy operator is approximately diagonal in the molecular basis, allowing us to use a projection approach to predict the level alignments. Our results indicate that the metallic substrate reduces the HOMO-LUMO gap by 3.5–4.0 eV, depending on the molecular coverage/presence of Au adatoms. Our GW results are further compared with those of a simple image charge model that describes the level alignment in physisorbed systems.

<sup>1</sup>SYQ and YC acknowledge grant NRF-NRFF2013-07 and the medium-sized centre program from the National Research Foundation, Singapore.

**4:18PM P24.00008 Nonequilibrium transport in the Anderson-Holstein model with interfacial screening<sup>1</sup>**, ENRICO PERFETTO, GIANLUCA STEFANUCCI, University of Rome Tor Vergata — Image charge effects in nanoscale junctions with strong electron-phonon coupling open the way to unexplored physical scenarios. Here we present a comprehensive study of the transport properties of the Anderson-Holstein model in the presence of dot-lead repulsion. We propose an accurate many-body approach to deal with the simultaneous occurrence of the Franck-Condon blockade and the screening-induced enhancement of the polaron mobility. Remarkably, we find that a novel mechanism of negative differential conductance originates from the competition between the charge blocking due to the electron-phonon interaction and the charge deblocking due to the image charges. An experimental setup to observe this phenomenon is discussed. References [1] E. Perfetto, G. Stefanucci and M. Cini, Phys. Rev. B 85, 165437 (2012). [2] E. Perfetto and G. Stefanucci, Phys. Rev. B 88, 245437 (2013). [3] E. Perfetto and G. Stefanucci, Journal of Computational Electronics 14, 352 (2015).

<sup>1</sup>E.P. and G.S. acknowledge funding by MIUR FIRB Grant No. RBFR12SW0J

**4:30PM P24.00009 Many-body effects and ultraviolet renormalization in three-dimensional Dirac materials<sup>1</sup>**, ROBERT THROCKMORTON, University of Maryland, JOHANNES HOFMANN, University of Cambridge, EDWIN BARNES, Virginia Tech — We develop a theory for electron-electron interaction-induced many-body effects in three dimensional (3D) Weyl or Dirac semimetals, including interaction corrections to the polarizability, electron self-energy, and vertex function, up to second order in the effective fine structure constant of the Dirac material. These results are used to derive the higher-order ultraviolet renormalization of the Fermi velocity, effective coupling, and quasiparticle residue, revealing that the corrections to the renormalization group (RG) flows of both the velocity and coupling counteract the leading-order tendencies of velocity enhancement and coupling suppression at low energies. This in turn leads to the emergence of a critical coupling above which the interaction strength grows with decreasing energy scale. In addition, we identify a range of coupling strengths below the critical point in which the Fermi velocity varies non-monotonically as the low-energy, non-interacting fixed point is approached. Furthermore, we find that while the higher-order correction to the flow of the coupling is generally small compared to the leading order, the corresponding correction to the velocity flow carries an additional factor of the Dirac cone flavor number relative to the leading-order result.

<sup>1</sup>Supported by LPS-MPO-CMTC.

**4:42PM P24.00010 Electron-electron interactions in Dirac and Weyl semimetals: collective modes and stability of the ground state<sup>1</sup>**, JOHN TOLSMA, ALLAN MACDONALD, Department of Physics, University of Texas at Austin — Three-dimensional Dirac and Weyl semimetals host linearly dispersive low-energy electronic bands in the bulk, and exotic Fermi-Arc states at the surface. Following theoretical proposals of candidate material classes [1,2], experimental observation of anomalous transport [3] and Fermi-Arc surface states [4] have recently been reported. Using time-dependent Hartree-Fock and renormalization group methods, we study collective mode dispersion and the influence of electron-electron interactions on the stability of the ground state. This work was supported by the DOE Division of Materials Sciences and Engineering under grant DE-FG02-ER45118. [1] Z. Wang et al., Phys. Rev. B. 88, 125427 (2013) [2] S.-M. Huang et al., Nat. Comm. 6, 7373 (2015) [3] T. Liang et al., Nat. Mater. 14, 280 (2014) [4] S.-Y. Xu et al., Science 347, 294 (2015)

<sup>1</sup>This work was supported by the DOE Division of Materials Sciences and Engineering under grant DE-FG02-ER45118

**4:54PM P24.00011 First-principles DFT+GW study of oxygen doped CdTe<sup>1</sup>**, WALTER ORELLANA, Departamento de Ciencias Físicas, Universidad Andres Bello, MAURICIO A. FLORES, Departamento de Física and Departamento de Matemáticas, Facultad de Ciencias, Universidad de Chile, EDUARDO MENÉNDEZ-PROUPIN, Departamento de Física, Facultad de Ciencias, Universidad de Chile — The role of oxygen doping in CdTe is addressed by first-principles calculations. Formation energies, charge transition levels and quasiparticle defect states are calculated within the DFT+GW formalism. The formation of a new defect is identified, the  $(O_{Te} - Te_{Cd})$  complex. This complex is energetically favored over both isovalent  $(O_{Te})$  and interstitial oxygen  $(O_i)$ . We find that incorporation of oxygen passivates the harmful deep energy levels derived from Te antisites, suggesting an improvement in the efficiency of CdTe based solar cells. Our calculations indicate that both  $(O_{Te})$  and  $(O_i)$  have low formation energies. Moreover,  $(O_{Cd})$  is only stable in the neutral charge state and undergoes a Jahn-Teller distortion. The  $(V_{Cd} - O_{Te})$  complex is found to be a shallow acceptor with a high formation energy. We also report an oxygen-related interstitial defect, which plays a key role in the diffusion mechanism of oxygen in CdTe.

<sup>1</sup>Support by FONDECYT Grant No. 1130437 is acknowledged. Powered@NLHPC: This research was partially supported by the supercomputing infrastructure of the NLHPC (ECM-02).

**5:06PM P24.00012 Quasi-particle band structure of potassium-doped few-layer black phosphorus with GW approximation**, HAN-GYU KIM, SEUNG SU BAIK, HYOUNG JOON CHOI, Department of Physics, IPAP, and Center for Computational Studies of Advanced Electronic Material Properties, Yonsei University, Seoul, Korea — We calculate the quasi-particle band structure of pristine and potassium-doped black phosphorus (BP) by using the GW approximation. We obtain band gaps of pristine bulk and few-layer BP and compare them with the result of the density functional calculations and experimental measurements. For potassium-doped cases, we calculate the electronic band structure of potassium-doped few-layer BPs with various doping densities. We obtain the critical doping density for the band-gap closing, and the energy-band dispersions when the band gap is inverted. We discuss Dirac semimetal properties of doped few-layer BPs obtained by the GW approximation. This work was supported by NRF of Korea (Grant No. 2011-0018306) and KISTI supercomputing center (Project No. KSC-2015-C3-039).

**5:18PM P24.00013 Quasiparticle and optical band gaps of  $Sr_{n+1}Ti_nO_{3n+1}$  from *ab-initio* many-body perturbation theory**, SEBASTIAN E REYES-LILLO, TONATIUH RANGEL, Molecular Foundry, LBNL; Dept. of Physics, UC Berkeley, FABIEN BRUNEVAL, Molecular Foundry, LBNL; Dept. of Physics, UC Berkeley; CEA, DEN, SRMP, JEFFREY B NEATON, Molecular Foundry, LBNL; Dept. of Physics, UC Berkeley; Kavli ENSI — The Ruddlesden Popper homologous series  $Sr_{n+1}Ti_nO_{3n+1}$  provides a unique opportunity to study the effect of dimensionality and confinement on the band gap and absorption spectrum of the complex oxide  $SrTiO_3$ . In this work, we use many-body perturbation theory within the GW approximation and the Bethe-Salpeter equation (BSE) approach to study the electronic and optical properties of  $Sr_{n+1}Ti_nO_{3n+1}$ . We find that our GW/BSE direct and indirect band gaps are in excellent agreement with measured direct and indirect optical gaps. We discuss technical aspects of the calculations such as convergence and starting-point dependence, and compare to higher levels of theory. In addition, we find a relatively large exciton binding energy of 500 meV for  $Sr_2TiO_4$  ( $n = 1$ ). We explore the role of structural distortions and epitaxial strain in the properties of the localized exciton. Our work suggests that layered structures can provide a viable route for the design of complex oxide materials with desirable optoelectronic properties. This work is supported by DOE.

**Wednesday, March 16, 2016 2:30PM - 5:30PM –**

**Session P25 DCMP: Superconducting Tunneling: Josephson Effect and THz Emission 324 -**

Richard Klemm, University of Central Florida

**2:30PM P25.00001 Effect of impurities on the Josephson current through helical metals: Exploiting a neutrino paradigm**, POUYAN GHAEMI, V. PARAMESWARAN NAIR, City College of City University of New York — In this talk we present our results on the effect of time-reversal symmetric impurities on the Josephson supercurrent through two dimensional helical metals such as on topological insulator surface state. We show that contrary to the usual superconducting-normal metal-superconducting junctions, the suppression of supercurrent in superconducting-helical metal-superconducting junction is mainly due to fluctuations of impurities in the junctions. Our results, which is a condensed matter realization of a part of the MSW effect for neutrinos, shows that the relationship between normal state conductance and critical current of Josephson junctions is significantly modified for Josephson junctions on the surface of topological insulators. We also study the temperature-dependence of supercurrent and present a two fluid model which can explain some of recent experimental results in Josephson junctions on the edge of topological insulators.

**2:42PM P25.00002 "Hybrid" multi-gap/single-gap Josephson junctions: Evidence of macroscopic quantum tunneling in superconducting-to-normal switching experiments on  $\text{MgB}_2/\text{I}/\text{Pb}$  and  $\text{MgB}_2/\text{I}/\text{Sn}$  junctions**, STEVE CARABELLO, JOSEPH LAMBERT, Drexel University, WENQING DAI, QI LI, Penn State University, KE CHEN, DANIEL CUNNANE, X. X. XI, Temple University, ROBERTO RAMOS, University of the Sciences — We report results of superconducting-to-normal switching experiments on  $\text{MgB}_2/\text{I}/\text{Pb}$  and  $\text{MgB}_2/\text{I}/\text{Sn}$  junctions, with and without microwaves. These results suggest that the switching behavior is dominated by quantum tunneling through the washboard potential barrier, rather than thermal excitations or electronic noise. Evidence includes a leveling in the standard deviation of the switching current distribution below a crossover temperature, a Lorentzian shape of the escape rate enhancement peak upon excitation by microwaves, and a narrowing in the histogram of escape counts in the presence of resonant microwave excitation relative to that in the absence of microwaves. These are the first such results reported in "hybrid" Josephson tunnel junctions, consisting of multi-gap and single-gap superconducting electrodes.

**2:54PM P25.00003  $\text{YBa}_2\text{Cu}_3\text{O}_7$  Nanowire Josephson Junctions Directly Written with a Focused Helium Ion Beam<sup>1</sup>**, SHANE A. CYBART, ETHAN Y. CHO, YUCHAO W. ZHOU, ROBERT C. DYNES, University of California - San Diego — We will present electrical transport measurements for superconducting nanowire Josephson junctions with widths ranging from 500 to 25 nm. The junctions were fabricated by using a 500-pm diameter helium ion beam to pattern superconducting nanowires, into 25-nm thick  $\text{YBa}_2\text{Cu}_3\text{O}_7$  (YBCO) thin films. The key to this direct-write method is that irradiated regions of the YBCO turn insulating for moderate ion doses which allows for very fine features to be defined ( $\sim 2$  nm). Nanowire junctions were fabricated with the length of the nanowire oriented along different crystallographic directions in the  $a-b$  plane. They exhibit a large increase in the anisotropy of the Josephson critical current and voltage state conductance as the nanowire width is decreased. In the narrowest of wires, the conductance changes by an order of magnitude. We interpret these observations to be due to the Josephson junctions being smaller than the granularity of the films. Measuring these single grains reveals characteristics of the  $a-b$  plane  $d$ -wave symmetry of superconductivity in YBCO.

<sup>1</sup>This work is funded by AFOSR.

**3:06PM P25.00004 Superconducting quantum interference devices made with normal metal and insulator barrier Josephson junctions in Y-Ba-Cu-O directly written with a focused helium beam**, ETHAN CHO, MENG MA, Univ of California - San Diego, CHUONG HUYNH, Carl Zeiss Microscopy LLC, KEVIN PRATT, DOUG PAULSON, Tristan Technologies Inc., VICTOR GLYANTSEV, Superconductor Technologies Inc., ROBERT DYNES, SHANE CYBART, Univ of California - San Diego — We will present electrical transport data for Y-Ba-Cu-O superconducting quantum interference devices (SQUIDS) with focused helium ion damage Josephson junctions. The junctions were directly written with a 30 keV focused helium ion beam, which locally creates disorder in Y-Ba-Cu-O that induces a superconducting-insulator transition. SQUIDS with Josephson junctions written with a dose of  $4 \times 10^{16} \text{ He}^+/\text{cm}^2$  have metallic barriers and show a current-voltage characteristic (I-V) well-described by the resistively shunted junction model. The spectral density of the flux noise is  $10 \mu\Phi_0/\sqrt{\text{Hz}}$  at 10 Hz and the white noise at higher frequencies is  $2 \mu\Phi_0/\sqrt{\text{Hz}}$ . SQUIDS with junctions written with higher ion doses ( $\sim 9 \times 10^{16} \text{ He}^+/\text{cm}^2$ ) have insulating Josephson barriers with a critical current of  $22 \mu\text{A}$  and a resistance of  $12 \Omega$  at 4 K. The I-V for all of these devices is not hysteretic due to the small capacitance and the resistance. At higher voltage the junction I-V curve shows tunnel-junction behavior and a superconducting energy gap edge at 20 mV. We will discuss how these results are a promising step forward for sensitive magnetic sensors made from high temperature superconductors at various temperatures.

**3:18PM P25.00005 Engineering the parity lifetime of  $\text{NbTiN}$  Cooper-pair transistors**, ATTILA GERESDI, DAVID VAN WOERKOM, TAMAS KRIVACHY, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, 2600 GA Delft, The Netherlands, SEBASTIAN RUBBERT, ANTON R. AKHMEROV, Kavli Institute of Nanoscience, Delft University of Technology, 2600 GA Delft, The Netherlands, LEO P. KOUWENHOVEN, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, 2600 GA Delft, The Netherlands — Controlling the quasiparticle occupation of a superconducting island is of fundamental importance for superconducting circuits as single electron tunneling results in decoherence. Thus far, engineering superconducting tunnel junctions for quantum bits was done exclusively based on aluminum, which limits integration with systems requiring finite magnetic field, such as topological superconductors based on spin-orbit coupled nanowires or spin ensembles. Here we present parity modulation of the switching current of a niobium titanium nitride ( $\text{NbTiN}$ ) Cooper-pair transistor coupled to aluminum (Al) leads for the first time. Owing to the gap profile  $\Delta_{\text{island}} \gg \Delta_{\text{leads}}$ , we observe a parity lifetime exceeding 1 minute in combination with a Josephson energy of  $50 \mu\text{eV}$ . We link this value to the finite subgap density of states of  $\text{NbTiN}$ , which is consistent with the subgap conductance measured by DC transport. We discuss our design of quasiparticle trapping and radiation shielding techniques, which resulted in a non-saturated parity lifetime down to a fridge temperature of 12 mK. Finally, we show that this circuit is compatible with magnetic fields in the range of 100 mT.

**3:30PM P25.00006 The cavity resonance mode of  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$  mesa terahertz sources as probed by scanning laser thermal microscopy<sup>1</sup>**, TIMOTHY BENSEMAN, Queens College CUNY, ALEXEI KOSHELEV, VITALII VLASKO-VLASOV, ULRICH WELP, WAI-KWONG KWOK, Argonne National Laboratory, YANG HAO, University of Illinois at Chicago, BORIS GROSS, MATTHIAS LANGE, DIETER KOELLE, REINHOLD KLEINER, University of Tuebingen, KAZUO KADOWAKI, University of Tsukuba — Stacked Intrinsic Josephson Junctions (IJJs) in the extremely anisotropic high- $T_c$  superconductor  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$  are a promising solid-state source of coherent terahertz radiation in the so-called "THz gap" range. In these devices, a geometric resonant mode of a stack of IJJs of typical dimensions  $300 \times 60 \times 1$  microns<sup>3</sup> acts to synchronize the individual junctions, resulting in coherent far-field THz emission. This resonance can be probed by scanning laser thermal microscopy, in which a modulated optical laser beam is rastered across the top surface of a stack. The resulting thermal perturbation to the stack's cavity mode can thus be mapped via the resulting xy-dependent modulation of the stack's electrical resistance. Here we discuss the experimentally measured scanning laser pattern of such a THz cavity mode, and the implications of its symmetry for the mechanism of IJJ synchronization in these devices.

<sup>1</sup>This research was supported by the Department of Energy, Office of Basic Energy Sciences, under Contract No. De-AC02-06CH11357.

**3:42PM P25.00007 Artificially induced hotspots in  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$  mesa terahertz sources<sup>1</sup>**, YANG HAO, University of Illinois at Chicago, ULRICH WELP, ALEXEI KOSHELEV, VITALII VLASKO-VLASOV, WAI-KWONG KWOK, Argonne National Laboratory, KAZUO KADOWAKI, University of Tsukuba, TIMOTHY BENSEMAN, Queens College CUNY — Mesa-shaped devices comprising stacked Intrinsic Josephson Junctions (IJJs) in the high-temperature superconductor  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$  can be used as compact sources of coherent terahertz radiation. Achieving high emission levels of THz emission power from these devices depends on efficient synchronization of the approximately 600 IJJs in the stack. Theoretical simulations of stacked IJJs, as well as some empirical results, suggest that thermal inhomogeneity of the stack may enhance THz emission power. There are a number of possible mechanisms by which this might occur, including a hotspot acting as a local resistive shunt for the IJJs (thus altering the spread of bias voltages in the stack and the junction damping dynamics) or by local self-heating reducing the phase-stiffness of the superconducting condensate in critical locations. Here we report results of artificially inducing local heating in these devices with thin film micro-heaters patterned on their surfaces, in order to determine which mechanism(s) could be responsible for self-heating-induced THz emission enhancement.

<sup>1</sup>Sample patterning was performed at the Center for Nanoscale Materials, an Office of Science user facility, supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

**3:54PM P25.00008 Scattering to different vortex polarity in coupled long Josephson junctions**, WALTRAUT WUSTMANN, KEVIN D. OSBORN, Laboratory for Physical Sciences, College Park, MD — We theoretically study the motion of flux vortices (fluxons) in structures made from discrete long Josephson junctions (DLJJs) which may have applications in the fields of reversible and low-power computing. We investigate the scattering of fluxons at specially designed interfaces where multiple DLJJs meet. Once fluxons approach the interface, flux oscillations at the interface can be temporarily excited before the fluxons continue along to another DLJJ. Under some conditions the fluxons will change their polarity (to antifluxons) and in other cases the fluxon continues without a change in polarity. We explain the dynamics through the resonant interaction of the soliton with bound states at the interface. We also study a controlled polarity gate, where the polarity of the target fluxon depends on a control fluxon which enters and exits the interface through separate DLJJs.

**4:06PM P25.00009 Instability of Driven Josephson Vortices in Long Underdamped Junctions<sup>1</sup>**, AHMAD SHEIKHZADA, ALEX GUREVICH, Department of Physics and Center for Accelerator Science, Old Dominion University — We show that a Josephson vortex driven by a dc current can become unstable due to strong Cherenkov radiation resulting from intrinsic nonlocal electrodynamics of long underdamped Josephson junctions. This instability is not captured by the conventional sine-Gordon equation but is described by a more general integro-differential equation for the phase difference,  $\theta(x, t)$ . Our numerical simulations of this nonlinear dynamic equation for different junction geometries have shown that, as the vortex reaches a critical velocity, it triggers a cascade of expanding vortex-antivortex pairs. As a result, vortices and antivortices become spatially separated and accumulate continuously on the opposite sides of expanding dissipative domain. This effect is most pronounced in thin film edge Josephson junctions at low temperatures where a single vortex can switch the whole junction into a resistive state at currents well below the Josephson critical current. Our results suggest that a rapidly moving Josephson vortex can destroy the superconducting long-range order in a way that is similar to the crack propagation in solids.

<sup>1</sup>This work was supported by DOE under grant No. DE-SC0010081.

**4:18PM P25.00010 Terahertz emission from a stack of intrinsic Josephson junctions in  $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10+\delta}$** , MANABU TSUJIMOTO, University of Tsukuba, ITSUHIRO KAKEYA, Kyoto University, SHINTARO ADACHI, TAKAO WATANABE, Hirosaki University, TAKANARI KASHIWAGI, HIDETOSHI MINAMI, KAZUO KADOWAKI, University of Tsukuba — Terahertz radiation in the 0.3–10 THz frequency range is a technologically attractive form of electromagnetic radiation, because it has applications in numerous fields. Terahertz generation from stacks of intrinsic Josephson junctions fabricated from  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$  (Bi-2212) has become a major focus of both experimental and theoretical research [U. Welp *et al.*, Nat. Photonics **7**, 702 (2013)]. Here, we observe continuous terahertz emission from a stack of intrinsic Josephson junctions made of  $\text{Bi}_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_{10+\delta}$  (Bi-2223). We investigate how triple  $\text{CuO}_2$  planes affect the c-axis current-voltage and emission characteristics. The terahertz emission spectra are measured by Fourier-transform infrared spectroscopy.

**4:30PM P25.00011 Josephson radiation from InSb-nanowire junction<sup>1</sup>**, DAVID VAN WOERKOM, ALEXANDER PROUTSKI, TAMAS KRIVACHY, DANIEL BOUMAN, RUBEN VAN GULIK, ONDER GUL, MAJA CASSIDY, Delft Univ. of Tech., The Netherlands, DIANA CAR, ERIK BAKKERS, Eindhoven Univ. of Tech., The Netherlands, LEO KOUWENHOVEN, ATTILA GERESDI, Delft Univ. of Tech., The Netherlands — Semiconducting nanowire Josephson junctions has recently gained interest as building blocks for Majorana circuits and gate-tuneable superconducting qubits. Here we investigate the rich physics of the Andreev bound state spectrum of InSb nanowire junctions utilizing the AC Josephson relation  $2eV_{\text{bias}} = \hbar f$ . We designed and characterized an on-chip microwave circuit coupling the nanowire junction to an  $\text{Al}/\text{AlO}_x/\text{Al}$  tunnel junction. The DC response of the tunnel junction is affected by photon-assisted quasiparticle current, which gives us the possibility to measure the radiation spectrum of the nanowire junction up to several tens of GHz in frequency. Our circuit design allows for voltage or phase biasing of the Josephson junction enabling direct mapping of Andreev bound states. We discuss our fabrication methods and choice of materials to achieve radiation detection up to a magnetic field of few hundred milliTesla, compatible with Majorana states in spin-orbit coupled nanowires.

<sup>1</sup>This work has been supported by the Netherlands Foundations FOM, Abstract NWO and Microsoft Corporation Station Q

**4:42PM P25.00012 Interaction between fractional Josephson vortices in multi-gap superconductor tunnel junctions**, JU H. KIM, Department of Physics, University of Houston-Clear Lake — In a long Josephson junction (LJJ) with two-band superconductors, fractionalization of Josephson vortices (fluxons) can occur in the broken time reversal symmetry state when spatial phase textures (i-solitons) are excited. Excitation of i-solitons in each superconductor layer of the junction, arising due to the presence of two condensates and the interband Josephson effect, leads to spatial variation of the critical current density between the superconductor layers. Similar to the situation in a  $Y\text{Ba}_2\text{Cu}_3\text{O}_{7-x}$  superconductor film grain boundary [1], this spatial dependence of the critical current density can self-generate magnetic flux in the insulator layer, resulting in fractional fluxons with large and small fraction of flux quantum. Similar to fluxons in one-band superconductor LJJ, these fractional fluxons are found to interact with each other. The interaction between large and small fractional fluxons determines the size of a fluxon which includes two (one large and one small) fractional fluxons. We discuss the nature of interaction between fractional fluxons and suggest that i-soliton excitations in multi-gap superconductor LJJ may be probed by using magnetic flux measurements.

1. R. Mint and I. Papiashvili, Phys. Rev. B **64**, 134501 (2001).

**4:54PM P25.00013 The emission mechanism of THz electromagnetic waves from Bi2212 mesa device**, CHI HARU WATANABE, HIDETOSHI MINAMI, TAKEO KITAMURA, TAKANARI KASHIWAGI, University of Tsukuba, RICHARD KLEMM, University of Central Florida, KAZUO KADOWAKI, University of Tsukuba — From the detailed study of the severe temperature inhomogeneity of the Bi2212 IJJ mesa structure often forming "hot-spot" at relatively higher bias current region, while the electromagnetic waves are emitted, multi terminal potential measurement of the mesa device has revealed that the equipotential part of the mesa can only give universal ac-Josephson relationship between the potential difference and the frequency measured by the FT-IR spectrometer, and it is violated as the potential is measured in the region where the hot-spot is formed. This means that the deviation of the emission frequency from the ac-Josephson effect comes from a gradient of the electrical potential distribution. This strongly suggests that the electromagnetic waves at THz frequency may be generated in the superconducting part of the mesa, where the static electric potential is uniform, satisfying the ac-Josephson relation universally no matter how much temperature gradient is.

**5:06PM P25.00014 Tunable plasma edge in Josephson junction loaded wire array metamaterial<sup>1</sup>**, MELISSA TREPANIER, DAIMENG ZHANG, University of Maryland, College Park, V. P. KOSHELETS, IREE, STEVEN ANLAGE, University of Maryland, College Park — It is desirable to have a tunable negative permittivity medium that operates in the microwave domain. The effective plasma frequency of a JJ-loaded wire array can be tuned as a function of dc current and temperature in the low current limit. To demonstrate this effect we observe a change in transmission through a single layer of 8 superconducting Nb wires that spans a rectangular waveguide. A simple model that treats the wires as an artificial dielectric with a tunable effective permittivity shows good agreement with measured results for tuning of the plasma edge. In addition we have observed interesting behavior at higher current and rf input power. The dynamics are very rich, highly hysteretic, and nonlinear.

<sup>1</sup>This work is supported by the NSF-GOALI and OISE programs through grant ECCS-1158644, and CNAM.

**5:18PM P25.00015 A high  $T_c$  superconducting terahertz emitter operated from 0.5 to 2.4 THz**,<sup>1</sup> T. KASHIWAGI, K. SAKAMOTO, H. KUBO, Y. SHIBANO, T. ENOMOTO, T. KITAMURA, K. ASANUMA, T. YASUI, C. WATANABE, K. NAKADE, Y. SAIWAI, T. KATSURAGAWA, T. TANAKA, T. YUASA, Univ. of Tsukuba, M. TSUJIMOTO, Kyoto Univ., R. YOSHIKAWA, Univ. of Tsukuba, T. YAMAMOTO, Ulm Univ., H. MINAMI, Univ. of Tsukuba, R.A. KLEMM, Univ. of Central Florida, K. KADOWAKI, Univ. of Tsukuba — According to our previous studies, the efficiency of the THz radiation from a high  $T_c$  superconducting emitter can be improved greatly when the stand-alone mesa structure of Bi2212 single crystal is used for the emitter<sup>1)</sup>. The principal reason for that lies in the heat removal from the mesa. Recently, we developed a new device structure with high heat exhaust from the stand-alone mesa structures and studied the radiation characteristics from the different shape of mesa structures. The results obtained from a cylindrical stand alone mesa show very wide the radiation frequencies ranging from 0.5 to 2.4 THz. Strong emission power peaks were observed at about 1.0 THz and 1.6 THz<sup>2)</sup>. 1) T. Kitamura *et al.*, Appl. Phys. Lett. **105**, 202603 (2014) 2) T. Kashiwagi *et al.*, Appl. Phys. Lett. **107**, 082601 (2015)

<sup>1</sup>T. K. is supported by Futaba Electronics Memorial Foundation and JSPS KAKENHI Grant No. 15K20897. This work is in part performed in collaboration with Dr. Wai Kwok and his group in Argonne National Lab.

## Wednesday, March 16, 2016 2:30PM - 4:42PM —

Session P26 DCMP DMP FIAP: Insulators: Ferroelectrics and Applications 325 - Mina Yoon, Oak Ridge National Laboratory

**2:30PM P26.00001 Relative stability of ferroelectric and antiferroelectric states in  $(\text{Na}_{0.5}\text{Bi}_{0.5})\text{TiO}_3$ -based solid solutions**, V. SOBOLEV, South Dakota School of Mines & Technology, Rapid City, SD 57701, USA, V. M. ISHCHUK, L. G. GUSAKOVA, N. G. KISEL, D. V. KUZENKO, N. A. SPIRIDONOV, Science & Technology Center ReactivElectron of the National Academy of Sciences of Ukraine, 83049 Donetsk, Ukraine — Influence of the B-site ion substitutions on the of relative stability of the antiferroelectric and ferroelectric phases in  $[(\text{Na}_{0.5}\text{Bi}_{0.5})_{0.80}\text{B}_{0.20}](\text{Ti}_{1-x}\text{B}_x)\text{O}_3$  (NBT-BT) solid solutions has been investigated. Zirconium and tin ions along with  $(\text{In}_{0.5}\text{Nb}_{0.5})$ ,  $(\text{Fe}_{0.5}\text{Nb}_{0.5})$ , and  $(\text{Al}_{0.5}\text{V}_{0.5})$  ion complexes have been used for substitutions. It is found that an increase of content of the substituting ion results in a near linear variation in the size of the crystal lattice unit cell. The relative stability of the antiferroelectric and ferroelectric phases changes according to the variation of the tolerance factor of solid solution which in turn varies with the change of solid solution composition cause by substitutions. Obtained results demonstrate a predominant influence of the size of substituting ions on the relative stability of the antiferroelectric and ferroelectric states in  $(\text{Na}_{0.5}\text{Bi}_{0.5})\text{TiO}_3$ -based solid solutions. Our results open a new option for raising the temperature of the ferroelectric to antiferroelectric phase transition NBT-BT compounds.

**2:42PM P26.00002 Visible light absorption in La, Cr co-doped  $\text{SrTiO}_3$  and  $\text{BaTiO}_3$  for ferroelectric photovoltaics**, RYAN COMES, MARTIN MCBRIARTY, PHUONG-VU ONG, Pacific Northwest National Lab, STEVE HEALD, Argonne National Lab, GERARD CARROLL, DANIEL GAMELIN, University of Washington, KEREN FREEDY, University of Virginia, SERGEY SMOLIN, JASON BAXTER, Drexel University, TIFFANY KASPAR, MARK BOWDEN, PETER SUSHKO, SCOTT CHAMBERS, Pacific Northwest National Lab — Ferroelectric materials offer intriguing possibilities as photovoltaic materials, as their built-in electric field is ideal for separation of optically-excited electron-hole pairs without the need for a p-n junction. However, the majority of ferroelectrics suffer from a wide optical band gap outside the visible range. By co-doping La and Cr into epitaxial  $\text{SrTiO}_3$  and  $\text{BaTiO}_3$  (SLTCO/BLTCO) thin films, we show that absorption in the visible light regime can be achieved with a band gap of ~2.3 eV while preserving ideal stoichiometry. Through x-ray photoelectron spectroscopy, spectroscopic ellipsometry, photoconductivity and ultrafast pump-probe transient reflectance measurements, we show that visible light excitation of Cr 3d valence electrons into the Ti 3d conduction band produces optical carriers. Using piezoresponse force microscopy and polarized x-ray absorption fine structure measurements, we measure the ferroelectric polarization of the doped BLTCO films. These results are compared to density functional theory models to understand the optical and structural properties of the materials.

## 2:54PM P26.00003 ABSTRACT WITHDRAWN —

**3:06PM P26.00004 Strain effect on the visible emission in ferroelectric nanotubes: template and wall-thickness effect**, YUNSANG LEE, Soongsil University, SANGDON BU, JINKYU HAN, Chonbuk National University — We investigated the strain effect on temperature-dependent photoluminescence property in the clamped (with template) and free-standing (without template)  $\text{PbTiO}_3$  (PTO) nanotubes. The wall-thickness of nanotubes was varied from 25 to 80 nm with the outer diameter fixed to 420 nm. While all nanotubes show sizable green/yellow emission, the temperature dependent shift of the emission energy is significantly suppressed in the clamped PTO nanotubes, which is attributed to the lattice strain driven by the template clamping. This clamping effect is more significant for thinner nanotubes. Even in the free-standing PTO nanotubes the temperature-dependence of emission is affected by the wall-thickness. The similar behavior is identified in the  $\text{Pb}(\text{Zr,Ti})\text{O}_3$  nanotubes. Our finding is the clear manifestation of the template and geometrical shape effect on the optical property of the nanotubes.

**3:18PM P26.00005 Negative Refractive Index Materials for Optical Range of Spectrum**, VLADIMIR SOBOLEV, South Dakota School of Mines and Technology, Rapid City, SD 57701, VALERII ISHCHUK, Science & Technology Center Reaktivelektron, of the National Academy of Sciences of Ukraine, Donesk, Ukraine — A new method of manufacturing of negative refractive index media is presented. It is demonstrated that one can use of the controlled decomposition of solid solutions of oxides with perovskite crystal structure in the state of coexisting domains of the antiferroelectric and ferroelectric phases for manufacturing of such materials. The lead zirconate titanate based solid solutions are considered as an example of substances suitable for creation of such materials. Manufactured composites constitute a dielectric antiferroelectric matrix with a structure of conducting interphase boundaries separating domains of the ferroelectric and antiferroelectric phases. The electric conductivity of the interphase boundaries occurs as a result of the local decomposition of the solid solutions in the vicinity of these boundaries. The decomposition process and consequently the conductivity of the interphase boundaries can be controlled by means of external influences.

**3:30PM P26.00006 Incommensurate lattice modulations in Potassium Vanadate<sup>1</sup>**, BRYAN CHAKOUMAKOS, ARNAB BANERJEE, LUMSDEN MARK, HUIBO CAO, Quantum Condensed Matter Div., Oak Ridge National Laboratory, Oak Ridge, TN - 37830, JONG-WOO KIM, Advanced Photon Source, Argonne National Laboratory, Lemont, IL - 60439, CHRISTINA HOFFMAN, XIAOPING WANG, Chem. & Mat. Sci. Div., Oak Ridge Nat. Lab. Oak Ridge, TN - 37830 — Potassium Vanadate ( $K_2V_3O_8$ ) is an  $S = 2D$  square lattice antiferromagnet that shows spin reorientation indicating a strong coupling between the magnetism and its dielectric properties with a promise of rich physics that promises multiferroicity. These tangible physical properties are strongly tied through a spin-lattice coupling to the underlying lattice and superlattice behavior. It has a superlattice (SL) onset below  $T_c = 115$  K with an approximate  $[3 \times 3 \times 2]$  modulation. Here we present our recent experiments at TOPAZ beamline at SNS which for the first time proves conclusively that the lattice modulations are incommensurate, with an in-plane  $Q$  of 0.315. We will also show our attempts to refine the data using JANA which requires a redefinition of the lattice, as well as the temperature and  $Q$  dependence of the superlattice modulation measured using neutrons at HFIR and synchrotron x-rays at APS. Our results are not only relevant for the ongoing search of multifunctional behavior in  $K_2V_3O_8$  but also generally for the superlattice modulations observed in a large family of fersenoites.

<sup>1</sup>Work performed at ORNL and ANL is supported by U.S. Dept. of Energy, Office of Basic Energy Sciences and Office of User Facilities Division.

**3:42PM P26.00007 Properties of Transition Metal Doped Alumina<sup>1</sup>**, ERIK NYKWEST, Univ of Connecticut - Storrs, KRISTA LIMMER, RAY BRENNAN, VICTORIA BLAIR, Army Research Lab, RAMPI RAMPRASAD, Univ of Connecticut - Storrs — Crystallographic texture can have profound effects on the properties of a material. One method of texturing is through the application of an external magnetic field during processing. While this method works with highly magnetic systems, doping is required to couple non-magnetic systems with the external field. Experiments have shown that low concentrations of rare earth (RE) dopants in alumina powders have enabled this kind of texturing. The magnetic properties of RE elements are directly related to their  $f$  orbital, which can have as many as 7 unpaired electrons. Since  $d$ -block elements can have as many as 5 unpaired electrons the effects of substitutional doping of 3d transition metals (TM) for Al in alpha (stable) and theta (metastable) alumina on the local structure and magnetic properties, in addition to the energetic cost, have been calculated by performing first-principles calculations based on density functional theory. This study has led to the development of general guidelines for the magnetic moment distribution at and around the dopant atom, and the dependence of this distribution on the dopant atom type and its coordination environment. It is anticipated that these findings can aid in the selection of suitable dopants help to guide parallel experimental efforts.

<sup>1</sup>This project was supported in part by an internship at the Army Research Laboratory, administered by the Oak Ridge Institute for Science and Education, along with a grant of computer time from the DoD High Performance Computing Modernization Program.

**3:54PM P26.00008 Incursion of water and Cu ions into porous low dielectric constant (LKD) thin films and interconnects resulting in damage, time dependent dielectric breakdown (TDDB) and decreased lifetime and reliability.**, ROBERT LAIBOWITZ, ARCHANA RAJA, Columbia University, THOMAS SHAW, ERIC LINIGER, STEPHAN COHEN, IBM Research Division, COLUMBIA UNIVERSITY COLLABORATION, IBM RESEARCH DIVISION COLLABORATION — Porous dielectrics, their interfaces and related processing details provide many opportunities for water and Cu incursion. The Cu typically starts as part of the electrode and needs a liner to keep it away from the dielectric. As scaling continues thinner liners and imperfections in the liner layer can expose the Cu to the LKD. This will lead to TDDB with greatly reduced lifetimes. Water exposure can come from processing or through defects in the passivation layer. Most studies of these breakdown effects have been accomplished using accelerated DC measurements in which the sample is destroyed. Dielectric relaxation provides a new set of measurements at low fields, low temperatures and reusable samples. In this way we have observed the presence of both physisorbed and chemisorbed water, determined their activation energy of motion and removal of the water by various annealing protocols. Initial measurements of Cu incursion have also been made. Preliminary measurement of samples containing Cu and water and processing damage show reduced reliability. We also have begun studies to determine the minimum liner thickness. .

**4:06PM P26.00009 Strong Red Luminescent Twin ZnO Nanorods for Nano-thermometry and Phonon Tunnel Device Application**, AVANENDRA SINGH, KARTIK SENAPATI, NISER, KARUNAKAR NANDA, IISC, BISWARUP SATPATI, SINP, PRATAP SAHOO, NISER — Two segments of horizontally grown crystalline ZnO nanorods (NRs) connected with an amorphous layer have been successfully synthesized using aqueous growth technique. The amorphous layer between the crystalline ZnO sections is tunable with growth parameters and confirmed by transmission electron microscopy. The confocal photoluminescence (PL) imaging and spectroscopy of twin ZnO NRs at different temperature shows stable and intense red emission with comparably weak UV emission. Red emission from the twin NRs are the consequence of surface defect and structural imperfections of lattice disorder. The disappearance of asymmetry in UV emission after 293K indicates the weak exciton-phonon coupling at higher temperature while the coupling is stronger at lower temperatures. An indirect analysis from phonon bands of PL shows that the amorphous layer acts as a phonon barrier beyond certain thickness. Such crystalline-amorphous-crystalline architecture may be suitable for fundamental studies of the phonon tunneling in nanostructure. We also show that the individual NRs can be used for sensing and mapping of temperature in a wide range of 80-373 K with an accuracy of 0.1K with good sensitivity. These NRs may have suitable application for non-contact nano-thermometry.

**4:18PM P26.00010 Analysis of metastable ultrasmall titanium oxide clusters using a hybrid global search algorithm and first-principles approach<sup>1</sup>**, ERIC INCLAN, Georgia Institute of Technology, Atlanta, GA 30332, JACK LASSESTER, Middle Tennessee State University, Murfreesboro, TN 37130, DAVID GEOHEGAN, MINA YOON, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831 — Research in  $TiO_2$  materials is highly relevant to energy and device applications, however, precise control of their morphologies and characterization are still a grand challenge in the field. We developed and applied a hybrid optimization algorithm to explore configuration spaces of energetically metastable  $TiO_2$ . Our approach was to minimize the total energy of  $TiO_2$  clusters in order to identify the energy landscape of plausible  $(TiO_2)_n$  ( $n = 1-100$ ). The hybrid algorithm retained good agreement with a regression on structures published in literature up to  $n = 25$ . Using first-principles density functional theory, we analyze basic properties of the hybrid-algorithm generated  $TiO_2$  nanoparticles. Our results show the expected convergence to bulk material characteristics as the cluster size increases in that the band gap varies with respect to the size of the nanocluster. The nanoclusters trended toward compact, low surface area structures that share characteristics of the bulk, namely octahedral microstructures as the nanoclusters increased in size. Our study helps in better identifying and characterizing experimentally observed structures.

<sup>1</sup>This work is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

**4:30PM P26.00011 Low energy THz excitations in distorted perovskites under strong magnetic fields and low temperature.** , N. E. MASSA, LANAIS EFO-CEQUINOR, UNLP, La Plata, Argentina, K. HOLLDAK, HZB-BESSY II, Berlin, Germany , V. TA PHUOC, R. SOPRACASE, GREMAN, Tours, France, L. DEL CAMPO, D. DE SOUSA MENESES, P. ECHEGUT, CNRS-CEMHTI, Orlans, France, J.A. ALONSO, ICMN-CSIC, Madrid, Spain — We report on the magnetic field evolution of distinctive absorption bands in several zero field cooled polycrystalline  $\text{RMO}_3$  ( $\text{R} = \text{Pr, Nd, Sm, Er, Tm, Lu}$ ;  $\text{M} = \text{Cr, Mn, Fe, Ni}$ ) at low temperatures. Measurements below  $120 \text{ cm}^{-1}$  were done in an 11 T magnet combined with a Bruker IFS125-HR interferometer at the THz beamline of the BESSY II storage ring. At the reordering spin temperature, the spectra of  $\text{ErCrO}_3$  show an Er-Kramers doublet at  $\sim 55 \text{ cm}^{-1}$  following a second order continuous reorientation. It suggests strong anisotropic  $\text{Er}^{3+}$ - $\text{Cr}^{3+}$  magnetic exchange interactions. The band strength of its triplet excited states decreases upon increasing the magnetic field. Non-Kramers Pr in  $\text{PrCrO}_3$  implies a magnetic field induced quasi-doublet system. Spin wave modes AF and F are also tentatively assigned. In  $\text{ErFeO}_3$ , the spin reordering of the canted transition metal, and the  $\text{Er}^{3+}$  exchange, is monitored emerging above 80 K. Temperature dependent multiplet transitions centered at  $50 \text{ cm}^{-1}$  and  $110 \text{ cm}^{-1}$  appear as asymmetric field dependent broad lines. The absence of activity at  $\sim 4 \text{ K}$  in  $\text{SmCrO}_3$ , shared by  $\text{SmMO}_3$  ( $\text{M} = \text{Fe, Ni}$ ), is consequence of near Cr-canted-Rare-Earth-opposite moment compensation juxtaposed to random micrograin orientation. We will also comment on observed only in  $\text{ErNiO}_3$  field dependent Er transitions and band profiles.

## Wednesday, March 16, 2016 2:30PM - 5:30PM –

Session P27 DCMP: VO<sub>2</sub>: Experiment and Theory 326 - Mengkun Liu, State University of New York, Stonybrook

**2:30PM P27.00001 Ultrafast Pump-Probe Studies of the Light-Induced MIT and Recovery of Niobium Dioxide Thin Films** , MELISSA BEEBE, College of William & Mary, J. MICHAEL KLOPF, Helmholtz-Zentrum Dresden-Rossendorf, SALINPORN KITTIWATANAKUL, JIWEI LU, STUART A. WOLF, University of Virginia, R. ALEJANDRA LUKASZEW, College of William & Mary — Niobium dioxide ( $\text{NbO}_2$ ) is a highly correlated binary oxide that, like vanadium dioxide ( $\text{VO}_2$ ), exhibits a first-order insulator-to-metal transition (IMT) at a material-dependent critical temperature, accompanied by a structural transformation from monoclinic to rutile. The nature of the IMT in  $\text{VO}_2$  has been discussed at length, while fewer studies have been carried out on  $\text{NbO}_2$ . Previous studies show that the IMT can also be optically induced in  $\text{VO}_2$  on a sub-picosecond timescale; here, we present the first ultrafast pump-probe studies showing this optically-induced transition in  $\text{NbO}_2$  thin films and compare these results to similar ones carried out on  $\text{VO}_2$  thin films.

**2:42PM P27.00002 OPTICAL SPECTROSCOPY OF THE  $M_2$  AND T PHASES OF VANADIUM DIOXIDE** , T.J. HUFFMAN, M.M. QAZILBASH, C. HENDRIKS, E.J. WALTER, H. KRAKAUER, College of William and Mary, JOONSEOK YOON, HONGLYOUL JU, Yonsei University, R. SMITH, G.L. CARR, Brookhaven National Laboratory — The salient feature of the familiar structural transition that accompanies the metal-insulator transition in bulk  $\text{VO}_2$  is a pairing of all of the vanadium ions in the  $M_1$  insulating phase. This pairing has long been thought critical to the emergence of insulating behavior. However, there exist two less familiar insulating states,  $M_2$  and T. These phases notably exhibit distinctly different V-V pairing. In the  $M_2$  phase, only half of the vanadium ions exhibit pairing while the other half carry local spin 1/2 magnetic moments and are equally spaced in quasi-one dimensional chains. The T phase has two types of inequivalent vanadium chains, each consisting of V-V pairs but with different spacing between V ions in the pairs. The  $M_1$  phase has been studied extensively with optical spectroscopy. By studying the two less familiar insulating phases,  $M_2$  and T, one can investigate how changes in V-V pairing affect the properties of the  $\text{VO}_2$  insulating state. We performed infrared and optical spectroscopy on the  $M_2$  and T phases in the same sample. Despite a clear change in the lattice structure, the inter-band transitions are insensitive to changes in the V-V pairing. This result conclusively establishes that intra-atomic Coulomb repulsion between electrons provides the dominant contribution to the energy gap in all insulating phases of  $\text{VO}_2$ . Our work highlights the necessity of considering the  $M_2$  and T phases of  $\text{VO}_2$  in future experimental and theoretical research.

**2:54PM P27.00003 Photoinduced phase transitions in narrow-gap Mott insulators: the case of  $\text{VO}_2$** <sup>1</sup> , ZHUORAN HE, ANDREW MILLIS, Columbia University — The nonequilibrium dynamics of strongly correlated electrons in photoexcited  $\text{VO}_2$  is studied using the quantum Boltzmann equation and nonequilibrium Hartree-Fock methods applied to a band structure given by extended density functional theory (DFT+ $U$ + $V$ ) and realistic dynamical interactions. The initial equilibration of electrons occurs in hundreds of femtoseconds. For physically reasonable parameters, our Hartree-Fock calculation sustains a new metastable  $M_1$  metal phase that is qualitatively consistent with the recent experiment of Morrison et al [1]. The long-term stability of the  $M_1$  metal phase will also be considered. [1] V. R. Morrison, R. P. Chatelain, K. L. Tiwari, A. Hendaoui, A. Bruhács, M. Chaker, and B. J. Siwick, Science 346, 445 (2014).

<sup>1</sup>This work is supported by the Department of Energy under grant number DE-SC0012375.

**3:06PM P27.00004 Random Field Driven Spatial Complexity at the Mott Transition in  $\text{VO}_2$**  , ERICA CARLSON, SHUO LIU, BENJAMIN PHILLABAUM, Purdue University, West Lafayette, IN, USA, KARIN DAHMEN, University of Illinois at Urbana-Champaign, Urbana, IL, USA, NARSIMHAMURTHY VIDHYADHIRAJA, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, INDIA , MUMTAZ QAZILBASH, College of William and Mary, Williamsburg, VA, USA , DIMITRI BASOV, University of California San Diego, La Jolla, CA, USA — We report the first application of critical cluster techniques to the Mott metal-insulator transition in vanadium dioxide. We show that the geometric properties of the metallic and insulating puddles observed by scanning near-field infrared microscopy are consistent with the system passing near criticality of the random field Ising model as temperature is varied. The resulting large barriers to equilibrium may be the source of the unusually robust hysteresis phenomena associated with the metal-insulator transition in this system.

**3:18PM P27.00005 Field-Effect Modulation of Ambipolar Doping and Domain Wall Band Alignment in P-type Vanadium Dioxide Nanowires** , YASEN HOU, XINGYUE PENG, YIMING YANG, DONG YU, Univ of California - Davis — The sub-picosecond metal-insulator phase transition in vanadium dioxide ( $\text{VO}_2$ ) has attracted extensive attention with potential applications in ultrafast Mott transistors. However, the development of  $\text{VO}_2$ -based transistors lags behind, owing to the lack of an efficient and hysteresis-free electrostatic doping control. Here we report the first synthesis of p-type single crystalline  $\text{VO}_2$  nanowires via catalyst-free chemical vapor deposition. The p-type doping was unambiguously confirmed by both solid and electrochemical gating methods, and further evidenced by the scanning photocurrent microscopic measurements. Interestingly, we observed that the photocurrent spot polarity at the metal-insulator domain walls was reversibly switched by electrochemical gating, which indicates a band bending flipping. Furthermore, we eliminated the common hysteresis in gate sweep and greatly shortened the transistor response time via a hybrid gating method, which combines the merits of liquid ionic and solid gating. The capability of efficient field effect modulation of ambipolar conduction and band alignment offers new opportunities on understanding the phase transition mechanism and enables novel electronic applications based on  $\text{VO}_2$ .

**3:30PM P27.00006 Electric Field-induced Resistance Switching in VO<sub>2</sub> Channels using Hybrid Gate Dielectric of High-*k* Ta<sub>2</sub>O<sub>5</sub>/Organic material Parylene-C.** , TINGTING WEI, TERUO KANKI, Institute of Scientific and Industrial Research, Osaka University, KOHEI FUJIWARA, Institute for Materials Research, Tohoku University, MASASHI CHIKANARI, HIDEKAZU TANAKA, Institute of Scientific and Industrial Research, Osaka University — Electrostatic approach utilizing field-effect transistor (FET) with correlated electron materials provides an avenue to realize the novel devices (Mott-transistor) and to clarify condensed matter physics. In this study, we have prepared Mott-transistors using vanadium dioxide (VO<sub>2</sub>) channels and employed hybrid gate dielectric consisted of high-*k* material Ta<sub>2</sub>O<sub>5</sub> and organic polymer parylene-C to trigger carrier transport modulation in VO<sub>2</sub>. Obvious resistance modulations were observed in insulating regime through time-dependent resistance measurement at varied square-shaped gate bias ( $V_G$ ). Contrasting to the hysteretic response in electric double layer transistor (EDLT), an abrupt resistance switching in less than of 2-second-interval enables us to attribute such immediate modulation to pure electrostatic effect. Moreover, the maximum of resistance change was identified to appear around phase transition temperature ( $T_{MI}$ ), which confirmed the disordered heterogeneous regime at  $T_{MI}$ . Taking advantage of systematic modulation using VO<sub>2</sub>-based devices, we demonstrated the pronounced shifts of  $T_{MI}$  by gate bias. Another fascinating behavior on asymmetric drop in  $T_{MI}$  by hole-electron carrier doping was observed.

**3:42PM P27.00007 Resistance modulation in VO<sub>2</sub> nanowires induced by an electric field *via* air-gap gates** , TERUO KANKI, MASASHI CHIKANARI, TINGTING WEI, HIDEKAZU TANAKA, Osaka University, THE INSTITUTE OF SCIENTIFIC AND INDUSTRIAL RESEARCH TEAM — Vanadium dioxide (VO<sub>2</sub>) shows huge resistance change with metal-insulator transition (MIT) at around room temperature. Controlling of the MIT by applying an electric field is a topical ongoing research toward the realization of Mott transistor. In this study, we have successfully switched channel resistance of VO<sub>2</sub> nano-wire channels by a pure electrostatic field effect using a side-gate-type field-effect transistor (SG-FET) *via* air gap and found that single crystalline VO<sub>2</sub> nanowires and the channels with narrower width enhance transport modulation rate. The rate of change in resistance ( $(R_0-R)/R$ , where  $R_0$  and  $R$  is the resistance of VO<sub>2</sub> channel with off state and on state gate voltage ( $V_G$ ), respectively) was 0.42 % at  $V_G = 30$  V in in-plane poly-crystalline VO<sub>2</sub> channels on Al<sub>2</sub>O<sub>3</sub>(0001) substrates, while the rate in single crystalline channels on TiO<sub>2</sub> (001) substrates was 3.84 %, which was 9 times higher than that using the poly-crystalline channels. With reducing wire width from 3000 nm to 400 nm of VO<sub>2</sub> on TiO<sub>2</sub> (001) substrate, furthermore, resistance modulation ratio enhanced from 0.67 % to 3.84 %. This change can not be explained by a simple free-electron model. In this presentation, we will compare the electronic properties between in-plane polycrystalline VO<sub>2</sub> on Al<sub>2</sub>O<sub>3</sub> (0001) and single crystalline VO<sub>2</sub> on TiO<sub>2</sub> (001) substrates, and show experimental data in detail..

**3:54PM P27.00008 Resistance noise spectroscopy across the thermally and electrically driven metal-insulator transitions in VO<sub>2</sub> nanobeams<sup>1</sup>** , ALI ALSAQQA, COLIN KILCOYNE, SUJAY SINGH, State Univ of NY - Buffalo, GREGORY HORROCKS, PETER MARLEY, SARBAJIT BANERJEE, Texas AM University, College Station, G. SAMBANDAMURTHY, State Univ of NY - Buffalo — Vanadium dioxide (VO<sub>2</sub>) is a strongly correlated material that exhibits a sharp thermally driven metal-insulator transition at  $T_c \sim 340$  K. The transition can also be triggered by a DC voltage in the insulating phase with a threshold ( $V_{th}$ ) behavior. The mechanisms behind these transitions are hotly discussed and resistance noise spectroscopy is a suitable tool to delineate different transport mechanisms in correlated systems. We present results from a systematic study of the low frequency ( $1 \text{ mHz} < f < 10 \text{ Hz}$ ) noise behavior in VO<sub>2</sub> nanobeams across the thermally and electrically driven transitions. In the thermal transition, the power spectral density (PSD) of the resistance noise is unchanged as we approach  $T_c$  from 300 K and an abrupt drop in the magnitude is seen above  $T_c$  and it remains unchanged till 400 K. However, the noise behavior in the electrically driven case is distinctly different: as the voltage is ramped from zero, the PSD gradually increases by an order of magnitude before reaching  $V_{th}$  and an abrupt increase is seen at  $V_{th}$ . The noise magnitude decreases above  $V_{th}$ , approaching the  $V = 0$  value. The individual roles of percolation, Joule heating and signatures of correlated behavior will be discussed.

<sup>1</sup>This work is supported by NSF DMR 0847324.

**4:06PM P27.00009 Strain-dependent ultrafast dynamics of insulator-to-metal phase transition in VO<sub>2</sub><sup>1</sup>** , SERGIY LYSENKO, ARMANDO RUA, JOSE FIGUEROA, FELIX FERNANDEZ, Department of Physics, University of Puerto Rico, Mayaguez, Puerto Rico 00681, USA — Much attention has been devoted recently to visualize and understand the strain effects in phase transition dynamics of vanadium oxide materials. In this study, using femtosecond angle-resolved light scattering technique we show strong influence of internal misfit strain in epitaxial VO<sub>2</sub>(M1) films on insulator-to-metal phase transition within less than 1 ps. Anisotropic strain in twinned domains and in domains of different size results mostly in antiphase oscillatory dynamics of coherent phonons. Depending on domain pattern and type of the substrate, this dynamics was found to be dependent on azimuthal angle and/or on spatial frequency of surface roughness. The origin of observed photoinduced antiphase oscillations is associated with compressive and tensile strain in VO<sub>2</sub> domains which alters the initial phase of the oscillations. In contrast to pure VO<sub>2</sub>(M1), the Cr-doped VO<sub>2</sub>(M2) shows strong phonon scattering signatures with noticeable random component in the phase of coherent phonons.

<sup>1</sup>This material is based upon work supported by the U. S. Army Research Laboratory and the U. S. Army Research Office under contract number W911NF-15-1-0448

**4:18PM P27.00010 Straining to observe the M2 phase in epitaxial VO<sub>2</sub> films<sup>1</sup>** , NICHOLAS QUACK-ENBUSH, MATTHEW WAHILA, LOUIS PIPER, Dept. of Physics, Binghamton University, HANJONG PAIK, MEGAN HOLTZ, XIN HUANG, JOEL BROCK, DAVID MULLER, DARRELL SCHLOM, Dept. of Materials Science and Engineering, Cornell University, JOSEPH WOICK, Materials Science and Engineering Laboratory, National Institute of Standards and Technology, DARIO ARENA, Dept. of Physics, University of South Florida — It has been more than a decade since it was shown that the transition temperature  $T_{MIT}$  of VO<sub>2</sub> in epitaxial thin films can be tuned by compressive and tensile strain along the rutile c-axis. Since this discovery, uniaxial strain studies of VO<sub>2</sub> nanobeams have demonstrated that compressive strain indeed lowers  $T_{MIT}$ , thus stabilizing the metallic rutile phase. However, even minor tensile strain induces an intermediate insulating monoclinic M2 phase. Whether this phase can be stabilized in thin films remains contentious owing to the constraints of sample and/or interface quality. Here, we present hard x-ray photoelectron spectroscopy and temperature-dependent soft x-ray absorption spectroscopy of high quality ultrathin epitaxial VO<sub>2</sub> films on TiO<sub>2</sub> (001) and (100) substrates. The VO<sub>2</sub>/TiO<sub>2</sub>(001) are absent of intermediate phases and maintain a MIT similar to unstrained VO<sub>2</sub>, while the VO<sub>2</sub>/TiO<sub>2</sub>(100) films display a stable M2 phase between the M1 and rutile endpoint phases. We discuss our findings in terms of differences between uniaxial and biaxial strain.

<sup>1</sup>This research is supported by the National Science Foundation under DMR-1409912

**4:30PM P27.00011 Metallic bubbles nucleation and growth in VO<sub>2</sub> nanofilms: insights from TDDFT+DMFT<sup>1</sup>**, VOLODYMYR TURKOWSKI, Dep. of Physics, Univ. of Central Florida, Orlando, FL 32816, JOSE MARIO GALICIA-HERNANDEZ, Inst. of Physics, Univ. of Puebla, Puebla 72550, Mexico and Univ. of Central Florida, Orlando, FL 32816, GREGORIO HERNANDEZ-COCOLETZI, Inst. of Physics, Univ. of Puebla, Puebla 72550, Mexico, TALAT S. RAHMAN, Dep. of Physics, Univ. of Central Florida, Orlando, FL 32816 — We apply a time-dependent density-functional theory + dynamical mean-field theory (TDDFT+DMFT) approach to model the response of insulating nanofilms of VO<sub>2</sub> to perturbations by ultrafast laser pulses. We focus on the spatially-resolved metallization of the systems, and especially on the process of nucleation and time-dependence of the size of the "surface" and "bulk" metallic domains (bubbles) as a function of film width. In particular, we find that the initial universal (parameter-independent) growth of the domains (radius  $R \sim t^{1/2}$ ), changes by the bubbles shrinking ( $R \sim t^{-a}$ ,  $a \sim 1$ ) as a result of Coulomb scattering effects, and eventually by post-femto-second phonon-involved relaxation of the systems to the equilibrium accompanied by infrared photoemission. The time-dependent conductivity obtained from the above results is in a good agreement with available experimental data.[1,2] [1] D.J. Hilton et al., PRL 99, 226401 (2007); [2] T.L. Cocker et al., PRB 85, 155120 (2012).

<sup>1</sup>Work supported in part by DOE Grant No. DOE-DE-FG02-07ER46354 and by CONACYT Scholarship 23210 (J.M.G.H.).

**4:42PM P27.00012 Observation of impact ionization in vanadium dioxide<sup>1</sup>**, JOSHUA HOLLEMAN, Florida State University/NHMFL, MICHAEL BISHOP, National High Magnetic Field Laboratory, CARLOS GARCIA, CHRISTIANNE BEEKMAN, Florida State University/NHMFL, SHINBUHM LEE, HO NYUNG LEE, Oak Ridge National Laboratory, EFSTRATIOS MANOUSAKIS, Florida State University/NHMFL, STEPHEN MCGILL, National High Magnetic Field Laboratory — Pump-probe optical spectroscopy was used to investigate the possibility of charge carrier multiplication by impact ionization in a 100 nm film of VO<sub>2</sub> in the M<sub>1</sub> insulating phase. The film was excited by pump pulses with energies above and below twice the band gap energy and observed with two different probe wavelengths. The transient reflectivities of the film were then compared. We observed an enhancement of the reflectivity for the higher energy pump pulses near zero delay compared to the reflectivity for the lower energy pump pulses for both probe wavelengths. Additionally, we identified and described multiple timescales within the charge dynamics. This experiment demonstrated that impact ionization acts as a carrier multiplication process in this prototypical strongly-correlated system.

<sup>1</sup>This work was supported by NSF DMR-1229217

**4:54PM P27.00013 Visualization of local phase transition behaviors in ultrathin VO<sub>2</sub>/TiO<sub>2</sub> thin films**, AHRUM SOHN, Ewha womans university, TEROU KANKI, HIDEKAZU TANAKA, Osaka university, DONG-WOOK KIM, Ewha womans university — VO<sub>2</sub> undergoes the first order phase transition and two electronic phases can coexist near the critical temperature. We investigated evolution of the surface work function maps of epitaxial VO<sub>2</sub>/TiO<sub>2</sub> thin films (thickness: 15, 30, and 45 nm) using Kelvin probe force microscopy (KPFM) measurements in the temperature range of 285-330 K. Fully strained thin films were almost free of grain boundaries and thicker films had dislocations caused by strain relaxation. The sample's work function decreases, while spanning the metal-insulator transition (MIT). The work function maps clearly revealed coexistence of the two distinct phase domains. The surface area fraction of the insulating phase near the dislocations was higher than that in other regions. Thicker films have complicated domain patterns; hence, the three-dimensional percolation model properly described the MIT behaviors. In contrast, the two-dimensional percolation model well explained the transition behaviors of uniformly strained thinner films.

**5:06PM P27.00014 A Microscopic Model for the Strongly Coupled Electron-Ion System in VO<sub>2</sub><sup>1</sup>**, TIMOTHY LOVERN, SANJOY SARKER, Department of Physics and Astronomy, University of Alabama — The metal-insulator transition (MIT) in vanadium dioxide (VO<sub>2</sub>) near 340 K is accompanied by a structural transition, suggesting strong coupling between electronic and lattice degrees of freedom [1]. To help elucidate this relationship, we construct and analyze a microscopic model in which electrons, described by a tight-binding Hamiltonian, are dynamically coupled to Ising-like ionic degrees of freedom. A mean-field decoupling leads to an interacting two-component (pseudo) spin-1 Ising model describing the ions. An analysis of the minimal ionic model reproduces the observed M1 and M2 dimerized phases and rutile metal phase, occurring in the observed order with increasing temperature. All three transitions are first order, as observed. We further find that both dimerization and correlations play crucial roles in describing the insulating M1 phase. We discuss why dynamical coupling of electrons and ions is key to obtain a full understanding of the phenomenology of VO<sub>2</sub>, particularly in the context of the phase coexistence [2] observed near the MIT.

[1] D. Paquet and P. Leroux-Hugon, Phys. Rev. B **22**, 5284 (1980).

[2] M. M. Qazilbash et al., Science **318**, 1750 (2007).

<sup>1</sup>This research was supported by the National Science Foundation (DMR-1508680).

**5:18PM P27.00015 Controlling Oxygen Vacancy Creation In Ionic Liquid Gated Vanadate Nanostructures**, COLIN KILCOYNE, SUJAY SINGH, State Univ of NY - Buffalo, GREGORY HORROCKS, PETER MARLEY, SARBAJIT BANERJEE, Texas AM University, College Station, G. SAMBANDAMURTHY, State Univ of NY - Buffalo — Vanadium dioxide (VO<sub>2</sub>) is a correlated material with a transition from a monoclinic insulator to a rutile metal at  $\sim 340$  K. Through ionic liquid gating, oxygen vacancies can be electrochemically induced in VO<sub>2</sub> and it is found that the vacancies formation is greatly facilitated in the rutile phase, leading to the suppression of the metal-insulator transition. The reversibility, the rate and kinetics of the electrochemical reaction can be readily controlled with the gate voltage sweeps suggesting a potential defect engineering route to tune the electrical and structural properties of VO<sub>2</sub>. Vanadium pentoxide (V<sub>2</sub>O<sub>5</sub>) is a related system with diverse structural and electronic phases that can be obtained by intercalation of various cations. The electrochemical role of ionic liquid gating in creating new phases and modulating conductance in exfoliated thin flakes of V<sub>2</sub>O<sub>5</sub> will also be presented. This work is supported by NSF DMR 0847324.

**Wednesday, March 16, 2016 2:30PM - 5:30PM —**

**Session P28 DMP: Advances in Topological Materials I** 327 - Anton Burkov, University of Waterloo

### **2:30PM P28.00001 Quantum Transport of Spin-helical Dirac Fermion Topological Surface States in Topological Insulators**

**YONG P. CHEN**, Purdue University — Three-dimensional (3D) topological insulators (TI) are a novel class of electronic materials with topologically-nontrivial band structure such that the bulk is gapped and insulating yet the surface has topologically protected gapless conducting states. Such topological surface states (TSS) give helically spin polarized Dirac fermions, and offer a promising platform to realize various other novel physics such as topological magnetoelectric effects and Majorana fermions. However, it is often challenging to unambiguously access and study the transport properties of TSS in many practical TI materials due to non-negligible bulk conducting states. I will discuss our recent experiments on high-quality intrinsic TIs with insulating bulk and surface-dominated conduction that allow us to reveal a number of characteristic transport properties of spin-helical Dirac fermion topological surface states. We have observed, for example, a thickness-independent and surface-dominated conductance (even at room temperature) in exfoliated TI thin films [1] and well-developed half-integer Dirac fermion quantum Hall effect (QHE) arising from TSS (observed up to 40K) [1]; fully-tunable two-species Dirac fermion QHE and other intriguing states in dual gated devices where both top and bottom surfaces can be independently controlled [2]; current-induced helical spin-polarization detected by spin sensitive transport measurements using magnetic electrodes [3]; and in TI nanoribbons, Shubnikov-de Haas (SdH) oscillations showing gate-tunable Berry phase and ultra-relativistic Dirac mass [4]; and a half-integer Aharonov-Bohm effect (ABE) unique to the circumferentially quantized spin helical Dirac fermion surface state modes (sub-bands), with a gate-tunable conductance oscillation and alternation between the half-integer ABE and regular ABE periodic in fermi momentum [5]. Such TIs and related devices may enable promising future applications in spintronics, thermoelectrics and various topological quantum devices. References: [1] Y. Xu et al., Nature Physics 10, 956 (2014); [2] Y. Xu et al., arXiv:1511.04597 (2015); [3] J. Tian et al., Scientific Reports 5, 14293 (2015); [4] L. A. Jauregui et al., Scientific Reports 5, 8452 (2015); [5] L. A. Jauregui et al., Nature Nanotechnology, in press, arxiv:1503.00685 (2015).

### **3:06PM P28.00002 Large linear magnetoresistance and high carrier mobility in a new Dirac semimetal candidate**

**JOHNPIERRE PAGLIONE**, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, **KEFENG WANG**, Center for Nanophysics and Advanced Materials Department of Physics, University of Maryland, **DAVID GRAF**, National High Magnetic Field Laboratory, Florida State University, **LIMIN WANG**, Center for Nanophysics and Advanced Materials Department of Physics, University of Maryland, **F. BOSCHINI**, **A. DAMASCELLI**, Department of Physics & Astronomy, University of British Columbia — We report experimental results on a new potential Dirac semimetal, the skutterudite material RhSb<sub>3</sub>. Together with a very large magnetoresistance and carrier mobility, the linear dispersion of the electronic band structure suggests properties similar to other recently reported Dirac and Weyl semimetals that deserve further investigation. Together with angle-resolved photoemission data, we present high field transport and quantum oscillations measurements that point to very large Fermi velocity and aspects of Berry's curvature that warrant further investigation.

### **3:18PM P28.00003 Temperature-Induced Lifshitz Transition in WTe<sub>2</sub>**

**NA HYUN JO**, **YUN WU**, Ames Laboratory/ISU, **MASAYUKI OCHI**, **RIKEN**, **LUNAN HUANG**, **DAIXIANG MOU**, **SERGEY L. BUD'KO**, **P.C. CANFIELD**, Ames Laboratory/ISU, **NANDINI TRIVEDI**, Ohio State University, **RYOTARO ARITA**, **RIKEN/Tohoku University**, **ADAM KAMINSKI**, Ames Laboratory/ISU — We use thermoelectric power (TEP), temperature- and field-dependent resistivity, and ultrahigh resolution, tunable, vacuum ultraviolet laser-based, angle-resolved photoemission spectroscopy (ARPES) measurements to study the electronic properties of WTe<sub>2</sub>, a compound that manifests exceptionally large, temperature-dependent magnetoresistance. The Fermi surface consists of two pairs of electron and two pairs of hole pockets along the  $X-\Gamma-X$  direction. We find a rare example of a temperature-induced Lifshitz transition at  $T \approx 160$  K. Temperature dependent TEP shows a change of slope at  $T \approx 175$  K and Kohler's rule was breakdown in the 70-140 K range. ARPES temperature scans confirm that the hole pockets completely disappear around 160 K. Our electronic structure calculations show a clear and substantial shift of the chemical potential  $\mu(T)$  due to the semimetal nature of this material driven by modest changes in temperature. [PRL 115, 166602 (2015)]

<sup>1</sup>This work is supported by the US DOE, Basic Energy Sciences under Contract No. DE-AC02-07CH11358; Betty Moore Foundation EPiQS Initiative (Grant No. GBMF4411); and CEM, a NSF MRSEC, under Grant No. DMR-1420451.

### **3:30PM P28.00004 High-field magnetoconductivity of topological semimetals**

**HAI-ZHOU LU**, South University of Science and Technology of China, **SONG-BO ZHANG**, **SHUN-QING SHEN**, The University of Hong Kong — The chiral anomaly has been widely believed to give a positive magnetoconductivity or negative magnetoresistivity in strong and parallel fields in topological semimetals. However, several recent experiments on both Weyl and Dirac topological semimetals show a negative magnetoconductivity in high fields. Here, we study the magnetoconductivity of Weyl and Dirac semimetals in a strong magnetic field applied along the direction that connects the Weyl nodes, we find that the conductivity along the field direction is not only determined by the Landau degeneracy, but also depends on the Fermi velocity and scattering potentials. We identify several scenarios in which the high-field magnetoconductivity is negative. It shows that the high-field positive magnetoconductivity may not be a compelling signature of the chiral anomaly. The quantum linear magnetoresistance will also be discussed.

### **3:42PM P28.00005 Orbital and anisotropy effects on the itinerant exchange interaction in 3D Dirac semimetals**

**SERGIO ULLOA**, Ohio University, **DIEGO MASTROGIUSEPPE**, Instituto de Fisica Rosario, **NANCY SANDLER**, Ohio University — Dirac semimetals are new materials that can be considered analogues of graphene in three dimensions. Their band structure exhibits robust Dirac points that are protected by crystalline symmetry, and strong spin-orbit interaction. These unusual properties suggest that magnetic impurities may reveal exotic behavior with potential technological importance. In metallic hosts, magnetic impurities interact through the electron gas via the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction that depends strongly on the band structure of the material. We report on the RKKY interaction in 3D Dirac semimetals, such as Na<sub>3</sub>Bi and Cd<sub>3</sub>As<sub>2</sub> [1, 2]. We discuss asymptotic expressions for the interaction corresponding to settings with magnetic impurities at different distances and relative angle with respect to high symmetry directions on the lattice. We show that the Fermi velocity anisotropy produces a strong renormalization of the magnitude of the interaction, and a correction to the frequency of oscillation in real space. Hybridization of the impurities to different conduction electron orbitals results in interesting anisotropic interactions which can generate spiral spin structures in doped samples. [1] Z. Liu et al., Science 343, 864 (2014); [2] Z. Liu et al., Nat. Mater. 13, 677 (2014)

### **3:54PM P28.00006 Study of angle dependent magnetoresistance in half-Heusler YPtBi**

**HYUNSOO KIM**, **KEFENG WANG**, **HALYNA HODOVANETS**, **JOHNPIERRE PAGLIONE**, Univ of Maryland-College Park — Semimetallic half-Heusler compounds (RTBi, R = rare earth, T = Pd, Pt) have been attracting much attention because multiple theoretical calculations predicted the topologically non-trivial band structure. However, the detail band structure near the  $\Gamma$  point depends on the specific calculation methods, and also the band structure inferred from experimental results show discrepancy from the theoretical one. Particularly in RPtBi (R=Y, Lu, Dy, Gd), the surface metallic states, which is absent in most of the theoretical results, were evident by recent ARPES measurements, but there has not been any detailed study on the metallic surface states. Moreover, the observation of topological nodal superconductivity in YPtBi makes the knowledge of Fermiology crucial to understand the pairing mechanism in the half-Heusler superconductors. Here, we present experimental results on angular dependence of magnetoresistance at various temperatures in single crystals of YPtBi. Based on observation of the angular dependence of Shubnikov-de Haas quantum oscillations, we discuss possible topologies of the bulk as well as the surface Fermi surfaces.

**4:06PM P28.00007 Large transverse current in topological Dirac semimetal Cd<sub>3</sub>As<sub>2</sub>**, WEI-LI LEE, SHIH-TING GUO, R. SANKAR, YUNG-YU CHIEN, Institute of Physics, Academia Sinica, Taipei 11529, Taiwan, TAY-RONG CHANG, HORNG-TAY JENG, Department of Physics, National Tsing Hua University, Hsinchu 30013, Taiwan, GUANG-YU GUO, Department of Physics, National Taiwan University, Taipei 10617, Taiwan, F. C. CHOU, Center for Condensed Matter Sciences, National Taiwan University, Taipei 10617, Taiwan — Cadmium arsenide (Cd<sub>3</sub>As<sub>2</sub>) is known for its inverted band structure and ultra-high electron mobility. It has been theoretically predicted and also confirmed by ARPES experiments to exhibit a 3D Dirac semimetal phase containing degenerate Weyl nodes. From magneto-transport measurements in high quality single crystals of Cd<sub>3</sub>As<sub>2</sub>, a small effective mass  $m^* \approx 0.05 m_e$  is determined from the Shubnikov-de Haas (SdH) oscillations. In certain field orientations, we find a splitting of the SdH oscillation frequency in the FFT spectrum suggesting a possible lifting of the double degeneracy in accord with the helical spin texture at outer and inner Fermi surfaces with opposite chirality predicted by our *ab initio* calculations. Strikingly, a large antisymmetric magnetoresistance with respect to the applied magnetic fields is uncovered over a wide temperature range in needle crystal of Cd<sub>3</sub>As<sub>2</sub> with its long axis along [112] crystal direction. It reveals a significant contribution of intrinsic anomalous velocity term in the transport equation intimately related to the unique 3D Rashba-like spin splitted bands in defected Cd<sub>3</sub>As<sub>2</sub>.

**4:18PM P28.00008 Magnetic Torque Anomaly in the Quantum Limit of Weyl and Dirac Semimetals**, NITYAN L. NAIR, PHILIP J.W. MOLL, ANDREW C. POTTER, Univ of California - Berkeley, BRAD RAMSHAW, KIMBERLY MODIC, National High Magnetic Field Laboratory, Los Alamos, SCOTT RIGGS, BIN ZENG, National High Magnetic Field Laboratory, Tallahassee, NIRMAL GHIMIRE, ERIC BAUER, Los Alamos National Laboratory, ROBERT KEALHOFFER, ZHENGLU LI, STEVEN LOUIE, Univ of California - Berkeley, FILIP RONNING, Los Alamos National Laboratory, JAMES G. ANALYTIS, Univ of California - Berkeley — Three dimensional Dirac and Weyl semimetals, characterized by bulk quasiparticles that behave as massless, linearly dispersing Dirac or Weyl fermions, have excited physicists with their unique topological properties and potential for applications. The experimental signatures of Weyl or Dirac fermions, however, are often subtle and indirect, especially in systems where they coexist with trivial electrons. Here, we report a novel method by which these topological systems can be unambiguously experimentally identified. Magnetic torque measurements were performed on the Weyl semimetal NbAs in high magnetic field, showing a large anomaly upon entering the quantum limit. The torque exhibits a striking sign reversal, corresponding to a change in the magnetic anisotropy that is a direct result of the topological properties of the charge carriers. This result can be generalized to other Dirac and Weyl semimetal systems and establishes quantum limit torque measurements as a simple and direct experimental method of distinguishing topologically non-trivial Weyl and Dirac systems from trivial semiconductors.

**4:30PM P28.00009 Large magnetoresistance and electronic anisotropy in NbAs<sub>2</sub>**<sup>1</sup>, BING SHEN, SHAN JIANG, NI NI, UCLA — Recently, extremely large magnetoresistance (XMR) was discovered in semimetal such as WTe<sub>2</sub> LaSb and so on, triggering extensive research on these materials and the origin of XMR. In this talk, we will report the transport properties of non-magnetic layered pnictide material NbAs<sub>2</sub>. Large transverse magnetoresistance is observed. At 10 K, the magnetoresistance is around 13000 % in the field of 9 T and shows no saturation behavior. The temperature dependent resistivity at various fields exhibits metal-to-semiconductor transition behavior around 100 K, which is coincident with the sudden increase of the Hall signal in the same temperature region. The angle dependent magnetoresistance at various temperatures follows the 3D scaling behavior with the mass anisotropy around 1.3-1.4, indicative of its 3D electron structure. Quantum oscillation data reveal the existence of at least three Fermi pockets in this material.

<sup>1</sup>Work at UCLA was supported by the U.S. Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences (BES) under Award Number DE-SC0011978.

**4:42PM P28.00010 Magnetic torque study of Weyl semimetal compounds TaP and NbP up to 45 Tesla**, GANG LI, TOMOYA ASABA, COLIN TINSMAN, FAN YU, BENJAMIN LAWSON, University of Michigan, YULIN CHEN, University of Oxford, LU LI, University of Michigan — Weyl semimetal is a recently proposed new state in condensed matter physics, in which the bulk bands could have three dimensional linear dispersion but the degeneracy at the cross point is lifted into a pair of Weyl points with opposite chirality. Among the predicted candidates, Tantalum monophosphide (TaP) and Niobium monophosphide (NbP) have the simplest composition and do not require extrinsic tuning. Photoemission data is accumulating and the unique Fermi-arc surface state is observed. Magnetotransport experiments has shown highly anisotropic magnetoresistance and quantum oscillations has been observed. Because both linear dispersive bands and conventional bands exist in these materials, a detailed study of the electronic structure of the bulk is highly desirable. We use torque magnetometry to study quantum oscillations of TaP and NbP down to 300 mK, and up to 45 Tesla, with focus on the angular dependence of oscillation frequencies. Our comparison shows clear difference in geometry of different bulk bands in these materials. Besides, a discussion will be made on high field torque data since 45 Tesla is high enough to push several of the bands into quantum limit.

**4:54PM P28.00011  $\pi$  Berry phase and Zeeman splitting of Weyl semimetal TaP**<sup>1</sup>, JIN HU, JINYU LIU, Tulane University, DAVID GRAF, National High Magnetic Field Laboratory, SEYED RADMANESH, DANIEL ADAMS, University of New Orleans, ALYSSA CHUANG, YU WANG, Tulane University, IRINEL CHIORESCU, Florida State University, JIANG WEI, Tulane University, LEONARD SPINU, University of New Orleans, ZHIQIANG MAO, Tulane University — The recent breakthrough in the discovery of Weyl fermions in mononitride semimetals provides opportunities to explore the exotic properties of relativistic fermions in condensed matter. The chiral anomaly-induced negative magnetoresistance and  $\pi$  Berry phase are two fundamental transport properties associated with the topological characteristics of Weyl semimetals. Since mononitride semimetals are multiple-band systems, resolving clear  $\pi$  Berry phase for each Fermi pocket remains a challenge. We report the determination of Berry phases of multiple Fermi pockets of Weyl semimetal TaP through high field quantum transport measurements. We show our TaP single crystal has the signatures of a Weyl state, including light effective quasiparticle masses, ultrahigh carrier mobility, as well as negative longitudinal magnetoresistance. Furthermore, we have generalized the Lifshitz-Kosevich (LK) formula for multiple-band Shubnikov-de Haas (SdH) oscillations and extracted the Berry phases of  $\pi$  for multiple Fermi pockets in TaP through the direct fits of the modified LK formula to the SdH oscillations. In high fields, we also probed signatures of Zeeman splitting, from which the Landé  $g$ -factor is extracted.

<sup>1</sup>Supported by the DOE (DE-SC0012432) and the NSF (EPS- 1003897)

**5:06PM P28.00012 Quantum Oscillations from generic surface Fermi arcs in Weyl semi-metals**, YI ZHANG, DANIEL BULMASH, PAVAN HOSUR, Stanford University, ANDREW POTTER, ASHVIN VISHWANATH, University of California, Berkeley — We re-examine the semiclassical derivation of quantum oscillations, and emphasize the correct definition of the chemical potential from the energy-time quantization perspective. In particular, for a Weyl semi-metal with surface Fermi arcs, the most natural energy reference point does not necessarily coincide with the energy of the bulk Weyl nodes. This results in several important amendments to previous conclusions for generic Weyl semi-metals. We also propose a simple lattice realization of Weyl semi-metals following the layered prescription and verify our theoretical conclusions with exact numerical studies.

**5:18PM P28.00013 Thermo-electric transports in double-Weyl semimetals**, QI CHEN, GREGORY A. FIETE, The University of Texas at Austin — Topological Weyl semimetals with linearly dispersing nodal points have received a surge of interest due to their experimental realization in real materials. Another nontrivial type of band crossing whose dispersion is not simply linear is the double Weyl point, around which the spectrum disperses linearly along one momentum direction but quadratically along the two remaining directions. In this work, we apply the semi-classical Boltzmann transport theory to study the thermo-electric conductivity of a double-Weyl fermion model. We find that the transport quantities exhibit an interesting dependence on the chemical potential and spatial anisotropic model parameters, differing from a simple quadratically or linearly dispersing electron gas. By applying a static magnetic field, we find that the double-Weyl point is only stable for a magnetic field along the linearly dispersing direction. The longitudinal and transverse electrical and thermal magneto-conductivity show a similar dependence on the in-plane cyclotron frequency to the linearly dispersing Weyl nodes. In the extreme quantum limit of chemical potential being much smaller than the cyclotron energy, we find that the lowest Landau levels are both chiral and doubly degenerate. The chiral anomaly contribution to the longitudinal magneto-conductivity is double that of a linearly dispersing Weyl node.

## Wednesday, March 16, 2016 2:30PM - 5:30PM –

Session P29 DCMP: Optical Spectroscopy on 3D Topological Insulators 328 - Dennis Drew, University of Maryland

**2:30PM P29.00001 Infrared studies of topological insulator systems**, KIRK POST, BRIAN CHAPLER, ALEX SCHAFGANS, Univ of California - San Diego, MENGKUN LIU, SUNY - Stonybrook, JIH-SHENG WU, Univ of California - San Diego, ANTHONY RICHARDELLA, JOON SUE LEE, Pennsylvania State University, ANJAN REIJNDERS, University of Toronto, YUN SANG LEE, Soongsil University, LIANG HE, XUFENG KOU, Univ of California - Los Angeles, MARIO NOVAK, ALEXEY TASKIN, KOUJI SEGAWA, Osaka University, MICHAEL GOLDFLAM, H. THEODORE STINSON, Univ of California - San Diego, XIAO LIANG QI, Stanford University, KENNETH BURCH, Boston College, KANG WANG, Univ of California - Los Angeles, MICHAEL FOGLER, Univ of California - San Diego, NITIN SAMARTH, Pennsylvania State University, YOICHI ANDO, Osaka University, DIMITRI BASOV, Univ of California - San Diego — The theoretical prediction, and subsequent experimental realization, of topological insulator (TI) systems, has vaulted this new class of materials to the vanguard of condensed matter physics. Since their discovery, we have carried out a number of infrared studies on various TI systems, including  $\text{Bi}_2\text{Se}_3$ ,  $\text{Bi}_{1-x}\text{Sb}_x$ , and  $\text{Bi}_{2-x}\text{Sb}_x\text{Te}_{3-y}\text{Se}_y$  crystals as well as  $\text{Bi}_2\text{Se}_3$  and  $(\text{Bi,Sb})_2\text{Te}_3$  thin films. A key element of these works is the revelation that the infrared response of  $\text{Bi}_{1-x}\text{Sb}_x$  crystals and  $(\text{Bi,Sb})_2\text{Te}_3$  thin films possess a significant, or even dominant, component from the topologically protected surface states. I will review these works and discuss future prospects of measuring the surface state response through optical spectroscopy techniques

**2:42PM P29.00002 Cyclotron resonance and Faraday rotation in topological insulator  $(\text{Bi,Sb})_2\text{Te}_3$** , YINMING SHAO, KIRK POST, JIH-SHENG WU, Univ of California - San Diego, ANTHONY RICHARDELLA, JOON SUE LEE, The Pennsylvania State University, MICHAEL FOGLER, Univ of California - San Diego, NITIN SAMARTH, The Pennsylvania State University, DIMITRI BASOV, Univ of California - San Diego — Using magneto-optical spectroscopy, we have explored the complex electronic structure of  $(\text{Bi,Sb})_2\text{Te}_3$  (BST) film. From the magneto-optical transmission spectra, we extracted the cyclotron resonance (CR) energy, and subsequently measured the broadband Faraday rotation spectra (FR). From these complementary FR-CR datasets, we were able to identify the conducting channels associated with the topological surface states of the film at the interface with the substrate and with the amorphous capping layer on top of the film. According to the FR data the two surfaces are dominated by carriers of opposite sign, in accord with earlier transport measurements. These results elucidate the origin of the zero-field optical response, observed previously, and give direct evidence of significant SS contribution using a bulk sensitive probe.

**2:54PM P29.00003 Terahertz Faraday Rotation in the Quantum Anomalous Hall System V-doped  $(\text{Bi,Sb})_2\text{Te}_3$** , OZGE OZEL, Massachusetts Inst of Tech-MIT, ALEX FRENZEL, UCSD, CUI-ZU CHANG, DANIEL PILON, JAGADEESH MOODERA, NUH GEDIK, Massachusetts Inst of Tech-MIT, GEDIK GROUP TEAM, MOODERA GROUP COLLABORATION — Time-reversal symmetry breaking in a topological insulator (TI) can be achieved by introducing ferromagnetism, which opens up a gap in the Dirac surface states. When the chemical potential is tuned to lie within the surface gap, the quantum anomalous Hall state emerges, which can be regarded as the quantum Hall state at zero external magnetic field. Recently, this state has been observed by static transport measurements in thin films of magnetically doped TIs. Time-domain terahertz spectroscopy has been demonstrated to be an effective probe of surface states and Hall effects in topological materials. Here, we use polarization modulation terahertz spectroscopy to study the intrinsic properties of massive Dirac electrons in V-doped  $(\text{Bi,Sb})_2\text{Te}_3$  via Faraday rotation measurements.

**3:06PM P29.00004 Quantized Faraday rotation of surface states in 3D topological insulator thin films**, LIANG WU, Department of Physics and Astronomy, The Johns Hopkins University, MARYAM SALEHI, Department of Materials Science and Engineering, Rutgers, The State University of New Jersey, NIKESH KOIRALA, SEONGSHIK OH, Department of Physics and Astronomy, Rutgers, The State University of New Jersey, N. PETER ARMITAGE, Department of Physics and Astronomy, The Johns Hopkins University, JOHNS HOPKINS UNIVERSITY TEAM, RUTGERS, THE STATE UNIVERSITY OF NEW JERSEY TEAM — Axion electrodynamics of topological surface states have been predicted a while ago, but the experimental observation has not been realized yet. One of the consequences of axion electrodynamics is a topological magneto-electric effect. In my talk, I will talk about utilizing a charge-transfer-doping method to lower the chemical point near the Dirac point in thin films of the topological insulator  $\text{Bi}_2\text{Se}_3$ . Using time-domain THz spectroscopy, we observed a crossover from semi-classical cyclotron resonances from topological surface states in the low field regime to a quantum regime at higher fields. A quantized Faraday rotation in the units of the fine structure constant was observed at high fields, which may provide the evidence for the topological magneto-electric effect.

**3:18PM P29.00005 Nonlinear optical properties of bismuth selenide**, DEREK BAS, SERCAN BABAKIRAY, TUDOR STANESCU, DAVID LEDERMAN, ALAN BRISTOW, West Virginia University — Bismuth selenide ( $\text{Bi}_2\text{Se}_3$ ) is a topological insulator with many interesting photonic properties. Much research has been done involving various types of photocurrents in an attempt to highlight the differences between the bulk electronic states and massless conducting surface states. Here,  $\text{Bi}_2\text{Se}_3$  films varying in thickness from 6 to 40 quintuple layers have been produced via molecular beam epitaxy as a means to vary the relative contributions of bulk and surface. On these samples, optical measurements were performed at around 1.6 eV, which is enough energy to stimulate transitions from the Fermi level to a region near the second Dirac cone. Z-scan was used to measure saturable absorption, time-resolved two-color pump-probe was used to measure two-photon absorption, and a Fourier transform infrared spectrometer was used to measure linear absorption. Results were examined and analyzed with respect to thickness. Thickness-dependent band structures were produced using a tight-binding model and used to compare with experimental results.

**3:30PM P29.00006 Fano  $q$  reversal in topological insulator  $\text{Bi}_2\text{Se}_3$** , S.V. DORDEVIC, G.M. FOSTER, M.S. WOLF, The University of Akron, N. STOJILOVIC, University of Wisconsin Oshkosh, H. LEI, C. PETROVIC, Brookhaven National Lab, Z. CHEN, Z.Q. LI, National High Magnetic Field Lab, L.C. TUNG, University of North Dakota — We studied magneto-optical response of a canonical topological insulator  $\text{Bi}_2\text{Se}_3$  with the goal of addressing a controversial issue of electron-phonon coupling. Magnetic-field induced modifications of reflectance are very pronounced in the infrared part of the spectrum, indicating strong electron-phonon coupling. This coupling causes an asymmetric line-shape of the  $60\text{ cm}^{-1}$  phonon mode, and is analyzed within the Fano formalism. The analysis reveals that the Fano asymmetry parameter ( $q$ ) changes sign when the cyclotron resonance is degenerate with the phonon mode. To the best of our knowledge this is the first example of magnetic field driven  $q$ -reversal.

### 3:42PM P29.00007 Evolving optical second-harmonic anisotropy at the cleaved $\text{Bi}_2\text{Se}_3$ surface.<sup>1</sup>

, YONG AN, AVERY GREEN, ALAIN DIEBOLD, SUNY Polytechnic Institute — Bismuth selenide ( $\text{Bi}_2\text{Se}_3$ ) is a centrosymmetric topological insulator with conducting surface states. The surface states have been studied by various electrical and optical techniques in air, but ambience effects and surface aging have not been adequately addressed. Optical second-harmonic generation (SHG) is a suitable probe for the  $\text{Bi}_2\text{Se}_3$  surface because SHG arises from symmetry breaking at the surface and thus should detect surface states preferentially over bulk states. However, a strong time dependence of SHG is often observed, hampering the detection and investigation of the surface states. Here we find a new phenomenon in which the major and minor intensity lobes of a measured rotational-anisotropy SHG pattern from a cleaved  $\text{Bi}_2\text{Se}_3$  (111) surface can significantly change with time and eventually switch their amplitudes. This switching provides a means for tracking the progress of surface oxidation inside a quintuple layer of  $\text{Bi}_2\text{Se}_3$ . We also perform pump-probe SHG experiments, comparatively on freshly cleaved and oxidized  $\text{Bi}_2\text{Se}_3$  surfaces, to study charge dynamics at the oxide/ $\text{Bi}_2\text{Se}_3$  interface and to detect spin polarization of photoexcited surface states in the  $\text{Bi}_2\text{Se}_3$  topological insulator.

<sup>1</sup>This work was supported by the SRC NRI Institute for Nanoelectronics Discovery and Exploration (INDEX)

### 3:54PM P29.00008 Tight-binding theory of NMR shifts in topological insulators<sup>1</sup>, ION GARATE,

SAMUEL BOUTIN, Université de Sherbrooke, JORGE RAMIREZ RUIZ, Universidad Autónoma de México — To date, most experiments in topological insulators have focused on probing the surface states of these materials and suppressing the often inevitable contribution from bulk states. However, the latter are of interest on their own and contain useful information that can be extracted with a local probe like nuclear magnetic resonance (NMR). Recently,  $^{77}\text{Se}$  NMR experiments on  $\text{Bi}_2\text{Se}_3$  single crystals have reported unusual field-independent linewidths and short spin-echo decays [1]. It is likely that an unexpectedly strong indirect internuclear coupling, characteristic of some inverted band structures, is the cause of these peculiar results. Motivated by this hypothesis, we report on a microscopic theory of NMR shifts and linewidths in  $\text{Bi}_2\text{Se}_3$  and  $\text{Bi}_2\text{Te}_3$ . Our theory provides quantitative estimates for the Knight shift, the orbital shift, the Ruderman-Kittel-Kasuya-Yoshida coupling and the Bloembergen-Rowland coupling. We will compare our findings with the available experimental data. [1] N. Georgieva, D. Rybicki, R. Guhne, G. Williams, S. Chong, I. Garate and J. Haase, arXiv:1511.01727 (2015)

<sup>1</sup>Funded by the National Science and Engineering Research Council of Canada, Fonds de Recherche Québécois Nature et Technologies, and Mitacs-Globalink.

### 4:06PM P29.00009 Gate Tunable Infrared Optical Response of $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ Topological

Insulators, WILLIAM WHITNEY, VICTOR BRAR, California Institute of Technology, YUNBO OU, Institute of Physics, Chinese Academy of Sciences, KE HE, QI-KUN XUE, Tsinghua University, HARRY ATWATER, California Institute of Technology — The electronic properties of topological insulators – narrow band-gap semiconductors that exhibit insulating bulk and semimetallic Dirac surface states – have been the subject of intense study over the past several years. The optical and optoelectronic behavior of these materials, however, remain widely uncharacterized. It has previously been shown that electrostatic gating can be used to tune the Fermi level in the Dirac semimetal graphene, modifying interband transitions and free carrier absorption. We report here experiments that demonstrate electronic control of the optical properties of 5-20 nm thick  $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$  films grown by Van der Waals epitaxy and transferred to silicon dioxide on silicon via an epitaxial lift off process. We find that infrared transmission and reflection from 3 to 10 microns are consistent with modulation of free-carrier absorption and bulk interband transitions in  $(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_3$ . We discuss transport results as well as the contributions that bulk and topological surface electronic transitions make to the optical response of these materials.

### 4:18PM P29.00010 Optical Second Harmonic Generation Study of Topological Insulator

$\text{Bi}_{2-x}\text{Sb}_x\text{Se}_3$ <sup>1</sup>, JISUN KIM, ZHENYU ZHANG, MATTHEW T. CURTIS, LOUIS H. HABER, RONGYING JIN, Louisiana State University — Second-order nonlinear optical spectroscopy such as second harmonic generation (SHG) is well-established and versatile technique for surface and interface studies. We apply this technique to study the surface symmetry of topological insulator  $\text{Bi}_{2-x}\text{Sb}_x\text{Se}_3$  in reflection geometry under four possible polarization configurations. By measuring the azimuthal angular dependence of SHG from the (111) surface of  $\text{Bi}_{2-x}\text{Sb}_x\text{Se}_3$  single crystals, we identify responses from both in-plane Se-Se bonds and out-of-plane Se-Bi/Sb bonds. This provides us information about the doping effect on the surface crystalline structure, which is critical for understanding the surface properties. The transition from topological to trivial insulator upon Sb doping will be discussed based on SHG data. Future work using sum frequency generation on these crystals will be considered as well.

<sup>1</sup>Funded by NSF and LSU ORED

### 4:30PM P29.00011 Current induced Optical Activity in Topological Insulator $\text{Bi}_2\text{Te}_2\text{Se}_1$ ,

NIRAJAN MANDAL<sup>1</sup>, IREK MITKOWSKI, Department of Physics and Astronomy, Purdue University, West Lafayette, IN 47907, MIKHAIL GLAZOV, Ioffe Institute, Polytechnicheskaya 26, 194021 St. Petersburg, Russia, YONG CHEN<sup>2</sup>, Department of Physics and Astronomy, Purdue University, West Lafayette, IN 47907 — Current induced polarization rotation of light (provided by a laser with wavelength=635nm) was studied from topological insulator (TI),  $\text{Bi}_2\text{Te}_2\text{Se}_1$ , grown by Bridgman method. The magnitude of the observed response increases linearly with the applied current and reverses sign upon reversing the current direction. Possible origins of the rotation can include the linear electro-optic Pockels effect (linear birefringence) and spin-Kerr effect due to the current induced spin polarization (e.g. resulting from the spin momentum locking of the surface states) at the sample surface. At room temperature, the rotation was measured as a function of the angle of incidence and laser polarization. Dependence of the rotation angle on the polarization of light (S or P) was used to isolate contributions from these two effects. The contribution from the electro optic effect was found to dominate over that from the current-induced spin- Kerr effect.

<sup>1</sup>Birck Nanotechnology Center, Purdue University, West Lafayette, IN 47907

<sup>2</sup>Birck Nanotechnology Center, Purdue University, West Lafayette, IN 47907 School of Electrical and Computer Engineering, Purdue University, West Lafayette, IN 47907

### 4:42PM P29.00012 STM studies of topological phase transition in $(\text{Bi},\text{In})_2\text{Se}_3$ <sup>1</sup>, WENHAN ZHANG,

XUEYUN WANG, SANG-WOOK CHEONG, WEIDA WU, Rutgers Univ, WEIDA WU TEAM, SANG-WOOK CHEONG COLLABORATION — Topological insulators (TI) are a class of materials with insulating bulk and metallic surface state, which is the result of band inversion induced by strong spin-orbit coupling (SOC). The transition from topological phase to non-topological phase is of great significance. In theory, topological phase transition is realized by tuning SOC strength. It is characterized by the process of gap closing and reopening. Experimentally it was observed in two systems:  $\text{TlBi}(\text{S}_{1-x}\text{Se}_x)_2$  and  $(\text{Bi}_{1-x}\text{In}_x)_2\text{Se}_3$  where the transition is realized by varying isovalent elements doping concentration. However, none of the previous studies addressed the impact of disorder, which is inevitable in doped systems. Here, we present a systematic scanning tunneling microscopy/spectroscopy study on  $(\text{Bi}_{1-x}\text{In}_x)_2\text{Se}_3$  single crystals with different In concentrations across the transition. Our results reveal an electronic inhomogeneity due to the random distribution of In defects which locally suppress the topological surface states. Our study provides a new angle of understanding the topological transition in the presence of strong disorders.

<sup>1</sup>This work is supported by NSF DMR-1506618.

**4:54PM P29.00013 First-Principle Calculations and Raman Studies of Surface Phonons in the Topological Insulators  $\text{Bi}_2\text{Se}_3$  and  $\text{Bi}_2\text{Te}_3$ .** , IBRAHIM BOULARES, GUANGSHA SHI, CTIRAD UHER, EMMANOUIL KIOUPAKIS, ROBERTO MERLIN, U. Michigan, PETR LOSTAK, U. Pardubice - Czech Republic — Raman [1-2], helium scattering [3] and photoemission experiments [4] on the topological insulators  $\text{Bi}_2\text{Se}_3$  and  $\text{Bi}_2\text{Te}_3$  show features in the range  $\sim 50$ -150  $\text{cm}^{-1}$ , which have been assigned to Raman-forbidden, infrared modes due to symmetry breaking at the surface [1-2] or surface phonons [3,4], which couple to the topologically protected electronic states [4]. We present first-principle LDA calculations and temperature-dependent Raman studies showing strong evidence of the existence of surface phonons in both  $\text{Bi}_2\text{Se}_3$  and  $\text{Bi}_2\text{Te}_3$ . The calculations reveal that these modes are quite insensitive to spin-orbit coupling, an indication that their occurrence is unrelated to the topological properties of these materials. [1] K. M. F. Shahil et al., Appl. Phys. Lett. 96, 153103 (2010). [2] V. Gnezdilov et al., Phys. Rev. B 84, 195118 (2011). [3] X. Zhu et al., Phys. Rev. Lett. 107, 186102 (2011). [4] J. A. Sobota et al., Phys. Rev. Lett. 113, (2014).

**5:06PM P29.00014 Optical helicity control of surface current in  $\text{SmB}_6$** <sup>1</sup>, SANJAY ADHIKARI, West Virginia University, YANJUN MA, CHANG-BEOM EOM, University of Wisconsin-Madison, CHENG CEN, West Virginia University —  $\text{SmB}_6$  is a promising candidate for topological Kondo insulator. One hallmark signature of topological states is the helical Dirac dispersion with perfect momentum-spin lockage. Here, we report current injection in  $\text{SmB}_6$  thin film with circularly polarized light at oblique incidence. A polarization-independent photovoltage was also detected. Both signals exhibited strong temperature dependences. While the polarization-independent photovoltage is likely due to thermoelectric effects, the circular photogalvanic effect (CPGE) has two possible origins: topological surface states or regular surface states with strong Rashba type spin-orbit coupling. The drastically different penetration depths of topological and regular surface states in  $\text{SmB}_6$  provide an opportunity to distinguish them by investigating films with different thicknesses. The strong correlation observed between the film thickness and CPGE photovoltage strongly supports the topological origin of the surface states. This research enhances our knowledge in controlling the spin and orbital degrees of freedom at  $\text{SmB}_6$  surface, and can also lead to exciting spintronic applications using optical tools.

<sup>1</sup>This work is supported by the Department of Energy Grant No. DE-SC-0010399

**5:18PM P29.00015 Photoinduced Anomalous Hall Effects in Weyl Semimetals**, CHING-KIT CHAN, PATRICK A. LEE, Massachusetts Institute of Technology, KENNETH S. BURCH, Boston College, JUNG HOON HAN, Sungkyunkwan University, YING RAN, Boston College — We examine theoretically the interplay between chiral photons and chiral electrons in Weyl semimetals. Owing to its monopole nature, a three-dimensional Weyl node is topologically-robust against a circularly polarized light. A driven Weyl system exhibits node shifts in the momentum space, in sharp contrast to the gap opening in a driven two-dimensional Dirac system. We show that the node shift leads to a change of the Chern vector which gives arise to a net photoinduced anomalous Hall conductivity, in the plane perpendicular to the light propagation. We shall describe the basic idea behind this generic photoinduced Hall effect, illustrate it with a concrete microscope model, and estimate its feasibility based on current optical experimental techniques.

## Wednesday, March 16, 2016 2:30PM - 5:30PM –

Session P30 DMP: Advances in Complex Oxide Film Growth 329 - Steven May, Drexel University

**2:30PM P30.00001 Oxygenation Dependence of the Resistance Upturn in  $\text{LaAlO}_3/\text{SrTiO}_3$  Heterostructures**<sup>1</sup>, H. ZHANG, University of Toronto, K. A. MAJLAN, J. H. NGAI, University of Texas at Arlington, C. MCMAHON, D. G. HAWTHORN, University of Waterloo, J. Y. T. WEI, University of Toronto & Canadian Institute for Advanced Research — Among the phenomena exhibited by  $\text{LaAlO}_3/\text{SrTiO}_3$  (LAO/STO) heterostructures, the appearance of a low-temperature resistance upturn has attracted much recent debate [1-4]. This phenomenon has been observed to co-occur with both nonlinear Hall effect and anisotropic magnetoresistance, and attributed to either Kondo effect, multiband conduction, or localization. It is primarily seen in samples grown by pulsed laser deposition, and is sensitive to film thickness, growth condition and electrostatic gating, all of which could affect the oxygen content. In this work, we study the effect of post-growth oxygenation on the resistance upturn in samples grown by molecular beam epitaxy, and how the Hall conductance and magnetoresistance are related to the occurrence of the upturn. X-ray photoelectron spectroscopy is used to monitor the valence states of Ti ions, in an effort to correlate them with the conduction and magnetic properties. Our results are analyzed in terms of oxygen vacancies in the presence of polar charge transfer, and the effect of these vacancies on the resistance upturn in LAO/STO heterostructures. [1] S. Das et al., PRB 90 (2014). [2] V. K. Guduru et al., PRB 88 (2013). [3] Z. Huang et al., PRB 88 (2013). [4] C. Bell et al., APL 94 (2009).

<sup>1</sup>Work supported by NSERC, CFI/OIT, and the Canadian Institute for Advanced Research.

**2:42PM P30.00002 Controlling Kondo Scattering at the Conducting Oxide Interfaces via Lattice Mismatch and Growth Oxygen Pressure**, KUN HAN, Physics department & NUSNNI-NanoCore, NUS, Singapore, SHENGWEI ZHENG, ZHEN HUANG, CHANGJIAN LI, NUSNNI-NanoCore, NUS, Singapore, WENXIONG ZHOU, NUSNNI-NanoCore, NUS, Singapore, T VENKATESAN, NUSNNI-NanoCore, NUS, Singapore, ARIANDO ARIANDO, Physics department NUSNNI-NanoCore, NUS, Singapore, ARIANDO TEAM — The interface magnetism, such as Kondo effect and ferromagnetism at the conducting interfaces between nonmagnetic oxides, has attracted great attention in recent years. In this report, we show that the interfacial Kondo scattering is enhanced by large lattice mismatch and high growth oxygen pressure. For the (001)  $\text{LaAlO}_3/\text{SrTiO}_3$  interface with 3.0% lattice mismatch, the sheet resistance upturn appears around 40 K when the growth oxygen pressure  $P_{\text{O}_2}$  is beyond 1 mTorr. By contrast, for the (001)  $(\text{La}_{0.3}\text{Sr}_{0.7})(\text{Al}_{0.65}\text{Ta}_{0.35})\text{O}_3/\text{SrTiO}_3$  interface with 1.0% lattice mismatch, no resistance upturn is observed until  $P_{\text{O}_2}$  is increased to 100 mTorr. Moreover, the magnetoresistance data confirm the resistance upturn is caused by Kondo scattering. We propose that the interface disorders, which can be induced by a large lattice mismatch and high  $P_{\text{O}_2}$ , are important for forming localized  $\text{Ti}^{3+}$  ions. These  $\text{Ti}^{3+}$  ions can be spin-polarized and scatter electrons that are confined near the interface by high  $P_{\text{O}_2}$ . This explains why the stronger magnetic interaction is observed at the  $\text{SrTiO}_3$ -based interfaces with the higher  $P_{\text{O}_2}$  and larger lattice mismatch, paving the way for manipulating the interface magnetism at the functional oxide interface.

**2:54PM P30.00003 Metal-insulator transition at lanthanum aluminate-strontium titanate interface induced by oxygen plasma treatment.**, WEITAO DAI, CHENG CEN, West Virginia Univ — The formation of two-dimensional electron gas (2DEG) at lanthanum aluminate (LAO)-strontium titanate (STO) interface, as well as the 2DEG's unique characters in metal-insulator transition, have evoked widespread interest. Highly insulating interfaces are obtained for the structures with LAO thickness below 3 unit cell (uc) and abrupt transition from an insulating to conducting interface was observed for samples with thicker LAO layers. For 3uc LAO/STO samples, reversible nanoscale control of the metal-insulator transition was implemented by a conductive AFM writing. Our research furtherly discovered a very stable metal-insulator transition can be achieved by oxygen plasma (OP) treatment for samples with thicker LAO layers. AFM imaging and XPS measurement demonstrated the low energy OP treatment altered only the surface bonds, which confirmed the importance of surface properties in the heterostructures. Then microscale Hall bars were patterned at the interface and imaged by electrostatic force microscope. Their transport and magnetic properties were measured. This research will promote deeper understanding about the interfacial metal-insulator transition mechanism and open new device opportunities. This work is supported by the Department of Energy Grant No. DE-SC-0010399 and National Science Foundation Grant No. NSF-1454950.

### 3:06PM P30.00004 On the Growth of Complex Oxides by Molecular Beam Epitaxy , DILLON FONG,

Argonne Natl Lab — Functional materials based on complex oxides in thin film form offer new and exciting strategies for meeting many of our outstanding energy challenges through systematic control of layer sequencing, strain, etc. However, the synthesis of such oxide films can be a major challenge even when utilizing reactive molecular-beam epitaxy (MBE), a powerful deposition technique that allows the construction of materials atomic plane by atomic plane. To understand the fundamental physics of oxide growth by reactive MBE, we present *in situ* surface x-ray diffraction results on the growth of SrTiO<sub>3</sub> and SrO-SrTiO<sub>3</sub> thin films on (001)-oriented SrTiO<sub>3</sub> substrates. For homoepitaxy, we compare sequential deposition (alternating Sr and Ti monolayer doses) with that of co-deposition of Sr and Ti, both in a background of oxygen pressure, and observe drastically different growth pathways due to the presence of a TiO<sub>2</sub> double layer. For heteroepitaxial growth of Ruddlesden-Popper SrO-SrTiO<sub>3</sub> films, we find that layers rearrange dynamically, resulting in layer sequences distinct from the shutter sequence. In general, the starting surface structure and composition, in combination with local thermodynamic considerations, strongly influence our ability to atomically construct new complex oxides.

### 3:42PM P30.00005 Self-regulating MBE growth of stoichiometric BaSnO<sub>3</sub> films *via* reactive radical mechanism<sup>1</sup> , ABHINAV PRAKASH, JOHN DEWEY, HWANHUI YUN, JONG SEOK JEONG, K. ANDRE MKHOYAN, BHARAT JALAN,

Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN 55455 — Growth of thin films comprising of element with low oxidation potential such as Sn often requires reactive oxidants such as ozone or high-pressure oxygen plasma. By utilizing the chemistry of highly reactive radical of Sn, we will present on the growth of phase-pure, epitaxial BaSnO<sub>3</sub> films using a hybrid molecular beam epitaxy (MBE) approach with scalable growth rates. The notable finding was that Sn radicals are very reactive to yield phase-pure BaSnO<sub>3</sub> films even in molecular oxygen [1]. In this approach, we use hexamethylditin (HMDT) as a tin source, a solid effusion cell for Ba and either molecular oxygen or an rf oxygen plasma source. Phase-pure BaSnO<sub>3</sub> films were grown at 900 °C, and oxygen pressure of 5x10<sup>-6</sup> Torr as a function Sn:Ba ratio. *In-situ* time-dependent RHEED intensity oscillations were observed establishing a layer-by-layer growth mode and a critical thickness of ≈1 nm for strain relaxation [1]. Rutherford backscattering spectrometry and lattice constant determined using high-resolution X-ray diffraction was used to optimize cation stoichiometry. “MBE growth window” was identified where films show bulk-like lattice parameter (4.116 Å) over a wide-range of cation flux ratios. A correlation between RHEED patterns, stoichiometry, and surface morphology was established. [1] A. Prakash *et al.*, J. Vac. Sci. & Technol. A **33**, 060608 (2015).

<sup>1</sup>This work is supported primarily by NSF (DMR-1410888)

### 3:54PM P30.00006 Single phase growth of materials with high polar mismatch at the interface<sup>1</sup> , MOHAMMAD SAGHAYEZHIAN, ZHEN WANG, HANGWEN GUO, GAOMIN WANG, LINA CHEN, WARD PLUMMER, JIANDI ZHANG, Louisiana State Univ - Baton Rouge, LA, 70803 — Growing thin films on polar surfaces has always been a challenge. An even greater challenge though, has been growing thin films on polar surfaces with polar mismatch at the interface. The divergence of surface free energy inhibits appearance of a sharp interface in these materials. Here for the first time, we report successful growth of LaNiO<sub>3</sub> on SrTiO<sub>3</sub> in (111) direction with correct phase. We show that by controlling the substrate's electronic and stoichiometric properties along with careful tune of thermodynamic parameters during the growth, it is possible to grow a single phase thin film of LaNiO<sub>3</sub>. Using RHEED, LEED, STM and TEM, we show that the interface is sharp and there is no structural discontinuity, and the surface of the film preserves its symmetry during the growth. In addition, angle-resolved core-level photoelectron spectroscopy confirms the single phase growth.

<sup>1</sup>Supported by U.S. DOE under Grant No. DOE DE-SC0002136

### 4:06PM P30.00007 Surface structural reconstruction of SrVO<sub>3</sub> thin films on SrTiO<sub>3</sub> (001)<sup>1</sup> , GAOMIN WANG, MOHAMMAD SAGHAYEZHIAN, LINA CHEN, HANGWEN GUO, JIANDI ZHANG, Louisiana State University — Paramagnetic metallic oxide SrVO<sub>3</sub> (SVO) is an itinerant system known to undergo thickness-induced metal-insulator-transition (MIT) in ultrathin film form, which makes it a prototype system for the study of the mechanism behind metal-insulator-transition like structure distortion, electron correlations and disorder-induced localization. We have grown SrVO<sub>3</sub> thin film with atomically flat surface through the layer-by-layer deposition by laser Molecular Beam Epitaxy (laser-MBE) on SrTiO<sub>3</sub> (001) surface. Low Energy Electron Diffraction (LEED) measurements reveal that there is a ( $\sqrt{2}\times\sqrt{2}$ ) R45 surface reconstruction independent of film thickness. By using LEED-I(V) structure refinement, we determine the surface structure. In combination with X-ray Photoelectron Spectroscopy (XPS) and Scanning Tunneling Microscopy (STM), we discuss the implication on the MIT in ultrathin films below 2-3 unit cell thickness.

<sup>1</sup>This work is supported by the National Science Foundation under the NSF EPSCoR Cooperative Agreement No. EPS-1003897 with additional support from the Louisiana Board of Regents

### 4:18PM P30.00008 Van der Waals Epitaxy of Functional Oxide Heterostructures , YING-HAO CHU,

National Chiao Tung University — In the diligent pursuit of low-power consumption, multifunctional, and environmentally friendly electronics, more sophisticated requirements on functional materials are on demand. Recently, the discovery of 2D layered materials has created a revolution to this field. Pioneered by graphene, these new 2D materials exhibit abundant unusual physical phenomena that is undiscovered in bulk forms. These materials are characterized with their layer form and almost pure 2D electronic behavior. The confinement of charge and heat transport at such ultrathin planes offers possibilities to overcome the bottleneck of present device development in thickness limitation, and thus push the technologies into next generation. Van der Waals epitaxy, an epitaxial growth method to combine 2D and 3D materials, is one of current reliable manufacturing processes to fabricate 2D materials by growing these 2D materials epitaxially on 3D materials. Then, transferring the 2D materials to the substrates for practical applications. In the mean time, van der Waals epitaxy has also been used to create free-standing 3D materials by growing 3D materials on 2D materials and then removing them from 2D materials since the interfacial bonding between 2D and 3D materials should be weak van der Waals bonds. In this study, we intend to take the same concept, but to integrate a family of functional materials in order to open new avenue to flexible electronics. Due to the interplay of lattice, charge, orbital, and spin degrees of freedom, correlated electrons in oxides generate a rich spectrum of competing phases and physical properties. Recently, lots of studies have suggested that oxide heterostructures provide a powerful route to create and manipulate the degrees of freedom and offer new possibilities for next generation devices, thus create a new playground for researchers to investigate novel physics and the emergence of fascinating states of condensed matter. In this talk, we use a 2D layered material as the substrate. And we take several oxides as examples to demonstrate a pathway to integrate 3D functional oxides on 2D layered materials.

### 4:54PM P30.00009 Atomic-level sculpting in STEM for studies of thickness dependent structural behavior in oxide thin films , ALBINA BORISEVICH, QIAN HE, STEPHEN JESSE, Oak Ridge National Lab, ANDREW AKBASHEV, JONATHAN SPANIER, Drexel University, MIGUEL FUENTES-CABRERA, BOBBY SUMPTER, Oak Ridge National Lab — Oxide thin films offer a rich playground for fundamental physics and possible applications due to a wide variety of electronic and magnetic properties and control of chemistry and strain conditions during growth. Scanning Transmission Electron Microscopy (STEM) studies of thin films often demonstrate that film structure is highly dependent on thickness; changes in overall symmetry at a two-atomic-layer scale have been reported. At the same time it was recently shown that crystalline oxide nanostructures can be grown locally during a STEM experiment from amorphous precursors. This method can be used for producing crystalline structures as small as 1-2 nm and the process can be observed *in situ* with atomic resolution. Here we utilize the sculpting approach to study size effects in ultrathin films of oxides as they are being grown inside a microscope. Transitions such as emergence of tilted structure, misfit defects and rotational domains can now be pinpointed with single atomic layer precision. Atomistic molecular dynamics simulations are used to establish theoretical underpinnings of the beam-induced growth mechanism. This work is funded by DMSE of the DOE BES (QH, AB), and by CNMS, which is funded at ORNL by SUFD of the DOE BES.

**5:06PM P30.00010 Electrical properties of solid-solution  $\text{SrZr}_x\text{Ti}_{1-x}\text{O}_3$  grown epitaxially on Ge by molecular beam epitaxy**, REZA MOGHADAM, KAMYAR AHMADI, University of Texas at Arlington, Z.-Y. XIAO, XIA HONG, University of NebraskaLincoln, JOSEPH NGAI, University of Texas at Arlington — The epitaxial growth of crystalline oxides on semiconductors enables new functionalities to be introduced to semiconductor devices. In particular, dielectric and ferroelectric oxides grown epitaxially on semiconductors provide a pathway to realize ultra-low power logic and memory devices. Here we present electrical characterization of solid-solution  $\text{SrZr}_x\text{Ti}_{1-x}\text{O}_3$  grown epitaxially on Ge through oxide molecular beam epitaxy.  $\text{SrZr}_x\text{Ti}_{1-x}\text{O}_3$  is of particular interest since the band offset with respect to the semiconductor can be tuned through Zr content  $x$ . We will present current-voltage, capacitance-voltage and piezoforce microscopy characterization of  $\text{SrZr}_x\text{Ti}_{1-x}\text{O}_3$ -Ge heterojunctions. In particular, we will discuss how the electrical characteristics of  $\text{SrZr}_x\text{Ti}_{1-x}\text{O}_3$ -Ge heterojunctions evolve with respect to composition, annealing and film thickness.

**5:18PM P30.00011 First principles study of Al/ $\text{SrTiO}_3$  interface formation**, ALI HAMZE, AGHAM POSADAS, KRISTY KORMONDY, ALEXANDER DEMKOV, Univ of Texas, Austin — Two-dimensional electron gases (2DEGs) at the interfaces of oxides have been the subject of much interest in recent years due to their relatively high carrier mobilities and potential for use in all-oxide devices. In particular, the  $\gamma\text{-Al}_2\text{O}_3$  ( $\gamma$ -alumina)- $\text{SrTiO}_3$  (STO) system has been the focus of much research. It exhibits a 2DEG at the interface with a carrier mobility ranging from  $10^3$ - $10^5$   $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ , depending on the thickness of the STO and how the  $\gamma$ -alumina film was grown. It is believed that Al atoms steal oxygen from the STO substrate at growth temperature and thus create a conductive channel in STO near the interface. We investigate the initial studies of the interface formation using density functional theory. The results of first principles calculations are compared with those of x-ray photoemission spectroscopy (XPS) performed in situ on thin Al films deposited on STO by molecular beam epitaxy. Analysis of the Al 2p XPS spectrum shows one layer of aluminum is fully oxidized during growth at 400C and 4 layers of aluminum are fully oxidized during growth at 600C. Furthermore, the Ti 2p XPS spectrum shows the titanium atoms are reduced, which is consistent with the presence of oxygen vacancies in STO.

## Wednesday, March 16, 2016 2:30PM - 5:30PM —

**Session P31 DCP: Water at Interfaces: From Spectroscopy Techniques to Computer Simulations** 331 - Songi Han

**2:30PM P31.00001 Water at surfaces with tunable surface chemistries and the chiral imprint of water around DNA.**<sup>1</sup>, POUL PETERSEN, Cornell University — Aqueous interfaces are ubiquitous in atmospheric chemistry and biological systems but are notoriously hard to probe experimentally. Surface-specific vibrational spectroscopy offers an avenue to directly probe the vibrational modes of the water OH stretching band but this method is challenging to implement to buried surfaces. Here we present results from sum-frequency generation (SFG) spectroscopy probing the buried interface between a functionalized surface and aqueous solutions. Studying such buried surfaces offers the advantage of being able to systematically tune the surface chemistry using self-assembled monolayers, i.e. the hydrophobic and hydrophilic character, and examine the effect on the interfacial water. In addition to water at these controlled surfaces, we have initiated studying water at biological surfaces. This includes the solvation structure around DNA. X-ray experiments at cryogenic temperatures have found crystallographic water in the minor groove of DNA giving rise to the notion of a spine of hydration surrounding DNA. Such structured water should exhibit a chiral structure adapted from DNA. We investigate if such a chiral water structure exist around DNA at room temperature using chiral SFG.

<sup>1</sup>This work was supported by the National Science Foundation under a NSF CAREER grant (CHE-1151079)

**3:06PM P31.00002 Molecular Views of Water at the Water/Air and Water/Lipid Interface**, MISCHA BONN, Max Planck Inst — At the surface of water, the water hydrogen-bonded network is interrupted, conferring properties on interfacial water different from bulk water. We elucidate, using a combined experimental and computational molecular dynamics approach, how the water hydrogen bond network is terminated at a phospholipid interface, and how this is different from conventional surfactant interface [1]. Moreover, for the water/air interface, we show that the evaporation of water – i.e. the release of individual water molecules from the bulk into the gas phase – is not a purely stochastic event. Rather, the evaporation follows one specific pathway, involving a delicately timed, concerted motion of several water molecules to 'launch' a single molecule from the surface [2]. [1] Lipid Carbonyl Groups Terminate the Hydrogen-Bond Network of Membrane-Bound Water, T. Ohto, E.H.G. Backus, C. Hsieh, M. Sulpizi, M. Bonn, Y. Nagata, J. Phys. Chem. Lett. J. Phys. Chem. Lett. 6, 4499–4503 (2015). [2] Molecular Mechanism of Water Evaporation, Nagata, Y.; Usui, K.; Bonn, M., Phys. Rev. Lett. 2015, in print.

**3:42PM P31.00003 Correlation between Pyroelectricity and Alignment of Interfacial Water**, DAVID EHRE, ELENA MEIRZADEH, ALIK BELITZKY, ERAN MISHUK, MEIR LAHAV, IGOR LUBOMIRSKY, Weizmann Institute of Science — In this work we investigate the connection between arrangement of water and pyroelectricity. Before the current work, pyroelectricity was attributed only to polar materials. Nevertheless, nonpolar Amino acid crystals and Yttrium doped Barium Zirconate ceramics exhibit pyroelectricity. Experimental results with MD simulation suggest that the source of pyroelectricity is polar arrangement of water molecules at the crystal surface, which leads to the formation of a deformed polar layer in the crystal. This makes the surface pyroelectricity an important surface characterization tool. Another phenomenon suggests that the converse effect to surface pyroelectricity is also exists i.e. alignment of water by pyroelectricity. We demonstrated that polar crystals in general and specifically positive pyroelectric charge can catalyze the freezing of supercooled water (SCW). Our studies show that pyroelectric effect increases the freezing point of SCW by 2 to 8 degrees. The fact that the freezing point is correlated to the amount of the surface charge together with the relative low electric field, implying that the surface charge aligns the interfacial water molecules or stabilizes sub-critical ice nuclei.

**3:54PM P31.00004 High-resolution imaging and spectroscopy of interfacial water at single bond limit**, YING JIANG, International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, P. R. China — Hydrogen bond is one of the most important weak interactions in nature and plays an essential role in a broad spectrum of physics, chemistry, biology, energy and material sciences. The conventional methods for studying hydrogen-bonding interaction are all based on spectroscopic or diffraction techniques. However, those techniques have poor spatial resolution and only measure the average properties of many hydrogen bonds, which are susceptible to the structural inhomogeneity and local environments, especially when interfacial systems are concerned. The spatial variation and inter-bond coupling of the hydrogen bonds leads to significant spectral broadening, which prohibits the accurate understanding of the experimental data. In this talk, I will present our recent progress on the development of new-generation scanning probe microscopy/spectroscopy (SPM/S) with unprecedentedly high sensitivity and resolution [1,2], for addressing weak inter- and intra-molecular interactions, such as hydrogen bonds and van der Waals force. Based on a qPlus sensor, we have succeeded to push the real-space study of a prototypical hydrogen-bonded system, i.e. water, down to single bond limit. Combined with state-of-the-arts quantum simulations, we have discovered exotic nuclear quantum effects (NQE) in interfacial water and revealed the quantum nature of the hydrogen bond from a completely new perspective [3]. [1] J. Guo et al., Nature Materials 13, 184 (2014). [2] J. Chen et al., Nature Communications 5, 4056 (2014). [3] X. Meng et al., Nature Physics 11, 235 (2015).

**4:30PM P31.00005 Water at lipid and surfactant interfaces—structure, dynamics, and spectroscopy**, JAMES SKINNER, University of Wisconsin — I will consider water confined by reverse micelles, multi-bilayers, and gyroid phases of a number of lipids and surfactants. Theoretical and simulation results will be compared with several non-linear IR experiments, including 2DIR and pump-probe anisotropy. In addition, I will discuss water near lipid and surfactant monolayers, especially making the connection with SFG and 2DSFG experiments.

**5:06PM P31.00006 Orientational dynamics of water at an extended hydrophobic interface<sup>1</sup>**, FLORIAN FIGGE, SHUNHAO XIAO, JOHN A. MCGUIRE, Department of Physics and Astronomy, Michigan State University, GUILLAUME STIRNEMANN, Institut de Biologie Physico-Chimique, Univ. Paris Diderot, DAMIEN LAAGE, Département de Chimie, École Normale Supérieure — Aqueous interfaces are central to many physical processes, but the dynamics of interfacial water molecules have been little studied. We have measured the orientational dynamics of water at its interface with a self-assembled monolayer of octadecylsilane on fused silica. A surface-sensitive sum-frequency probe generated by mixing a visible and a vibrationally resonant infrared (IR) pulse is used to monitor the dangling (non-hydrogen-bonded) OH stretch vibration after excitation with a resonant IR pump pulse. By measuring pure and isotopically diluted water with orthogonal pump polarizations, we find that relaxation of the dangling OH stretch excitation is dominated by the out-of-plane jump from a dangling to a hydrogen-bonded configuration and the subsequent redistribution of energy from the surface hydrogen-bonded OH stretch excitation. The out-of-plane jump time is 1.5(1)ps, 30% slower than that reported for the air-water interface and twice as short as the jump time between hydrogen bonded configurations in the bulk. Molecular dynamics simulations indicate that the slower dynamics at the hydrophobic interface compared to the water-air interface are due to the hydrogen bonds at the hydrophobic interface being stronger than those at the water-air interface.

<sup>1</sup>The authors acknowledge support from the National Science Foundation (Grant No. CHE- 1151590).

**5:18PM P31.00007 Water Adsorption on the LaMnO<sub>3</sub> Surface**, CHRIS BILLMAN, Physics Department and Quantum Theory Project, University of Florida, YAN WANG, Materials Science and Engineering, Massachusetts Institute of Technology, HAI-PING CHENG, Dept. of Physics and Quantum Theory Project, University of Florida — Studying the adsorption of water on the metallic LaMnO<sub>3</sub> surface can provide insight into this complicated surface-adsorbate interaction. Using density functional theory, we investigated the adsorption of a water monomer, dimer, trimer and a monolayer on the surface. The electronic structure of ground state configurations is explored using analysis of density of states, charge density, and crystal orbital overlap populations. We found that the interaction between the surface and water molecules is stronger than hydrogen bonding between molecules, which facilitates wetting of the surface. Adsorbed water molecules form very strong hydrogen bonds, with substantially shifted OH stretch modes. For the monolayer of adsorbed water, a hint of a bilayer is observed with a height separation of only 0.2 Å. However, simulated scanning tunneling microscopy (STM) images and vibrational spectra suggest a significant difference between the two layers due to intermolecular bonding and interaction with the substrate.

## Wednesday, March 16, 2016 2:30PM - 5:30PM —

Session P32 DMP GERA FIAP: Quantum Thermoelectric Systems 332 - Jeff Urban, Molecular Foundry, UC Berkeley

**2:30PM P32.00001 Evolutionary structure search of efficient thermoelectric compounds**, MARIBEL NÚÑEZ VALDEZ, Moscow Institute of Physics and Technology, ARTEM OGANOV, Skolkovo Inst Sci and Tech; Moscow Inst of Phys and Tech; SUNY Stony Brook, Dept Geosci Ctr Mat Design; SUNY Stony Brook, Inst Adv Computat — Thermoelectric materials, which are used to harvest waste heat to generate power, are taking an important role for energy solutions. However, it is of fundamental significance the optimization of a variety of conflicting properties in order to obtain a high efficiency thermoelectric device to be cost-effective for applications. This efficiency or figure of merit ( $ZT$ ), which depends on the Seebeck coefficient, electrical resistivity and heat conductivity, is restricted by currently available materials and fabricating technologies. Therefore, the main objective of our study is the identification of thermodynamically stable compounds and their crystal structures with high  $ZT$  given just a set of elements by using an evolutionary algorithm in which the figure of merit is a degree of freedom to be optimized. We test the performance of our methods within the system Bi<sub>2</sub>Te<sub>3</sub>-Sb<sub>2</sub>Te<sub>3</sub>. These compounds are well known for their large  $ZT$ 's and their use in technological applications. Our results indicate a high feasibility for the employment of our evolutionary algorithm search using a wide variety of elements for optimizing and designing new thermoelectric materials.

**2:42PM P32.00002 High-throughput screening for thermoelectric sulphides by using crystal structure features as descriptors<sup>1</sup>**, RUIZHI ZHANG, BAOLI DU, KAN CHEN, MIKE REECE, Queen Mary University of London, MATERIALS RESEARCH INSTITUTE TEAM — With the increasing computational power and reliable databases, high-throughput screening is playing a more and more important role in the search of new thermoelectric materials. Rather than the well established density functional theory (DFT) calculation based methods, we propose an alternative approach to screen for new TE materials: using crystal structural features as descriptors. We show that a non-distorted transition metal sulphide polyhedral network can be a good descriptor for high power factor according to crystal field theory. By using Cu/S containing compounds as an example, 1600+ Cu/S containing entries in the Inorganic Crystal Structure Database (ICSD) were screened, and of those 84 phases are identified as promising thermoelectric materials. The screening results are validated by both electronic structure calculations and experimental results from the literature. We also fabricated some new compounds to test our screening results. Another advantage of using crystal structure features as descriptors is that we can easily establish structural relationships between the identified phases. Based on this, two material design approaches are discussed: 1) High-pressure synthesis of metastable phase; 2) In-situ 2-phase composites with coherent interface.

<sup>1</sup>This work was supported by a Marie Curie International Incoming Fellowship of the European Community Human Potential Program

**2:54PM P32.00003 Thermal Conductivities in Solids from First Principles: Accurate Computations and Rapid Estimates**, CHRISTIAN CARBOGNO, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — In spite of significant research efforts, a first-principles determination of the thermal conductivity  $\kappa$  at high temperatures has remained elusive. Boltzmann transport techniques that account for anharmonicity perturbatively become inaccurate under such conditions. *Ab initio* molecular dynamics (MD) techniques using the *Green-Kubo* (GK) formalism capture the full anharmonicity, but can become prohibitively costly to converge in time and size. We developed a formalism that accelerates such GK simulations by several orders of magnitude and that thus enables its application within the limited time and length scales accessible in *ab initio* MD. For this purpose, we determine the *effective* harmonic potential occurring during the MD, the associated temperature-dependent phonon properties and lifetimes. Interpolation in reciprocal and frequency space then allows to extrapolate to the macroscopic scale. For both force-field and *ab initio* MD, we validate this approach by computing  $\kappa$  for Si and ZrO<sub>2</sub>, two materials known for their particularly harmonic and anharmonic character. Eventually, we demonstrate how these techniques facilitate reasonable estimates of  $\kappa$  from existing MD calculations at virtually no additional computational cost.

**3:06PM P32.00004 Local thermoelectric probes of nonequilibrium quantum systems<sup>1</sup>**, CHARLES STAFFORD, University of Arizona — A theory of local temperature and voltage measurement in an interacting quantum system far from equilibrium is developed. We prove that a steady-state measurement by a floating thermoelectric probe is unique if it exists. Furthermore, we show that a solution exists provided there is no net local population inversion. In the case of population inversion, the system may be assigned a (unique) negative temperature. An expression for the local entropy of a nonequilibrium quantum system is introduced that, together with the local temperature and voltage, allows for a complete analysis of the local thermodynamics of the thermoelectric processes in the system. The Clausius form of the second law and the third law are shown to hold exactly locally, while the zeroth and first laws are shown to be valid to leading order in the Sommerfeld expansion. The local quantum thermodynamics underlying the enhancement of thermoelectricity by quantum interference is discussed.

<sup>1</sup>Work supported by the U.S. Department of Energy, Office of Science, Award No. DE-SC0006699.

**3:42PM P32.00005 Nanoelectronic primary thermometry below 4 millikelvin**, MATTHEW SARSBY, RICHARD HALEY, DAVID IAN BRADLEY, RICHARD GEORGE, YURI PASHKIN, JONATHAN PRANCE, University of Lancaster, UK, DAVID GUNNARSSON, HANNELE HEIKKINEN, MIKA PRUNNILA, VTT Technical Research Centre of Finland, PENTTIL JARI, LEIF ROSCHIER, Aivon Oy, Finland. — We present measurements of nanoelectronic Coulomb Blockade Thermometers that are optimised for operation below 10 mK. Their design incorporates on-chip electronic filters and cooling fins with a high electron-phonon coupling. By immersing the devices in the 3He/4He mixture of a dilution refrigerator, and by minimising electrical noise in the measurement circuit, the on-chip electron temperature reaches a value of 3.7 mK, the lowest yet measured in any nanoelectronic device. Above 7 mK the devices are in good thermal contact with their environment and are not susceptible to self-heating. Below 7 mK the device continues to provide accurate thermometry of the on-chip electron temperature, which is seen to diverge from the ambient temperature. In this regime the device provides valuable information about noise and heat-leaks from the environment, which points the way towards cooling nanoelectronic structures to lower temperatures.

**3:54PM P32.00006 Thermoelectric Corrections to Quantum Measurement**, JUSTIN BERGFELD, Department of Physics, Department of Chemistry, Illinois State University, MARK RATNER, Department of Chemistry, Northwestern University, CHARLES STAFFORD, Department of Physics, University of Arizona, MASSIMILIANO DI VENTRA, Department of Physics, University of California — The voltage and temperature measured by a floating probe of a nonequilibrium quantum system is shown to exhibit nontrivial thermoelectric corrections at finite temperature. Using a realistic model of a scanning thermal microscope to calculate the voltage and temperature distributions, we predict quantum temperature variations along graphene nanoribbons subject to a thermal bias which are not simply related to the local density of states. Experimentally, the wavelength of the oscillations can be tuned over several orders of magnitude by gating/doping, bringing quantum temperature oscillations within reach of the spatial resolution of existing measurement techniques. We also find that the Peltier cooling/heating which causes the temperature oscillations can lead to significant errors in voltage measurements for a wide range of system.

**4:06PM P32.00007 Deciphering the Landauer-Büttiker Transmission Function from Single Molecule Break Junction Experiments**, MATTHEW REUTER, Department of Applied Mathematics and Statistics and Institute for Advanced Computational Science, Stony Brook University, STEPHEN TSCHUDI, Stony Brook University — When investigating the electrical response properties of molecules, experiments often measure conductance whereas computation predicts transmission probabilities. Although the Landauer-Büttiker theory relates the two in the limit of coherent scattering through the molecule, a direct comparison between experiment and computation can still be difficult. Experimental data (specifically that from break junctions) is statistical and computational results are deterministic. Many studies compare the most probable experimental conductance with computation, but such an analysis discards almost all of the experimental statistics. In this work we develop tools to decipher the Landauer-Büttiker transmission function directly from experimental statistics and then apply them to enable a fairer comparison between experimental and computational results.

**4:18PM P32.00008 A simple Quantum heat engine operating between two negative temperatures<sup>1</sup>**, TOLASA A DIMA, PhD Student, MULUGETA BEKELE, Associate Professor of Physics — We study a heat engine that operates between two reservoirs at negative temperatures. A system of spin-half particles, in the thermodynamic limit, subject to a time dependent external magnetic field, is used as a working substance because of its capability to demonstrate negative absolute temperature. We explored the finite-time quantities: period, power and efficiency. The engine is explored in its maximum power and optimum mode of operation from which its figure of merit is defined as the product of scaled power and scaled efficiency. We found that power-wise the engine provides better performance under its maximum power mode of operation than the optimized mode; however, efficiency-wise, the optimized mode of operation is better than its maximum mode operation.

<sup>1</sup>We thank the International Science programme, IPS, Uppsala, Sweden for the support to this research?

**4:30PM P32.00009 Thermal Memristive Devices**, LUKE SHAPIRO, KAMIL WALCZAK, Pace University — We examine heat transfer via Coulomb Blockaded quantum systems connected to two heat reservoirs (thermal baths). Specifically, we propose simple models for negative differential thermal conductance and pinched hysteretic loops in the heat fluxes as functions of temperature. Our computational method is based on the theory of propagators, where additional mechanisms of shifting and blocking specific energy levels is incorporated. Those devices may play a major role in the future thermal management.

**4:42PM P32.00010 Density of States for Warped or non-Warped Energy Bands<sup>1</sup>**, NICHOLAS MECHOLSKY, LORENZO RESCA, IAN PEGG, Catholic Univ of America, MARCO FORNARI, Central Michigan University — The goal of this talk is to investigate when band warping affects density-of-states effective mass. Further, band "corrugation," a form of band warping referring to energy dispersions that deviate "more severely" from being twice-differentiable at isolated critical points, may also correlate in different ways with density-of-states effective masses and other band warping parameters. In this talk, an angular effective mass formalism is developed and used to study the electronic density of states of warped and non-warped energy bands towards an application in thermoelectric transport design. We demonstrate effects of band warping and prove the superiority of the angular effective mass treatment for valence energy bands in cubic materials. We explore examples that can also be critical to precisely distinguish the contributions due to band warping and to band non-parabolicity in non-degenerate bands of thermoelectric materials that have a consequent practical interest.

<sup>1</sup>The presenter wished to thank the Vitreous State Laboratory

**4:54PM P32.00011 A generalized Sommerfeld expansion for thermopower calculation**, JIE GU, XIAO GUANG ZHANG, HAI-PING CHENG, Univ of Florida - Gainesville — Kelvin formula relates the thermopower to the temperature derivative of the chemical potential. The latter can be evaluated using the Sommerfeld expansion as a standard approximation at low temperatures. We present a generalized expansion with improved accuracy at intermediate and high temperatures. We apply the formula to sodium cobaltate  $\text{Na}_x\text{CoO}_2$  and other thermoelectric materials to verify its validity over a wide temperature range.

**5:06PM P32.00012 Temperature Dependent Structure of Thermoelectric  $\text{Ca}_3\text{Co}_4\text{O}_9$** , TAO WU, TREVOR TYSON, HAN ZHANG, NJIT, MILINDA ABEYKOON, Photon Sciences, BNL — Structural studies of thermoelectric “ $\text{Ca}_3\text{Co}_4\text{O}_9$ ” have been conducted for a broad range of temperatures using probes covering multiple length scales. Details on the structure and its connection to the electron transport and thermal properties will be discussed. This work is supported by DOE Grant DE-FG02-07ER46402.

**5:18PM P32.00013 DYNAMICAL CORRECTION OF THERMOELECTRIC COEFFICIENTS FOR STRONGLY INTERACTING ELECTRONS IN THE COULOMB BLOCKADE REGIME**, KAIKE YANG, Universidad del Pais Vasco, San Sebastian, Spain — FOR MOLECULES WEAKLY COUPLED TO LEADS THE EXACT ZERO-BIAS KOHN-SHAM CONDUCTANCE CAN BE ORDERS OF MAGNITUDE LARGER THAN THE TRUE CONDUCTANCE DUE TO THE LACK OF DYNAMICAL EXCHANGE-CORRELATION (XC) EFFECTS. RECENTLY, IT HAS BEEN SHOWN [1] HOW THESE DYNAMICAL XC CORRECTIONS CAN BE CALCULATED USING ONLY QUANTITIES OBTAINED FROM STATIC DENSITY FUNCTIONAL THEORY. HERE, WE INVESTIGATE THE THERMOELECTRIC TRANSPORT AND DERIVE THE XC CORRECTION TO THE SEEBECK COEFFICIENT. WE FIND THAT THE DYNAMICAL CORRECTION TO THE SEEBECK COEFFICIENT IS DETERMINANT IN EVALUATING THE THERMOPOWER: THE ABSOLUTE VALUE OF THE DYNAMICAL CORRECTION FOR THE SEEBECK COEFFICIENT IS, FOR CERTAIN VALUES OF GATE VOLTAGE, MUCH LARGER THAN THAT OF THE KOHN-SHAM TERM. FINALLY, WE COMPARE OUR DENSITY FUNCTIONAL CALCULATIONS TO THE RATE EQUATION [2] AND THE EXPERIMENTAL RESULTS [3]. [1] S. KURTH, ET AL., PRL, 030601 (2013). [2] C. W. J. BEENAKKER, ET AL., PRB, 9667 (1992). [3] J. P. SMALL, ET AL., PRL, 256801 (2003).

## Wednesday, March 16, 2016 2:30PM - 5:30PM –

### Session P33 DPOLY: Organic Electronics and Photonics - Structure-Property Relationships 336

- Diru Ratnaweera, University of Sri Jayewardenepura, Sri Lanka

**2:30PM P33.00001 Molecular dynamics simulations for the study of optical properties in conjugated semiconducting molecules**, JACK WILDMAN, JEAN-CHRISTOPHE DENIS, PETER REPIŠČÁK, MARTIN J. PATERSON, IAN GALBRAITH, Heriot-Watt University — Conformational disorder of conjugated polymers strongly influences their optical and electronic properties. Molecular Dynamics (MD) simulations can provide a quantitative understanding of these effects. Given the ever-expanding range of molecules with potential for device applications, it is critical to systematically establish accurate MD parameters for such simulations. We present an experimentally verified, general and optimised procedure, based on a computationally inexpensive methodology for generating the required MD parameters for conjugated molecules. By combining a large sample (~1000) of MD generated conformations with DFT calculations for the resulting electronic states we can explore the influence of conformational disorder on the optical properties. Using this scheme, we determine the effect of conformational variation on both linear and two-photon absorption spectra in a number of different conjugated semiconducting oligomers. Our results indicate that, while there exists significant inhomogeneous broadening in the linear absorption, there is only a weak conformational influence on the two-photon absorption spectrum.

**2:42PM P33.00002 Directed self-assembly of  $\pi$ -conjugated oligopeptides for supramolecular electronics.**, BO LI, SONGSONG LI, YUECHENG ZHOU, University of Illinois at UrbanaChampaign, JOHN TOVAR, Johns Hopkins University, WILLIAM WILSON, Harvard University, CHARLES SCHROEDER, University of Illinois at UrbanaChampaign — The directed mesoscale engineering of nanoscale building blocks holds enormous promise to catalyze a revolution in new functional materials for advanced electronics. Bio-inspired systems can play a key role in this effort due to their inherent “programmable” function. In this work, oligopeptide with defined flanking sequences was appended to  $\pi$ -conjugated units, thereby directing their assembly processes in a designed manner. By utilizing custom-designed microfluidic devices and controlled acid vapor diffusion, the self-assembly rate was directed and precisely tuned. Notably, the kinetics was found to play a key role in the morphology of self-assembled  $\pi$ -conjugated oligopeptides. The influence of flanking peptide sequences and  $\pi$ -conjugated core-core interactions on the self-assembly nanostructure was systematically investigated. Importantly, the electronic properties of the synthetic peptide assembly was explored by integration as the active layer of a field effect transistor. The presented study offers insights to the design and fabrication of supramolecular electronics.

**2:54PM P33.00003 In-situ observation of dynamic processes during organic semiconductor thin film deposition and strain-stabilization of metastable states**, YANG LI, JING WAN, Department of Physics and Materials Science Program, University of Vermont, DETLEF-M. SMILGIES, Cornell High Energy Synchrotron Source, Cornell University, NICOLE BOUFFARD, Microscopy Imaging Center, College of Medicine, University of Vermont, RICHARD SUN, Angstrom Sun Technologies Inc., RANDALL HEADRICK, Department of Physics and Materials Science Program, University of Vermont — In-situ optical spectromicroscopy in reflection mode is used to study the growth mechanisms and thermal stability of 6,13- bis(trisopropylsilyl)ethynyl-pentacene (TIPS-pentacene) thin films. The results show that the films form in a supersaturated state before transforming to a solid film. Molecular aggregates are observed by optical spectroscopy in this supersaturated region corresponding to subcritical nuclei in the crystallization process. During deposition on a heated substrate, a progressive blue shift of optical absorption peaks of the solid film is observed at higher deposition temperatures due to a continuous thermally driven change of the crystalline packing. As crystalline films are cooled to ambient temperature they become strained although cracking of thicker films is observed, which allows the strain to partially relax. Below a critical thickness of 30 nm, cracking is not observed and the films are constrained to the lattice constants corresponding to the temperature at which they were deposited. An high averaged hole mobility about  $2\text{ cm}^2\text{V}^{-1}\text{s}^{-1}$  is obtained for strained TIPS-pentacene thin films deposited at 135C.

**3:06PM P33.00004 Transient phases during crystallization of solution-processed organic thin films<sup>1</sup>**, JING WAN, YANG LI, JEFFERY ULBRANDT, Department of Physics, University of Vermont, DETLEF-M SMILGIES, Cornell High Energy Synchrotron Source, JONATHAN HOLLIN, ADAM WHALLEY, Department of Chemistry, University of Vermont, RANDALL HEADRICK, Department of Physics, University of Vermont — We report an in-situ study of 2,7-diethyl[1]benzothieno[3,2-b][1]benzothiophene ( $\text{C}_8$ -BTBT) organic semiconductor thin film deposition from solution via hollow pen writing, which exhibits multiple transient phases during crystallization. Under high writing speed (25 mm/s) the films have an isotropic morphology, although the mobilities range up to  $3.0\text{ cm}^2/\text{V}\cdot\text{s}$ . To understand the crystallization in this highly non-equilibrium regime, we employ in-situ microbeam grazing incidence wide-angle X-ray scattering combined with optical video microscopy at different deposition temperatures. A sequence of crystallization was observed in which a layered liquid-crystalline (LC) phase of  $\text{C}_8$ -BTBT precedes inter-layer ordering. For films deposited above 80°C, a transition from LC phase to a transient crystalline state that we denote as Cr1 occurs after a temperature-dependent incubation time, which is consistent with classical nucleation theory. After an additional  $\approx 0.5\text{s}$ , Cr1 transforms to the final stable structure Cr2. Based on these results, we demonstrate a method to produce large crystalline grain size and high carrier mobility during high-speed processing by controlling the nucleation rate during the transformation from the LC phase.

<sup>1</sup>NSF DMR-1307017, NSF DMR-1332208

**3:18PM P33.00005 Critical Role of Processing on the Thermoelectric Performance of Doped Semiconducting Polymers**, SHRAYESH PATEL, UC Santa Barbara - Materials Research Lab, ANNE GLAUDELL, MICHAEL CHABINYC, UC Santa Barbara - Materials Department — The ability to convert excess waste heat into useable energy can significantly help meet the global energy demands. One may capture this waste heat through thermoelectrics devices. In a thermoelectric material, the charge carriers transport both electrical current and heat. Consequently, under a temperature difference ( $\Delta T$ ), a carrier concentration gradient results in a voltage ( $\Delta V$ ), which is related to the Seebeck coefficient,  $\alpha = -\Delta V / \Delta T$ . One of the challenges lies in finding materials that simultaneously have low thermal conductivity ( $\kappa$ ), high electrical conductivity ( $\sigma$ ), and high Seebeck coefficient ( $\alpha$ ). Conjugated semiconducting polymers can potentially meet this demand due to their inherent low thermal conductivity and high electrical conductivity through sufficient doping. Here, we report on the critical role of thermal processing on the enhancement of thermoelectric properties of conjugated polymer thin films. These films were doped using three different mechanisms: acid (toluene sulfonic acid), charge transfer ( $F_4$ TCNQ), and vapor (fluorinated-alkyl trichlorosilane). These thermoelectrics properties will be correlated to the structural and morphological properties of the doped thin-films through various synchrotron X-ray scattering techniques. Lastly, to further elucidate the charge transport mechanism driving the thermoelectric performance, we report on the temperature-dependent measurements of both the Seebeck coefficient and electrical conductivity.

**3:30PM P33.00006 Influence of Molecular Shape on Molecular Orientation and Stability of Vapor-Deposited Organic Semiconductors**, DIANE M. WALTERS, NOAH D. JOHNSON, M. D. EDIGER, University of Wisconsin-Madison — Physical vapor deposition is commonly used to prepare active layers in organic electronics. Recently, it has been shown that molecular orientation and packing can be tuned by changing the substrate temperature during deposition, while still producing macroscopically homogeneous films. These amorphous materials can be highly anisotropic when prepared with low substrate temperatures, and they can exhibit exceptional kinetic stability; films retain their favorable packing when heated to high temperatures. Here, we study the influence of molecular shape on molecular orientation and stability. We investigate disc-shaped molecules, such as TCTA and m-MTDATA, nearly spherical molecules, such as Alq<sub>3</sub>, and linear molecules covering a broad range of aspect ratios, such as p-TTP and BSB-Cz. Disc-shaped molecules have preferential horizontal orientation when deposited at low substrate temperatures, and their orientation can be tuned by changing the substrate temperature. Alq<sub>3</sub> forms stable, amorphous films that are optically isotropic when vapor deposited over a broad range of substrate temperatures. This work may guide the choice of material and deposition conditions for vapor-deposited films used in organic electronics and allow for more efficient devices to be fabricated.

**3:42PM P33.00007 Selective crystallization of conjugated polymers into nanowires from graphene coated surfaces.**, DANIEL ACEVEDO-CARTAGENA, JIAXIN ZHU, Univ of Mass - Amherst, ELVIRA TRABANINO, None, EMILY PENTZER, Case Western Reserve University, TODD EMRICK, ALEJANDRO BRISEO, Univ of Mass - Amherst, STEPHEN NONNENMANN, RYAN HAYWARD, Univ of Mass, Amherst — Solution-based crystallization of conjugated polymers offers a scalable and attractive route to develop hierarchical structures for organic electronic devices, especially solar cells. The introduction of well-defined nucleation sites into metastable supersaturated solutions provides a way to regulate the crystallization behavior, and therefore the morphology of the material. We focus on metastable solutions of poly(3-hexylthiophene) (P3HT) dissolved in mixtures of m-xylene, a marginal solvent, and chlorobenzene, a good solvent. Appropriate levels of supersaturation are identified to suppress homogenous nucleation of crystals at room temperature, while allowing for crystallization on heterogeneous nucleation sites. We show that in these metastable solutions, P3HT selectively crystallizes on graphene-coated surfaces. Through in situ atomic force microscopy, we confirm that nanowires grow vertically in a face-on orientation from highly oriented pyrolytic graphite and graphene. Moreover, this method can be successfully extended to other conjugated polymers with superior electronic properties, such as poly[2,5-bis(3-tetradecylthiophen-2-yl)thieno[3,2-b] thiophene]. Therefore, this method is a promising route to improve the performance of organic electronics.

**3:54PM P33.00008 Surface induced alignment for semiflexible polymers**, WENLIN ZHANG, ENRIQUE GOMEZ, SCOTT MILNER, Pennsylvania State University — The interfacial structure of semiflexible polymers can largely affect the overall performance of applications, such as organic electronics. Due to backbone stiffness, semiflexible polymers, including conjugated polymers, tend to align parallel to an impenetrable surface. The segmental alignment near the wall creates a quadrupolar aligning field, which can interact with the polymer backbones and enhance the chain alignment. In the present work, we combine molecular dynamic (MD) simulations and a lattice version of self-consistent field theory (SCFT) to investigate the surface induced alignment for semiflexible polymers. Using MD simulations of bead-spring chains, we demonstrate that the thickness of the aligned layer is about a persistence length  $L_p$  for semiflexible polymers in the isotropic phase. Using the SCFT lattice model, we predict that the amplitude and range of the alignment increase with increasing nematic coupling, quantified by the nematic coupling constant  $\alpha$ . The impenetrable surface acts as a perturbation on the chain alignment, and the nematic coupling  $\alpha$  amplifies the perturbation. By comparing the SCFT results for chains near an impenetrable surface to MD simulations, we can also qualitatively estimate  $\alpha$  for semiflexible polymers.

**4:06PM P33.00009 Revealing molecular order inside and between PBTTT nanoribbons through the polarized X-ray scattering**, BRIAN COLLINS, Washington State University, DEAN DELONGCHAMP, National Institute of Standards and Technology — Electronic and optical properties of conjugated polymers emerge not only through molecular architecture, but also through hierarchical ordering from the molecular to the mesoscale. Characterizing aspects of that ordering critical to properties can be challenging, however. For example, local molecular orientation within and connectivity between ordered structures is considered paramount for charge transport in conjugated polymer films. While some of these aspects can be imaged with state-of-the-art microscopy measurements, true statistical measurements of molecular order and connectivity remain elusive due to the low levels of crystalline packing that limit diffractive and other techniques capable of statistical analysis. Recently, we demonstrated how resonant scattering with polarized soft X-rays (PSoXS) is sensitive to molecular orientation and that such measurements could be used to locate sources and types of ordering within larger nanostructures on a statistical basis. Here we combine forward simulation and measurements of PSoXS on PBTTT nanoribbon films to extract critical information such as the average level of molecular alignment within nanoribbon structures and the level of connectivity between ribbons that promote the dominant charge transport mechanisms in these films. Further development of PSoXS will enable crucial insight into internal molecular order within organic materials tied to optical and electronic properties and how to control these properties for use in novel devices.

**4:18PM P33.00010 Charge Transport in Conjugated Block Copolymers**, BRANDON SMITH, THINH LE, YOUNGMIN LEE, ENRIQUE GOMEZ, Penn State University — Interest in conjugated block copolymers for high performance organic photovoltaic applications has increased considerably in recent years. Polymer/fullerene mixtures for conventional bulk heterojunction devices, such as P3HT:PCBM, are severely limited in control over interfaces and domain length scales. In contrast, microphase separated block copolymers self-assemble to form lamellar morphologies with alternating electron donor and acceptor domains, thereby maximizing electronic coupling and local order at interfaces. Efficiencies as high as 3% have been reported in solar cells for one block copolymer, P3HT-PFTBT, but the details concerning charge transport within copolymers have not been explored. To fill this gap, we probed the transport characteristics with thin-film transistors. Excellent charge mobility values for electron transport have been observed on aluminum source and drain contacts in a bottom gate, bottom contact transistor configuration. Evidence of high mobility in ordered PFTBT phases has also been obtained following thermal annealing. The insights gleaned from our investigation serve as useful guideposts, revealing the significance of the interplay between charge mobility, interfacial order, and optimal domain size in organic block copolymer semiconductors.

**4:30PM P33.00011 Selective crystallization of regioregularity controlled polythiophene for enhancing mechanical stability and electronic performance.** , HYEONG JUN KIM, KAIST, HOJEONG YU, POSTECH, JAE HAN KIM, JIN-SUNG KIM, TAEK SOO KIM, KAIST, JOON HAK OH, POSTECH, BUMJOON KIM, KAIST — Considering the many potential applications of organic electronics in portable electronic devices, it is of great importance to develop an electro-active material that possesses mechanical stability and high electronic performance. Coexistence of both properties, however, is very difficult to achieve because good electronic performance is associated with long conjugation length, and high crystallinity often results in stiffness and brittleness. Herein, we utilize P3HT with two different regioregularities: high RR (98%) P3HT has high electronic properties but poor mechanical resilience, and low RR P3HT (68%) exhibits high elasticity and ductility but poor electronic performance. Selective crystallization of high RR P3HT induced by solution assembly allows construction of percolated networks of high RR P3HT nanowires (NWs) embedded in low RR P3HT matrix. Only 5 wt% high RR P3HT is required to reach a hole mobility comparable to that of high RR P3HT, and high RR NWs embedded in film exhibits 20 times higher elongation at break. Selective self-assembly allows us to overcome the fragile nature of highly crystalline conjugated polymers without losing their electronic properties.

**4:42PM P33.00012 Regio regularity effects on chain mobility and entanglement for poly(3-hexylthiophene)<sup>1</sup>** , RENXUAN XIE, ENRIQUE GOMEZ, Department of Chemical Engineering, Penn State University at University Park, RALPH COLBY, Department of Materials Science and Engineering, Penn State University at University Park — Poly(3-hexylthiophene-2,5-diyl) (P3HT) is a conjugated polymer that can serve as the active layer in a variety of electronic devices. However, its glass transition temperature ( $T_g$ ) and entanglement molecular weight ( $M_e$ ) are still in dispute. These parameters are essential for estimating the density of tie chains, which are hypothesized to limit the bulk charge transport. A wide range of molecular weights of both regiorandom (RRa) and regioregular (RRe) P3HT were studied by oscillatory shear rheology. Coupled with the molecular weight distribution from GPC,  $M_e$  was extracted by fitting the linear viscoelastic data of multiple MW samples using BoB software. Furthermore, two  $T_g$ 's were identified for both RRe and RRa P3HT.  $T_g$  corresponds to the segmental motion and follows Flory-Fox equation well for various MWs with  $2\text{ C} < T_g < 14\text{ C}$ , yielding high MW limit of  $T_{g\infty} = 21\text{ C}$ . RRe has a larger  $M_e$  than RRa, which might originate from their different  $T_{gPE}$  corresponding to the side chain packing. So, further investigation on their packing lengths via dilute solution light scattering will be crucial to understand entanglement in these semiflexible polymers.

<sup>1</sup>National Science Foundation

**4:54PM P33.00013 Controlling the out-of-plane orientation of solution-processed organic semiconductor crystals** , XIAOSHEN BAI, Department of Chemical Engineering and Materials Science, Stevens Institute of Technology, MEGAN HAND, Mechanical Engineering, Stevens Institute of Technology, JACK LY, ALEJANDRO BRISENO, Department of Polymer Science and Engineering, University of Massachusetts, Amherst, STEPHANIE LEE, Department of Chemical Engineering and Materials Science, Stevens Institute of Technology — We demonstrate the ability to control out-of-plane orientation of small-molecule bis(triisopropylsilyl)ethynyl pyranthrene (TIPS-PY) crystals drop cast from the solution phase onto SiO<sub>2</sub> substrates. By tuning solvent-molecule interactions through the incorporation of varying amounts of an anti-solvent during drop casting, we observed a systematic change in the crystal morphology from cross-shaped crystals to needle like crystals using optical microscopy and scanning electron microscopy. 2-D x-ray diffraction experiments revealed that this change in crystal morphology corresponded to a change in the crystallographic orientation of the crystals, from one in which the (100) plane is parallel to the substrate surface to one in which the (001) plane is parallel to the substrate surface. Tuning molecule-substrate interactions by modifying the surface energy of the underlying substrate was also found to affect the observed crystal orientation. Because organic semiconductor crystals display large charge transport anisotropies along different crystallographic directions, it is expected that the out-of-plane charge mobility will depend on the TIPS-PY crystal orientation.

**5:06PM P33.00014 Birefringence and Enhanced Stability in Stable Organic Glasses<sup>1</sup>** , TIANYI LIU, ANNEMARIE EXARHOS, KEVIN CHENG, TIEZHENG JIA, PATRICK WALSH, JAY KIKKAWA, ZAHRA FAKHRAAI, Univ of Pennsylvania — Stable glasses can be prepared by physical vapor depositing organic molecules onto a cold substrate at slow rates. These glasses have many exceptional properties such as high thermal stability, high density, and birefringence. Regardless of the molecular shape or intermolecular interactions, birefringence has been observed in various stable glasses produced at low temperatures (below 80% of the molecule's glass transition temperature,  $T_g$ ). Here we prepare stable glasses of an organic molecule, 9-(3,5-di(naphthalen-1-yl)phenyl)anthracene, that possesses a nearly isotropic shape and intrinsic fluorescence. Ellipsometry is used to show that all stable glasses prepared in the temperature range from 73%  $T_g$  to 97%  $T_g$  show positive birefringence. Angle- and polarization- dependent photoluminescence measurements show isotropic molecular orientation in these optically birefringent glasses. Furthermore, the values of birefringence are strongly correlated with the enhanced density, implying a general origin of the observed anisotropy in stable glasses. This correlation can elucidate the role of packing in the formation of such high-density glasses.

<sup>1</sup>The authors would like to acknowledge Ethan Alguire and Joe Subotnik for simulation. Z.F. acknowledges funding from NSF CAREER (DMR-1350044). P.J.W. acknowledges funding from NSF (CHE-1152488). J.M.K acknowledges funding from NSF (DMR-1206270).

**5:18PM P33.00015 Traversing the polymorphic landscape through tuning molecule-molecule, molecule-substrate and molecule-solvent interactions** , GEOFFREY PURDUM, Dept. of Chemical and Biological Engineering, Princeton University, THOMAS GESSNER, R. THOMAS WEITZ, BASF SE, GMV 67056, Germany, YUEH-LIN LOO, Dept. of Chemical and Biological Engineering, Princeton University — As subtle changes in the crystalline packing motif of molecular semiconductors can have a large impact on charge transport, a thorough understanding of the accessibility of polymorphs in thin films is needed. Using a series of core-chlorinated naphthalene tetracarboxylic diimides, we demonstrate that the choice of the alkyl substituents at the imide functionalities, as well as the choice of substrate and post-deposition processing conditions, tune the relative strengths of molecule-molecule, molecule-substrate and molecule-solvent interactions, providing a handle over polymorphic selection. We access the triclinic polymorph of NTCDI-CH<sub>2</sub>C<sub>3</sub>F<sub>7</sub> in thermally evaporated thin films; solvent-vapor annealing induces a reversible transformation to its monoclinic polymorph. The addition of a fluoromethylene group in the alkyl substituent increases molecule-molecule interactions and, accordingly, improves the stability of its triclinic polymorph; this derivative does not undergo a polymorphic transformation with any of the post-deposition conditions we have explored.

**Wednesday, March 16, 2016 2:30PM - 5:30PM —**

**Session P34 DPOLY: Biopolymers and Biohybrid Polymers - Assembly and Thermodynamics**

337 - Muzhou Wang, NIST

**2:30PM P34.00001 Thermodynamics, morphology, and kinetics of early- stage self-assembly of pi-conjugated oligopeptides<sup>1</sup>** , BRYCE THURSTON, Univ of Illinois - Urbana, JOHN TOVAR, Johns Hopkins University, ANDREW FERGUSON, Univ of Illinois - Urbana — Synthetic oligopeptides containing  $\pi$ -conjugated cores self-assemble novel materials with attractive electronic and photophysical properties. All-atom, explicit solvent molecular dynamics simulations of Asp-Phe-Ala-Gly-OPV3-Gly-Ala-Phe-Asp peptides were used to parameterize an implicit solvent model to simulate self-assembly. At low-pH conditions, peptides assemble into  $\beta$ -sheet-like stacks with strongly favorable monomer association free energies of  $\Delta F \approx -25k_B T$ . Aggregation at high-pH produces disordered aggregates destabilized by Coulombic repulsion between negatively charged Asp termini. We model simulations of hundreds of monomers as a continuous-time Markov process. We infer transition rates between different aggregate sizes and microsecond relaxation times for early-stage assembly. Our data suggests a hierarchical model of assembly in which peptides coalesce into small clusters over tens of nanoseconds followed by structural ripening and diffusion limited aggregation on longer time scales. This work provides new molecular-level understanding of early-stage assembly, and a means to study the impact of peptide chemistry upon the thermodynamics, assembly kinetics, and morphology of the supramolecular aggregates.

<sup>1</sup>Supported by U.S. Department of Energy, Office of Science, Basic Energy Sciences, Award DE-SC0004857. Molecular simulations partially conducted on University of Illinois Computational Science and Engineering Program parallel computing resources

**2:42PM P34.00002 Bridging Length Scales to Study Self-Assembly and Self-Organization** , BRYAN KAYE, DANIEL NEEDLEMAN, Harvard University — A variety of proteins can assemble into large polymers as an integral part of their biological function. Studying the biochemistry and biophysics of polymer formation often involves time-resolvable measurements of the amount of polymer. Non-invasive measurements of polymer can be divided into two categories: short (spectroscopy) and large (microscopy) length scale measurements. Microscopy-based estimates of polymer amount are often dependent on spatial non-uniformity of polymer, whereas spectroscopy-based estimates of polymer amount are often based on models that are difficult to test. Here we show how both large and small length scale measurements can be combined to validate the assumptions behind both measurements while incorporating both measurements to make more accurate estimates of polymer amount. We utilize this approach with two-photon microscopy and FRET to measure the amount of tubulin (monomer) in microtubules (polymer) in order to study microtubule nucleation in cell extracts. In addition, this approach may be useful to study a wide variety of polymers, including actin filaments, viruses, lipid membranes, and other protein aggregates.

**2:54PM P34.00003 Creating Ordered Antibody Arrays with Antibody-Polymer Conjugates.** , XUEHUI DONG, ALLIE OBERMEYER, BRADLEY OLSEN, Massachusetts Institute of Technology — Antibodies are a category of functional proteins that play crucial roles in the immune system and have been widely applied in the area of cancer therapeutics, targeting delivery, signal detection, and sensors. Due to the extremely large size and lack of specific functional groups on the surface, it is challenging to functionalize antibodies and manipulate the ordered packing of antibodies in an array with high density and proper orientation, which is critical to achieve outstanding performance in materials. In this work, we demonstrate an efficient and facile approach for preparing antibody-polymer conjugates with two-step sequential “click” reaction to form antibody-polymer block copolymers. Highly ordered nanostructures are fabricated based on the principles of block copolymer self-assembly. The nanostructures are studied with both small angle X-ray scattering (SAXS) and transmission electron microscopy (TEM). Lamellae with alternating antibody domain and polymer domain are observed with an overall domain size of  $\sim 50$  nm. The nanostructure not only increases the packing density and promotes proper orientation of the antibody, but also provides possible channel to facilitate substrate transportation and improves the stability of the antibody.

**3:06PM P34.00004 Self-assembly of Artificial Actin Filaments** , CHRISTOPHER GROSENICK, SHENG FENG CHENG, Virginia Polytechnic Institute and State University — Actin Filaments are long, double-helical biopolymers that make up the cytoskeleton along with microtubules and intermediate filaments. In order to further understand the self-assembly process of these biopolymers, a model to recreate actin filament geometry was developed. A monomer in the shape of a bent rod with vertical and lateral binding sites was designed to assemble into single or double helices. With Molecular Dynamics simulations, a variety of phases were observed to form by varying the strength of the binding sites. Ignoring lateral binding sites, we have found a narrow range of binding strengths that lead to long single helices via various growth pathways. When lateral binding strength is introduced, double helices begin to form. These double helices self-assemble into substantially more stable structures than their single helix counterparts. We have found double helices to form long filaments at about half the vertical binding strength of single helices. Surprisingly, we have found that triple helices occasionally form, indicating the importance of structural regulation in the self-assembly of biopolymers.

**3:18PM P34.00005 Intermediate-filaments: from disordered building blocks to well-ordered cells.** , MICHA KORNREICH, ETI MALKA-GIBOR, ADI LASER-AZOGUI, OFER DORON, RAM AVINERY, Tel Aviv University, HARALD HERRMANN, German Cancer Research Center, Heidelberg, ROY BECK, Tel Aviv University — In the past decade it was found that  $\approx 50\%$  of human proteins contain long disordered regions, which play significant functional roles. As these regions lack a defined 3D folded structure, their ensemble conformations can be studied using polymer physics statistical-mechanics arguments. We measure the structure and mechanical response of hydrogels composed of neuronal intermediate filaments proteins. In the nervous system, these proteins provide cells with their mechanical support and shape, via interactions of their long, highly charged and disordered protein chains. We employ synchrotron small-angle X-ray scattering and various microscopy techniques to investigate such hydrogels from the nano- to the macro-scale. In contrast to previous polymer physics theories and experiments, we find that shorter and less charged chains can promote network expansion. The results are explained by intricate interactions between specific domains on the interacting chains, and also suggest a novel structural justification for the changing protein compositions observed during neuronal development. We address the following questions: Can protein disorder have an important role in cellular architecture? Can structural disorder in the micro-scale induce orientational and translational order on the macro-scale? How do the physical properties of disordered protein regions, such as charge, length, and hydrophobicity, modulate the cellular super-structure?

**3:30PM P34.00006 The effect of local melting of DNA on DNA loop formation** , JIYOUN JEONG, HAROLD KIM, Georgia Inst of Tech — Statistical mechanics of double-stranded DNA (dsDNA) is well described by the wormlike chain model (WLC) which assumes a harmonic bending potential. Such smooth bending potential may no longer be valid for large bending angles to form small loops ( $<100$  bp). Instead, DNA may rely on rare structural transitions such as local melting (opening) of base pairs to lower the energetic cost. In theory, open base pairs called bubbles can increase the looping probability of short DNA molecules by a few orders of magnitude, but a robust experimental validation of this theoretical prediction is lacking. Here, we investigated the correlation between local melting probability and looping dynamics of dsDNA using single-molecule fluorescence resonance energy transfer (FRET). We designed two groups of short DNA molecules with low and high melting probabilities around their center and measured their looping and unlooping rates in equilibrium. Our data allow rigorous tests of meltable wormlike chain (MWLC) models at short length scales for setting ranges of acceptable free energy cost of bubble formation and flexibility values of a bubble.

**3:42PM P34.00007 Effect of Backbone Design on Hybridization Thermodynamics of Oligo-nucleic Acids: A Coarse-Grained Molecular Dynamics Simulation Study**, AHMADREZA F. GHOBADI, Department of Chemical and Biomolecular Engineering, University of Delaware, Newark DE 19716, ARTHI JAYARAMAN, Department of Chemical and Biomolecular Engineering, Department of Material Science and Engineering, University of Delaware, Newark DE 19716 — DNA hybridization is the basis of various bio-nano technologies, such as DNA origami and assembly of DNA-functionalized nanoparticles. A hybridized double stranded (ds) DNA is formed when complementary nucleobases on hybridizing strands exhibit specific and directional hydrogen bonds through canonical Watson-Crick base-pairing interactions. In recent years, the need for cheaper alternatives and significant synthetic advances have driven design of DNA mimics with new backbone chemistries. However, a fundamental understanding of how these backbone modifications in the oligo-nucleic acids impact the hybridization and melting behavior of the duplex is still lacking. In this talk, we present our recent findings on impact of varying backbone chemistry on hybridization of oligo-nucleic acid duplexes. We use coarse-grained molecular dynamics simulations to isolate the effect of strand flexibility, electrostatic interactions and nucleobase spacing on the melting curves for duplexes with various strand sequences and concentrations. Since conjugation of oligo-nucleic acids with polymers serve as building blocks for thermo-responsive polymer networks and gels, we also present the effect of such conjugation on hybridization thermodynamics and polymer conformation.

**3:54PM P34.00008 Pore Diameter Dependence and Segmental Dynamics of Poly-Z-L-lysine and Poly-L-alanine Confined in 1D Nanocylindrical Geometry**, EYLUL TUNCEL, TOBB UET, YASUHIITO SUZUKI, Max Planck Institute for Polymer Research, AGATHAGGELOS IOSSIFIDIS, University of Ioannina, MARTIN STEINHART, University of Osnabruck, HANS-JURGEN BUTT, Max Planck Institute for Polymer Research, GEORGE FLOUDAS, University of Ioannina, HATICE DURAN, TOBB UET — Structure formation, thermodynamic stability, phase and dynamic behaviors of polypeptides are strongly affected by confinement. Since understanding the changes in these behaviors will allow their rational design as functional devices with tunable properties, herein we investigated Poly-Z-L-lysine (PZLL) and Poly-L-alanine (PALa) homopolypeptides confined in nanoporous alumina containing aligned cylindrical nanopores as a function of pore size by differential scanning calorimetry (DSC), Fourier Transform Infrared Spectroscopy, Solid-state NMR, X-ray diffraction, Dielectric spectroscopy(DS). Bulk PZLL exhibits a glass transition temperature ( $T_g$ ) at about 301K while PZLL nanorods showed slightly lower  $T_g$  (294K). The dynamic investigation by DS also revealed a decrease (4K) in  $T_g$  between bulk and PZLL nanorods. DS is a very sensitive probe of the local and global secondary structure relaxation through the large dipole to study effect of confinement. The results revealed that the local segmental dynamics, associated with broken hydrogen bonds, and segmental dynamics speed-up on confinement.

**4:06PM P34.00009 Effects of spermine binding on Taxol-stabilized microtubules**, SHENGFENG CHENG, CHOLA REGMI, Virginia Polytechnic Institute and State University — Previous studies have shown that polyamines such as spermine present in cells at physiological concentrations can facilitate the polymerization of tubulins into microtubules (MTs). A recent experiment demonstrates that in the presence of high-concentration spermine, Taxol-stabilized MTs undergo a shape transformation into inverted tubulin tubules (ITTs), the outside surface of which corresponds to the inside surface of a regular MT. However, the molecular mechanism underlying the shape transformation of MTs into ITTs is unclear. We perform all atom molecular dynamics simulations on Taxol-stabilized MT sheets containing two protofilaments surrounded by spermine ions. The spermine concentration is varied from 0 to 25mM to match the range probed experimentally. We identify important spermine binding regions on the MT surface and the influence of the spermine binding on the structure and dynamics of MTs. In contrast to Taxol, our results show that spermine binding seems to decrease the flexibility of tubulin proteins, resulting in weaker tubulin-tubulin contacts and promoting the bending of protofilaments into curved protofilaments, inverted rings, and eventually inverted tubules.

**4:18PM P34.00010 Tuning the entropic spring to dictate order and functionality in polymer conjugated peptide biomaterials**, SINAN KETEN, Northwestern University — Hybrid peptide-polymer conjugates have the potential to combine the advantages of natural proteins and synthetic polymers, resulting in biomaterials with improved stability, controlled assembly, and tailored functionalities. However, the effect of polymer conjugation on peptide structural organization and functionality, along with the behavior of polymers at the interface with biomolecules remain to be fully understood. This talk will summarize our recent efforts towards establishing a modeling framework to design entropic forces in helix-polymer conjugates and polymer-conjugated peptide nanotubes to achieve hierarchical self-assembling systems with predictable order. The first part of the talk will discuss how self-assembly principles found in biology, combined with polymer physics concepts can be used to create artificial membranes that mimic certain features of ion channels. Thermodynamics and kinetics aspects of self-assembly and how it governs the growth and stacking sequences of peptide nanotubes will be discussed, along with its implications for nanoscale transport. The second part of the talk will review advances related to modeling polymer conjugated coiled coils at relevant length and time scales. Atomistic simulations combined with sampling techniques will be presented to discuss the energy landscapes governing coiled-coil stability, revealing cascades of events governing disassembly. This will be followed by a discussion of mechanisms through which polymers can stabilize small proteins, such as shielding of solvents, and how specific peptide sequences can reciprocate by altering polymer conformations. Correlations between mechanical and thermal stability of peptides will be discussed. Finally, coarse-grained simulations will provide insight into how the location of polymer attachment changes entropic forces and higher-level organization in helix bundle assemblies. Our findings set the stage for a materials-by-design capability towards dictating complex topologies of polymer-peptide conjugate systems.

**4:54PM P34.00011 Thermal Properties of Silk Fibroin Using Fast Scanning Calorimetry<sup>1</sup>**, PEGGY CEBE, BENJAMIN PARTLOW, DAVID KAPLAN, Tufts University, ANDREAS WURM, EVGENY ZHURAVLEV, CHRISTOPH SCHICK, University of Rostock — We performed fast scanning chip-based calorimetry of silk protein using the Mettler Flash DSC1. We suggest the methodology by which to obtain quantitative information on the very first scan to high temperature, including the melting endotherm of the beta pleated sheets. For proteins, this first scan is the most important one, because the crystalline secondary structural features, the beta pleated sheets, melt after the first heating and cannot be thermally reintroduced. To obtain high quality data, the samples must be treated to drying and enthalpy relaxation sequences. The heat flow rates in heating and cooling must be corrected for asymmetric heat losses. We evaluate methods to obtain an estimate of the sample mass, finally choosing internal calibration using the known heat capacity increment at the glass transition. We report that even heating at rates of 2000 K/s, thermal degradation of silk cannot be totally avoided, though it can be minimized. Using a set of nineteen samples, we successfully determine the liquid state heat capacity of silk as:  $C_p^{liquid}(T) = (1.98 \pm 0.06) \text{ J/gK} + T(6.82 \pm 1.4) \times 10^{-4} \text{ J/gK}^2$ . Methods for estimation of the sample mass will be presented and compared.

<sup>1</sup>National Science Foundation, Polymers Program DMR-1206010; DAAD; Tufts Faculty Supported Leave

**5:06PM P34.00012 Long-term Controlled Drug Release from bi-component Electrospun Fibers**, SHANSHAN XU, ZIXIN ZHANG, QINGHUA XIA, CHARLES HAN, Chinese Academy of Sci (CAS) — Multi-drug delivery systems with timed programmed release are hard to be produced due to the complex drug release kinetics which mainly refers to the diffusion of drug molecules from the fiber and the degradation of the carrier. This study focused on the whole life-time story of the long-term drug releasing fibrous systems. Electrospun membrane utilizing FDA approved polymers and broad-spectrum antibiotics showed specific drug release profiles which could be divided into three stages based on the profile slope. With throughout morphology observation, cumulative release amount and releasing duration, releasing kinetics and critical factors were fully discussed during three stages. Through changing the second component, approximately linear drug release profile and a drug release duration about 13 days was prepared, which is perfect for preventing post-operative infection. The addition of this semi-crystalline polymer in turn influenced the fiber swelling and created drug diffusion channels. In conclusion, through adjusting and optimization of the blending component, initial burst release, delayed release for certain duration, and especially the sustained release profile could all be controlled, as well as specific anti-bacterial behavior could be obtained.

**5:18PM P34.00013 Correlation Between Chain Architecture and Hydration Water Structure in Polysaccharides** , MICHAEL GROSSUTTI, JOHN DUTCHER, University of Guelph — The physical properties of confined water can differ dramatically from those of bulk water. Hydration water associated with polysaccharides provides a particularly important example of confined water, with differences in polysaccharide structure providing different spatially confined environments for water adsorption. We have used attenuated total reflection infrared (ATR-IR) spectroscopy to investigate the structure of hydration water in films of three different polysaccharides under controlled relative humidity (RH) conditions. We compare the results obtained for films of highly branched, monodisperse phytyglycogen nanoparticles to those obtained for two unbranched polysaccharides, hyaluronic acid (HA) and chitosan. We find similarities between water structuring in the two linear polysaccharides, and significant differences for phytyglycogen. In particular, the phytyglycogen nanoparticles exhibited high network water connectivity, and a large increase in the fraction of multimer water clusters with increasing RH, whereas the water structure for HA and chitosan was found to be insensitive to changes in RH. These measurements provide unique insight into the relationship between the chain architecture and hydration of polysaccharides.

**Wednesday, March 16, 2016 2:30PM - 5:18PM –**  
**Session P35 DBIO: Physics of Sensorimotor Neural Circuits II** 338 - Alex Koulakov, Cold Springs Harbor Laboratory

**2:30PM P35.00001 Old and new news about single-photon sensitivity in human vision<sup>1</sup>** , PHILIP NELSON, University of Pennsylvania — It is sometimes said that “our eyes can see single photons,” when in fact the faintest flash of light that can reliably be reported by human subjects is closer to 100 photons. Nevertheless, there is a sense in which the familiar claim is true. Experiments conducted long after the seminal work of Hecht, Schlaer, and Pirenne in two distinct realms, those of human psychophysics and single-cell physiology, now admit a more precise conclusion to be drawn about our visual apparatus. Finding a single framework that accommodates both kinds of result is a nontrivial challenge, and one that sets severe quantitative constraints on any model of dim-light visual processing. I will present one such model and compare it to a recent experiment.

<sup>1</sup>Partially supported by the NSF under Grants EF-0928048 and DMR-0832802.

**2:42PM P35.00002 Matching tutors and students: effective strategies for information transfer between circuits** , TIBERIU TESILEANU, CUNY - Graduate Center, VIJAY BALASUBRAMANIAN<sup>1</sup>, University of Pennsylvania, BENEC OLVECKY, Harvard University — Many neural circuits transfer learned information to downstream circuits: hippocampal-dependent memories are consolidated into long-term memories elsewhere; motor cortex is essential for skill learning but dispensable for execution; anterior forebrain pathway (AFP) in songbirds drives short-term improvements in song that are later consolidated in pre-motor area RA. We show how to match instructive signals from tutor circuits to synaptic plasticity rules in student circuits to achieve effective two-stage learning. We focus on learning sequential patterns where a timebase is transformed into motor commands by connectivity with a ‘student’ area. If the sign of the synaptic change is given by the magnitude of tutor input, a good teaching strategy uses a strong (weak) tutor signal if student output is below (above) its target. If instead timing of tutor input relative to the timebase determines the sign of synaptic modifications, a good instructive signal accumulates the errors in student output as the motor program progresses. We demonstrate song learning in a biologically-plausible model of the songbird circuit given diverse plasticity rules interpolating between those described above. The model also reproduces qualitative firing statistics of RA neurons in juveniles and adults.

<sup>1</sup>Also affiliated to CUNY - Graduate Center.

**2:54PM P35.00003 Sensory stimuli reduce the dimensionality of cortical activity** , LUCA MAZZUCATO, ALFREDO FONTANINI, GIANCARLO LA CAMERA, State Univ of NY- Stony Brook — Neural ensembles in alert animals generate complex patterns of activity. Although cortical activity unfolds in a space whose dimension is equal to the number of neurons, it is often restricted to a lower dimensional subspace. Dimensionality is the minimal number of dimensions that accurately capture neural dynamics, and may be related to the computational tasks supported by the neural circuit. Here, we investigate the dimensionality of neural ensembles from the insular cortex of alert rats during periods of ‘ongoing’ (spontaneous) and stimulus-evoked activity. We find that the dimensionality grows with ensemble size, and does so significantly faster during ongoing compared to evoked activity. We explain both results using a recurrent spiking network with clustered architecture, and obtain analytical results on the dependence of dimensionality on ensemble size, number of clusters, and pair-wise noise correlations. The theory predicts a characteristic scaling with ensemble size and the existence of an upper bound on dimensionality, which grows with the number of clusters and decreases with the amount of noise correlations. To our knowledge, this is the first mechanistic model of neural dimensionality in cortex during both spontaneous and evoked activity.

**3:06PM P35.00004 Patterns in nature shape human visual perception.** , ANN HERMUNDSTAD, University of Pennsylvania — The statistical regularities of natural signals are known to shape the first stages of sensory processing. In the visual system, an efficient representation of light intensity begins in retina, where statistical redundancies are removed via spatiotemporal decorrelation. Much less is known, however, about the efficient representation of complex features in higher visual areas. I will discuss how the central visual system, operating with different goals and under different constraints, makes efficient use of resources to extract meaningful features from complex visual stimuli.

**3:42PM P35.00005 Nonlinear Bayesian cue integration explains the dynamics of vocal learning<sup>1</sup>** , BAOHUA ZHOU, SAMUEL SOBER, ILYA NEMENMAN, Emory University — The acoustics of vocal production in songbirds is tightly regulated during both development and adulthood as birds progressively refine their song using sensory feedback to match an acoustic target. Here, we perturb this sensory feedback using headphones to shift the pitch (fundamental frequency) of song. When the pitch is shifted upwards (downwards), birds eventually learn to compensate and sing lower (higher), bringing the experienced pitch closer to the target. Paradoxically, the speed and amplitude of this motor learning decrease with increases in the introduced error size, so that birds respond rapidly to a small sensory perturbation, while seemingly never correcting a much bigger one. Similar results are observed broadly across the animal kingdom, and they do not derive from a limited plasticity of the adult brain since birds can compensate for a large error as long as the error is imposed gradually. We develop a mathematical model based on nonlinear Bayesian integration of two sensory modalities (one perturbed and the other not) that quantitatively explains all of these observations. The model makes predictions about the structure of the probability distribution of the pitches sung by birds during the pitch shift experiments, which we confirm using experimental data.

<sup>1</sup>This work was supported in part by James S. McDonnell Foundation Grant 220020321, NSF Grant IOS/1208126, NSF Grant IOS/1456912 and NIH Grants R01NS084844.

**3:54PM P35.00006 Neurocontrol in sensory cortex<sup>1</sup>**, JASON RITT, Boston University, ANIRBAN NANDI, Washington University, St. Louis, JOSEPH SCHROEDER, Boston University, SHINUNG CHING, Washington University, St. Louis — Technology to control neural ensembles is rapidly advancing, but many important challenges remain in applications, such as design of controls (e.g. stimulation patterns) with specificity comparable to natural sensory encoding. We use the rodent whisker tactile system as a model for active touch, in which sensory information is acquired in a closed loop between feedforward encoding of sensory information and feedback guidance of sensing motions. Motivated by this system, we present optimal control strategies that are tailored for underactuation (a large ratio of neurons or degrees of freedom to stimulation channels) and limited observability (absence of direct measurement of the system state), common in available stimulation technologies for freely behaving animals. Using a control framework, we have begun to elucidate the feedback effect of sensory cortex activity on sensing in behaving animals. For example, by optogenetically perturbing primary sensory cortex (SI) activity at varied timing relative to individual whisker motions, we find that SI modulates future sensing behavior within 15 msec, on a whisk by whisk basis, changing the flow of incoming sensory information based on past experience.

<sup>1</sup>J.T.R. and S.C. hold Career Awards at the Scientific Interface from the Burroughs Wellcome Fund

**4:06PM P35.00007 Dynamical encoding of looming, receding, and focussing.** <sup>1</sup>, ANDRE LONGTIN, STEPHEN ELISHA CLARKE, LEONARD MALER, University of Ottawa, CENTER FOR NEURAL DYNAMICS COLLABORATION — This talk will discuss a non-conventional neural coding task that may apply more broadly to many senses in higher vertebrates. We ask whether and how a non-visual sensory system can focus on an object. We present recent experimental and modeling work that shows how the early sensory circuitry of electric sense can perform such neuronal focusing that is manifested behaviorally. This sense is the main one used by weakly electric fish to navigate, locate prey and communicate in the murky waters of their natural habitat. We show that there is a distance at which the Fisher information of a neuron's response to a looming and receding object is maximized, and that this distance corresponds to a behaviorally relevant one chosen by these animals. Strikingly, this maximum occurs at a bifurcation between tonic firing and bursting. We further discuss how the invariance of this distance to signal attributes can arise, a process that first involves power-law spike frequency adaptation. The talk will also highlight the importance of expanding the classic dual neural encoding of contrast using ON and OFF cells in the context of looming and receding stimuli.

<sup>1</sup>The authors acknowledge support from CIHR and NSERC.

**4:18PM P35.00008 Songbird Respiration is Controlled by Multispike Patterns at Millisecond Temporal Resolution<sup>1</sup>**, CAROLINE HOLMES, KYLE SRIVASTAVA, Emory University, MICHEL VELLEMA, COEN ELEMANS, University of Southern Denmark, ILYA NEMENMAN, SAMUEL SOBER, Emory University — Although the importance of precise timing of neural action potentials (spikes) is well known in sensory systems, approaches to motor control have focused almost exclusively on firing rates. Here we examined whether precise timing of spikes in multispike patterns has an effect on the motor output in the respiratory system of the Bengalese finch, a songbird. By recording from single motor neurons and the muscle fibers they innervate in freely behaving birds, we find that the spike trains are significantly non-Poisson, suggesting that the precise timing of spikes is tightly controlled. We further find that even a one millisecond shift of an individual spike in a multispike pattern predicts a significantly different air sac pressure. Finally, we provide evidence for the causal relation between precise spike timing and the motor output in this organism by stimulating the motor system with precisely timed patterns of electrical impulses. We observe that shifting a single pulse by as little as two milliseconds elicits differences in resulting air sac pressure. These results demonstrate that the precise timing of spikes does play a role in motor control.

<sup>1</sup>This work was partially supported by NSF Grant IOS/1208126, NIH Grant 5R90DA033462, NIH Grant R01NS084844, and NIH Grant F31DC013753

**4:30PM P35.00009 The primary visual cortex in the neural circuit for visual orienting<sup>1</sup>**, LI ZHAOPING, University College London — The primary visual cortex (V1) is traditionally viewed as remote from influencing brain's motor outputs. However, V1 provides the most abundant cortical inputs directly to the sensory layers of superior colliculus (SC), a midbrain structure to command visual orienting such as shifting gaze and turning heads. I will show physiological, anatomical, and behavioral data suggesting that V1 transforms visual input into a saliency map to guide a class of visual orienting that is reflexive or involuntary. In particular, V1 receives a retinotopic map of visual features, such as orientation, color, and motion direction of local visual inputs; local interactions between V1 neurons perform a local-to-global computation to arrive at a saliency map that highlights conspicuous visual locations by higher V1 responses. The conspicuous location are usually, but not always, where visual input statistics changes. The population V1 outputs to SC, which is also retinotopic, enables SC to locate, by lateral inhibition between SC neurons, the most salient location as the saccadic target. Experimental tests of this hypothesis will be shown. Variations of the neural circuit for visual orienting across animal species, with more or less V1 involvement, will be discussed.

<sup>1</sup>Supported by the Gatsby Charitable Foundation

**4:42PM P35.00010 Distributed multisensory integration in a recurrent network model through supervised learning**, HE WANG, K. Y. MICHAEL WONG, Hong Kong University of Science and Technology — Sensory integration between different modalities has been extensively studied. It is suggested that the brain integrates signals from different modalities in a Bayesian optimal way. However, how the Bayesian rule is implemented in a neural network remains under debate. In this work we propose a biologically plausible recurrent network model, which can perform Bayesian multisensory integration after trained by supervised learning. Our model is composed of two modules, each for one modality. We assume that each module is a recurrent network, whose activity represents the posterior distribution of each stimulus. The feedforward input on each module is the likelihood of each modality. Two modules are integrated through cross-links, which are feedforward connections from the other modality, and reciprocal connections, which are recurrent connections between different modules. By stochastic gradient descent, we successfully trained the feedforward and recurrent coupling matrices simultaneously, both of which resembles the Mexican-hat. We also find that there are more than one set of coupling matrices that can approximate the Bayesian theorem well. Specifically, reciprocal connections and cross-links will compensate each other if one of them is removed. Even though trained with two inputs, the network's performance with only one input is in good accordance with what is predicted by the Bayesian theorem.

**4:54PM P35.00011 Learning tinnitus<sup>1</sup>**, J. LEO VAN HEMMEN, Physik Department, TU Munich — Tinnitus, implying the perception of sound without the presence of any acoustical stimulus, is a chronic and serious problem for about 2% of the human population. In many cases, tinnitus is a pitch-like sensation associated with a hearing loss that confines the tinnitus frequency to an interval of the tonotopic axis. Even in patients with a normal audiogram the presence of tinnitus may be associated with damage of hair-cell function in this interval. It has been suggested that homeostatic regulation and, hence, increase of activity leads to the emergence of tinnitus. For patients with hearing loss, we present spike-timing-dependent Hebbian plasticity (STDP) in conjunction with homeostasis as a mechanism for "learning" tinnitus in a realistic neuronal network with tonotopically arranged synaptic excitation and inhibition. In so doing we use both dynamical scaling of the synaptic strengths and altering the resting potential of the cells. The corresponding simulations are robust to parameter changes. Understanding the mechanisms of tinnitus induction, such as here, may help improving therapy.

<sup>1</sup>Work done in collaboration with Julie Goulet and Michael Schneider. JLvH has been supported partially by BCCN – Munich.

**5:06PM P35.00012 Simulating Visual Learning and Optical Illusions via a Network-Based Genetic Algorithm**, THEODORE SIU, Rutgers University Department of Physics, MIGUEL VIVAR, Rutgers University Department of Biomedical Engineering, TROY SHINBROT, Rutgers University Department of Physics — We present a neural network model that uses a genetic algorithm to identify spatial patterns. We show that the model both learns and reproduces common visual patterns and optical illusions. Surprisingly, we find that the illusions generated are a direct consequence of the network architecture used. We discuss the implications of our results and the insights that we gain on how humans fall for optical illusions

**Wednesday, March 16, 2016 2:30PM - 5:30PM –**

**Session P36 GSOFT: Frontiers of Liquid Crystals: From Colloids to Chiral Liquid Crystals** 339

- Randy Kamien, University of Pennsylvania

**2:30PM P36.00001 Directed self-assembly of colloidal particles onto the chemically anchoring patterned surface in a nematic liquid crystal**, XIAO LI, JULIO ARMAS-PÉREZ, JUAN HERNANDEZ-ORTIZ, JUAN DE PABLO, PAUL NEALEY, University of Chicago — The defects assisted assembly of colloidal particles works are more focused on the defects created in the bulk or the interface of nematic liquid crystal, which usually observe a group of particles spontaneously forming a chain or aggregating over the defects. The confining surface with specific 3D sculptured structures, such as pyramid or zig-zag grooves, offers the opportunity to isolate the trapped particles into certain position. Here, we explore a new method to direct self-assemble the colloidal particles through manipulating defects on the 2D geometry confined anchoring surface. Since the director of the preferred planar orientation of LCs could be manipulated by the pattern geometry and dimension, the topological defects could be engineered based on multi-stable orientation by designed 2D geometry pattern of different controllable direction at sub-micrometer dimension. We demonstrate that the designed one single middle straight stripe with disjoint two groups of straight stripe array on both side of the middle stripe as 45 angle of different orientation director could control the distortion of the disjoint gap space thus acting as defects template to trap the colloidal particles directed self-assembly at the designed positions. Through anchoring distribution on the pattern areas, geometry design of pattern, and also the external electric field applied on the system, those defects areas could be generate, erase, resume or even correct.

**2:42PM P36.00002 Self-assembly and separation of nematic colloids through photo-patterned molecular orientation<sup>1</sup>**, CHENHUI PENG, YUBING GUO, Liquid Crystal Institute and Chemical Physics Interdisciplinary Program, Kent State University, Kent, OH 44242, USA, CHRISTOPHER CONKLIN, JORGE VIALS, School of Physics and Astronomy and Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, MN 55455, USA, SERGIJ SHYANOVSKII, QI-HUO WEI, OLEG LAVRETOVICH, Liquid Crystal Institute and Chemical Physics Interdisciplinary Program, Kent State University, Kent, OH 44242, USA, OLEG D. LAVRETOVICH TEAM, JORGE VIALS COLLABORATION — Design and control of particles self-assembly is an important theme in colloidal science. Dispersions of colloids in a nematic liquid crystal (LC) show a diversity of self-assembled structures guided by long-range interactions. Here we describe a versatile approach to control colloidal structures through surface-patterned molecular orientation and dynamic processes of LC-enabled electrokinetics (LCEK). In presence of the electric field, the surface-imprinted pattern of molecular orientation triggers LCEK flows which transport the colloidal aggregates to specified locations. The aggregation is directed by the director gradients. Colloids that differ in surface anchoring or shape are guided into different areas of the cell, thus being sorted. The dynamic approach to control colloidal systems through LCEK in cells with patterned director field opens the opportunities in the microfluidic and lab on a chip applications.

<sup>1</sup>This work was supported by NSF grants DMR-1507637, DMS-1434185 and CMMI-1436565

**2:54PM P36.00003 Directed Self-assembly of Colloidal Particles on a Blue Phase I Interface<sup>1</sup>**, JOSE MARTINEZ-GONZALEZ, YE ZHOU, MONIRO SADAT SADATI, Univ of Chicago, NICHOLAS ABBOTT, University of Wisconsin, JUAN DE PABLO, Univ of Chicago — Blue phases are liquid states of matter with a highly ordered defect structure which confers unique properties among complex fluids. In this work, a free energy model of chiral liquid crystals is used to consider the self-assembly of colloids and nanoparticles on the interface of a Blue Phase I. It is shown that the crystalline defect structure of the blue phase produces intricate, two-dimensional hexagonal and Kagome structures among the nanoparticle arrangements, with lattice parameters that depend on the type of anchoring of the liquid crystal at the particles surface. These parameters can be tuned via the chirality of the material, thereby offering intriguing possibilities for the creation of hierarchical materials based on the directed assembly of particles in chiral liquid crystals.

<sup>1</sup>This work is supported by the Department of Energy, Basic Energy Sciences, Materials Science and Engineering Division, Biomaterials Program, through DE-SC004025.

**3:06PM P36.00004 Three-Dimensional Topological Solitons in Chiral Liquid Crystals and Ferromagnetic Colloids.**, IVAN SMALYUKH<sup>1</sup>, University of Colorado Boulder — Three-dimensional knotted solitons - often called “hopfions” - have continuous physical fields classified by the Hopf index topological invariant and behave like particles. These hopfions arise in theories in many branches of physics, but their structure and stability are rarely accessible to direct experimental studies. We realize and characterize such static solitons in the molecular alignment fields of chiral liquid crystals and in the magnetization field of colloids with long-range ferromagnetic ordering. Our experiments agree with predictions of numerical modeling based on free energy minimization. By exploiting facile response of the soft matter host media, we demonstrate exquisite control of structure and tunable self-assembly of such solitonic “particles”. This lecture will discuss how liquid crystals and colloids can serve as soft matter model systems in studies of structure, topology and dynamics of three-dimensional topological solitons.

<sup>1</sup>GSoft Early Career

**3:42PM P36.00005 Brownian Dynamics of Colloidal Particles in Lyotropic Chromonic Liquid Crystals<sup>1</sup>**, ANGEL MARTINEZ, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PETER J. COLLINGS, Department of Physics and Astronomy, Swarthmore College, Swarthmore, ARJUN G. YODH, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia — We employ video microscopy to study the Brownian dynamics of colloidal particles in the nematic phase of lyotropic chromonic liquid crystals (LCLCs). These LCLCs (in this case, DSCG) are water soluble, and their nematic phases are characterized by an unusually large elastic anisotropy. Our preliminary measurements of particle mean-square displacement for polystyrene colloidal particles (~5 micron-diameter) show diffusive and sub-diffusive behaviors moving parallel and perpendicular to the nematic director, respectively. In order to understand these motions, we are developing models that incorporate the relaxation of elastic distortions of the surrounding nematic field. Further experiments to confirm these preliminary results and to determine the origin of these deviations compared to simple diffusion theory are ongoing; our results will also be compared to previous diffusion experiments in nematic liquid crystals [1-3]. 1. G. J. Krüger, *Physics Reports* **82**, 229 (1982). 2. J. C. Loudet, P. Hanusse, P. Poulin, *Science* **306**, 1525 (2004) 3. T. Turiv, I. Lazo, A. Brodin, B. I. Lev, V. Reiffenrath, V. G. Nazarenko, O. D. Lavrentovich, *Science* **342**, 1351 (2013).

<sup>1</sup>We gratefully acknowledge financial support through NSF DMR12-05463, MRSEC DMR11-20901, and NASA NNX08AO0G.

**3:54PM P36.00006 Dielectric Anisotropy of Gold Nanoparticle Colloids in Nematic Liquid Crystals**, ANGELO VISCO, JON FOUST, RIZWAN MAHMOOD, JOSEPH BELOBRADICH, Slippery Rock Univ — We present electrical and optical studies of hexanethiol-treated gold nanoparticle (GNPs) colloids in 4-cyano-4'-pentyl-biphenyl (5CB) liquid crystals. Preliminary data analysis suggests an unusual behavior of sudden drop and then rise in the dielectric anisotropy at a critical concentration of 0.0862% by wt. GNPs and a sudden rise and then drop in the nematic to isotropic transition temperature. Above the critical concentration the data level off to within the uncertainty of the experimental errors. This colloidal system will help us to understand the interaction and the effects of nanoparticles on the self-assembly of LC molecules and the manner in which these particles organize in LC. This study is important for further developments in nanotechnology, sharp and fast display panels, and within the medical field.

**4:06PM P36.00007 Colloidal Transport within Nematics with Arrays of Obstacles**, KUI CHEN, OLIVIA GEBHARDT, Johns Hopkins Univ, GERMAN DRAZER, Rutgers University, DANIEL REICH, ROBERT LEHENY, Johns Hopkins Univ — We have investigated the transport behavior of spherical colloidal particles suspended in the nematic liquid crystal 4-cyano-4'-pentylbiphenyl (5CB) within microfluidic arrays of cylindrical obstacles arranged in a square lattice. Homeotropic anchoring at the surfaces of the obstacles created periodic director-field patterns that strongly influenced the trajectories of the colloids, which had both planar and homeotropic anchoring, as they traversed the arrays under gravity. When the applied force was along a symmetry direction of the lattice, the particles moved parallel to the force but with pronounced modulations in their velocity due to the liquid-crystal-mediated interactions with the posts. With increasing angle between the force and symmetry direction, the particle trajectories underwent a transition in which their average velocity no longer followed the force and instead was parallel to the lattice symmetry direction. The point of this transition was dictated by the particle-post interactions, suggesting a potential new mechanism for particle separations.

**4:18PM P36.00008 Colloidal interactions and self-assembly of plasmonic metal pyramids in nematic liquid crystals.**, SUNGOH PARK, IVAN SMALYUKH, Department of Physics, University of Colorado at Boulder — Combining ordered structure of soft matter systems, such as liquid crystals, with the unique optical properties of metal nano- and micro-particles is a promising approach of designing and realizing mesostructured composites with pre-engineered properties. In this work, we disperse nanofabricated pyramid-shaped plasmonic particles in a nematic host fluid and demonstrate that the particles spontaneously align with respect to the uniform far-field liquid crystal director. This alignment is driven by minimization of the surface anchoring and bulk elastic free energies of the nematic host. Interestingly, multiple stable and metastable orientations of these particles can be controllably observed. Using laser tweezers and video microscopy, we explore inter-particle pair interaction forces as well as the ensuing colloidal self-assembly. We analyze this experimentally observed rich physical behavior of our soft matter composite by invoking electrostatic multipole analogy of elastic distortions induced by the particles in a nematic liquid crystal host and discuss potential practical uses.

**4:30PM P36.00009 Co-dispersion of plasmonic nanorods in thermotropic nematic liquid crystals<sup>1</sup>**, GHADAH SHEETAH, PhD student, QINKUN LIU, PostDoc, IVAN SMALYUKH, Professor — Colloidal dispersions of plasmonic metal nanoparticles in liquid crystals promise the capability of pre-engineering tunable optical properties of mesostructured metal-dielectric composites. Recently, concentrated dispersions of anisotropic gold, silver, and metal alloy nanoparticles in nematic hosts have been achieved and successfully controlled by low-voltage fields [1, 2]. However, to enable versatile designs of material behavior of the composites, simultaneous co-dispersion of anisotropic particles with different shapes, alignment properties, and compositions are often needed. We achieve such co-dispersions and explore their switching characteristics in response to external stimuli like light and electric fields. We demonstrated that spectral characteristics of co-dispersions of multiple types of anisotropic nanoparticles in a common nematic host provides unprecedented variety of electrically- and optically-tunable material behavior, with a host of potential practical applications in electro-optic devices and displays. [1] Liu, Q., Yuan, Y., & Smalyukh, I. I. (2014). *Nano letters*, 14(7), 4071-4077. [2] Zhang, Y., Liu, Q., Mundoor, H., Yuan, Y., & Smalyukh, I. I. (2015). *ACS nano*, 9(3), 3097-3108.

<sup>1</sup>Ghadah acknowledges support from the King Faisal University (KFU) graduate fellowship

**4:42PM P36.00010 Tactoids of chiral liquid crystals<sup>1</sup>**, VIVIANA PALACIO-BETANCUR, STIVEN VILLADA-GIL, Departamento de Materiales y Minerales. Universidad Nacional de Colombia, Sede Medellín., YE ZHOU, JULIO C. ARMAS-PREZ, Institute for Molecular Engineering. University of Chicago, JUAN JOS DE PABLO, Institute for Molecular Engineering. University of Chicago. Argonne National Laboratory., JUAN PABLO HERNANDEZ-ORTIZ, Departamento de Materiales y Minerales. Universidad Nacional de Colombia, Sede Medellín. — The phase diagram of chiral liquid crystals confined in ellipsoids is obtained, by following a theoretically informed Monte Carlo relaxation of the tensor alignment field  $\mathbf{Q}$ . The free energy of the system is described by a functional in the framework of the Landau-de Gennes formalism. This study also includes the effect of anchoring strength, curvature, and chirality of the system. In the low chirality region of the phase diagram we found the twist bipolar (BS) phase and some cholesteric phases such as the radial spherical structure (RSS), twist cylinder (TC) and double twist cylinder (DTC) whose axis of rotation is not necessarily aligned with the major axis of the geometry. For high chirality scenarios, the disclination lines are twisted or bent near the surface preventing the formation of symmetric networks of defects, although an hexagonal pattern is formed on the surface which might serve as open sites for collocation of colloids. By analyzing the free energies of isochoric systems, prolate geometries tend to be more favorable for high chirality and low anchoring conditions.

<sup>1</sup>Universidad Nacional de Colombia Ph.D. grant and COLCIENCIAS under the Contract No. 110-165-843-748. CONACYT for Postdoctoral Fellowships Nos. 186166 and 203840.

**4:54PM P36.00011 Chiral liquid crystals: the vestigial chiral phases of  $T$ ,  $O$ ,  $I$  matter<sup>1</sup>**, JAAKKO NISSINEN, KE LIU, ROBERT-JAN SLAGER, Lorentz Institute for Theoretical Physics, Leiden University, the Netherlands, KAI WU, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory and Stanford University, USA, JAN ZAAANEN, Lorentz Institute for Theoretical Physics, Leiden University, the Netherlands — We show how chiral order develops in vestigial isotropic phases of  $T$ ,  $O$  and  $I$  liquid crystalline systems in three dimensions. The liquid crystal phases are realized in a lattice model of orientational degrees of freedom with point group symmetries  $G \subset O(3)$ , represented as  $O(3)$ -rotors coupled to  $G$  gauge fields. The model incorporates also disclinations via the gauge fields, features an ordered nematic phase with unbroken  $G$  rotations at low temperatures and a high temperature isotropic liquid phase. We observe an intermediate phase with spontaneous chirality but isotropic  $SO(3)$  symmetry (a liquid) for the gauge groups  $T$ ,  $O$ , and  $I$ , the proper symmetry groups of the tetrahedron, cube and icosahedron, respectively. For the other subgroups of  $SO(3)$ ,  $C_{n \leq \infty}$  and  $D_{n \leq \infty}$ , there is generically only a single phase transition from the nematic phase to the isotropic liquid. We discuss the nature of the phase transitions and conditions under which the chiral phase is stabilized by the nematic order parameter fluctuations. The nature of the vestigial chiral phase is reminiscent of the so-called Ising nematic phase in iron based superconductors.

<sup>1</sup>Research supported by the Netherlands foundation for Fundamental Research of Matter (FOM)

**5:06PM P36.00012 Structures of cholesteric liquid crystals confined in rectangular microchannels<sup>1</sup>**, QI-HUO WEI, YUBING GUO, JIE XIANG, OLEG LAVRETOVICH, Kent State University — When cholesteric liquid crystals are confined in various geometries, the interplays between the boundary conditions, the bulk structures and different length scales (pitch, penetration depth, and confinement size) may cause frustration and formation of intriguing topological defects and disclination lines. This paper presents our recent studies on the structures of cholesteric liquid crystals confined in rectangular microchannels with homeotropic alignments. The rectangular microchannels with various sizes and aspect ratios are made in glass substrates by using modern nanofabrication techniques. Detailed liquid crystal structures and their optical characterizations will be presented as a function of the channel depth and width.

<sup>1</sup>Work was supported by ACS PRF 53018-ND7

**5:18PM P36.00013 Cooking skyrmions: modeling temperature dependence of defect textures in cholesteric liquid crystals<sup>1</sup>**, SAJEDEH AFGHAH, ANDREW KONYA, JONATHAN SELINGER, ROBIN SELINGER, Liquid Crystal Institute, Kent State University — Using 3-d simulations and analytical calculations, we study temperature dependence of defect structures in liquid crystals in confined geometries. We model a cholesteric liquid crystal confined in a microchannel with homeotropic anchoring, and investigate resulting defect structures—skyrmions, alone or in periodic arrays (bubble domains), and striped textures—as a function of microchannel dimensions, cholesteric pitch, and surface anchoring strength. We model temperature dependence by varying Frank constants and pitch using functions fit to experimental values. Experiments by the Qihuo Wei group show that skyrmion arrays in a microchannel appear to “pop” at a threshold temperature, transforming into elongated defects that span the microchannel’s width. We explore this behavior using simulation and show that skyrmions elongate when their spacing is below a critical distance. Implementation of the simulation code in CUDA for a GPU-equipped computer produces highly efficient performance. We also carry out analytical calculations of free energy to determine optimal/stable structures for skyrmions and other defect textures in thin cells. Both simulation and analytical results are compared to recent experiments by the Qihuo Wei group.

<sup>1</sup>Supported by NSF CMMI-1436565. Acknowledgment is made to the Donors of the American Chemical Society Petroleum Research Fund for partial support of this research.

**Wednesday, March 16, 2016 2:30PM - 5:30PM –**  
**Session P37 GSOFD DPOLY: Soft Matter Interfaces: Blo-, Dielectrics, Transport and Other Phenomena** 340 - Silvina Matysiak, University of Maryland, College Park

**2:30PM P37.00001 Nonlinear transport of soft droplets in pore networks**, FRANCK VERNEREY, EDUARD BENET CERDA, KANGHYEON KOO, University of Colorado - Boulder — A large number of biological and technological processes depend on the transport of soft colloidal particles through porous media; this includes the transport and separation of cells, viruses or drugs through tissues, membranes and microfluidic devices. In these systems, the interactions between soft particles, background fluid and the surrounding pore space yield complex, nonlinear behaviors such as non-Darcy flows, localization and jamming. We devise a computational strategy to investigate the transport of non-wetting and deformable water droplets in a microfluidic device made of a random distribution of cylindrical obstacles. We first derive scaling laws for the entry of the droplet in a single pore and discuss the role of surface tension, contact angle and size in this process. This information is then used to study the transport of multiple droplets in an obstacle network. We find that when the droplet size is close to the pore size, fluid flow and droplet trafficking strongly interact, leading to local redistributions in pressure fields, intermittent clogging and jamming. Importantly, it is found that the overall droplet and fluid transport display three different scaling regimes depending on the forcing pressure, and that these regimes can be related to droplet properties.

**2:42PM P37.00002 Simulation of non-ionic surfactant micelle formation across a range of temperature and pressure**, GREGORY CUSTER, University of Maryland, PAYEL DAS, IBM Thomas J. Watson Research Center, SILVINA MATYSIAK, University of Maryland — Non-ionic surfactants can, at certain concentrations and thermodynamic conditions, aggregate into micelles due to their amphiphilic nature. Our work looks at the formation and behavior of micelles at extremes of temperature and pressure. Due to the large system size and simulation time required to study micelle formation, we have developed a coarse-grained (CG) model of our system. This CG model represents each heavy atom with a single CG bead. We use the multibody Stillinger-Weber potential, which adds a three-body angular penalty to a two-body potential, to emulate hydrogen bonds in the system. We simulate the linear surfactant  $C_{12}E_5$ , which has a nonpolar domain of 12 carbons and a polar domain of 5 ethers. Our CG model has been parameterized to match structural properties from all-atom simulations of single and dimer surfactant systems. Simulations were performed using a concentration above the experimental critical micelle concentration at 300K and 1atm. We observe an expected region of stable micelle formation at intermediate temperature, with a breakdown at high and low temperature, as well as at high pressure. The driving forces behind the destabilization of micelles and the mechanism of micelle formation at different thermodynamic conditions will be discussed.

**2:54PM P37.00003 On the pH of Aqueous Attoliter-Volume Droplets<sup>1</sup>**, KIERAN P. RAMOS, SAMSON S. VELPULA, TREVOR B. DEMILLE, RYAN PAJELA, LORI S. GOLDNER, Department of Physics, University of Massachusetts Amherst — Droplets of water dispersed in perfluorinated liquids have widespread use including microfluidics, drug delivery and single-molecule measurements. Perfluorinated liquids are distinctly biocompatible due to their stability, low surface tension, lipophobicity, and hydrophobicity. For this reason, the effect of the perfluorinated surface on droplet contents is usually ignored. However, as the droplet diameter is reduced, we expect that any effect of the water/oil interface on droplet contents will become more obvious. We studied the pH of attoliter-volume aqueous droplets in perfluorinated liquids using pH-sensing fluorescent dyes. Droplets were prepared either by sonication or extrusion from buffer and perfluorinated liquids (FC40 or FC77). A non-ionic surfactant was used to stabilize the droplets. Buffer strength, ionic strength, and pH of the aqueous phase were varied and resulting droplet pH compared to the pH of the buffer from which they were formed. Preliminary data are consistent with a pH in droplets that depends on the concentration of non-ionic surfactant. At low surfactant concentrations, the pH in droplets is distinctly lower than the stock buffer. However, as the concentration of non-ionic surfactant is increased the change in pH decreases.

<sup>1</sup>This work was funded by NSF/DBI-1152386.

**3:06PM P37.00004 Electrolyte-mediated adsorption to neutral and dielectric interfaces**, JOS ZWANIKKEN, University of Massachusetts, Lowell, YUFEI JING, Northwestern University, VIKRAM JADHAO, Johns Hopkins University, MONICA OLVERA DE LA CRUZ, Northwestern University — Biology relies on electrolytes to regulate molecular interactions and to support functionality in numerous vital processes. Although the role of the electrolyte is generally categorized into two tendencies, namely “salting-out” and “salting-in”, the more versatile aspects can be revealed by a more detailed picture of the microscopic ionic structure. We use molecular dynamics simulations and numerical calculations based on liquid state theory, and obtain high-resolution, quantitative information about the spatial structure of primitive model electrolytes in dielectric confinement, up to high concentrations (0.9 M) and strong electrostatic coupling. The theoretical methods also quantify two relevant underlying thermal forces that are highly tunable by the specific selection of electrolytes. The results refine the understanding of the adsorption behavior of ions and macromolecular solutes, and identify tuning parameters for macromolecular assembly, based on ion size, valency, and ionic composition.

**3:18PM P37.00005 Dipolar fluids near a dielectric surface**, ZIWEI WANG, ERIK LUIJTEN, Northwestern University — The behavior of dipolar fluids near an interface is of fundamental importance in a broad variety of fields, including colloid chemistry, electrochemistry, biochemistry and surface science. The structural properties of such a fluid are affected not only by the presence of surface charge, but also by a dielectric mismatch across the interface. Using large-scale Monte Carlo simulations that explicitly take into account dielectric effects, we investigate a prototypical dipolar fluid. In addition to the organization of the fluid, characterized through the dipolar orientations and spatial correlations, we also calculate the surface tension by employing simulations in the grand-canonical ensemble.

**3:30PM P37.00006 Dielectric effects on the ion distribution near a Janus colloid**, HUANXIN WU, MING HAN, ERIK LUIJTEN, Northwestern University — Spherical Janus colloids, particles with two domains of different materials, are typically heterogeneous in permittivity. This dielectric heterogeneity will influence their behavior in electrolytes, ranging from their aggregation to their electrokinetics in external fields. We investigate the structure of the electric double layer around spherical Janus colloids immersed in solution via molecular dynamics simulations. Polarization of the colloidal surfaces by the surrounding ions is calculated dynamically with a boundary-element method based Poisson solver. One observation is that even neutral Janus colloids may carry a net dipole moment in the presence of asymmetric salts. Moreover, we extend this study to incorporate a *spatially varying permittivity of the solvent* near a charged Janus colloid, and demonstrate the effect of this dielectric variation on the electric double layer.

**3:42PM P37.00007 Preventing Oxide Adhesion of Liquid Metal Alloys to Enable Actuation in Microfluidic Systems**, ISHAN JOSHIPURA, ALEXANDER JOHNSON, HUDSON AYERS, MICHAEL DICKEY, North Carolina State University — This work explores the wetting behavior of an oxide-coated liquid metal, eutectic alloy of gallium and indium ('EGaln'), which remains a liquid at room temperature. Liquid metals uniquely combine fluidity with metallic properties. Combined, these properties enable soft, stretchable, and shape reconfigurable electronics with 'softer than skin' interfaces. Ga forms spontaneously a thin surface oxide that alters its wetting behavior and makes it difficult to move across surfaces without leaving residue behind. We examine the effects of surface roughness (i.e., Cassie-Baxter state) and lubrication to minimize adhesion of Ga oxide to surfaces. Lubricated surfaces create a 'slip-layer' of liquid between the metal and surface that also inhibits wetting. This slip layer allows the metal to move reversibly through microchannels by preventing adhesion of the oxide. The metal may be pumped or moved by using low voltages or pneumatic actuation. Optical microscopy confirms the importance of the slip-layer, which enables non-stick motion of the metal through capillaries. Finally, electrochemical impedance spectroscopy characterizes the electrohydrodynamic motion of EGaln in capillary systems.

**3:54PM P37.00008 Confining capillary waves to control aerosol droplet size from surface acoustic wave nebulisation<sup>1</sup>**, ELIJAH NAZARZADEH, JULIEN REBOUD, RAB WILSON, JONATHAN M. COOPER, University of Glasgow — Aerosols play a significant role in targeted delivery of medication through inhalation of drugs in a droplet form to the lungs. Delivery and targeting efficiencies are mainly linked to the droplet size, leading to a high demand for devices that can produce aerosols with controlled sizes in the range of 1 to 5  $\mu\text{m}$ . Here we focus on enabling the control of the droplet size of a liquid sample nebulised using surface acoustic wave (SAW) generated by interdigitated transducers on a piezoelectric substrate (lithium niobate). The formation of droplets was monitored through a high-speed camera (600,000 fps) and the sizes measured using laser diffraction (Spraytec, Malvern Ltd). Results show a wide droplet size distribution (between 0.8 and 400  $\mu\text{m}$ ), while visual observation (at fast frame rates) revealed that the large droplets (>100  $\mu\text{m}$ ) are ejected due to large capillary waves (80 to 300  $\mu\text{m}$ ) formed at the free surface of liquid due to leakage of acoustic radiation of the SAWs, as discussed in previous literature (Qi et al. Phys Fluids, 2008). To negate this effect, we show that a modulated structure, specifically with feature sizes, typically 200  $\mu\text{m}$ , prevents formation of large capillary waves by reducing the degrees of freedom of the system, enabling us to obtain a mean droplet size within the optimum range for drug delivery (<10  $\mu\text{m}$ ).

<sup>1</sup>This work was supported by an EPSRC grant (EP/K027611/1) and an ERC Advanced Investigator Award (340117Biophononics)

**4:06PM P37.00009 Scaling Laws for liquid and ion transport in nanochannels grafted with polyelectrolyte brushes**, GUANG CHEN, SHAYANDEV SINHA, SIDDHARTHA DAS, Univ of Maryland-College Park, SOFT MATTER, INTERFACES, AND ENERGY LABORATORY (SMIEL) TEAM — Grafting nanochannels with polyelectrolyte (PE) brushes renders tremendous functionality to the nanochannels, making them capable of applications such as ion manipulation, ion sensing, current rectification, nanofluidic diode fabrication, and flow control. PE brush is a special case of polymers at interfaces; such brush-like structure is possible only when the grafting density ( $\sigma$ ) is beyond a critical value. In this study, we shall propose scaling laws that identify  $\sigma$ -N (N is the size of the PE molecule) combination that simultaneously ensure that the grafted PE molecules adopt "brush"-like configuration and the height of the PE brushes are smaller than the nanochannel half height. Secondly, we pinpoint the scaling conditions where the electrostatic effects associated with the PE brushes can be decoupled from the corresponding PE excluded volume and elastic effects; such de-coupling has tremendous connotation in context of modeling of electrostatics and transport at PE-brush-covered interfaces. Thirdly, we provide scaling arguments to quantify the dependence of the flow penetration depth into the PE brush as a function of the  $\sigma$ -N combination. Finally, our scaling estimates pinpoint the conditions where the flow or electric field induced deformation of the grafted nanochannel PE brushes can be neglected while modeling the pressure-driven or electroosmotic transport or ionic current in such nanochannels.

**4:18PM P37.00010 Entropic changes in liquid gallium clusters: understanding the anomalous melting temperatures**, NICOLA GASTON, MacDiarmid Institute for Advanced Materials and Nanotechnology, KRISTA STEENBERGEN, Massey University — Melting in finite-sized materials differs in two ways from the solid-liquid phase transition in bulk systems. First, there is an inherent scaling of the melting temperature below that of the bulk, known as melting point depression. Secondly, at small sizes, changes in melting temperature become non-monotonic, and show a size-dependence that is sensitive to the structure of the particle. Melting temperatures that exceed those of the bulk material have been shown to occur in vacuum, but have still never been ascribed a convincing physical explanation. Here we find answers in the structure of the aggregate liquid phase in small gallium clusters, based on molecular dynamics simulations that reproduce the greater-than-bulk melting behavior observed in experiments, and demonstrate the critical role of a lowered entropy in destabilising the liquid state.

**4:30PM P37.00011 Thermocapillary Technique for Shaping and Fabricating Optical Ribbon Waveguides**, KEVIN FIEDLER<sup>1</sup>, SANDRA TROIAN, California Institute of Technology — The demand for ever increasing bandwidth and higher speed communication has ushered the next generation optoelectronic integrated circuits which directly incorporate polymer optical waveguide devices. Polymer melts are very versatile materials which have been successfully cast into planar single- and multimode waveguides using techniques such as embossing, photolithography and direct laser writing. In this talk, we describe a novel thermocapillary patterning method for fabricating waveguides in which the free surface of an ultrathin molten polymer film is exposed to a spatially inhomogeneous temperature field via thermal conduction from a nearby cooled mask pattern held in close proximity. The ensuring surface temperature distribution is purposely designed to pool liquid selectively into ribbon shapes suitable for optical waveguiding, but with rounded and not rectangular cross sectional areas due to capillary forces. The solidified waveguide patterns which result from this non-contact one step procedure exhibit ultrasmooth interfaces suitable for demanding optoelectronic applications. To complement these studies, we have also conducted finite element simulations for quantifying the influence of non-rectangular cross-sectional shapes on mode propagation and losses.

<sup>1</sup>KF gratefully acknowledges support from a NASA Space Technology Research Fellowship.

**4:42PM P37.00012 Relaxations of star-shaped polystyrene melts approaching the colloidal limit**, KYLE JOHNSON, University of Michigan, EMMANOUIL GLYNOS, Foundation for Research and Technology-Hellas, GEORGIOS SAKELLARIOU, University of Athens, PETER GREEN, University of Michigan — The dynamics of star-shaped polystyrene melts with functionalities ranging from  $8 < f < 64$  and arm molecular weights ranging from 9 kg/mol  $< M < 80$  kg/mol were investigated using small amplitude oscillatory shear measurements. The frequency dependent storage,  $G'$ , and loss,  $G''$ , moduli were measured in the linear viscoelastic regime in order to characterize the terminal relaxation behavior of the macromolecules. Our studies reveal gradual, low-frequency deviations away from the Milner-McLeish theory for arm retraction indicating more elastic behavior as functionality is increased. The magnitudes of these deviations diminish with increasing arm molecular weight. These elastic deviations are consistent with the emergence of a relaxation representing cooperative structural rearrangements and colloidal behavior. Our results indicate that changes in the size of the core region for low molecular weight arms leads to a transition in the dynamics from an arm retraction mechanism to a cooperative, structural relaxation mechanism.

**4:54PM P37.00013 The origin of star-shaped oscillations of Leidenfrost drops**, XIAOLEI MA, JUSTIN C. BURTON, Department of Physics, Emory University — We experimentally investigate the oscillations of Leidenfrost drops of water, liquid nitrogen, ethanol, methanol, acetone and isopropyl alcohol. The drops levitate on a cushion of evaporated vapor over a hot, curved surface which keeps the drops stationary. We observe star-shaped modes along the periphery of the drop, with mode numbers  $n = 2$  to 13. The number of observed modes is sensitive to the properties of the liquid. The pressure oscillation frequency in the vapor layer under the drop is approximately twice that of the drop frequency, which is consistent with a parametric forcing mechanism [1]. However, the Rayleigh and thermal Marangoni numbers are of order 10,000, indicating that convection should play a dominating role as well. Surprisingly, we find that the wavelength and frequency of the oscillations only depend on the thickness of the liquid, which is twice the capillary length, and do not depend on the mode number, substrate temperature, or the substrate curvature. This robust behavior suggests that the wavelength for the oscillations is set by thermal convection inside the drop, and is less dependent on the flow in the vapor layer under the drop. [1] P. Brunet and J. H. Snoeijer, Eur. Phys. J. Spec. Top. 192, 207 (2011).

**5:06PM P37.00014 The intrinsic structure of liquid interfaces<sup>1</sup>**, MARCELLO SEGA, University of Vienna, Austria, PAL JEDLOVSKY, Department of Chemistry, EKF, Eger, Hungary, BALAZS FABIÁN, Institut UTINAM, Université de Franche-Comté, Besançon, France, GEORGE HORVAI, Budapest University of Technology and Economics, Budapest, Hungary — Thermal capillary waves develop spontaneously at fluid/fluid interfaces, and modulate their shapes on scales much larger than the molecular one, thus smearing any density profile measured or calculated using only a global coordinate system<sup>2</sup>. In this contribution we present a local picture of several thermodynamic quantities (density, energy, free energy, surface tension) at liquid/vapour interfaces, analyzing them both on a molecular layer-by-layer basis<sup>3</sup>, and as a function of the intrinsic distance from the interface<sup>4</sup>, revealing their true, intrinsic structure.

<sup>1</sup>ETN-COLLDENSE (H2020-MCSA-ITN-2014, Grant No. 642774)

<sup>2</sup>E. Chacon and P. Tarazona, Phys. Rev. Lett. 91, 166103 (2003)

<sup>3</sup>M. Segá, B. Fabian and P. Jedlovsky, J. Chem. Phys. 143, 114709 (2015)

<sup>4</sup>L. B. Partay, G. Hantal, P. Jedlovsky, A. Vincze, and G. Horvai, J. Comput. Chem. 29, 945 (2008).

**5:18PM P37.00015 Out of equilibrium GigaPa Young modulus of water nanobridge probed by Force Feedback Microscopy**, SIMON CARPENTIER, CNRS, Inst NEEL, F-38042 Grenoble, France, MARIO S. RODRIGUES, MIGUEL VITORINO, University of Lisboa, Faculty of Sciences, BioISI-Biosystems & Integrative Sciences Institute, Campo Grande, Lisboa, P-1749-016, Portugal, LUCA COSTA, ESRF, The European Synchrotron, 71 Rue des Martyrs, 38000 Grenoble, France, ELISABETH CHARLAIX, CNRS, LIPhy, Grenoble, F-38402, France, JOEL CHEVRIER, CNRS, Inst NEEL, F-38042 Grenoble, France — Because of capillary condensation, water droplets appear in nano/micropores. We report that dynamical properties of such nanobridge dramatically change when probed at different time scales [1]. Using a Force Feedback Microscope [2], the gap between the nano-tip and the surface is continuously varied, and we observe this change in the simultaneous measurements, at different frequencies, of the stiffness  $G'$  (N/m), the dissipative coefficient  $G''$  (kg/sec) together with the static force. This is made possible thanks to feedback force which cancels in real time the force acting on the tip. It avoids the mechanical instabilities due to the nucleation of the nanobridge. As the measuring time approaches the microsecond, the liquid droplet exhibits a large positive stiffness (it is small and negative in the long time limit). Although clearly controlled by surface effects, it compares to the stiffness of a solid nanobridge with a 1 GigaPa Young modulus. [1] Carpentier et al. arXiv preprint arXiv:1503.06756, 2015. [2] Rodrigues et al. Applied Physics Letters, 101(20):203105, 2012.

## Wednesday, March 16, 2016 2:30PM - 5:30PM –

Session P38 DPOLY GSOFT: Glasses Altered by Interfaces II 341 - Mesfin Tsige, University of Akron

**2:30PM P38.00001 In Situ Analysis of the Glass Transition Temperature of Irreversibly Adsorbed Polymer Nanolayers**, MARY BURROUGHS, RODNEY PRIESTLEY, Department of Chemical and Biological Engineering, Princeton University — When a polymer thin film is adsorbed in the melt state, individual chains can strongly adsorb to the supporting substrate in a manner that appears to be irreversible. This irreversible adsorption of polymer chains results from the large number of individual contacts made between monomer units and the substrate that stabilize the polymer from desorption. The formation and development of irreversibly adsorbed layers with increased annealing time has been shown to correlate with changes in their structure and dynamic properties and may impact the properties of thin polymer films. Here we investigate the link between deviations in the glass transition temperature ( $T_g$ ) of polymer thin films from the bulk value and the growth of irreversibly adsorbed nanolayers. Through the use of fluorescence spectroscopy, we are able to directly measure  $T_g$  of polystyrene adsorbed nanolayers in an exposed geometry and in situ. The results allow us to examine the influences of interfaces and molecular weight on the  $T_g$  of adsorbed nanolayers throughout their development. By undertaking these studies, critical information is obtained that assists in the design and processing of technologies in which thin polymer films are placed in contact with solid interfaces.

**2:42PM P38.00002 Tailoring Glassy Dynamics on the Nanoscale: Covalent Bonding versus Physical Adsorption in Polymer-based Nanocomposites**, ADAM HOLT, Univ of Tennessee, Knoxville, VERA BOCHAROVA, SHIWANG CHENG, Chemical Science Division, Oak Ridge National Laboratory, ALEXANDER KISLIUK, ADAM IMEL, THUSITHIA ETAMPAWALA, Univ of Tennessee, Knoxville, TYLER WHITE, TOMONORI SAITO, Chemical Science Division, Oak Ridge National Laboratory, NICOLE SIKES, Columbus State University, MARK DADMUN, ALEXEI SOKOLOV, Univ of Tennessee, Knoxville — Polymer grafted nanoparticles (PGNs) offer improved miscibility, stability, and most importantly dispersibility in a polymer matrix over traditional nanoparticle fillers. However, despite the large interest in the miscibility and dispersibility of PGNs within polymer melts, few attempts have been made to study the material properties of solvent-free PGNs and specifically how they compare to traditional polymer nanocomposites (PNCs). In this experiment, the structure and dynamical properties of PGNs of three different molecular weights with identical grafting densities are directly compared to PNCs with similar polymer volume fraction. We find that the segmental dynamics in the interfacial layer are more strongly influenced by the covalent bonding than in the composite system (chain adsorption) and ascribe this to highly stretched chain conformations near the interface, similar to a polymer brush. These results show that the chain conformations in a polymer melt near an interface, especially on the nanoscale, can strongly influence segmental dynamics and offers an explanation to many of the disputed results in the polymer nanocomposite literature.

**2:54PM P38.00003 Polymer Dynamics Effects on Solute Transport in Hairy Nanoparticle Membranes<sup>1</sup>**, EILEEN BUENNING, CONNOR BILCHAK, CHRISTOPHER DURNING, Columbia University, BRIAN BENICEWICZ, University of South Carolina, ALEXEI SOKOLOV, University of Tennessee/Oak Ridge National Laboratory, SANAT KUMAR, Columbia University — Molecular transport measurements in matrix-free grafted nanoparticle (MFGNP) films have shown remarkable enhancement of permeability and ideal selectivity of small condensable molecules and simple gases over the neat polymer melts and conventional, dispersed nanoparticle composites. Films comprised of covalently-attached poly(methyl acrylate) PMA chains to the surface of 14nm silica particles self-assemble into ordered arrays, and we postulate this structure plays an important role in regulating solute transport. This self-assembly creates interstitial spaces between the nanoparticle cores, which the polymer chains can only fill by stretching. Here we use small-angle neutron scattering (SANS), broadband dielectric spectroscopy (BDS), rheology and temperature-modulated differential scanning calorimetry (TMDSC) to probe polymer chain and segmental dynamics and investigate this hypothesis of chain stretching in MFGNP materials. We found that grafting slows both chain and segmental relaxation, and increases fragility, indicating that the chains are more “frustrated” in the grafted systems. We propose that the effects of the chain/surface interactions on chain dynamics leads to an increase in available free volume and thus enhances transport properties in MFGNP systems.

<sup>1</sup>Special thanks to the NSF GRFP and the DOE SCGSR programs

**3:06PM P38.00004 Effect of Molecular Architecture on Polymer Melt Surface Dynamics**, MARK FOSTER, The University of Akron Dept. of Polymer Science — The dynamics of the thermally stimulated surface height fluctuations in a polymer melt dictate wetting, adhesion, and tribology at that surface. These surface fluctuations can be profoundly altered by tethering of the chains. One type of tethering is the tethering of one part of a molecule to another part of the same molecule. This tethering is found in both long chain branched polymers and in macrocycles. We have studied the surface fluctuations with X-ray Photon Correlation Spectroscopy for melts of well-defined, anionically polymerized polystyrenes of various architectures, including linear, 6 arm star, pom-pom, comb and cyclic architectures. For linear chains, the variation of surface relaxation time with in-plane scattering vector can be fit using a hydrodynamic continuum theory (HCT) of thermally stimulated capillary waves that knows nothing of the chain architecture. Assuming the theory is applicable, apparent viscosities of the films may then be inferred from the XPCS data. For unentangled linear chains, the viscosity inferred from XPCS data in this manner is the same as that measured by conventional bulk rheometry. The HCT does a reasonable job of describing the variation of relaxation time with scattering vector for long branched chains also, but only if a viscosity much larger than that of the bulk is assumed. The discrepancy between the viscosity inferred from surface relaxation times using the HCT and that derived from conventional rheometry grows larger as the bulk  $T_g$  is approached and is different for each long chain branched architecture. However, for densely branched combs and cyclic chains different behaviors are found. Acknowledgement: Thanks to NSF (CBET 0730692) and the Advanced Photon Source, supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Science, under contract No. W-31-109-ENG-38.

**3:42PM P38.00005 Relaxation processes and glass transition in confined 1,4-polybutadiene films: A Molecular Dynamics study**, WOLFGANG PAUL, Martin-Luther-University, 55099 Halle, MATHIEU SOLAR, INSA, Strasbourg, France — We will present results from Molecular Dynamics simulations of a chemically realistic model of 1,4-polybutadiene (PB) chains confined by graphite walls. Relaxation processes in this system are heterogeneous and anisotropic. We will present evidence for a slow additional relaxation process related to chain desorption from the walls. We also study the structural relaxation resolved with respect to the distance from the graphite walls and show the influence of structural changes on the relaxation behavior. The temperature dependence of the dielectric relaxation in layers of different thickness near the walls shows no indication of a shift of  $T_g$  as a function of thickness when analyzed with a Vogel-Fulcher fit. We explain this by the importance of intramolecular dihedral barriers for the glass transition in PB which dominate over the density changes next to a wall except for a 1 nm thick layer directly at the wall.

**3:54PM P38.00006 Unusual Molecular Weight Dependence to the Physical Aging of Thin Polystyrene Films**, MICHAEL THEES, CONNIE ROTH, Emory University — Physical aging and the glass transition are intimately related, with the physical aging rate providing a measure of the stability of the glassy state formed. Previously, we have investigated the physical aging rate in thin supported polystyrene (PS) films finding that the local aging rate is correlated with the local glass transition temperature [Pye et al., *Macromolecules* 43, 8296 (2010)]. These studies were able to provide a measure of the depth to which bulk glassy dynamics are perturbed by the free surface interface, a distance much further than similar measures of liquid-like dynamics. Here, we present physical aging measurements of thin PS films using ellipsometry. Surprisingly, we observe a distinctive molecular weight dependence to the physical aging behavior of thin (30 nm thick) films not present in bulk (1000 nm thick) films for very high molecular weights ( $M_w > 3000$  kg/mol). These results indicate that chain connectivity plays a subtle, but important role in how gradients of glassy dynamics are propagated between the free surface and substrate interfaces

**4:06PM P38.00007 Effects of molecular weight and tacticity on the  $T_g$  of poly(methyl methacrylate) films supported by silica<sup>1</sup>**, KUN GENG, FEI CHEN, OPHELIA TSUI, Boston University Physics Department — The glass transition temperature ( $T_g$ ) of poly(methyl methacrylate) (PMMA) films supported by silica is studied as a function of film thickness at different molecular weights ( $M_w$ ) for different polymer tacticities. The  $T_g$  confinement effect is found to depend on the  $M_w$  and tacticity. For the films with a low  $M_w$  of 2.5 kg/mol,  $T_g$  is depressed for the atactic films, consistent with previous results. In contrast, the films with a higher syndiotactic content exhibit  $T_g$  enlargement as thickness decreases. We tentatively suggest this to be caused by the influence of chain stiffness on the  $T_g$  that dominates at low  $M_w$  and varies with tacticity. For sufficiently high  $M_w$ , the effect of chain stiffness is expected to be small. At  $M_w = 50$  kg/mol, the  $T_g$  confinement effect of the atactic and more syndiotactic films reverses from that observed of the low- $M_w$  counterpart films. We suggest the chain stiffness effect to be negligible at this  $M_w$ , and attribute the opposite  $T_g$  confinement effect to be caused by a competition between the surface  $T_g$  and the substrate  $T_g$  in these films. The  $T_g$  found of bilayers made of the atactic and more syndiotactic PMMAs with this  $M_w$  supports our attribute.

<sup>1</sup>We are grateful to the support of NSF through the project DMR-1310536.

**4:18PM P38.00008 Chain conformation near the substrate interface in nanoparticle stabilized polymer thin films<sup>1</sup>**, DEBORAH BARKLEY, MANI SEN, NAISHENG JIANG, MAYA ENDOH, TADANORI KOGA, Stony Brook University, GUANGCUI YUAN, SUSHIL SATIJA, Center for Neutron Research, NIST, YUGANG ZHANG, OLEG GANG, Brookhaven National Lab, ALAMGIR KARIM, University of Akron — When nanoparticles (NPs) are added to polymer thin films, they often migrate to the film-substrate interface and form a “diffused immobile interfacial layer”, which serves to screen the polymer-substrate interaction and suppress dewetting. The fundamental, but unsolved question is how the conformations of the polymer chains in the layer are affected by the NPs and how that impacts the enhancement of film stability. To address the question, we used dodecane thiol-functionalized gold NPs (2.4 nm diameter) and polystyrene (PS,  $M_w=30$ kDa). We found that the critical concentration of the Au NPs to induce complete dewetting suppression of 20 nm-thick PS/Au thin films on cleaned Si substrates is 5 wt% (wt of particle/wt of polymer). To investigate the interfacial structures at the polymer-solid interface, we rinsed the annealed PS/Au thin films with toluene and characterized the residual interfacial layers by using various x-ray and neutron scattering techniques. The results indicate that the conformation of the polymer chains closer to the substrate becomes less flattened with the addition of gold NPs, allowing chains at the substrate to entangle more effectively with free chains comprising the bulk film. The detailed mechanism will be discussed.

<sup>1</sup>T.K. acknowledges funding from NSF Grant (CMMI-1332499)

**4:30PM P38.00009 The Effect of Acid-Base Interactions on Conformation of Adsorbed Polymer Chains**, NISHAD DHOPATKAR, HE ZHU, Graduate Student, ALI DHINOJWALA, Professor — Adsorption of polymer chains from solutions is of fundamental interest in polymer science. This adsorption process is governed by the complex interplay between the solvent-polymer, polymer-substrate, and solvent-substrate interaction energies. In early 1970's, Fowkes and his coworkers have introduced the concept of acid base interactions in explaining why PMMA (basic) adsorption was extremely low on acidic substrates from acidic solvents. The acidic solvent molecules compete with the surface for binding with the basic polymer sites and this reduces the adsorption of PMMA. Here, by using interface-selective sum frequency generation spectroscopy (SFG) and attenuated-total-reflectance (ATR)-FTIR spectroscopy we directly measure whether the solvent or polymer molecules interact with the substrate in acidic, basic, and neutral solvents. Surprisingly, we find that the surface acidic site (hydroxyl) groups are still covered with PMMA chains in acidic solvent. The PMMA chains in acidic solvent adsorb with much higher fraction of chains as trains in comparison to loops and tails. Such differences in the static and dynamic conformations have consequences in understanding the exchange kinetics, colloidal stabilization, chromatographic separations, adhesion and friction, and stabilization of nanocomposites.

**4:42PM P38.00010 Surfactants at Single-Walled Carbon Nanotube-Water Interface: Physics of Surfactants, Counter-Ions, and Hydration Shell**<sup>1</sup>, KETAN S. KHARE, MSED, NIST, Gaithersburg, MD 20899 and Physics, Georgetown Univ., DC 20057, FREDERICK R. PHELAN JR., MSED, NIST, Gaithersburg, MD 20899 — Specialized applications of single-walled carbon nanotubes (SWCNTs) require an efficient and reliable method to sort these materials into monodisperse fractions with respect to their defining metrics (chirality, length, etc.) while retaining their physical and chemical integrity. A popular method to achieve this goal is to use surfactants that individually disperse SWCNTs in water and then to separate the resulting colloidal mixture into fractions that are enriched in monodisperse SWCNTs. Recently, experiments at NIST have shown that subtle point mutations of chemical groups in bile salt surfactants have a large impact on the hydrodynamic properties of SWCNT-surfactant complexes during ultracentrifugation. These results provide strong motivation for understanding the rich physics underlying the assembly of surfactants around SWCNTs, the structure and dynamics of counter ions around the resulting complex, and propagation of these effects into the first hydration shell. Here, all-atom molecular dynamics simulations are used to investigate the thermodynamics of SWCNT-bile salt surfactant complexes in water with an emphasis on the buoyant characteristics of the SWCNT-surfactant complexes. Simulation results will be presented along with a comparison with experimental data.

<sup>1</sup>Official contribution of the National Institute of Standards and Technology; not subject to copyright in the United States.

**4:54PM P38.00011 Polyethylene oxide hydration in grafted layers.**<sup>1</sup>, ELENA DORMIDONTOVA, ZILU WANG, Physics Department and Institute of Materials Science, University of Connecticut, Storrs, CT — Hydration of water soluble polymers is one of the key-factors defining their conformation and properties, similar to biopolymers. Polyethylene oxide (PEO) is one of the most important biomedical-applications polymers and is known for its reverse temperature solubility due to hydrogen bonding with water. As in many practical applications PEO chains are grafted to surfaces, e.g. of nanoparticles or planar surfaces, it is important to understand PEO hydration in such grafted layers. Using atomistic molecular dynamic simulations we investigate the details of molecular conformation and hydration of PEO end-grafted to gold surfaces. We analyze polymer and water density distribution as a function of distance from the surface for different grafting densities. Based on a detailed analysis of hydrogen bonding between polymer and water in grafted PEO layers, we will discuss the extent of PEO hydration and its implication for polymer conformation, mobility and layer properties.

<sup>1</sup>This research is supported by NSF (DMR-1410928)

**5:06PM P38.00012 The Unusual Conformational Behavior of Polyzwitterionic Brushes in Aqueous Solutions**, JUN MAO, Univ of Chicago, WEI CHEN, Argonne National Laboratory, GUANGCUI YUAN, NIST Center for Neutron Research, National Institute of Standards and Technology, JING YU, Argonne National Laboratory, MATTHEW TIRRELL, Univ of Chicago — Polyzwitterions constitute a peculiar class of polyelectrolytes, which are electrically neutral polymers containing both a positive and a negative charge on each repeating unit. Surfaces coated with polyzwitterionic brushes are resistant to the nonspecific accumulation of proteins and microorganisms, making them excellent candidates for a wide range of antifouling applications, from biocompatible medical devices to marine coatings. The surrounding environment can dramatically influence the conformational behavior of polyzwitterionic brushes. High-density polyzwitterionic brushes poly(2-methacryloyloxyethyl phosphorylcholine) (PMPC) were synthesized using surface initiated atom-transfer radical polymerization, and neutron reflectivity (NR) measurements were performed to investigate the ionic strength dependence of the conformational behaviors of PMPC brushes in monovalent salt solutions. Despite the numerous observations of normal pure polyelectrolyte brushes, NR results showed that both the densely concentrated layer near the substrate surface and the relatively swollen layer into the solution have been observed in different  $q$  range in a single neutron reflectivity profile. These results will definitely help us to better understand the relationship between the solution behaviors of zwitterionic polymer brushes and their antifouling properties.

**5:18PM P38.00013 Homopolymer Adsorption on Hexagonal Surfaces: A Replica-Exchange Monte Carlo Study**, BENJAMIN LIEWEHR, MICHAEL BACHMANN, The University of Georgia — The adsorption behavior and thermodynamic properties of a coarse-grained flexible homopolymer, grafted on a hexagonal patterned surface, are investigated by means of parallel-tempering replica-exchange Monte Carlo simulations. In this study, the strength of the polymer-surface interaction, which is based on a standard Lennard-Jones potential, is changed systematically, mimicking different hexagonally patterned substrate materials. Specific order parameters are introduced to discriminate structural phases, at different surface adsorptions strengths and temperatures, into classes of expanded, globular, droplet, and compact conformations. Finally, we provide a complete structural hyperphase diagram for a polymer with 55 monomers and discuss representative polymer structures.

**Wednesday, March 16, 2016 2:30PM - 5:18PM –**

**Session P39 DBIO GSNP: Information Processing in Cellular Signaling and Gene Regulation**

342 - Andrew J. Mugler, Purdue University

**2:30PM P39.00001 Towards a predictive theory for genetic regulatory networks**, GASPER TKACIK, IST Austria — When cells respond to changes in the environment by regulating the expression levels of their genes, we often draw parallels between these biological processes and engineered information processing systems. One can go beyond this qualitative analogy, however, by analyzing information transmission in biochemical “hardware” using Shannon’s information theory. Here, gene regulation is viewed as a transmission channel operating under restrictive constraints set by the resource costs and intracellular noise. We present a series of results demonstrating that a theory of information transmission in genetic regulatory circuits feasibly yields non-trivial, testable predictions. These predictions concern strategies by which individual gene regulatory elements, e.g., promoters or enhancers, read out their signals; as well as strategies by which small networks of genes, independently or in spatially coupled settings, respond to their inputs. These predictions can be quantitatively compared to the known regulatory networks and their function, and can elucidate how reproducible biological processes, such as embryonic development, can be orchestrated by networks built out of noisy components. Preliminary successes in the gap gene network of the fruit fly *Drosophila* indicate that a full ab initio theoretical prediction of a regulatory network is possible, a feat that has not yet been achieved for any real regulatory network. We end by describing open challenges on the path towards such a prediction.

### 3:06PM P39.00002 Theory of optimal information transmission in E. coli chemotaxis pathway

, GABRIELE MICALI, ROBERT G. ENDRES, Imperial College London — Bacteria live in complex microenvironments where they need to make critical decisions fast and reliably. These decisions are inherently affected by noise at all levels of the signaling pathway, and cells are often modeled as an input-output device that transmits extracellular stimuli (input) to internal proteins (channel), which determine the final behavior (output). Increasing the amount of transmitted information between input and output allows cells to better infer extracellular stimuli and respond accordingly. However, in contrast to electronic devices, the separation into input, channel, and output is not always clear in biological systems. Output might feed back into the input, and the channel, made by proteins, normally interacts with the input. Furthermore, a biological channel is affected by mutations and can change under evolutionary pressure. Here, we present a novel approach to maximize information transmission: given cell-external and internal noise, we analytically identify both input distributions and input-output relations that optimally transmit information. Using E. coli chemotaxis as an example, we conclude that its pathway is compatible with an optimal information transmission device despite the ultrasensitive rotary motors.

### 3:18PM P39.00003 BMP4 density gradient in disk-shaped confinement

, BEHNAZ BOZORGUI, HAMID TEIMOURI, ANATOLY B. KOLOMEISKY, Rice University — We present a quantitative model that explains the scaling of BMP4 gradients during gastrulation and the recent experimental observation that geometric confinement of human embryonic stem cells is sufficient to recapitulate much of germ layer patterning. Based on a assumption that BMP4 diffusion rate is much smaller than the diffusion rate of its inhibitor molecules, our results confirm that the length-scale which defines germ layer territories does not depend on system size.

### 3:30PM P39.00004 Mechanical Feedback and Arrest in Gene Expression

, STUART SEVIER, HERBERT LEVINE, Rice Univ — The ability to watch biochemical events at the single-molecule level has increasingly revealed that stochasticity plays a leading role in many biological phenomena. One important and well known example is the noisy, “bursty” manner of transcription. Recent experiments have revealed relationships between the level and noise in gene expression hinting at deeper stochastic connections. In this talk we will discuss how the mechanical nature of transcription can explain this relationship and examine the limits that the physical aspects of transcription place on gene expression.

### 3:42PM P39.00005 Information processing in multi-step signaling pathways

, AMBHI GANESAN, IBM, ARCHER HAMIDZADEH, Yale University, JIN ZHANG, UCSD, ANDRE LEVCHENKO, Yale University — Information processing in complex signaling networks is limited by a high degree of variability in the abundance and activity of biochemical reactions (biological noise) operating in living cells. In this context, it is particularly surprising that many signaling pathways found in eukaryotic cells are composed of long chains of biochemical reactions, which are expected to be subject to accumulating noise and delayed signal processing. Here, we challenge the notion that signaling pathways are insulated chains, and rather view them as parts of extensively branched networks, which can benefit from a low degree of interference between signaling components. We further establish conditions under which this pathway organization would limit noise accumulation, and provide evidence for this type of signal processing in an experimental model of a calcium-activated MAPK cascade. These results address the long-standing problem of diverse organization and structure of signaling networks in live cells.

### 3:54PM P39.00006 Towards Predictive Modeling of Information Processing in Microbial Ecosystems With Quorum-Sensing Interactions

, TAHIR YUSUFALY, JAMES BOEDICKER, University of Southern California — Bacteria communicate using external chemical signals in a process known as quorum sensing. However, the efficiency of this communication is reduced by both limitations on the rate of diffusion over long distances and potential interference from neighboring strains. Therefore, having a framework to quantitatively predict how spatial structure and biodiversity shape information processing in bacterial colonies is important, both for understanding the evolutionary dynamics of natural microbial ecosystems, and for the rational design of synthetic ecosystems with desired computational properties. As a first step towards these goals, we implement a reaction-diffusion model to study the dynamics of a LuxI/LuxR quorum sensing circuit in a growing bacterial population. The spatiotemporal concentration profile of acyl-homoserine lactone (AHL) signaling molecules is analyzed, and used to define a measure of physical and functional signaling network connectivity. From this, we systematically investigate how different initial distributions of bacterial populations influence the subsequent efficiency of collective long-range signal propagation in the population. We compare our results with known experimental data, and discuss limitations and extensions to our modeling framework.—/abstract—

### 4:06PM P39.00007 Thermodynamics of nuclear transport<sup>1</sup>

, CHING-HAO WANG, PANKAJ MEHTA, Department of Physics, Boston University, Boston, MA 02215, MICHAEL ELBAUM, Department of Materials and Interfaces, Weizmann Institute of Science, Rehovot, Israel — Molecular transport across the nuclear envelope is important for eukaryotes for gene expression and signaling. Experimental studies have revealed that nuclear transport is inherently a nonequilibrium process and actively consumes energy. In this work we present a thermodynamics theory of nuclear transport for a major class of nuclear transporters that are mediated by the small GTPase Ran. We identify the molecular elements responsible for powering nuclear transport, which we term the “Ran battery” and find that the efficiency of transport, measured by the cargo nuclear localization ratio, is limited by competition between cargo molecules and RanGTP to bind transport receptors, as well as the amount of NTF2 (i.e. RanGDP carrier) available to circulate the energy flow. This picture complements our current understanding of nuclear transport by providing a comprehensive thermodynamics framework to decipher the underlying biochemical machinery.

<sup>1</sup>PM and CHW were supported by a Simons Investigator in the Mathematical Modeling in Living Systems grant (to PM).

### 4:18PM P39.00008 Vector Encoding in Biochemical Networks

, GARRETT POTTER, BO SUN, Oregon State University — Encoding of environmental cues via biochemical signaling pathways is of vital importance in the transmission of information for cells in a network. The current literature assumes a single cell state is used to encode information, however, recent research suggests the optimal strategy utilizes a vector of cell states sampled at various time points. To elucidate the optimal sampling strategy for vector encoding, we take an information theoretic approach and determine the mutual information of the calcium signaling dynamics obtained from fibroblast cells perturbed with different concentrations of ATP. Specifically, we analyze the sampling strategies under the cases of fixed and non-fixed vector dimension as well as the efficiency of these strategies. Our results show that sampling with greater frequency is optimal in the case of non-fixed vector dimension but that, in general, a lower sampling frequency is best from both a fixed vector dimension and efficiency standpoint. Further, we find the use of a simple modified Ornstein-Uhlenbeck process as a model qualitatively captures many of our experimental results suggesting that sampling in biochemical networks is based on a few basic components.

### 4:30PM P39.00009 Deciphering the Minimal Algorithm for Development and Information-

genesis. , ZHIYUAN LI, Princeton Center for Theoretical Science, Princeton University, CHAO TANG, Center for Quantitative Biology, Peking University, HAO LI, Dept. of Biochemistry and Biophysics and California Institute for Quantitative Biosciences, University of California, San Francisco — During development, cells with identical genomes acquire different fates in a highly organized manner. In order to decipher the principles underlying development, we used C.elegans as the model organism. Based on a large set of microscopy imaging, we first constructed a “standard worm” in silico: from the single zygotic cell to about 500 cell stage, the lineage, position, cell-cell contact and gene expression dynamics are quantified for each cell in order to investigate principles underlying these intensive data. Next, we reverse-engineered the possible gene-gene/cell-cell interaction rules that are capable of running a dynamic model recapitulating the early fate decisions during C.elegans development. We further formulated the C.elegans embryogenesis in the language of information genesis. Analysis towards data and model uncovered the global landscape of development in the cell fate space, suggested possible gene regulatory architectures and cell signaling processes, revealed diversity and robustness as the essential trade-offs in development, and demonstrated general strategies in building multicellular organisms.

**4:42PM P39.00010 Reliable Signal Transduction** , ROY WOLLMAN, Dept of Chemistry and Biochemistry, University of California, San Diego — Stochasticity inherent to biochemical reactions (intrinsic noise) and variability in cellular states (extrinsic noise) degrade information transmitted through signaling networks. We analyzed the ability of temporal signal modulation - that is dynamics - to reduce noise-induced information loss. In the extracellular signal-regulated kinase (ERK), calcium ( $\text{Ca}^{2+}$ ), and nuclear factor kappa-B ( $\text{NF-}\kappa\text{B}$ ) pathways, response dynamics resulted in significantly greater information transmission capacities compared to nondynamic responses. Theoretical analysis demonstrated that signaling dynamics has a key role in overcoming extrinsic noise. Experimental measurements of information transmission in the ERK network under varying signal-to-noise levels confirmed our predictions and showed that signaling dynamics mitigate, and can potentially eliminate, extrinsic noise-induced information loss. By curbing the information-degrading effects of cell-to-cell variability, dynamic responses substantially increase the accuracy of biochemical signaling networks.

## Wednesday, March 16, 2016 2:30PM - 5:30PM –

**Session P40 GSNP GSOF: More Geometry and Dynamics: Wrinkling, Folding, Snapping, etc.**

343 - Dominic Vella, Oxford University

**2:30PM P40.00001 Rolling Wrinkles on Elastic Substrates** , MICHAEL IMBURGIA, ALFRED CROSBY, Univ of Mass - Amherst — The mechanics of rolling contact between an elastomer layer and a thin film present unique opportunities for taking advantage of elastic instabilities, such as surface wrinkling, to create patterned surfaces. Here we present a plate-to-roll (P2R) geometry to laminate a thin film onto an elastomer layer in order to induce surface wrinkling. First, a poly(dimethylsiloxane) (PDMS) layer is draped around a roller and pressed into contact with a poly(styrene) (PS) film supported on a plate. Once rolling begins, the PS film preferentially laminates onto the PDMS layer. During this process, the deformation of the PDMS layer can induce wrinkling when the contact load exceeds a critical value. Wrinkle feature size consists of amplitudes of  $0.2 - 4\mu\text{m}$  and wavelengths of  $15 - 20\mu\text{m}$ . Wrinkle amplitude can be controlled by contact load and roller curvature, as well as the mechanical properties and thickness of the film and elastomer. We develop semi-empirical equations to describe the effect of contact load and roller curvature on the wrinkle aspect ratio. Finite-element modeling of an elastomer layer in rolling contact with a rigid plate is used to support experimental results. Using these models, wrinkle-based technologies such as optoelectronics and enhanced adhesives can be envisioned.

**2:42PM P40.00002 Slow frictional waves** , Koushik Viswanathan, Purdue University, Narayan Sundaram, Indian Institute of Science, Srinivasan Chandrasekar, Purdue University — Stick-slip, manifest as intermittent tangential motion between two dry solid surfaces, is a friction instability that governs diverse phenomena from automobile brake squeals to earthquakes. We show, using high-speed in situ imaging of an adhesive polymer interface, that low velocity stick-slip is fundamentally of three kinds, corresponding to passage of three different surface waves — separation pulses, slip pulses and the well-known Schallamach waves. These waves, traveling much slower than elastic waves, have clear distinguishing properties. Separation pulses and Schallamach waves involve local interface separation, and propagate in opposite directions while slip pulses are characterized by a sharp stress front and do not display any interface detachment. A change in the stick-slip mode from separation to slip pulse is effected simply by increasing the normal force. Together, these three waves constitute all possible stick-slip modes in adhesive friction and are shown to have direct analogues in muscular locomotory waves in soft bodied invertebrates. A theory for slow wave propagation is also presented which is capable of explaining the attendant interface displacements, velocities and stresses.

**2:54PM P40.00003 Poking around: how indentation reveals wrinkly isometries** , DOMINIC VELLA, University of Oxford, Hamid Ebrahimi, Northeastern University , Joseph Paulsen, Syracuse University, Ashkan Vaziri, Northeastern University, Narayanan Menon, Benny Davidovitch, UMass Amherst — When deforming extremely thin objects, deformation via stretching is relatively expensive. It is therefore natural to seek deformations that preserve lengths, or isometries. Two common examples of such isometries in mechanics are the 'd'-cone (for a plate) and 'mirror buckling' (for a shell). I will show two examples for which the presence of a weak tension means that these isometries are not obtained experimentally. Instead, the systems in question wrinkle and tend to new 'wrinkly isometries': isometries that are only available to a wrinkled object.

**3:06PM P40.00004 Curvature-induced stiffness and the spatial variation of wavelength in wrinkled sheets** , Narayanan Menon, JD Paulsen, Evan Hoffeld, Hunter King, Jiangshui Huang, Thomas Russell, Zhanlong Qiu, Benny Davidovitch, U of Massachusetts, Amherst, Dominic Vella, Mathematical Institute, Oxford University — Natural wrinkle patterns often inhabit surfaces of curved substrates, and typically are spatially nonuniform. However, the unified understanding of wrinkle wavelength [1] in terms of a competition between the bending energy of a sheet and the stiffness provided by the tension or potential energy of the supporting substrate, applies only to nearly-planar, parallel, and spatially uniform wrinkle patterns. We describe theory and experiment that extend this understanding in two major directions. The first is to show that the underlying curvature may be treated as a distinct term in the substrate stiffness. The second is to demonstrate in two very different settings that the local value of the wavelength is determined by the local stiffness of the subphase. Both results are encapsulated in a simple, local law for the wavelength that has greatly expanded applicability. We acknowledge support from the WM Keck Foundation 1. Cerda, E., & Mahadevan, L. (2003). *Physical review letters*, 90, 074302.

**3:18PM P40.00005 Geometry-driven folding transitions in floating thin films** , Joseph D. Paulsen, Syracuse University, Vincent Démery, PCT-ESPCI, France, K. Bugra Toga, Eastman Chemical Company, Zhanlong Qiu, Benny Davidovitch, Thomas P. Russell, Narayanan Menon, Univ of Mass - Amherst — When a thin elastic sheet is compressed, it forms wrinkles to gather excess material, while deforming the fluid or solid substrate by only a small amount. Upon further compression, the sheet may fold, in order to lower the mechanical energy of the system<sup>1</sup>. Here we demonstrate a folding transition that is independent of the mechanical properties of the sheet. We study the deformations of a thin polymer film that has an annular shape, floating on a planar air-water interface. By controlling the concentration of a surfactant outside the film, we vary the tension pulling on the outer boundary of the annulus. The sheet spontaneously folds at a threshold ratio of inner to outer surface tension that depends on the geometry of the sheet, but is independent of its bending rigidity. Our results are consistent with a simple geometric principle: the sheet adopts the unstretched shape that minimizes the interfacial energy of the exposed liquid<sup>2</sup>. Finally, we consider the application of this geometric principle to the folding of a floating indented film.

1. Pocivavsek et al., *Science* 320, 912 (2008).
2. Paulsen et al., *Nature Materials*, doi:10.1038/nmat4397 (2015).

**3:30PM P40.00006 Ribbon curling** , Anne Juel, University of Manchester, UK, Chris Prior, University of Durham, UK, Julien Moussou, ENS Paris, France, Buddhapriya Chakrabarti, University of Durham, UK, Oliver Jensen, University of Manchester, UK — The procedure of curling a ribbon by running it over a sharp blade is commonly used when wrapping presents. Despite its ubiquity, a quantitative explanation of this everyday phenomenon is still lacking. We address this using experiment and theory, examining the dependence of ribbon curvature on blade curvature, the longitudinal load imposed on the ribbon and the speed of pulling. Experiments in which a ribbon is drawn steadily over a blade under a fixed load show that the ribbon curvature is generated over a restricted range of loads, the curvature/load relationship can be non-monotonic, and faster pulling (under a constant imposed load) results in less tightly curled ribbons. We develop a theoretical model that captures these features, building on the concept that the ribbon under the imposed deformation undergoes differential plastic stretching across its thickness, resulting in a permanently curved shape. The model identifies factors that optimize curling and clarifies the physical mechanisms underlying the ribbon's nonlinear response to an apparently simple deformation.

**3:42PM P40.00007 Periodic Buckling Patterns On Constrained Elastic Shells.** , JOEL MARTHELOT, ANNA LEE, PIERRE-THOMAS BRUN, FRANCISCO LOPEZ JIMENEZ, PEDRO M. REIS, MIT — Thin spherical shells range from nanometer-sized viruses to space vehicles. A pressure differential between the inner and outer part of the shell can result in the buckling and catastrophic failure of the structure. We revisit this classic buckling problem, depressurizing thin elastic shells, which are arrested from within by a concentric spherical mandrel. As a result, buckling is constrained to occur within the gap between the two. Above a critical pressure, dimples appear sequentially on the surface of the shell to form a robust periodic pattern. We perform precision desktop experiments to construct the bifurcation diagram of the process, and explore a range of geometric and material properties. A scaling analysis enables us to rationalize the dependence of the size of the dimples on both the radius of the shell and the radial gap between the shell and the inner rigid mandrel. Moreover, we characterize the process of nucleation and progression of the dimpled pattern front. Particular emphasis is given to the patterns obtained in the strongly nonlinear post-buckling regime where a network of sharp ridges forms.

**3:54PM P40.00008 Defect-controlled buckling of depressurized elastic shells** , ANNA LEE, JOEL MARTHELOT, FRANCISCO LPEZ JIMNEZ, PIERRE-THOMAS BRUN, PEDRO REIS, Massachusetts Institute of Technology — We revisit the classic problem of buckling of spherical elastic shells under pressure loading, with an emphasis on determining the role that engineered imperfections have on the critical buckling pressure. Since the 1960s numerous theoretical and computational studies have addressed this canonical problem in engineering mechanics, but there is a striking lack of precision experiments to corroborate these predictions. We perform an experimental investigation where thin shells of nearly uniform thickness are fabricated by the coating of hemispherical molds with a polymer solution, which upon curing yields the elastic structure. Moreover, our manufacturing technique allows us to introduce a single dimple-like defect with controllable geometric properties. By systematically varying the amplitude of this defect (smaller than the thickness of the shell) we study the effect that these imperfections have on the buckling strength of our spherical shells. Small deviations from the spherical geometry result in large reductions in the buckling pressure and our experimental results agree well with the existing theories. We then perform a broader exploration for other classes of defects, for which theoretical predictions are yet to be developed.

**4:06PM P40.00009 Stress Localization in Elastic Shells** , SARAH SELDEN, ARTHUR EVANS, NAKUL BENDE, RYAN HAYWARD, CHRISTIAN SANTANGELO, Univ of Mass - Amherst — Upon indentation, thin shells react by localizing strain energy in polygonal structures as opposed to a uniform axisymmetric distribution. While the formation of these localized structures are well-characterized for perfect shells, a change in shell thickness or the introduction of a crease fundamentally changes the nature of the shell deformation. We perform finite element simulations, in tandem with experiments to explore the effect of different shell geometries on the energy landscape. We find that the crease induces a new symmetry-breaking localization that does not appear in perfect shells, and we explore the deformation characteristics of the creased shell over a wide range of crease radii, and crease orientations.

**4:18PM P40.00010 Regularizing rigidifying curves to understand the low-energy deformations of thin shells** , SALEM AL MOSLEH, CHRISTIAN SANTANGELO, Univ of Mass - Amherst, GEOMETRY OF MATERIALS TEAM — It is much harder to stretch a piece of paper than bend it. We exploit this fact to simplify the elastic energy of a thin shell. We accomplish this by extending the linear isometric displacements, displacements that do not cause stretching to lowest order, to low energy Nambu-Goldstone modes. This approach fails in an interesting way in the vicinity of “rigidifying curves,” curves with zero normal curvature, because half of the linear isometries are divergent there. We use a renormalization group methods to show that nonlinearities in the strain regularize these divergences. We explore the relationship between these modes and folding along curves of zero normal curvature.

**4:30PM P40.00011 Hunting for ghosts in elastic snap-through** , MICHAEL GOMEZ, DEREK E. MOULTON, DOMINIC VELLA, Mathematical Institute, University of Oxford — Elastic ‘snap-through’ is a striking instability often seen when an elastic system loses bistability, e.g. due to a change in geometry or external loading. The switch from one state to another is generally rapid and hence is used to generate fast motions in biology and engineering. While the onset of instability has been well studied, the dynamics of the transition itself remain much less well understood. For example, the dynamics exhibited by children’s jumping popper toys, or the leaves of the Venus flytrap plant, are much slower than would be expected based on a naive estimate of the elastic timescales. To explain this discrepancy, the natural conclusion has been drawn that some other effect, such as viscoelasticity, must play a role. We demonstrate here that purely elastic systems may show similar ‘slow’ dynamics during snap-through. This behaviour is due to a remnant (or ‘ghost’) of the snap-through bifurcation underlying the instability, analogously to bottleneck phenomena in 1-D dynamical systems. This slowness is a generic consequence of being close to bifurcation — it does not require dissipation. We obtain scaling laws for the length of the delay and compare these to numerical simulations and experiments on real samples.

**4:42PM P40.00012 One Bend, Two Bend: Stepping Towards a Complex Folded Object.** , ANDREW CROLL, DAMITH ROZAIRO, North Dakota State Univ — Crumpled thin films form a very unique jammed state of matter. They are both lightweight and ridged, suggesting broad industrial relevance. While researchers have theorized over the origins of these properties, very little experimental work has been performed directly collecting both structural and material properties in concert. Without testing the strength and interplay of the basic structures making up the larger object (bends, folds, and d-cones) it is difficult if not impossible to completely trust the origin of various material properties and processes (modulus, aging behaviour). Here we show that laser scanning confocal microscopy can be used to image geometry directly in concert with the recording of traditional macroscopic measurements (e.g. force vs displacement). Specifically, we examine the force/displacement behaviour in systems of 1 to N folds created with well understood polymeric materials.

**4:54PM P40.00013 Wrinkling Instability Induced by Imposed Gaussian Curvature in the Zero-tension Limit<sup>1</sup>** , YIWEI SUN, BENNY DAVIDOVITCH, GREGORY GRASON, Univ of Mass - Amherst — The adhesion of thin stiff films onto spherical substrates introduces compressive stresses, which cause the laminated film to buckle out of plane. Previous studies addressed the emerging wrinkle pattern in the limit of zero bending modulus and the presence of surface tension at the boundary, and found the radius of the inner unwrinkled zone scales with the tension. Here we study another fundamental limit: finite bending modulus and zero exerted tension. In this limit, subtlety will arise from the fact that the singular expansion, which previous studies relied on, becomes ill-defined. To reveal the morphology in the zero-tension limit, we employ numerical simulations based on bead-bond model. Surprisingly, we find that the scaling law for the radius of the unwrinkled zone can be generalized from the finite tension to the zero tension limit, by applying a bending modulus dependent term to the tension dominated scale. The simulation results also highlight the residual compressive hoop stress, which is scaled by bending modulus in the absence of tension. The findings suggest the existence of a new, yet unstudied process, by which the deformed shape of the sheet approaches isometry as the bending modulus vanishes, in the absence of boundary loads.

<sup>1</sup>ACS PRF 54513-ND5

**5:06PM P40.00014 Geometry of Thin Nematic Elastomer Sheets** , HILLEL AHARONI, Univ of Pennsylvania, ERAN SHARON, RAZ KUPFERMAN, Hebrew University of Jerusalem — A thin sheet of nematic elastomer attains 3D configurations depending on the nematic director field upon heating. In this talk we describe the intrinsic geometry of such a sheet, and derive an expression for the metric induced by general smooth nematic director fields. Furthermore, we investigate the reverse problem of constructing a director field that induces a specified 2D geometry. We provide an explicit analytical recipe for constructing any surface of revolution using this method. We demonstrate how the design of an arbitrary 2D geometry is accessible using approximate numerical methods.

**5:18PM P40.00015 Unpredictable Motion and Post-chaotic Self-Organization of Flexible Structures.** , NICHOLAS NECHITAILO, Naval Surface Warfare Center, Dahlgren, Virginia — Two physical phenomena, “reverse buckling” and “post-chaotic self-organization”, were discovered by the author of this paper. The phenomena were analyzed using Newton’s mechanics, Euler bifurcation and buckling theory, and Poincaré’s theory of chaotic motion when “prediction becomes impossible.” However, our experimental and theoretical findings revealed a more complex nonlinear physics with some predictability of final states. Geometric and material nonlinearities in flexible plates, beams and shells lead to transient chaos and unexpected final shapes. In one experiment, an axisymmetric transverse pressure pulse was applied to a circular metal membrane. It buckled, lost axial symmetry and formed a folded six-corner star. In another test, an impulsively stretched rod buckled and obtained a final shape similar to that of a rod under static axial compression. “Reputable” finite element and finite difference codes could not reliably predict deformation of an aluminum beam under a transverse pressure pulse. The anomalous responses were observed in a narrow region of the load amplitude and duration. These were described by simple analytical equations. Similar phenomena were seen in nonlinear equations of motion representing various non-mechanical systems.

**Wednesday, March 16, 2016 2:30PM - 5:30PM –**  
**Session P41 DBIO DPOLY DCOMP: Physics of Proteins: Structure and Dynamics I** 344 - Corey O’Hearn, Yale University

**2:30PM P41.00001 Infrared Structural Biology: Detect Functionally Important Structural Motions of Proteins<sup>1</sup>** , AIHUA XIE, Oklahoma State University — Proteins are dynamic. Lack of dynamic structures of proteins hampers our understanding of protein functions. Infrared structural biology (IRSB) is an emerging technology. There are several advantages of IRSB for mechanistic studies of proteins: (1) its excellent dynamic range (detecting structural motions from picoseconds to  $\geq$  seconds); (2) its high structural sensitivity (detect tiny but functionally important structural motions such as proton transfer and changes in hydrogen bonding interaction); (3) its ability to detect different structural motions simultaneously. Successful development of infrared structural biology demands not only new experimental techniques (from infrared technologies to chemical synthesis and cell biology), but also new data processing (how to translate infrared signals into quantitative structural information of proteins). These topics will be discussed as well as examples of how to use IRSB to study structure-function relationship of proteins.

<sup>1</sup>This work was supported by NSF DBI1338097 and OCAST HR10-078

**3:06PM P41.00002 Quantifying the Energy Landscape Statistics in Proteins - a Relaxation Mode Analysis** , ZHIKUN CAI, YANG ZHANG, Univ of Illinois - Urbana — Energy landscape, the hypersurface in the configurational space, has been a useful concept in describing complex processes that occur over a very long time scale, such as the multistep slow relaxations of supercooled liquids and folding of polypeptide chains into structured proteins. Despite extensive simulation studies, its experimental characterization still remains a challenge. To address this challenge, we developed a relaxation mode analysis (RMA) for liquids under a framework analogous to the normal mode analysis for solids. Using RMA, important statistics of the activation barriers of the energy landscape becomes accessible from experimentally measurable two-point correlation functions, e.g. using quasi-elastic and inelastic scattering experiments. We observed a prominent coarsening effect of the energy landscape. The results were further confirmed by direct sampling of the energy landscape using a metadynamics-like adaptive autonomous basin climbing computation. We first demonstrate RMA in a supercooled liquid when dynamical cooperativity emerges in the landscape-influenced regime. Then we show this framework reveals encouraging energy landscape statistics when applied to proteins.

**3:18PM P41.00003 The Onset of Collective Structural Vibrations at the Protein Dynamical Transition** , MENGYANG XU, KATHERINE A. NIESSEN, YANTING DENG, NIGEL S. MICHKI, State Univ of NY - Buffalo, Buffalo, NY, EDWARD H. SNELL, Hauptman-Woodward Medical Research Institute, State Univ of NY - Buffalo, Buffalo, NY, ANDREA G. MARKELZ, State Univ of NY - Buffalo, Buffalo, NY — X-ray, neutron scattering and terahertz measurements [1,2] found a rapid increase in dynamics of critically hydrated proteins above 220 K, termed the protein dynamical transition. Protein function ceases below the DT. It has been suggested that protein dynamics is slaved to the solvent and the DT originates from thermally activated solvent motions. Since previous measurements did not distinguish local diffusive and librational motions from long-range collective vibrations of proteins, it has not been determined how long-range motions are affected by the DT. Using a recently developed technique, crystal anisotropy terahertz microscopy [3] we directly measured the long-range motions for lysozyme and examined the temperature dependence in the 180-290 K range. We find that the distinct intramolecular vibrations do not follow the expected phonon-like behavior of solid state systems where the vibrational bands sharpen and blue shift with decreasing temperature, rather decrease in intensity as the DT is approached and disappear below the DT. This suggests the surrounding solvent below the DT acts as a frozen cage preventing long-range motions. 1.Doster,W.,et al. Phys.Rev.Lett., 2010.104(9):098101. 2.Niessen,K.,et al. Biophys.Rev., 2015.7,201. 3.Acbas,G.,et al. Nat.Comm., 2014.5,3076.

**3:30PM P41.00004 Structural and Dynamic Analysis on IDPs by Modified AWSEM-MD** , HAO WU, GAREGIN PAPOIAN, Univ of Maryland-College Park, PAPOIAN THEORETICAL BIOPHYSICS GROUP TEAM — Unlike globular proteins, intrinsically disordered proteins (IDPs) lack both secondary and tertiary structures and can play key roles in various biological processes, including transcriptional regulation, molecular recognition and cellular signaling. These functions can be potentially elucidated by structural heterogeneity of IDPs. Because of their flexibility and disordered nature, it has been difficult to investigate IDPs both computationally and experimentally. In particular, it is desirable to develop coarse-grained, yet accurate models of IDPs, such that simulations exploring sufficient conformational ensembles could be carried out within feasible times. To achieve this goal, we modified the associative memory, water mediated, structure and energy model (AWSEM-MD), which is typically used for folding of globular proteins or binding studies. We tested modified AWSEM-MD on several well-studied IDPs and found the transient secondary structure propensity is consistent with NMR experimental results. The rugged free energy landscapes obtained also show structural heterogeneity of these IDPs. Our proposed extension of AWSEM-MD may allow simulating a wider range of IDPs with high accuracy and computational efficiency.

**3:42PM P41.00005 Capturing high temperature protein conformations for low-temperature study using ultra-fast cooling** , DAVID MOREAU, HAKAN ATAKISI, ROBERT THORNE, Cornell University — protocols for cooling biomolecular crystals for x-ray cryocrystallography are poorly controlled, leading to crystal-to-crystal and within-crystal non-isomorphism. Furthermore, cooling times below the protein-solvent glass transition of .1 s provide ample time for biological temperature conformations to depopulate and shift. To address these issues, methods and apparatus for cooling biomolecular crystals at rates approaching 100,000 K/s have been developed. These cooling rates are sufficient to eliminate ice formation on cooling without use of cryoprotectants, and to quench additional high-temperature conformations for low-temperature study. Time scales for conformational relaxation can be characterized using variable cooling rates. Possible extension of these methods to maximize conformational quenching will be discussed.

**3:54PM P41.00006 Protein Conformational Entropy is Independent of Solvent** , NATHANIEL NUCCI, Rowan University, VERONICA MOORMAN, JOHN GLEDHILL, KATHLEEN VALENTINE, A. JOSHUA WAND, University of Pennsylvania — Proteins exhibit most of their conformational entropy in individual bond vector motions on the ps-ns timescale. These motions can be examined through determination of the Lipari-Szabo generalized squared order parameter ( $O^2$ ) using NMR spin relaxation measurements. It is often argued that most protein motions are intimately dependent on the nature of the solvating environment. Here the solvent dependence of the fast protein dynamics is directly assessed. Using the model protein ubiquitin, the order parameters of the backbone and methyl groups are shown to be generally unaffected by up to a six-fold increase in bulk viscosity or by encapsulation in the nanoscale interior of a reverse micelle. In addition, the reverse micelle condition permits direct comparison of protein dynamics to the mobility of the hydration layer; no correlation is observed. The dynamics of aromatic side chains are also assessed and provide an estimate of the length- and timescale of protein motions where solvent dependence is seen. These data demonstrate the solvent independence of conformational entropy, clarifying a long-held misconception in the fundamental behavior of biological macromolecules. Supported by the National Science Foundation.

**4:06PM P41.00007 Moving in the Right Direction: Evolution of Protein Structural Vibrations with Functional State and Mutation** , KATHERINE NIESSEN, MENG YANG XU, SUNY University at Buffalo, Physics, EDWARD SNELL, Hauptman-Woodward Medical Research Institute, Buffalo, NY, ANDREA MARKELZ, SUNY University at Buffalo, Physics — Long-range intramolecular vibrations may enable efficient access to functionally important conformations. We examine how these motions change with inhibitor binding and mutation using terahertz anisotropic absorption and molecular modeling [1,2]. The measured anisotropic absorption dramatically changes with 3NAG inhibitor binding for wild type (WT) free chicken egg white lysozyme (CEWL). We examine the evolution of internal motions with binding using normal mode analysis to calculate an ensemble averaged vibrational density of states (VDOS) and isotropic and anisotropic absorptions for both WT and a two residue (R14 and H15) deletion mutant which has a 1.4 higher activity rate [3]. While the VDOS and isotropic response are largely unchanged with inhibitor binding, the anisotropic response changes dramatically with binding. However, for the mutant the calculated unbound anisotropic absorption more closely resembles its bound spectrum, and it has increased calculated mean squared fluctuations in regions overlapping those in its bound state. These results indicate that the mutant's enhanced activity may be due to a shift in the *direction* of vibrations toward those of the bound state, increasing the sampling rate of the bound conformation. [1] DOI: 10.1007/s12551-015-0168-4 [2] DOI: 10.1038/ncomms4076 [3] DOI: 10.1006/jmbi.1999.2572

**4:18PM P41.00008 The Molecular Dynamics Study of the Structural Conversions in the Transformer Protein RfaH** , JEEVAN GC, BERNARD GERSTMAN, PREM CHAPAGAIN, Florida International University — Recently, a class of multi-domain proteins such as RfaH transcription factor are labelled as the transformer proteins as they undergo major conformational transformation for performing multiple functions. In the absence of the inter-domain contacts, the C-terminal domain of RfaH transforms from its alpha-helix conformation to a beta-barrel structure. Each of these states have their own functional role: in its alpha-helix state, RfaH-CTD inhibits the transcription by masking the binding site of RNAP, but in its beta state it facilitates the translation. We used various molecular dynamics simulations to study its transformer-like behavior of full-RfaH and identified key amino acid residues that are important in modulating such behavior. Our results show that the inter domain interactions constitute the major barrier in the alpha-helix to beta-barrel conversion. Once the interfacial interactions are broken, structural conversion is easier. The structural conversion from beta-barrel to alpha-helix proceeds with the rearrangement of the hydrophobic residues followed by the inter domain contacts formation via non-native, transient salt-bridge formation, leading to the formation of the native inter domain salt-bridge and hydrophobic contacts to give the final alpha-helix structure.

**4:30PM P41.00009 Motional displacements in proteins incorporating dynamical diversity<sup>1</sup>** , DERYA VURAL, UT/ORNL Center for Molecular Biophysics, Oak Ridge National Laboratory, P.O. Box 2008, Tennessee 37831 , USA, JEREMY SMITH, UT/ORNL Center for Molecular Biophysics, Oak Ridge National Laboratory, P.O. Box 2008, Tennessee 37831, USA, HENRY GLYDE, Department of Physics and Astronomy, University of Delaware, Newark, Delaware 19716-2570, USA — The average mean square displacement (MSD),  $\langle r^2 \rangle$ , of hydrogen  $H$  in proteins is measured using incoherent neutron scattering methods. The observed MSD shows a marked increase in magnitude at a temperature  $T_D \simeq 240$  K. This is widely interpreted as a dynamical transition to large MSDs which make function possible in proteins. However, when the data is interpreted in terms of a single averaged MSD, the extracted  $\langle r^2 \rangle$  depends on the neutron momentum transfer,  $\hbar Q$ , used in the measurement. We have shown recently that this apparent dependence on  $Q$  arises because the dynamical diversity of the  $H$  in the protein is neglected[2]. We present models of the dynamical diversity of  $H$  in Lysozyme that when used in the analysis of simulated neutron data lead to consistent,  $Q$  independent values for the average MSD and for the diversity model. 2. D. Vural and L. Hong, J. C. Smith and H. R. Glyde. *Phys. Rev. E* **91**, 052705 (2015).

<sup>1</sup>Supported in part by Office of Basic Energy Sciences, USDOE, ER46680

**4:42PM P41.00010 Microsecond dynamics of mismatch repair proteins** , FREDDIE SALSURY, WILLIAM THOMPSON, Wake Forest University — We will present the results of long-time simulations (250ns-1microsecond) of the mismatch repair protein complexes Mutsalpha bound to various substrates, both normal and damaged. We do so to demonstrate the importance of long-range fluctuations and generalized allostery in such systems and how long-scale GPU-enabled simulations can enabled such analysis.

**4:54PM P41.00011 Intermediate State Dependence of Intramolecular Vibrations in Photoactive Yellow Protein** , YANTING DENG, MENG YANG XU, KATHERINE NIESSEN, SUNY Buffalo, Buffalo, NY, MARIUS SCHMIDT, University of Wisconsin, Milwaukee, WI, ANDREA MARKELZ, SUNY Buffalo, Buffalo, NY — Photoactive proteins provide a testbed for the role of long-range collective motions in protein function. Long-range intramolecular vibrations of the protein scaffold may provide efficient energy relaxation[1], enhancement of chromophore vibrations that promote structural transitions[2] and assistance in electron energy transfer[3]. Photoactive yellow protein (PYP) is a cytoplasmic photocycling protein associated with the negative phototactic response to blue light in halohodospira halophile. We measure the intramolecular vibrations of PYP using crystal anisotropy terahertz microscopy (CATM)[4] as a function of photoexcitation. Room temperature CATM measurements are performed in the dark and with continuous illumination at 488 nm, which is found to result in an approximately 20% steady photoexcited state (pB). We find a decrease in anisotropic absorption in frequency range 20-60  $\text{cm}^{-1}$  with photoexcitation. This result may be due to an increase in sample disorder associated with the structural change in pB state. We compare the measured and calculated spectra using molecular dynamics and normal mode/quasi-harmonic analysis to identify the nature of the motions giving rise to the resonant absorption bands. 1. Levantino, M., et al. Nat Commun, 2015. 6. 2. Mataga, N., et al. Chem. Phys. Lett., 2002. 352(3-4): p. 220-225. 3. Fokas, A.S., et al. Photosynth. Res., 2014. 122(3): p. 275-292. 4. Acbas, G., et al. Nat Commun, 2014. 5.

**5:06PM P41.00012 Structure and dynamics of Ebola virus matrix protein VP40 by a coarse-grained Monte Carlo simulation** , RAS PANDEY, University of Southern Mississippi, BARRY FARMER, Air Force Research Laboratory — Ebola virus matrix protein VP40 (consisting of 326 residues) plays a critical role in viral assembly and its functions such as regulation of viral transcription, packaging, and budding of mature virions into the plasma membrane of infected cells. How does the protein VP40 go through structural evolution during the viral life cycle remains an open question? Using a coarse-grained Monte Carlo simulation we investigate the structural evolution of VP40 as a function of temperature with the input of a knowledge-based residue-residue interaction. A number local and global physical quantities (e.g. mobility profile, contact map, radius of gyration, structure factor) are analyzed with our large-scale simulations. Our preliminary data show that the structure of the protein evolves through different state with well-defined morphologies which can be identified and quantified via a detailed analysis of structure factor.

**5:18PM P41.00013 Effects of pressure on the dynamics of a hyperthermophilic protein revealed by quasielastic neutron scattering<sup>1</sup>**, U. R. SHRESTHA, D. BHOWMIK, Wayne State Univ, J. R. D. COPLEY, M. TYAGI, J. B. LEO, NIST Center for Neutron Research, X.-Q. CHU, Wayne State Univ — Inorganic pyrophosphatase (IPPase) from *Thermococcus thioireducens* is a large oligomeric protein derived from hyperthermophilic microorganism that is found near hydrothermal vents deep under the sea, where the pressure is nearly 100 MPa. Here we study the effects of pressure on the conformational flexibility and relaxation dynamics of IPPase over a wide temperature range using quasielastic neutron scattering (QENS) technique. Two spectrometers were used to investigate the  $\beta$ -relaxation dynamics of proteins in time ranges from 2 to 25 ps, and from 100 ps to 2 ns. Our results reveal that, under the pressure of 100 MPa, IPPase displays much faster relaxation dynamics than a mesophilic model protein, hen egg white lysozyme (HEWL) [1], opposite to what we observed previously under the ambient pressure [2]. These contradictory observations imply that high pressure affects the dynamical properties of proteins by distorting their energy landscapes. Accordingly, we derived a general schematic denaturation phase diagram that can be used as a general picture to understand the effects of pressure on protein dynamics and activities. [1] Shrestha et al. (2015), *Proc Natl Acad Sci USA*, doi: 10.1073/pnas.1514478112. [2] Chu et al. (2012), *J Phys Chem B* 116(33): 9917-9921.

<sup>1</sup>Wayne State Univ Startup Fund

**Wednesday, March 16, 2016 2:30PM - 5:30PM –**  
**Session P42 DPOLY: Small Molecule Transport in Polymers and Polymer Nanocomposites I -**  
**Industry Day 345 - Praveen Agarwal, Dow Chemical Company**

**2:30PM P42.00001 Chemical and Temperature Effects on Diffusion in a Model Polymer/Nanoparticle Composite<sup>1</sup>**, DUSTIN JANES, U.S. Food and Drug Administration, CHRISTOPHER DURNING, Columbia University — Polymers and inks used in medical devices may be strengthened with nanoparticle fillers, so an understanding of how they may affect the release of residuals and additives via diffusion will help modernize biocompatibility testing. Transport of small molecules in polymers with increasing volume fraction of impermeable nanoparticles is often poorly predicted by the simple Maxwell model for heterogeneous media. In this presentation we will examine two diffusing classes, only one of which possesses hydrogen bonding interactions with the nanoparticle surface. Since similar reductions in mutual diffusion coefficients were observed in both cases we attribute the enhancement of the "blocking effect" in nanocomposites to a reduction in polymer mobility in the interfacial volume near the nanoparticle. The temperature and penetrant concentration dependence of the diffusion coefficients were examined in the context of a Vrentas-Duda free volume model that includes a thermally activated prefactor. While data obtained for rubbery poly(methyl acrylate) clearly obeys the expected Arrhenius scaling with  $E_A = 11$  kJ/mol, results for films containing  $d = 14$  nm spherical silica nanoparticles do not, providing more evidence that polymer free volume is perturbed in unexpected ways even for conceptually simple systems.

<sup>1</sup>National Science Foundation IGERT Program, Pall Corporation

**2:42PM P42.00002 Controlling Free Volume for Permeability enhancement in Polymer-Grafted Nanocomposites**, CONNOR BILCHAK, EILEEN BUENNING, SANAT KUMAR, CHRISTOPHER DURNING, Columbia University, BRIAN BENICEWICZ, University of South Carolina — Significant advances in polymer membrane technology have been made by exploring glassy materials with intrinsically high 'free volume', allowing for diffusion selectivity. However, the permeability of these materials is restricted by the Robeson Upper Bound and exhibits long-term aging. While nanofiller have been used to avoid the deleterious effect of aging, they further limit transport properties and can result in non-equilibrium structures that phase-separate. We here show that 14nm silica nanoparticles grafted with rubbery Poly(Methyl Acrylate) (PMA) chains form hexatic lattices, solving a common difficulty in this class of membrane constructs of controlled dispersion morphology. In addition, our results show that these materials have permeabilities elevated relative to the neat polymer matrix, offering surprising beneficial gas transport properties. We also show that the 'free volume' available for diffusion can be adequately controlled by tuning polymer chain length and graft density. We propose the morphology of these grafted nanoparticle systems may be manipulated to optimize these composites for a wide variety of vital gas separations.

**2:54PM P42.00003 Gas Transport in Polymer-Grafted Nanoparticles**, KAI ZHANG, SANAT KUMAR, Columbia University — The efficient separation of gases is crucial for clean energy technologies. With their intrinsic multiscale features and excellent self-assembly properties, polymer-grafted nanoparticles (PGNP) material makes a good candidate for effective gas separation, but the basic understanding of gas transport in PGNPs is still missing. While the nanoparticles cores are spherical, the corona of the PGNPs can be deformed into anisotropic space-filling polygons at high density that are commensurate with the crystal structures (Wigner-Seitz cells). Such deformation indicates that the polymer chains are extended or compressed along different directions and create cavities within the crystals that can help to improve the gas selectivity. We use coarse-grained computer simulations to study the solubility and diffusion of gas molecules inside the crystalline packing of the NP cores. By tuning the degree of polymerization, the surface density of grafting chains and the size of gas molecules, we systematically investigate the dependence of gas transport on these parameters. We find that the void formed by three contacting monomers imposes a critical lengthscale beyond which the transport becomes highly size selective.

**3:06PM P42.00004 Understanding transport in model water desalination membranes**, EDWIN CHAN, National Institute of Standards and Technology — Polyamide based thin film composites represent the the state-of-the-art nanofiltration and reverse osmosis membranes used in water desalination. The performance of these membranes is enabled by the ultrathin (~100 nm) crosslinked polyamide film in facilitating the selective transport of water over salt ions. While these materials have been refined over the last several decades, understanding the relationships between polyamide structure and membrane performance remains a challenge because of the complex and heterogeneous nature of the polyamide film. In this contribution, we present our approach to addressing this challenge by studying the transport properties of model polyamide membranes synthesized via molecular layer-by-layer (mLbL) assembly. First, we demonstrate that mLbL can successfully construct polyamide membranes with well-defined nanoscale thickness and roughness using a variety of monomer formulations. Next, we present measurement tools for characterizing the network structure and transport of these model polyamide membranes. Specifically, we used X-ray and neutron scattering techniques to characterize their structure as well as a recently-developed indentation based poromechanics approach to extrapolate their water diffusion coefficient. Finally, we illustrate how these measurements can provide insight into the original problem by linking the key polyamide network properties, i.e. water-polyamide interaction parameter and characteristic network mesh size, to the membrane performance.

**3:42PM P42.00005 Salt transport properties of model reverse osmosis membranes using electrochemical impedance spectroscopy**, KATHLEEN FELDMAN, EDWIN CHAN, GERY STAFFORD, CHRISTOPHER STAFFORD, NIST — With the increasing shortage of clean water, efficient purification technologies including membrane separations are becoming critical. The main requirement of reverse osmosis in particular is to maximize water permeability while minimizing salt permeability. Such performance optimization has typically taken place through trial and error approaches. In this work, key salt transport metrics are instead measured in model reverse osmosis membranes using electrochemical impedance spectroscopy (EIS). As shown previously, EIS can provide both the membrane resistance  $R_m$  and membrane capacitance  $C_m$ , with  $R_m$  directly related to salt permeability. The membranes are fabricated in a molecular layer by layer approach, which allows for control over such parameters as thickness, surface and bulk chemistry, and network geometry/connectivity.  $R_m$ , and therefore salt permeability, follows the expected trends with thickness and membrane area but shows unusual behavior when the network geometry is systematically varied. By connecting intrinsic material properties such as the salt permeability with macroscopic performance measures we can begin to establish design rules for improving membrane efficiency and facilitate the creation of next-generation separation membranes.

**3:54PM P42.00006 Using Indentation to Characterize Water Transport and Structure in Nafion Thin Films**<sup>1</sup>, ERIC DAVIS, Department of Chemical and Biomolecular Engineering, Clemson University, Clemson, SC 29634, NICHOLE NADERMANN, KIRT PAGE, CHRISTOPHER STAFFORD, EDWIN CHAN, Materials Science and Engineering Division, National Institute of Standards and Technology, Gaithersburg, MD 20899 — Perfluorinated ionomers, specifically Nafion, are the state-of-the-art polymer used in fuel cells. For this application, Nafion is utilized in both a bulk (hundreds of microns) and confined (tens of nanometers) state. For Nafion thin films in a confined state, i.e., Nafion as thin film coatings on catalyst particles, in-plane transport may play a critical role in the movement of water and protons through this catalysis layer. In this study, water transport was measured for a series of Nafion thin film thicknesses using poroelastic relaxation indentation (PRI). Unlike traditional through-thickness diffusion measurement techniques for thin polymer films (e.g., quartz crystal microbalance), PRI can be used to probe the in-plane water transport behavior. Relative to bulk Nafion, reduced in-plane water diffusion was observed in thin film Nafion, and below approximately 1 micron, water diffusivity and Nafion film thickness exhibited a logarithmic relationship. Equilibrium swelling measurements of water saturated Nafion thin films were used in conjunction with pore network theory to develop a picture of how the molecular-scale structure of Nafion changes with confinement to nanoscale film thicknesses.

<sup>1</sup>Using Indentation to Characterize Water Transport and Structure in Nafion Thin Films

**4:06PM P42.00007 Water and polymer dynamics in highly crosslinked polyamide membranes**, BRADLEY FRIEBERG, EDWIN CHAN, MADHU TYAGI, CHRISTOPHER STAFFORD, CHRISTOPHER SOLES, National Institute of Standards and Technology — Highly crosslinked polyamides for reverse osmosis are the state-of-the-art active material in membranes for desalination. The thin film composite membrane structure that is used commercially has been empirically designed to selectively allow the passage of water molecules and minimize the passage of solutes such as salt. However, due to the large roughness and variability of the polyamide layer, there is a limited understanding of the structure-property relationship for these materials as well as the transport mechanism. To better understand the water transport mechanism we measure the water and polymer dynamics of polyamide membranes using quasi-elastic neutron scattering (QENS). By hydrating the membrane with deuterated water, we are able to isolate the dynamics of the hydrogenated membrane on the pico- and nanosecond time scales. By subsequently hydrating the membranes with hydrogenated water, the QENS measurements on the same times scales reveal information about both the translational and rotational dynamics of water confined within the polyamide membrane. Further understanding of the water diffusion mechanism will establish design rules in which the performance of future membrane materials can be improved.

**4:18PM P42.00008 CO<sub>2</sub> adsorption in a hierarchically structured carbon by SANS**, LILIN HE, JITENDRA BAHADUR, YURI MELNICHENKO, CRISTIAN CONTESCU, NIDIA GALLEGO, Oak Ridge National Laboratory — This contribution investigated the high pressure adsorption behavior of CO<sub>2</sub> at T = 296 K in hierarchically structured carbon using small-angle neutron scattering (SANS) technique. We observed a strong densification of CO<sub>2</sub> in micropores accompanied by non-monotonic adsorption-induced pore deformation. Liquid-like density of CO<sub>2</sub> confined in the micropores was reached with increasing pressure to 20 bar, which corresponds to the relative pressure of  $P/P_{sat} \sim 0.3$ . At  $P > 20$  bar, density of confined CO<sub>2</sub> approached a plateau. The size of micropores first increases with pressure, reached a maximum at 20 bar, and then decreased with further increasing pressure. A complementary SANS experiment carried out on the same microporous carbon saturated with argon that is neutron-transparent and non-adsorbing inert shows no deformation of micropores at pressures up to  $\sim 200$  bars. This result proved that the observed deformation of micropores in CO<sub>2</sub> was an adsorption-induced phenomenon, caused by the solvation pressure - induced strain and strong densification of confined CO<sub>2</sub> in the micropores.

**4:30PM P42.00009 Characterization of nanoscale spatial distribution of small molecules in amorphous polymer matrices**, RALM RICARTE, MARC HILLMYER, TIMOTHY LODGE, University of Minnesota — Hydroxypropyl methylcellulose acetate succinate (HPMCAS) can significantly enhance the efficacy of active pharmaceutical ingredients (APIs). Yet, the interactions between species in HPMCAS-API blends are not understood. Elucidating these interactions is difficult because the spatial distributions of HPMCAS and API in the blends are ambiguous; the polymer and drug may be molecularly mixed or the species may form phase separated domains. As these phase separated domains may be less than 100 nm in size, traditional characterization techniques may not accurately evaluate the spatial distribution. To address this challenge, we explore the use of electron energy-loss spectroscopy (EELS) for detecting the model API phenytoin in an HPMCAS-phenytoin blend. Using EELS, we directly measured with high accuracy and precision the phenytoin concentrations in several blends. We present evidence that suggests phase separation occurs in blends that have a phenytoin loading of approximately 50 wt percent. Finally, we demonstrate that this technique achieves a sub-100 nm spatial resolution and can detect several other APIs.

**4:42PM P42.00010 Quantitative monitoring of membrane permeation via in-situ ATR FT-IR spectroscopy**<sup>1</sup>, BRYAN BECKINGHAM, Lawrence Berkeley National Laboratory; Auburn University, DANIEL MILLER, Lawrence Berkeley National Laboratory — Ion conducting membranes are of interest for various energy applications including fuel cells and artificial photosynthesis systems. Within the context of artificial photosynthesis, membranes are desired that facilitate the ion transport necessary to feed the electrochemical reactions while meeting various additional selectivity and permeability demands depending on the CO<sub>2</sub> reduction products. Herein, we demonstrate the use of in-situ ATR FT-IR spectroscopy to quantitatively resolve the concentration of single and multicomponent mixtures of various CO<sub>2</sub> reduction products including methanol, formate and acetate. We then apply this methodology to the in-situ monitoring of the permeation of single and multicomponent mixtures across commercially available membranes. Membrane permeabilities and selectivities calculated from the single component time-resolved concentration curves are compared to the multicomponent permeation experiments.

<sup>1</sup>This material is based upon work performed at the Joint Center for Artificial Photosynthesis, a DOE Energy Innovation Hub, supported through the Office of Science of the U.S. Department of Energy under Award Number DE-SC000493.

**4:54PM P42.00011 Transport of Water in Semicrystalline Block Copolymer Membranes**, DANIEL HALLINAN, ONYEKACHI OPARAJI, Florida State Univ — Poly(styrene)-block-poly(ethylene oxide) (PS-*b*-PEO) is a semicrystalline block copolymer (BCP) with interesting properties. It is mechanically tough, amphiphilic, and has a polar phase. The mechanical toughness is due to the crystallinity of PEO and the high glass transition temperature of PS, as well as the morphological structure of the BCP. The polymer has high CO<sub>2</sub>, water, and salt solubility that derive from the polar PEO component. Potential applications include CO<sub>2</sub> separation, water purification, and lithium air batteries. In all of the aforementioned applications, water transport is an important parameter. The presence of water can also affect thermal and mechanical properties. Water transport and thermal and mechanical properties of a lamellar PS-*b*-PEO copolymer have been measured as a function of water activity. Water transport can be affected by the heterogeneous nature of a semicrystalline BCP. Therefore, Fourier transform infrared - attenuated total reflectance (FTIR-ATR) spectroscopy has been employed, because water transport and polymer swelling can be measured simultaneously. The effect of BCP structure on transport has been investigated by comparing water transport in PS-*b*-PEO to a PEO homopolymer. The crystalline content of the PEO and the presence of glassy PS lamellae will be used to explain the transport results.

**5:06PM P42.00012 Elasticity dominated surface segregation of small molecules in polymer mixtures**, SALVATORE CROCE, Durham University, JAROSLAW KRAWCZYK, Durham University, Lodz University of Technology, TOM MCLEISH, BUDDHAPRIYA CHAKRABARTI, Durham University — When a binary polymer mixture with mobile components is left to equilibrate, the low molecular weight component migrates to the free surface. A balance between loss of translational entropy and gain in surface energy dictates the equilibrium partitioning ratio and the migrant fraction. Despite its ubiquity and several theoretical and experimental investigations, the phenomenon is not fully understood. Further, methods by which migration can be controlled are in its nascent stage of development. We propose a new phenomenological free energy functional that incorporates the elasticity of bulk polymer mixtures (reticulated networks and gels) and show (using mean field and self-consistent field theories) that the migrant fraction decreases with increasing the bulk modulus of the system. Further, a wetting transition observed otherwise for large values of miscibility parameter and polymerization index can be avoided by increasing the elastic modulus of the system. Estimated values of moduli (for the effect to be observable) are akin to those of rubbery polymers. Our work paves the way for controlling surface migration in complex industrial formulations with polymeric ingredients where this effect leads to decreased product stability and performance.

**5:18PM P42.00013 Anomalous Diffusion of Water in Lamellar Membranes Formed by Pluronic Polymers**<sup>1</sup>, ZHE ZHANG, Biology and Soft-Matter Division, Oak Ridge National Laboratory; Julich Center for Neutron Science., MICHAEL OHL, Oak Ridge National Laboratory; Julich Center for Neutron Science., YOUNGKYU HAN, GREGORY SMITH, CHANGWOO DO, Biology and Soft-Matter Division, Oak Ridge National Laboratory, BIOLOGY AND SOFT-MATTER DIVISION, OAK RIDGE NATIONAL LABORATORY TEAM, JULICH CENTER FOR NEUTRON SCIENCE TEAM — Water diffusion is playing an important role in polymer systems. We calculated the water diffusion coefficient at different layers along z-direction which is perpendicular to the lamellar membrane formed by Pluronic block copolymers (L62: (EO<sub>6</sub>-PO<sub>34</sub>-EO<sub>6</sub>)) with the molecular dynamics simulation trajectories. Water molecules at bulk layers are following the normal diffusion, while that at hydration layers formed by polyethylene oxide (PEO) and hydrophobic layers formed by polypropylene oxide (PPO) are following anomalous diffusion. We find that although the subdiffusive regimes at PEO layers and PPO layers are the same, which is the fractional Brownian motion, however, the dynamics are different, i.e. diffusion at the PEO layers is much faster than that at the PPO layers, and meanwhile it exhibits a normal diffusive approximation within a short time period which is governed by the localized free self-diffusion, but becomes subdiffusive after  $t > 8$  ps, which is governed by the viscoelastic medium.

<sup>1</sup>The Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy; and Zhe Zhang gratefully acknowledges financial support from Julich Center for Neutron Science

## Wednesday, March 16, 2016 2:30PM - 5:18PM –

Session P43 GSNP GSOF: Granular Materials 346 - Eric DeGiuli, cole Polytechnique Fdrale de Lausanne

**2:30PM P43.00001 A Phase Diagram Unifies Energy Dissipation, Kinetics, and Rheology in Inertial Granular Flows**, ERIC DEGIULI, Ecole Polytech Fed de Lausanne, JIM MCELWAINE, Durham University, MATTHIEU WYART, Ecole Polytech Fed de Lausanne — Flows of hard granular materials depend strongly on the interparticle friction coefficient  $\mu_p$  and on the inertial number  $I$ , which characterizes proximity to the jamming transition where flow stops. Guided by numerical simulations, we derive the phase diagram of dense inertial flow of spherical particles, finding three regimes for  $10^{-4} < I < 0.1$ : frictionless, frictional sliding, and rolling. These are distinguished by the dominant means of energy dissipation, changing from collisional to sliding friction, and back to collisional, as  $\mu_p$  increases from zero at constant  $I$ . The three regimes differ in their kinetics and rheology; in particular, the velocity fluctuations and the stress anisotropy both display non-monotonic behavior with  $\mu_p$ , corresponding to transitions between the three regimes of flow. We characterize the scaling properties of these regimes, show that energy balance yields scaling relations for each of them, and explain why friction qualitatively affects flow.

**2:42PM P43.00002 Enhanced Flow of Granular Material**, GEORGE MCMURDY, SCOTT FRANKLIN, CHARLES BACHMANN, Rochester Institute of Technology — We study a peculiar, anomalous weakening in wet sand brought about by the addition of small amounts of fine silt. The effect has been observed in uncontrolled field experiments, which we reproduce in the lab. Samples consist of sand from a local state park with a broad grain-size distribution between 300-600 microns, to which we add controlled amounts of silt, with a size distribution between 25-75 microns. Moisture contents range from 0-15% (by mass); we find our samples unable to hold much more than 15%. Samples are formed into free-standing cylinders and loaded from above until collapse. Mass fraction of silt varies from 0-20%, spanning the range observed in coastal sands. Results are compared with dynamic deflection moduli found in the field, and possible mechanisms are discussed.

**2:54PM P43.00003 Solid-liquid like phase transition in a confined granular suspension**, NARIAKI SAKAI, FREDERIC LECHENAULT, MOKHTAR ADDA BEDIA, Laboratoire de Physique Statistique - Ecole Normale Supérieure, Paris — We present an experimental study of a liquid-solid like phase transition in a two-dimensional granular media. Particles are placed in a vertical Hele-Shaw cell filled with a denser solution of cesium-chloride. Thus, when the cell is rotated around its axis, hydrostatic pressure exerts a centripetal force on the particles which confines them towards the center. This force is in competition with gravity, thus by modifying the rotation rate, it is possible to transform continuously and reversibly the sample from a disordered loose state to an ordered packed state. The system presents many similarities with thermal systems at equilibrium like density and interface fluctuations, and the transition between the two phases goes through a coexistence state, where there is nucleation and growth of locally ordered domains which are captured by the correlation function of the hexatic order parameter. We discuss the possibility to extend the grand-canonical formalism to out-of-equilibrium systems, in order to uncover a state equation between the density and the pressure in the medium.

**3:06PM P43.00004 Forces and Flows in Non-Newtonian Suspensions<sup>1</sup>**, MELODY LIM, JONATHAN BARES, ROBERT BEHRINGER, Duke University — Above a certain solid mass fraction, suspensions of dense granular particles in water exhibit non-Newtonian behavior, including impact-activated solidification. Although it has been suggested that solidification depends on interactions with the suspension boundary, quantitative experiments on the boundary forces have not been reported. In the present experiments, we determine the magnitude and timings of impactor-driven events in both the boundaries and body of the suspension using high-speed video, tracer particles, and photoelastic container boundaries. We observe a shock-like propagation in the cornstarch suspension during impact. The dynamics of the shockfront are strongly correlated to those of the intruder. We also observe a second extremely fast shockfront, associated with the propagation of forces to the boundaries of the suspension. The dynamics of this shockfront do not depend on the intruder dynamics, but are correlated to the volume fraction of cornstarch particles in the suspension. The observed shockfront propagates at a speed which is faster than the sound speed in the experiment container.

<sup>1</sup>We acknowledge funding from the W. M. Keck Foundation, and grants NSF-DMR1206351 and NASA NNX15AD38G.

**3:18PM P43.00005 Cooling of 3D Granular Gases: Experiments in Microgravity<sup>1</sup>**, KIRSTEN HARTH, SANDRA WEGNER, TORSTEN TRITTEL, RALF STANNARIUS, Institute of Experimental Physics and MARS, Otto von Guericke University Magdeburg — Granular gases are ensembles of macroscopic grains, which move randomly and interact through inelastic collisions. This non-equilibrium statistical system is easy to picture, but still insufficiently understood. Numerous theoretical treatments have been performed, favorably with spherical grains and periodic boundaries, starting from a homogeneous state. Experimentally, such a gas in 3D can only be realized with strong external forcing or in microgravity. We have recently demonstrated that the use of elongated grains facilitates the realization of 3D experiments beyond the Knudsen regime (1). Main findings in a sounding rocket experiment were non-Gaussian velocity distributions and a violation of the equipartition of kinetic energy in the steady state. Rotational degrees of freedom are under-excited. When the excitation is stopped, energy is dissipated, the granular gas is "cooling". We present the first quantitative study of the cooling of a granular gas, based on a 3D data evaluation, from drop tower experiments. The evolution of the kinetic energy in translational and rotational degrees of freedom is compared to Haff's law and recent numerical studies. Additionally, we analyze velocity and density distributions. (1) K. Harth et al., Phys. Rev. Lett. 110 144102 (2013)

<sup>1</sup>This research was funded by German Aerospace Center DLR grants 50WM1241 and 50WB1344 and by DFG grant STA-425/34-1.

**3:30PM P43.00006 ABSTRACT WITHDRAWN —**

**3:42PM P43.00007 Flying in a sandstorm: granular flow dynamics around an intruder**, YASIN KARIM, ERIC CORWIN, University of Oregon — Using high-speed imaging and direct force measurements, we study the flow dynamics around an intruder in a quasi-two dimensional granular gas. We also vary the geometry of the intruder and explore how changing the curvature, for instance, affects the lift force. For a given angle of attack, an intruder with a straighter side facing the flow experiences higher lift than one with a more convex side. We use particle image velocimetry to measure flow fields and correlate them with our direct force measurements to elaborate on how granular gas flows respond to changes in intruder geometry.

**3:54PM P43.00008 Collisional Model of the Stopping Force of 3D Granular Impact<sup>1</sup>**, CACEY STEVENS, JONATHAN BARES, ROBERT BEHRINGER, Department of Physics, Duke University — A dense granular packing can cause a free-falling intruding object to come to an abrupt stop as its momentum is dissipated to the grains. An empirical force law has been widely accepted to describe this process; it characterizes the stopping force as the sum of depth-dependent friction and velocity-dependent inertial drag.<sup>2</sup> However, a complete interpretation of this force, incorporating grain-scale interactions during impact, remains unresolved. Here, the momentum transfer is proposed to occur through sporadic collisions with clusters of high force-carrying grains at the intruder's surface.<sup>3</sup> To test this model in 3D impact experiments, we determine the forces acting on an intruder decelerating through a dense granular medium using high-speed video of its trajectory. By attaching a rod to the intruder and observing its motion from perpendicular angles, we obtain all translational and rotational dynamics. We vary the shape of the impeding object to infer intruder-grain interactions from its consequent path. As a result, we connect the inertial drag to the effect of intruder shape and rotation based on the collisional model.

<sup>1</sup>Supported by Duke University Provost's Postdoctoral Program and NASA grant NNX15AD38G

<sup>2</sup>H. Katsuragi et al, Nat. Phys. **3**, 6 (2007)

<sup>3</sup>Y. Takehara et al EPL **92**, 44003 (2010), A. Clark et al, PRE **89**, 012201 (2014)

**4:06PM P43.00009 Real-time magnetic resonance imaging of highly dynamic granular phenomena**, ALEXANDER PENN, Laboratory for Energy Science and Engineering, ETH Zurich and Institute for Biomedical Engineering, University and ETH Zurich, KLAAS P. PRUESSMANN, Institute for Biomedical Engineering, University and ETH Zurich, CHRISTOPH MLLER, Laboratory for Energy Science and Engineering, ETH Zurich — Probing non-intrusively the interior of three-dimensional granular systems is a challenging task for which a number of imaging techniques have been applied including positron emission particle tracking, X-ray tomography and magnetic resonance imaging (MRI). A particular advantage of MRI is its versatility allowing quantitative velocimetry through phase contrast encoding and tagging, arbitrary slice orientations and the flexibility to trade spatial for temporal resolution and vice versa during image reconstruction. However, previous attempts to image granular systems using MRI were often limited to (pseudo-) steady state systems due to the poor temporal resolution of conventional imaging methodology. Here we present an experimental approach that overcomes previous limitations in temporal resolution by implementing a variety of methodological advances, viz. parallel data acquisition through tailored multiple receiver coils, fast gradient readouts for time-efficient data sampling and engineered granular materials that contain signal sources of high proton density. Achieving a spatial and temporal resolution of, respectively, 2 mm x 2 mm and 50 ms, we were able to image highly dynamic phenomena in granular media such as bubble coalescence and granular compaction waves.

**4:18PM P43.00010 Investigation of the effect of wall friction on the flow rate in 2D and 3D Granular Flow<sup>1</sup>**, BRENDA CARBALLO-RAMIREZ, MOLLIE PLEAU, NALINI EASWAR, Smith College, SUMIT BIRWA, TCIS Hyderabad, NEIL SHAH, SHUBHA TEWARI, University of Massachusetts — We have measured the mass flow rate of spherical steel spheres under gravity in vertical, straight-walled 2 and 3-dimensional hoppers, where the flow velocity is controlled by the opening size. Our measurements focus on the role of friction and its placement along the walls of the hopper. In the 2D case, an increase in the coefficient of static friction from  $\mu = 0.2$  to 0.6 is seen to decrease the flow rate significantly. We have changed the placement of frictional boundaries/regions from the front and back walls of the 2D hopper to the side walls and floor to investigate the relative importance of the different regions in determining the flow rate. Fits to the Beverloo equation show significant departure from the expected exponent of 1.5 in the case of 2D flow. In contrast, 3D flow rates do not show much dependence on wall friction and its placement. We compare the experimental data to numerical simulations of gravity driven hopper granular flow with varying frictional walls constructed using LAMMPS\*. \*<http://lammps.sandia.gov>

<sup>1</sup>Supported by NSF MRSEC DMR 0820506

**4:30PM P43.00011 Normal coefficient of restitution of wet particles<sup>1</sup>** , KAI HUANG, THOMAS MUELLER, INGO REHBERG, Experimentalphysik V, University of Bayreuth — The normal coefficient of restitution (COR) for a spherical particle bouncing on a wet surface is investigated experimentally. The dependence of the COR on the impact velocity and various particle and liquid properties will be presented and discussed in terms of dimensionless numbers that characterize the interplay between inertial, viscous, and surface forces. At a fixed ratio of the liquid film thickness  $\delta$  to the particle diameter  $D$ , the wet COR is found to be inverse proportional to the Stokes number  $St$ , which measures the inertia of the particle to the viscous force from the liquid. This relation provides a convenient way of predicting wet COR with two fit parameters. For two different types of particles, we vary systematically the dimensionless film thickness  $\delta/D$  and discuss its influence on the fit parameters. Finally, we rationalize the observations with a model that considers possible sources of energy dissipation associated with a wet impact.

<sup>1</sup>KH and TM acknowledge the support from the DFG through Grant No. HU1939/2-1

**4:42PM P43.00012 Long-term behavior of granular chains held between walls is really equilibrium.<sup>1</sup>** , MICHELLE PRZEDBORSKI, Brock University, SURAJIT SEN, State University of New York at Buffalo, THAD HARROUN, Brock University — Granular chains have been the focus of a number of studies, in part due to their numerous applications, ranging from shock absorption and vibration reduction to energy localization. Force impulses to an unloaded granular chain result in a propagating solitary wave (SW), analogous to a soliton of the Korteweg-de Vries equation. When SWs collide with a boundary or another SW, secondary solitary waves (SSWs) are produced as grains break contact. A consequence of this process is the transition from a non-ergodic, SW dominant, phase to the stable “quasi-equilibrium” (QE) phase, thought to be distinct from true thermodynamic equilibrium due to the absence of equipartitioning of energy. We show that, in the absence of energy dissipation, when granular systems are allowed to evolve to extremely long times, the number of SSWs becomes sufficiently large that the system actually approaches a true equilibrium phase. In this extreme-time limit, energy in fact becomes equipartitioned among all grains, and we illustrate how the specific heat and kinetic energy fluctuations can be predicted by the generalized equipartition theorem, regardless of the degree of the interaction potential. This opens up the possibility that granular systems should be treated by equilibrium statistical mechanics.

<sup>1</sup>This work was supported by a Vanier Canada Graduate Scholarship

**4:54PM P43.00013 Experimental observations of root growth in a controlled photoelastic granular material** , SERGE MORA, JONATHAN BARES, LMGC Montpellier, JEAN-YVES DELENNE, INRA-UMR-IATE Montpellier, THIERRY FOURCAUD, CIRAD-UMR-AMAP Montpellier — The mechanism of root growth in soil is a key issue to understand both how to improve plant development and how to stabilize grounds. However, no experimental studies have been carried out to directly observe root development and surrounding stress while imposing specific grain configurations or mechanical loading. We present a novel set-up which permits to observe the development of chickpea root networks in a 2D granular material made of bidisperse photoelastic discs while imposing the position of the grains, the intergranular spacing and the nature of the system confinement: (i) open cell, (ii) confined cell (iii) sheared cell. In the experimental apparatus several root development cells are treated in parallel to increase the statistical meaning of the observations. Evolution of the root network is followed as well as position and pressure inside each disc by mean of a camera and classical photoelastic techniques. Preliminary results will be presented.

**5:06PM P43.00014 Topological interlocking provides stiffness to stochastically micro-cracked materials beyond the transport percolation limit.** , ANIRBAN PAL, CATALIN PICU, Department of Mechanical, Aerospace and Nuclear Engineering, Rensselaer Polytech Institute, MARIAN V. LUPULESCU, New York State Museum, Research and Collections — We study the mechanical behavior of two-dimensional, stochastically microcracked continua in the range of crack densities close to, and above the transport percolation threshold. We show that these materials retain stiffness up to crack densities much larger than the transport percolation threshold, due to topological interlocking of sample sub-domains. Even with a linear constitutive law for the continuum, the mechanical behavior becomes non-linear in the range of crack densities bounded by the transport and stiffness percolation thresholds. The effect is due to the fractal nature of the fragmentation process and is not linked to the roughness of individual cracks. We associate this behavior to that of itacolumite, a sandstone that exhibits unusual flexibility.

## Wednesday, March 16, 2016 2:30PM - 5:30PM –

Session P44 GQI: Quantum Error Correction 347 - Jacob Taylor, University of Maryland / NIST

**2:30PM P44.00001 A universal fault-tolerant gate set for the 5-qubit quantum code** , THEODORE YODER, RYUJI TAKAGI, ISAAC CHUANG, Massachusetts Institute of Technology — While the smallest single-error correcting classical code encodes one bit in just three, the smallest such quantum code requires five qubits to protect one qubit. Yet, the 5-qubit quantum code is widely regarded as useless when it comes to encoded quantum computation, as it supports just one non-Pauli transversal gate, the  $K = SH$  gate where  $H$  is Hadamard and  $S$  is the phase gate. However, transversal gates, though convenient, are not all there is to fault-tolerant computation. Here we develop non-transversal, fault-tolerant logical gates for the 5-qubit quantum code, including logical controlled-Z (CZ) and logical controlled-controlled-Z (CCZ). With  $K$ , we can then create fault-tolerant CNOT and Toffoli gates. Together, logical Toffoli and  $K$  imply that the 5-qubit code is capable of universal, fault-tolerant quantum computation. Moreover, we achieve our results without magic states. Indeed, no ancillary qubits beyond those needed for error-correction are necessary in any of our fault-tolerant constructions. We also report fault-tolerance thresholds for our new gates, calculated by exact computer simulation. In some cases, our logical gates on the 5-qubit code have better thresholds than the analogous constructions on the next smallest quantum code, the 7-qubit code.

**2:42PM P44.00002 Quantum fault-tolerant thresholds for universal concatenated schemes** , CHRISTOPHER CHAMBERLAND, TOMAS JOCHYM-O'CONNOR, Institute for Quantum Computing, University of Waterloo, RAYMOND LAFLAMME, Institute for Quantum Computing, University of Waterloo, Perimeter Institute — Fault-tolerant quantum computation uses ancillary qubits in order to protect logical data qubits while allowing for the manipulation of the quantum information without severe losses in coherence. While different models for fault-tolerant quantum computation exist, determining the ancillary qubit overhead for competing schemes remains a challenging theoretical problem. In this work, we study the fault-tolerance threshold rates of different models for universal fault-tolerant quantum computation. Namely, we provide different threshold rates for the 105-qubit concatenated coding scheme for universal computation without the need for state distillation. We study two error models: adversarial noise and depolarizing noise and provide lower bounds for the threshold in each of these error regimes. Establishing the threshold rates for the concatenated coding scheme will allow for a physical quantum resource comparison between our fault-tolerant universal quantum computation model and the traditional model using magic state distillation.

**2:54PM P44.00003 Critical parameters of a noise model that affect fault tolerant quantum computation on a single qubit** , PAVITHRAN IYER, Univ of Sherbrooke, MARCUS P DA SILVA, Raytheon BBN Technologies, DAVID POULIN, Univ of Sherbrooke — In this work, we aim to determine the parameters of a single qubit channel that can tightly bound the logical error rate of the Steane code. We do not assume any a priori structure for the quantum channel, except that it is a CPTP map and we use a concatenated Steane code to encode a single qubit. Unlike the standard Monte Carlo technique that requires many iterations to estimate the logical error rate with sufficient accuracy, we use techniques to compute the complete effect of a physical CPTP map, at the logical level. Using this, we have studied the predictive power of several physical noise metrics on the logical error rate, and show, through numerical simulations with random quantum channels, that, on their own, none of the natural physical metrics lead to accurate predictions about the logical error rate. We then show how machine learning techniques help us to explore which features of a random quantum channel are important in predicting its logical error rate.

**3:06PM P44.00004 Doubled Color Codes** , SERGEY BRAVYI, IBM Watson Research Center — Combining protection from noise and computational universality is one of the biggest challenges in the fault-tolerant quantum computing. Topological stabilizer codes such as the 2D surface code can tolerate a high level of noise but implementing logical gates, especially non-Clifford ones, requires a prohibitively large overhead due to the need of state distillation. In this talk I will describe a new family of 2D quantum error correcting codes that enable a transversal implementation of all logical gates required for the universal quantum computing. Transversal logical gates (TLG) are encoded operations that can be realized by applying some single-qubit rotation to each physical qubit. TLG are highly desirable since they introduce no overhead and do not spread errors. It has been known before that a quantum code can have only a finite number of TLGs which rules out computational universality. Our scheme circumvents this no-go result by combining TLGs of two different quantum codes using the gauge-fixing method pioneered by Paetznick and Reichardt. The first code, closely related to the 2D color code, enables a transversal implementation of all single-qubit Clifford gates such as the Hadamard gate and the  $\pi/2$  phase shift. The second code that we call a doubled color code provides a transversal T-gate, where T is the  $\pi/4$  phase shift. The Clifford+T gate set is known to be computationally universal. The two codes can be laid out on the honeycomb lattice with two qubits per site such that the code conversion requires parity measurements for six-qubit Pauli operators supported on faces of the lattice. I will also describe numerical simulations of logical Clifford+T circuits encoded by the distance-3 doubled color code. Based on a joint work with Andrew Cross.

**3:42PM P44.00005 Efficiently simulable approximations to realistic incoherent and coherent errors and their application to threshold estimation** , MAURICIO GUTIERREZ, KENNETH BROWN, Georgia Institute of Technology — Classical simulations of noisy stabilizer circuits are often used to estimate the threshold of a quantum error-correcting code (QECC). It is not completely clear how sensitive a code's threshold is to the error model, and whether or not a Pauli channel (PC) is a good approximation for realistic non-stabilizer errors. Within the stabilizer formalism, it has been shown that for a single qubit more accurate approximations can be obtained by expanding the PC. We now examine the feasibility of employing these error approximations at the single-qubit level to obtain better estimates of a QECC's threshold. We calculate the level-1 pseudo-threshold for the Steane  $[[7,1,3]]$  code for several error models. At the logical level, the Pauli twirled channel (PTC) provides an extremely accurate approximation for incoherent channels. However, for coherent channels, the PTC severely underestimates the magnitude of the error. By computing the effective 1-qubit process matrix for the whole circuit at low error rates, it becomes clear that this behavior is due to the stronger persistence of off-diagonal entries in the coherent channels. Therefore, if the main source of error in the quantum system is coherent, reliable stabilizer simulations should employ expanded Clifford channels.

**3:54PM P44.00006 Decoder for 3-D color codes** , KUNG-CHUAN HSU, TODD BRUN, University of Southern California — Transversal circuits are important components of fault-tolerant quantum computation. Several classes of quantum error-correcting codes are known to have transversal implementations of any logical Clifford operation. However, to achieve universal quantum computation, it would be helpful to have high-performance error-correcting codes that have a transversal implementation of some logical non-Clifford operation. The 3-D color codes<sup>1</sup> are a class of topological codes that permit transversal implementation of the logical  $\pi/8$ -gate. The decoding problem of a 3-D color code can be understood as a graph-matching problem on a three-dimensional lattice. Whether this class of codes will be useful in terms of performance is still an open question. We investigate the decoding problem of 3-D color codes and analyze the performance of some possible decoders.

<sup>1</sup>H. Bombín, New J. Phys. **17**, 083002 (2015).

**4:06PM P44.00007 High-threshold decoding algorithms for the gauge color code** , WILLIAM ZENG, Rigetti Computing, BENJAMIN BROWN, Niels Bohr Institute, University of Copenhagen — Gauge color codes are topological quantum error correcting codes on three dimensional lattices. They have garnered recent interest due to two important properties: (1) they admit a universal transversal gate set, and (2) their structure allows reliable error correction using syndrome data obtained from a measurement circuit of constant depth. Both of these properties make gauge color codes intriguing candidates for low overhead fault-tolerant quantum computation. Recent work by Brown et al. calculated a threshold of 0.31% for a particular gauge color code lattice using a simple clustering decoder and phenomenological noise. We show that we can achieve improved threshold error rates using the efficient Wootton and Loss Markov-chain Monte Carlo (MCMC) decoding. In the case of the surface code, the MCMC decoder produced a threshold close to that code's upper bound. While no upper bound is known for gauge color codes, the thresholds we present here may give a better estimate.

**4:18PM P44.00008 ABSTRACT WITHDRAWN —**

**4:30PM P44.00009 Potts glass reflection of the decoding threshold for qudit quantum error correcting codes<sup>1</sup>** , YI JIANG, University of California, Riverside, ALEXEY A. KOVALEV, University of Nebraska—Lincoln, LEONID P. PRYADKO, University of California, Riverside — We map the maximum likelihood decoding threshold for qudit quantum error correcting codes to the multicritical point in generalized Potts gauge glass models, extending the map constructed previously for qubit codes [1]. An  $n$ -qudit quantum LDPC code, where a qudit can be involved in up to  $m$  stabilizer generators, corresponds to a  $\mathbb{Z}_d$  Potts model with  $n$  interaction terms which can couple up to  $m$  spins each. We analyze general properties of the phase diagram of the constructed model, give several bounds on the location of the transitions, bounds on the energy density of extended defects (non-local analogs of domain walls), and discuss the correlation functions which can be used to distinguish different phases in the original and the dual models.

[1] A A Kovalev and L P Pryadko, Quant. Inf. & Comp. **15**, 0825 (2015).

<sup>1</sup>This research was supported in part by the grants: NSF PHY-1415600 (AAK), NSF PHY-1416578 (LPP), and ARO W911NF-14-1-0272 (LPP)

**4:42PM P44.00010 Fault-tolerant quantum computation in multiqubit block codes: performance and overhead**<sup>1</sup>, TODD BRUN, Univ of Southern California — Fault-tolerant quantum computation requires that quantum information remain encoded in a quantum error-correcting code at all times; that a universal set of logical unitary gates and measurements is available; and that the probability of an uncorrectable error is low for the duration of the computation. Quantum computation can in principle be scaled up to unlimited size if the rate of decoherence is below a threshold. The main constructions that have been studied involve encoding each logical qubit in a separate block (either a concatenated code or a block of the surface code), which typically requires thousands of physical qubits per logical qubit, if not more. To reduce this overhead, we consider using multiqubit codes to achieve much higher storage rates. We estimate performance and overhead for certain families of codes, and ask: how large a quantum computation can be done as a function of the decoherence rate for a fixed size code block? Finally, we consider remaining open questions and limitations to this approach.

<sup>1</sup>This work is supported by NSF Grant No. CCF-1421078.

**4:54PM P44.00011 Numerical Simulation of Coherent Error Correction**, DANIEL CROW, ROBERT JOYNT, MARK SAFFMAN, Univ of Wisconsin, Madison — A major goal in quantum computation is the implementation of error correction to produce a logical qubit with an error rate lower than that of the underlying physical qubits. Recent experimental progress demonstrates physical qubits can achieve error rates sufficiently low for error correction, particularly for codes with relatively high thresholds such as the surface code and color code. Motivated by experimental capabilities of neutral atom systems, we use numerical simulation to investigate whether coherent error correction can be effectively used with the 7-qubit color code. The results indicate that coherent error correction does not work at the 10-qubit level in neutral atom array quantum computers. By adding more qubits there is a possibility of making the encoding circuits fault-tolerant which could improve performance.

**5:06PM P44.00012 Noise Estimation and Adaptive Encoding for Asymmetric Quantum Error Correcting Codes**<sup>1</sup>, JAN FLORJANCZYK, TODD BRUN, Univ of Southern California, CENTER FOR QUANTUM INFORMATION SCIENCE AND TECHNOLOGY TEAM — We present a technique that improves the performance of asymmetric quantum error correcting codes in the presence of biased qubit noise channels. Our study is motivated by considering what useful information can be learned from the statistics of syndrome measurements in stabilizer quantum error correcting codes (QECC). We consider the case of a qubit dephasing channel where the dephasing axis is unknown and time-varying. We are able to estimate the dephasing angle from the statistics of the standard syndrome measurements used in stabilizer QECC's. We use this estimate to rotate the computational basis of the code in such a way that the most likely type of error is covered by the highest distance of the asymmetric code. In particular, we use the  $[[15, 1, 3]]$  shortened Reed-Muller code which can correct one phase-flip error but up to three bit-flip errors. In our simulations, we tune the computational basis to match the estimated dephasing axis which in turn leads to a decrease in the probability of a phase-flip error. With a sufficiently accurate estimate of the dephasing axis, our memory's effective error is dominated by the much lower probability of four bit-flips.

<sup>1</sup>ARO MURI Grant No. W911NF-11-1-0268

**5:18PM P44.00013 Details of  $[[7,1,3]]$  Syndrome Measurements**, YAAKOV WEINSTEIN, MITRE — We explore different aspects of syndrome measurements (SM) for the  $[[7,1,3]]$  quantum error correction code. This includes determining how often to apply SM, comparing the performance of different SM, rearranging the order in which SM are applied, and exploring the effects of improving SM ancilla state construction. Finally, we attempt to formulate gates and their attached SM as superoperators.

## Wednesday, March 16, 2016 2:30PM - 5:30PM –

Session P45 GQI: Semiconductor Qubits: Quantum Dot / Donor Devices and Readout 348 - John Gamble, Sandia National Laboratory

**2:30PM P45.00001 Nuclear-driven electron spin rotations in a coupled silicon quantum dot and single donor system**, PATRICK HARVEY-COLLARD, Univ of Sherbrooke, NOAH TOBIAS JACOBSON, MARTIN RUDOLPH, GREGORY A. TEN EYCK, JOEL R. WENDT, TAMMY PLUYM, MICHAEL P. LILLY, Sandia National Laboratories, MICHEL PIORO-LADRIRE, Univ of Sherbrooke, MALCOLM S. CARROLL, Sandia National Laboratories — Single donors in silicon are very good qubits. However, a central challenge is to couple them to one another. To achieve this, many proposals rely on using a nearby quantum dot (QD) to mediate an interaction. In this work, we demonstrate the coherent coupling of electron spins between a single  $^{31}\text{P}$  donor and an enriched  $^{28}\text{Si}$  metal-oxide-semiconductor few-electron QD. We show that the electron-nuclear spin interaction can drive coherent rotations between singlet and triplet electron spin states. Moreover, we are able to tune electrically the exchange interaction between the QD and donor electrons. The combination of single-nucleus-driven rotations and voltage-tunable exchange provides all elements for future all-electrical control of a spin qubit, and requires only a single dot and no additional magnetic field gradients. This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. DOE's National Nuclear Security Administration under contract DE-AC04-94AL85000.

**2:42PM P45.00002 All-electrical control of a singlet-triplet qubit coupled to a single nuclear spin**<sup>1</sup>, N. TOBIAS JACOBSON, Sandia National Laboratories, PATRICK HARVEY-COLLARD, Sandia National Laboratories and Universite de Sherbrooke, ANDREW BACZEWSKI, JOHN GAMBLE, MARTIN RUDOLPH, ERIK NIELSEN, RICHARD MULLER, MALCOLM CARROLL, Sandia National Laboratories — Donor nuclear spins in isotopically purified silicon have very long coherence times, suggesting that they may form high-quality quantum memories. We propose that coupling these nuclear spins to few-electron quantum dots could enable nuclear spin readout and two-qubit operations of the joint quantum dot and nuclear spin system without the need for electron spin resonance. As a step towards this goal, our group recently demonstrated coherent singlet/triplet electron spin rotations induced by the hyperfine interaction between electronic spin degrees of freedom and a single nuclear spin in isotopically purified silicon. In this talk, I will discuss the feasibility of universal all-electrical control of such a singlet/triplet electron spin qubit and explore the decoherence mechanisms that we expect to dominate. Finally, I will examine the relative merits of AC and pulsed DC gating schemes.

<sup>1</sup>Sandia is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the US Department of Energy National Nuclear Security Administration under Contract No. DE-AC04- 94AL85000.

**2:54PM P45.00003 Full Controllability of a Singlet-Triplet Qubit Coupled to a Nuclear Spin Qubit**, ANDREW D. BACZEWSKI, JOHN KING GAMBLE, N. TOBIAS JACOBSON, RICHARD P. MULLER, ERIK NIELSEN, STEPHEN M. CARR, MALCOLM S. CARROLL, Sandia National Laboratories, MATTHEW CURRY, Sandia National Laboratories and University of New Mexico, PATRICK HARVEY-COLLARD, Sandia National Laboratories and Universit  de Sherbrooke, RYAN M. JOCK, MARTIN RUDOLPH, Sandia National Laboratories — Recent experimental developments indicate that it is possible to drive coherent singlet-triplet rotations in a MOS quantum dot coupled to a single nearby phosphorus donor through the electron-nucleus hyperfine interaction. With the addition of NMR, we propose that it is possible to achieve universal 2-qubit control spanning i.) an electronic singlet-triplet subspace of the dot, ii.) the spin-1/2 donor nucleus, and iii.) entangling operations between them. We will assess the practicality of such an approach given realistic experimental conditions and constraints, including a comparison of pulsed and RF control of the detuning between the donor and dot. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Security Administration under contract DE-AC04-94AL85000.

**3:06PM P45.00004 Transport through an impurity tunnel coupled to a Si/SiGe quantum dot**, RYAN H. FOOTE, DANIEL R. WARD, University of Wisconsin-Madison, J.R. PRANCE, Lancaster University, JOHN KING GAMBLE, ERIK NIELSEN, Sandia National Laboratories, BRANDUR THORGRIMSSON, D.E. SAVAGE, University of Wisconsin-Madison, A.L. SARAIVA, Universidade Federal do Rio de Janeiro, MARK FRIESEN, S.N. COPPERSMITH, M.A. ERIKSSON, University of Wisconsin-Madison — Here we present measurements of transport through a gate-defined quantum dot formed in a Si/SiGe heterostructure, demonstrating controllable tunnel coupling between the quantum dot and a localized electronic state.<sup>1</sup> Combining experimental stability diagram measurements with 3D capacitive modeling based on the expected electron density profiles, we determine the most likely location of the localized state in the quantum well. This work is supported in part by NSF (DMR-1206915, IIA-1132804), ARO (W911NF-12-1-0607) and the William F. Vilas Estate Trust. Development and maintenance of the growth facilities used for fabricating samples supported by DOE (DE-FG02-03ER46028). This research utilized facilities supported by the NSF (DMR-0832760, DMR-1121288). The work of J.K.G. and E.N. was supported in part by the Laboratory Directed Research and Development program at Sandia National Laboratories. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

<sup>1</sup>Ryan H. Foote *et al.*, *Appl. Phys. Lett.* **107**, 103112 (2015)

**3:18PM P45.00005 Silicon quantum dots with counted antimony donor implants**, MEENAKSHI SINGH, JOSE PACHECO, DANIEL PERRY, JOEL WENDT, RONALD MANGINELL, JASON DOMINGUEZ, TAMMY PLUYM, DWIGHT LUHMAN, EDWARD BIELEJEC, MICHAEL LILLY, MALCOLM CARROLL, Sandia National Laboratory — Antimony donor implants next to silicon quantum dots have been detected with integrated solid-state diode detectors with single ion precision. Devices with counted number of donors have been fabricated and low temperature transport measurements have been performed. Charge offsets, indicative of donor ionization and coupling to the quantum dot, have been detected in these devices. The number of offsets corresponds to 10-50% of the number of donors counted. We will report on tunneling time measurements and spin readout measurements on the donor offsets. This work was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. DOE Office of Basic Energy Sciences user facility. The work was supported by Sandia National Laboratories Directed Research and Development Program. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a Lockheed-Martin Company, for the U. S. Department of Energy under Contract No. DE-AC04-94AL85000.

**3:30PM P45.00006 Detection of ion implanted patterns in silicon using STM**, HYUN-SOO KIM, Univ of Maryland-College Park, A.N. RAMANAYAKA, Joint Quantum Institute, Univ of Maryland-College Park, K.J. DWYER, Univ of Maryland-College Park, M.D. STEWART JR., J.M. POMEROY, National Institute of Standards and Technology — Ion implanted regions in silicon are scanned using STM to detect features which will facilitate in-situ overlay and alignment of STM hydrogen patterned nano-devices. STM hydrogen lithography is used to make atomically precise devices such as single electron transistors and single atom qubits. However, with currently available imaging techniques, we are limited to make devices on a single plane using STM lithography. In-situ detection of high local doping concentrations using STM will allow precise alignment between the multiple layers of buried nano-devices and metal electrodes.

**3:42PM P45.00007 Atomistic simulations of negatively charged donor states probed in STM experiments**, ARCHANA TANKASALA, Purdue University, USA, JOE SALFI, SVEN ROGGE, CQCCT, University of New South Wales, Australia, GERHARD KLIMECK, RAJIB RAHMAN, Purdue University, USA — A single donor in silicon binding two electrons ( $D^-$ ) is important for electron spin readout and two-qubit operations in a donor based silicon (Si) quantum computer, and has recently been probed in Scanning Tunneling Microscope (STM) experiments for sub-surface dopants. In this work, atomistic configuration interaction technique is used to compute the two-electron states of the donor taking into account the geometry of the STM-vacuum-silicon-reservoir device. While 45 meV charging energy is obtained for  $D^-$  in bulk Si, the electrostatics of the device reduces the charging energy to ~30 meVs. It is also shown that the reduced charging energy enables spin triplet states to be bound to the donor. The exchange splitting between the singlet and triplet states can be tuned by an external electric field. The computed wavefunctions of the  $D^-$  state helps to understand how the contribution of the momentum space valley states change with donor depth and electric field.

**3:54PM P45.00008 Atomic Precision Donor Devices Fabricated on Strained Silicon on Insulator (sSOI) with SiGe**, E. YITAMBEN, E. BUSSMANN, D.A. SCRYMGEOUR, M. RUDOLPH, S.M. CARR, D.R. WARD, M.S. CARROLL, Sandia National Laboratories — Recently, Si:P donor spin qubits have achieved coherence times (nuclear & e-) that underscore their quantum computing potential. One next major challenge is to integrate donors into a gated structure where electrons can be moved between P, or drawn off of the P to interact, e.g. to an interface as in Kane's proposal. A key constraint is limited thermal budget, to limit P thermal segregation, which precludes typical gate oxidation of Si. We are developing an alternative materials stack utilizing an interfacial barrier layer of relaxed epitaxial SiGe, with donors placed in a strained Si-on-insulator (sSOI) substrate. We fabricate atomic precision donor structures in sSOI via STM hydrogen lithography. Utilizing Si microfabrication and STM in tandem with our Si and Ge molecular beam epitaxy (MBE), we fabricated devices to test our SiGe/sSOI stack concept and atomic-precision fab techniques. To establish our donor-doping capability, we made Hall and Van der Pauw devices in P:sSOI delta-doped layers exhibiting  $n_e > 10^{14}/\text{cm}^2$  and mobilities of  $\sim 100 \text{ cm}^2/\text{Vs}$  ( $T=4\text{K}$ ) similar to results reported relaxed Si reported elsewhere. Second, we have grown our concept epitaxial SiGe/sSOI stack, evaluated the morphology using STM, and fabricated Hall devices to evaluate low-T transport in our first SiGe/sSOI. Here, we report on these advances in atomic precision donor fab, along with STM analysis our MBE SiGe/sSOI. This work extends STM-based atom precision fab on strained Si toward a vertically gated architecture.

#### 4:06PM P45.00009 Low-frequency conductance fluctuations in Si:P and Ge:P $\delta$ -layers , SAQUIB

SHAMIM, Department of Physics, Indian Institute of Science, Bangalore 560 012, India, SUDDHASATTA MAHAPATRA, GIORDANO SCAPPUCCI<sup>1</sup>, W. M. KLESSE, MICHELLE Y. SIMMONS, Centre for Quantum Computation and Communication Technology, University of New South Wales, Sydney NSW 2052, Australia, ARINDAM GHOSH, Department of Physics, Indian Institute of Science, Bangalore 560 012, India — Delta doped Si:P and Ge:P devices offer a formidable platform for application towards quantum computation. The fabrication of single donor devices by STM-lithography takes us forward to address the solid state quantum bits. The atomic scale control however makes the devices extremely sensitive to fluctuations and disorder which affect their long term stability. Hence, a study of low frequency  $1/f$  noise for these devices is desirable. We measure  $1/f$  noise in Si:P and Ge:P  $\delta$ -layers of varying doping density. Fluctuations in conductivity arise due to fluctuations in mobility and the Hooge parameter scales inversely with mobility as  $1/\mu^3$  for all devices. For highly doped Ge:P  $\delta$ -layer, the noise magnitude in a perpendicular magnetic field ( $B_{\perp}$ ) reduces by factors of two at the phase breaking field and the Zeeman field indicating universal conductance fluctuations (UCF). The phase breaking length  $l_{\phi}^{UCF}$  extracted by fitting the  $B_{\perp}$  dependence of noise to the crossover function matches well with  $l_{\phi}^{WL}$  extracted from weak localization (WL) fits to magnetoconductivity indicating that both UCF and WL are governed by same scattering rates.

<sup>1</sup>Present Address: QuTech, Delft University of Technology, P.O. Box 5046, 2600 GA Delft, The Netherlands

#### 4:18PM P45.00010 Weak measurement and quantum steering of spin qubits in silicon , ANDREA

MORELLO, JUHA MUHONEN<sup>1</sup>, STEPHANIE SIMMONS<sup>2</sup>, SOLOMON FREER, JUAN DEHOLLAIN, UNSW Australia, JEFFREY MCCALLUM, DAVID JAMIESON, Univ Melbourne, KOHEI ITOH, Keio University, ANDREW DZURAK, UNSW Australia — Single-shot, projective measurements have been demonstrated with very high fidelities on both the electron [1] and the nuclear [2] spin of single implanted phosphorus (<sup>31</sup>P) donors in silicon. Here we present a series of experiments where the measurement strength is continuously reduced, giving access to the regime of weak measurement of single spins. For the electron qubit, the measurement strength is set by the measurement time compared to the spin-dependent tunneling time between the <sup>31</sup>P donor and a charge reservoir. For the nuclear qubit, the measurement strength is set by the rotation angle of an ESR pulse.

We have demonstrated quantum steering of the spin states, with curious and useful applications. We can improve the fidelity of electron qubit initialization by steering it towards the ground state, thus bypassing thermal effects on the initialization process. We can also accurately measure the electron-reservoir tunnel coupling, without the electron ever tunneling away from the <sup>31</sup>P atom. Finally, these techniques allow the study of weak values and Leggett-Garg inequalities.

[1] A. Morello et al., Nature 467, 687 (2010)

[2] J.J. Pla et al., Nature 496, 334 (2013)

<sup>1</sup>Present address: AMOLF, Amsterdam, The Netherlands

<sup>2</sup>Present address: Simon Fraser University, Burnaby, Canada

#### 4:30PM P45.00011 Single-Shot Charge Readout Using a Cryogenic Heterojunction Bipolar Transistor Preamplifier Inline with a Silicon Single Electron Transistor at Millikelvin Temperatures<sup>1</sup> , MATTHEW CURRY, University of New Mexico, TROY ENGLAND, JOEL WENDT, TAMMY PLUYM, MICHAEL LILLY, STEPHEN

CARR, MALCOLM CARROLL, Sandia National Laboratories — Single-shot readout is a requirement for many implementations of quantum information processing. The single-shot readout fidelity is dependent on the signal-to-noise-ratio (SNR) and bandwidth of the readout detection technique. Several different approaches are being pursued to enhance read-out including RF-reflectometry, RF-transmission, parametric amplification, and transistor-based cryogenic preamplification. The transistor-based cryogenic preamplifier is attractive in part because of the reduced experimental complexity compared with the RF techniques. Here we present single-shot charge readout using a cryogenic Heterojunction-Bipolar-Transistor (HBT) inline with a silicon SET charge-sensor at millikelvin temperatures. For the relevant range of HBT DC-biasing, the current gain is 100 to 2000 and the power dissipation is 50 nW to 5  $\mu$ W, with the microfabricated SET and discrete HBT in an integrated package mounted to the mixing chamber stage of a dilution refrigerator. We experimentally demonstrate a SNR of up to 10 with a bandwidth of 1 MHz, corresponding to a single-shot time-domain charge-sensitivity of approximately  $10^{-4}$   $e/\sqrt{\text{Hz}}$ . This measured charge-sensitivity is comparable to the values reported using the RF techniques.

<sup>1</sup>Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a Lockheed-Martin Company, for the U. S. Department of Energy under Contract No. DE-AC04-94AL85000.

#### 4:42PM P45.00012 Flexible Low-power SiGe HBT Amplifier Circuits for Fast Single-shot Spin Readout<sup>1</sup> , TROY ENGLAND, MICHAEL LILLY, Sandia National Labs, MATTHEW CURRY, CQuIC and the Dept. of Physics and Astronomy, University

of New Mexico, STEPHEN CARR, MALCOLM CARROLL, Sandia National Labs — Fast, low-power quantum state readout is one of many challenges facing quantum information processing. Single electron transistors (SETs) are potentially fast, sensitive detectors for performing spin readout of electrons bound to Si:P donors. From a circuit perspective, however, their output impedance and nonlinear conductance are ill suited to drive the parasitic capacitance of coaxial conductors used in cryogenic environments, necessitating a cryogenic amplification stage. We will introduce two new amplifier topologies that provide excellent gain versus power tradeoffs using silicon-germanium (SiGe) heterojunction bipolar transistors (HBTs). The AC HBT allows in-situ adjustment of power dissipation during an experiment and can provide gain in the millikelvin temperature regime while dissipating less than 500 nW. The AC Current Amplifier maximizes gain at nearly 800 A/A. We will also show results of using these amplifiers with SETs at 4 K. This work was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. DOE Office of Basic Energy Sciences user facility. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation, a Lockheed-Martin Company, for the U. S. Department of Energy under Contract No. DE-AC04-94AL85000.

<sup>1</sup>Flexible Low-power SiGe HBT Amplifier Circuits for Fast Single-shot Spin Readout

#### 4:54PM P45.00013 Dispersively Detected Pauli Spin-Blockade in a Silicon Nanowire Field-Effect Transistor , ANDREAS BETZ, Hitachi Cambridge Laboratory, Cambridge, UK, R WACQUEZ, M. VINET, X. JEHL, CEA-LETI, Grenoble,

France, A.L. SARAIVA, Universidade Federal do Rio de Janeiro, Brasil, M. SANQUER, CEA-LETI, Grenoble, France, A.J. FERGUSON, Cavendish Laboratory, Cambridge, UK, M.F. GONZALEZ-ZALBA, Hitachi Cambridge Laboratory, Cambridge, UK — We report the dispersive readout of the spin state of a double quantum dot (DQD) formed at the corner states of a silicon nanowire FET. Two face-to-face topgate electrodes allow us to independently tune the charge occupation of the quantum dot system down to the few-electron limit. We measure the charge stability of the DQD in DC transport as well as dispersively via in situ gate-based radio frequency (rf) reflectometry, where one top-gate electrode is connected to a resonator. The latter removes the need for external charge sensors in quantum computing architectures and provides a compact way to readout the dispersive shift caused by changes in the quantum capacitance during inter-dot charge transitions. Here, we observe Pauli spin-blockade in the rf response of the circuit at finite magnetic fields between singlet and triplet states. The blockade is lifted at higher magnetic fields when intra-dot triplet states become the ground state configuration. A line shape analysis of the dispersive signal reveals furthermore an intra-dot valley-orbit splitting  $\Delta_{vo} \simeq 145 \mu\text{eV}$ . Our results open up the possibility to operate compact CMOS technology as a singlet-triplet qubit and make split-gate silicon nanowire architectures an ideal candidate for the study of spin dynamics.

**5:06PM P45.00014 Characterization and Monte Carlo simulation of single ion Geiger mode avalanche diodes integrated with a quantum dot nanostructure** , PETER SHARMA, J. B. S. ABRAHAM, G. TEN EYCK, K. D. CHILDS, E. BIELEJEC, M. S. CARROLL, Sandia National Laboratories — Detection of single ion implantation within a nanostructure is necessary for the high yield fabrication of implanted donor-based quantum computing architectures. Single ion Geiger mode avalanche (SIGMA) diodes with a laterally integrated nanostructure capable of forming a quantum dot were fabricated and characterized using photon pulses. The detection efficiency of this design was measured as a function of wavelength, lateral position, and for varying delay times between the photon pulse and the overbias detection window. Monte Carlo simulations based only on the random diffusion of photo-generated carriers and the geometrical placement of the avalanche region agrees qualitatively with device characterization. Based on these results, SIGMA detection efficiency appears to be determined solely by the diffusion of photo-generated electron-hole pairs into a buried avalanche region. Device performance is then highly dependent on the uniformity of the underlying silicon substrate and the proximity of photo-generated carriers to the silicon-silicon dioxide interface, which are the most important limiting factors for reaching the single ion detection limit with SIGMA detectors. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

**5:18PM P45.00015 Joint measurement of electron spin qubits via proximal conductance<sup>1</sup>** , JASON KESTNER, Department of Physics, UMBC — We propose a method to carry out joint measurements on spin qubits that are separated by several microns. Joint measurements, which reveal multi-qubit properties without determining anything about the individual qubits, are a key ingredient to performing quantum error correction and to producing measurement-based entanglement of non-interacting qubits. We presume that the qubits are capacitively coupled to a common conductance channel and are separated by a distance less than the phase coherence length of the semiconductor, and we calculate the tolerance of the procedure to various experimental imperfections. Conditions for carrying out  $N$ -qubit syndrome measurements are discussed.

<sup>1</sup>Support provided by UMBC Office of Research through an SRAIS award.

## **Wednesday, March 16, 2016 2:30PM - 5:30PM — Session P46 DCMP: Metals III 311 - Michael Mehl, NRL**

**2:30PM P46.00001 ABSTRACT WITHDRAWN —**

**2:42PM P46.00002 Orbital-free *ab initio* molecular dynamics study of the free liquid surface of Cd.** , BEATRIZ GONZALEZ DEL RIO, LUIS ENRIQUE GONZALEZ TESEDO, Fisica Teorica, Atomica y Optica, Universidad de Valladolid — We report results of an orbital-free *ab initio* molecular dynamics (OF-AIMD) study of the free liquid surface of Cd at 800 K. A key ingredient in the OF-AIMD method is the local ionic pseudopotential describing the ions-valence electrons interaction. We have developed a force-matching method [1] to derive a local ionic pseudopotential suitable to account for a rapidly varying density system, such as a free liquid surface. Results are reported for several structural properties. The calculated reflectivity shows a marked maximum whose origin is related to the surface layering, along with a shoulder located at a much smaller wavevector transfer. [1] B. G. del Rio and L. E. Gonzalez, J. Phys.: Condens. Matter **26**, 465102 (2014)

**2:54PM P46.00003 A parametric study of surface roughness and bonding mechanisms of aluminum alloys with epoxies: a molecular dynamics simulation.<sup>1</sup>** , RAJENDRA TIMILSINA, STEPHANIE TERMAATH, Univ of Tennessee, Knoxville — The marine environment is highly aggressive towards most materials. However, aluminium-magnesium alloys (Al-Mg, specifically, 5xxx series) have exceptionally long service life in such aggressive marine environments. For instance, an Al-Mg alloy, AA5083, is extensively used in naval structures because of its good mechanical strength, formability, seawater corrosion resistance and weldability. However, bonding mechanisms of these alloys with epoxies in a rough surface environment are not fully understood yet. It requires a rigorous investigation at molecular or atomic levels. We performed a molecular dynamics simulation to study an adherend surface preparation and surface bonding mechanisms of Al-Mg alloy (AA5083) with different epoxies by developing several computer models. Various distributions of surface roughness are introduced in the models and performed molecular dynamics simulations. Formation of a beta phase (Al<sub>3</sub>Mg<sub>2</sub>), microstructures, bonding energies at the interface, bonding strengths and durability are investigated.

<sup>1</sup>Office of Naval Research

**3:06PM P46.00004 ABSTRACT WITHDRAWN —**

**3:18PM P46.00005 Viscoelastic damping in crystalline composites and alloys** , RAGHAVAN RANGANATHAN, RAHMI OZISIK, PAWEL KEBLINSKI, Rensselaer Polytech Inst — We use molecular dynamics simulations to study viscoelastic behavior of model Lennard-Jones (LJ) crystalline composites subject to an oscillatory shear deformation. The two crystals, namely a soft and a stiff phase, individually show highly elastic behavior and a very small loss modulus. On the other hand, when the stiff phase is included within the soft matrix as a sphere, the composite exhibits significant viscoelastic damping and a large phase shift between stress and strain. In fact, the maximum loss modulus in these model composites was found to be about 20 times greater than that given by the theoretical Hashin-Shtrikman upper bound. We attribute this behavior to the fact that in composites shear strain is highly inhomogeneous and mostly accommodated by the soft phase, corroborated by frequency-dependent Grüneisen parameter analysis. Interestingly, the frequency at which the damping is greatest scales with the microstructural length scale of the composite. Finally, a critical comparison between damping properties of these composites with ordered and disordered alloys and superlattice structures is made.

**3:30PM P46.00006 A general and predictive model of anisotropic grain boundary energy and morphology for polycrystal-level simulations** , BRANDON RUNNELS, University of Colorado Colorado Springs, IRENE BEYERLEIN, Los Alamos National Laboratory, SERGIO CONTI, University of Bonn, MICHAEL ORTIZ, California Institute of Technology — In this work, a new model for anisotropic GB energy and morphology is formulated that is fast, general, dependent on only three material parameters, and is verified by comparison with more than 40 MD and experimental datasets for (a)symmetric, tilt/twist, FCC/BCC materials, as well as experimental measurements. A relaxation algorithm is presented that is able to efficiently compute the optimal facet pattern and corresponding relaxed energy. Finally, the GB model is implemented as an interface model in a polycrystal simulation to observe the effects of GB in conjunction with elastic and plastic deformation. The simulations are compared with those using an isotropic GB model, and the effect of the GB isotropy on the bulk properties and microstructure is determined. The results have applications towards, e.g., improved polycrystal simulations, understanding void nucleation, and GB engineering.

**3:42PM P46.00007 Atomic-Scale Imprinting into Amorphous Metals**, UDO SCHWARZ, RUI LI, GEORG SIMON, EMELY KINSER, ZE LIU, ZHENG CHEN, CHAO ZHOU, JONATHAN SINGER, CHINEDUM OSUJI, JAN SCHROERS, Yale University — Nanoimprinting by thermoplastic forming (TPF) has attracted significant attention in recent years due to its promise of low-cost fabrication of nanostructured devices. Usually performed using polymers, amorphous metals have been identified as a material class that might be even better suited for nanoimprinting due to a combination of mechanical properties and processing ability. Commonly referred to as metallic glasses, their featureless atomic structure suggests that there may not be an intrinsic size limit to the material's ability to replicate a mold. To study this hypothesis, we demonstrate atomic-scale imprinting into amorphous metals by TPF under ambient conditions. Atomic step edges of a SrTiO<sub>3</sub> (STO) single crystal used as mold were successfully imprinted into Pt-based bulk metallic glasses (BMGs) with high fidelity. Terraces on the BMG replicas possess atomic smoothness with sub-Angstrom roughness that is identical to the one measured on the STO mold. Systematic studies revealed that the quality of the replica depends on the loading rate during imprinting, that the same mold can be used multiple times without degradation of mold or replicas, and that the atomic-scale features on as-imprinted BMG surfaces has impressive long-term stability (months).

**3:54PM P46.00008 First principles study of lattice disordering and magnetic behavior in Cu-NiMnAl and CuNiMnSn Heusler alloys**, SHIFRAH ARON-DINE, Harvey Mudd College, GREGORY POMREHN, The Boeing Company, AURORA PRIBRAM-JONES, Lawrence Livermore National Lab, LORI BASSMAN, Harvey Mudd College — In this work we present density functional theory calculations on two new Heusler alloys, CuNiMnAl and CuNiMnSn, and explore how the electronic properties of these structures are affected by atomic disordering. Elements are disordered 1%-25% on constant and varying sublattices to explore changes in electronic structure and magnetization. We then use a Monte Carlo method to predict expected magnetic behavior and compare with experimental results.

**4:06PM P46.00009 First principles statistical mechanics of alloys and magnetism<sup>1</sup>**, MARKUS EISENBACH, SUFFIAN N. KHAN, YING WAI LI, Oak Ridge National Lab — Modern high performance computing resources are enabling the exploration of the statistical physics of phase spaces with increasing size and higher fidelity of the Hamiltonian of the systems. For selected systems, this now allows the combination of Density Functional based first principles calculations with classical Monte Carlo methods for parameter free, predictive thermodynamics of materials. We combine our locally selfconsistent real space multiple scattering method for solving the Kohn-Sham equation with Wang-Landau Monte-Carlo calculations (WL-LSMS). In the past we have applied this method to the calculation of Curie temperatures in magnetic materials. Here we will present direct calculations of the chemical order disorder transitions in alloys. We present our calculated transition temperature for the chemical ordering in CuZn and the temperature dependence of the short-range order parameter and specific heat. Finally we will present the extension of the WL-LSMS method to magnetic alloys, thus allowing the investigation of the interplay of magnetism, structure and chemical order in ferrous alloys.

<sup>1</sup>This research was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division and it used Oak Ridge Leadership Computing Facility resources at Oak Ridge National Laboratory.

**4:18PM P46.00010 First-principles Co database: Energetics of binary Co alloys and compounds<sup>1</sup>**, SHAHAB NAGHAVI, VINAY HEGDE, CHRIS WOLVERTON, Department of Materials Science and Engineering, Northwestern University, Evanston, Illinois 60208, USA — The field of superalloys has received a recent spike in interest with the discovery of metastable  $\gamma'$ -Co<sub>3</sub>(Al,W) precipitates with the L1<sub>2</sub> structures. We present density functional calculations for the first and second nearest-neighbor solute-vacancy binding energies of 27 substitutional solutes in fcc-cobalt. As by-products, we also calculate the dilute mixing energy, dilute volume of mixing, and solubility enthalpy. A modest correlation between the solute size and its binding to an accompanying vacancy has been found. Our calculations reveal that a vacancy not only relieves the strain associated with large solutes, but also mediates a weak bonding between the large solute and its next nearest-neighbor atoms, resulting in high solute-vacancy binding energies. We also find that the solute-vacancy binding energy is minimized for a half-filled *d*-band, in the middle of a transition metal series, and varies parabolically with the *d*-band filling. In general, 4*d* and their counterpart 5*d* transition metals have nearly similar solute-vacancy binding energies, but much larger than those of 3*d* transition metals, and the deviation increase by moving away from a half-filled band.

<sup>1</sup>Center for Hierarchical Materials Design (CHiMaD)

**4:30PM P46.00011 X-ray measurements of the self-organization of martensitic variants during thermal cycling**, DANIEL PEREZ, University of Ottawa, MARK SUTTON, McGill University, MICHAEL ROGERS, University of Ottawa — The deformation of most types of metals involves an irreversible flow of crystallographic dislocations. This allows for their ductility. The deformation of a metallic shape memory alloy (SMA), on the other hand, is accommodated by a solid-solid phase transition. If deformed in the low-temperature martensitic phase, an SMA can be returned to its original shape by raising its temperature to the point where it changes back to its high-temperature parent phase. When the reverse occurs and the transformation is from parent to martensitic phase, an SMA goes from a high-symmetry to a low-symmetry state in which a number of martensitic variants are produced. We monitored the self-organization of these variants during cycles of periodic thermal driving. This was done using in situ X-ray Photon Correlation Spectroscopy (XPCS), which uses correlation from X-ray speckle to quantify the degree of microstructural change in a material. Our measurements revealed enhanced reversibility in the organization of the martensitic variants as the system evolved during repeated thermal cycling.

**4:42PM P46.00012 Long-time atomistic evolution of grain boundary in nickel using the kinetic activation-relaxation technique**, SAMI MAHMOUD, MICKAL TROCHET, OSCAR RESTREPO, NORMAND MOUSSEAU, University of Montreal — The microscopic mechanisms associated with the evolution of metallic materials are still a matter of debate as both experimental and numerical approaches fail to provide a detailed atomic picture of their time evolution. Here, we use the kinetic activation-relaxation technique (k-ART) [1], an unbiased off-lattice kinetic Monte Carlo method with on-the-fly catalog building to overcome these limitations and follow the atomistic evolution of a 10,000-atom grain boundary Ni system over macroscopic time scales. We first characterize the kinetic properties of four different empirical potentials, the embedded atom method (EAM), the first and second modified embedded atom method (MEAM1NN and MEAM2NN respectively) and the Reax force field (ReaxFF) potentials. Comparing the energetics, the elastic effects and the diffusion mechanisms for systems with one to three vacancies and one to three self-interstitials in nickel simulated over second time scale, we conclude that ReaxFF and EAM potentials are closest to experimental values. We then proceed to study the long-time evolution of a grain boundary with the Reax forcefield and to offer a detailed description of its energy landscape, including the exact description of short and long-range effects on self-diffusion along the interface. [1] N. Mousseau *et al*, *Comput. Mater. Sci.*, vol. 100, pp. 111–123, 2015.

**4:54PM P46.00013 Fluid-like flows in large-strain deformation of metals** , HO YEUNG, National Institute of Standards and Technology, DINAKAR SAGAPURAM<sup>1</sup>, Koushik Viswanathan, Purdue University, NARAYAN SUNDARAM, Indian Institute of Science, ANIRBAN MAHATO, KEVIN TRUMBLE, SRINIVASAN CHANDRASEKAR, Purdue University — Laminar or smooth plastic flow, commonly observed in large deformation of metals, becomes unstable under certain conditions, resulting in inhomogeneous plastic flow. Using *in situ* imaging, we demonstrate the unique features of two inhomogeneous flow modes in metal plasticity — the well-known shear band flow and the recently discovered sinuous flow — and methods for suppressing them. Both modes occur via a two stage process — nucleation and flow development. The nucleation stage results in a weak material zone and the development stage involves imposition of significant strains. In the case of shear bands, using additional micro-marker techniques, we show that the second stage is well described by a viscous slider model. As a result, controlling the second stage causes band formation to cease. We demonstrate the use of this method — Passive Geometric Flow control — to form long strips from metallic alloys that are difficult to form conventionally. For sinuous flow, nucleation and flow formation kinematics show remarkable resemblance with flows in complex fluids. The nucleation stage can be altered using suitable ink coatings on the free surface or by surface pre-straining, and we use this idea to demonstrate complete sinuous flow suppression.

<sup>1</sup>Membership pending

**5:06PM P46.00014 Grain Growth in Cerium Metal** , JASON COOLEY, Los Alamos National Laboratory, MARTHA KATZ, None, CHARLES MIELKE, JOEL MONTALVO, Los Alamos National Laboratory — We report on grain growth in forged and rolled cerium plate for temperatures from 350 to 700 degrees C and times from 30 to 120 minutes. The cerium was made by arc-melting into a 25 mm deep by 80 mm diameter copper mold. The resulting disk was forged at room temperature to a 25% reduction of thickness four times with a 350 degree C strain relief heat treatment for 60 minutes between forging steps. The resulting 8 mm thick plate was cold rolled at room temperature to a 25% reduction of thickness three times with a 350 C strain relief heat treatment between steps resulting in a plate approximately 3 mm thick. 5 x 10 mm coupons were cut from the plate for the grain growth study.

**5:18PM P46.00015 Ab initio calculation of oxygen self-diffusion coefficient in uranium dioxide**  $\text{UO}_2$  , BORIS DORADO, CEA, DAM, DIF - Bruyeres-le-Chatel, France, PHILIPPE GARCIA, CEA, DEN, DEC - Cadarache, France, MARC TORRENT, CEA, DAM, DIF - Bruyeres-le-Chatel, France — Uranium dioxide  $\text{UO}_2$  is the most widely used nuclear fuel worldwide and its atomic transport properties are relevant to practically all engineering aspects of the material. Although transport properties have already been studied in  $\text{UO}_2$  by means of first-principles calculations, the ab initio determination of self-diffusion coefficients has up to now remained unreachable because the relevant computational tools were neither available or adapted. The present work reports our results related to the ab initio calculation of the oxygen self-diffusion coefficient in  $\text{UO}_2$ . We first determine the Gibbs free energies of formation of oxygen charged defects by calculating both the electronic and vibrational (hence entropic) contributions. Then, we use the transition state theory in order to compute the effective jump frequency of the defects, which in turn provides us with the value of the pre-exponential factor. The results are compared to self-diffusion data obtained experimentally with a careful monitoring of the relevant thermodynamic conditions (oxygen partial pressure, temperature, impurity content).

## Wednesday, March 16, 2016 2:30PM - 5:06PM – Session P47 FOEP: Beyond the Lab: Bringing History and Physics to the Public 312 -

**2:30PM P47.00001 Creating a Community to Strengthen the Broader Impacts of Condensed Matter Physics Research**<sup>1</sup> , SHIREEN ADENWALLA, JOCELYN BOSLEY, Dept of Physics, University of Nebraska, GREGORY VOTH, Dept of Physics, Wesleyan University, LEIGH SMITH, Dept of Physics, University of Cincinnati — The Broader Impacts (BI) merit criteria set out by the National Science Foundation are essential for building the public support necessary for science to flourish. Condensed matter physicists (CMP) have made transformative impacts on our society, but these are often invisible to the public. Communicating the societal benefits of our research can be challenging, because CMP consists of many independent research groups for whom effective engagement in the public arena is not necessarily a forte. Other BI activities, such as engaging K-12 students and teachers to increase scientific literacy and strengthen the STEM workforce, may be very effective, but these are often isolated and short in duration. To increase the visibility of CMP and to make the implementation of BI activities more efficient, we have created a website with two sides: a public side to communicate to a broad audience exciting scientific discoveries in CMP and the technologies they enable, and a private side for condensed matter researchers to communicate with one another about effective broader impact activities. Here we discuss the content of the new website, and the best practices we have identified for communicating the excitement of CMP research to the broadest possible audience.

<sup>1</sup>NSF-DMR 1550737, 1550724 and 1550681

**2:42PM P47.00002 Schrödinger's Magnetic Ambitions: His Attempts in the 1940s to Understand Terrestrial Magnetism through a Unitary Field Theory.** , PAUL HALPERN, University of the Sciences in Philadelphia — In 1943, Schrödinger presented several papers to the Royal Irish Academy outlining his efforts to unify electromagnetism, gravitation, and what is now known as the strong force in a Unitary Field Theory. To furnish experimental proof for his ideas, he suggested that variations in Earth's magnetic field might be understood through his theoretical notion that electromagnetism is attenuated by a kind of cosmological constant. We'll explore the nature and context of his proposal and examine reactions to his assertions.

**2:54PM P47.00003 The Schrödinger Sessions: Science for Science Fiction**<sup>1</sup> , CHAD ORZEL, Union College Dept. of Physics and Astronomy, EMILY EDWARDS, STEVEN ROLSTON, Joint Quantum Institute — In July 2015, we held a workshop for 17 science fiction writers working in a variety of media at the Joint Quantum Institute at the University of Maryland, College Park. "The Schrödinger Sessions," funded by an outreach grant from APS, provided a three-day "crash course" on quantum physics and technology, including lectures from JQI scientists and tours of JQI labs. The goal was to better inform and inspire stories making use of quantum physics, as a means of outreach to inspire a broad audience of future scientists. We will report on the contents of the workshop, reactions from the attendees and presenters, and future plans.

<sup>1</sup>Funded by an Outreach Mini-Grant from the APS

**3:06PM P47.00004 Layman friendly spectroscopy<sup>1</sup>**, STIPO SENTIC, SHARON SESSIONS, New Mexico Tech — Affordable consumer grade spectrometers (e.g. SCiO, Qualcomm Tricorder XPRIZE) are becoming more available to the general public. We introduce the concepts of spectroscopy to the public and K12 students and motivate them to delve deeper into spectroscopy in a dramatic participatory presentation and play. We use diffraction gratings, lasers, and light sources of different spectral properties to provide a direct experience of spectroscopy techniques. Finally, we invite the audience to build their own spectrometer—utilizing the APS SpectraSnapp cell phone application—and study light sources surrounding them in everyday life. We recontextualize the stigma that science is hard (e.g. Math, Science Popular Until Students Realize They're Hard, The Wall Street Journal) by presenting the material in such a way that it demonstrates the scientific method, and aiming to make failure an impersonal scientific tool—rather than a measure of one's ability, which is often a reason for shying away from science. We will present lessons we have learned in doing our outreach to audiences of different ages.

<sup>1</sup>This work is funded by the APS Outreach Grant "Captain, we have matter matters!" We thank New Mexico Tech Physics Department and Physics Club for help and technical equipment.

**3:18PM P47.00005 Value of Fundamental Science**, ALEXEY BUROV, Fermilab — Fundamental science is a hard, long-term human adventure that has required high devotion and social support, especially significant in our epoch of Mega-science. The measure of this devotion and this support expresses the real value of the fundamental science in public opinion. Why does fundamental science have value? What determines its strength and what endangers it? The dominant answer is that the value of science arises out of curiosity and is supported by the technological progress. Is this really a good, astute answer? When trying to attract public support, we talk about the mystery of the universe<sup>1</sup>. Why do these words sound so attractive? What is implied by and what is incompatible with them? More than two centuries ago, Immanuel Kant asserted an inseparable entanglement between ethics and metaphysics. Thus, we may ask: which metaphysics supports the value of scientific cognition, and which does not? Should we continue to neglect the dependence of value of pure science on metaphysics? If not, how can this issue be addressed in the public outreach? Is the public alienated by one or another message coming from the face of science? What does it mean to be politically correct in this sort of discussion?

**3:30PM P47.00006 Putting Research in the Classroom: A Partnership for Curriculum Building**, NATHAN TOMPKINS, ANIQUE OLIVIER-MASON, Brandeis University — Many science classes today are taught in a historical context as if scientific discovery was something that only happened in the past with textbooks focused on presenting facts and equations without conveying that the process of science is to ask and answer questions. To address these deficiencies we have developed a science outreach course to unite high school science educators with young researchers for a series of workshops to develop teaching modules. The modules connect specific textbook concepts and state standards to current materials science research in hands-on learning experiences for high school students. The idea is to make math, science, technology, and engineering concepts more exciting, accessible, and relevant to high school students through interactions with diverse researchers and instruction from curriculum based on cutting-edge materials science research. The goal is to demonstrate that science is a living, active process of inquiry and questioning; not simply a litany of facts, figures, and historical anecdotes. The ultimate aim is for the teaching modules prepared in this course to be packaged and prepared for dissemination to schools outside the immediate vicinity in order to expand the reach to communities underrepresented in the sciences.

**3:42PM P47.00007 Discover Science Initiative, outreach and professional development at the University of California, Irvine<sup>1</sup>**, JILL PESTANA, JAMES EARTHMAN, Univ of California - Irvine — Discover Science Initiative (DSI) is an unprecedented success in the Southern Californian community by reaching out to over 5,000 participants through eight hands-on workshops on topics from fungi to the physics of light, and two large events in the past year. The DSI vision is to provide an avenue for University of California, Irvine (UCI) students and faculty from all departments to engage with the local community through workshops and presentations on interdisciplinary, state-of-the-art STEM research unique to UCI. DSI provides professional development opportunities for diverse students at UCI, while providing outreach at one of the most popular educational centers in Southern California, the Discovery Cube, which hosts over 400,000 guests each year. In DSI, students engage in peer-to-peer mentoring with guidance from the UCI School of Education in designing workshops, leading meetings, and managing teams. Also, students practice science communication, coached by certified communications trainers. Students involved in DSI learn important skills to complement their academic degrees, and stay motivated to pursue their career goals.

<sup>1</sup>Support for DSI is from Diverse Educational and Doctoral Experience (DECADE) at UCI.

**3:54PM P47.00008 Texas A&M Physics Festival: bringing together the community, faculty, and students**, TATIANA ERUKHIMOVA, Texas A&M University — Texas A&M Physics Festival started in 2003 with a dozen of hands-on exhibits and an inaugural lecture by Stephen Hawking. Over the years it evolved into one of the largest STEM outreach events in the area. The Festival attracts over 4000 visitors annually from all over Texas and other states. It features over 100 interactive exhibits displayed by faculty and students, public lectures by world-renowned scientists and astronauts, professional bubble shows, and many other activities. I will report on the structure of the Festival as well as strategies for involving undergraduate and graduate students and faculty in public outreach. I will further discuss the results of an independent evaluation of the 2015 Festival by the NSF-funded EvalFest program.

**4:06PM P47.00009 Movie Physics: pirates, spies and other worlds.<sup>1</sup>**, BEATRIZ GONZALEZ DEL RIO, V. GONZALEZ-FERNANDEZ, Universidad de Valladolid and Physics League Association, J.L. MARTIN, Physics League Association, L. SANCHEZ-TEJERINA, Universidad de Valladolid and Physics League Association, G. PEREZ, L. ARES, E. VASALLO, P. MARTIN, V. VILLA, S. GARCIA, M. VARA, S. MARTIN, P. ALVAREZ, C. GONZALEZ, P. LOPEZ, Physics League Association, M.A. BURGOS, Universidad de Valladolid and Physics League Association, V.M. GONZALEZ, J. CARBAJO, Physics League Association, C. VELASCO-MERINO, F. HEVIA, Universidad de Valladolid and Physics League Association, F. MARTINEZ, J.F. MARTINEZ, Physics League Association, D. GONZALEZ-HERRERO, A.H. GLORIANI, D. MATEOS, Universidad de Valladolid and Physics League Association — Taking advantage of many popular films, the basics of many physical principles can be shown in a really attractive and stunning way. Five shows/workshops form this project attending the necessities of the target public: kids become pirates, high-school students are pushed to the limit and visit other fantasy worlds, and the general public discover the powers of physics and some terrifying secrets. By November 2015 we have obtained more than 2900 viewers. The activities have been presented in different national and international conferences, on an international science fair and have been published by several Spanish media. During 2015 the Physics League Association has received three international awards due to some activities from this project. Additional Authors: B. G. del Rio [1,2], V. Gonzalez-Fernandez [1,2], J. L. Martin [1], L. Sanchez-Tejerina [1,2], G. Prez [1], L. Ares [1], E. Vasallo [1], P. Martin [1], V. Villa [1], S. Garca [1], M. Vara [1], S. Martin [1], P. Alvarez [1], C. Gonzalez [1], P. Lopez [1], M.A. Burgos [1,2], V. M. Gonzalez [1], J. Carabajo [1], C. Velasco-Merino [1,2], F. Hevia [1,2], D. Gutiez [1], F. Martinez [1], J. F. Martinez [1], L. E. Vazquez [1], M. Bueno [1], M. Escribano [1], P. Guillem [1], R. Garca [1], D. Gonzalez [1], D. Gonzalez-Herrero [1,2], A. H. Gloriani [1,2], J. Ctores [1], J. Hernandez [1], A. Ivarez [1], M. Ivarez [1], D. Mateos [1,2]

[1] Physics League Association, SPAIN

[2] Universidad de Valladolid, SPAIN

<sup>1</sup>APS Mini Grants 2015, EPS Young Minds and OSA

**4:18PM P47.00010 Title: SCOAP<sup>3</sup>: Explanation and Current Status** , MATTHEW MARSTELLER, Carnegie Mellon University — The Sponsoring Consortium for Open Access Publishing in Particle Physics (SCOAP<sup>3</sup>) is a successful global partnership of libraries, funding agencies and research centers. SCOAP<sup>3</sup> has negotiated with journal publishers on behalf of libraries and institutions from around the world to produce open access literature in particle physics journals that were previously published in a traditional subscription-based model. This presentation will provide an overview of the process, an update of its status and some intriguing research metrics that have emerged.

**4:30PM P47.00011 First Megascience Experiment at Fermilab: Through Hardship to Protons** , VITALY PRONSKIKH, VALERIE HIGGINS, Fermi National Accelerator Laboratory — The E-36 experiment on the small angle proton-proton scattering that officially started in 1970, making use of the Main Ring beams and giving rise to a chain of similar experiments that continued after 1972, was the first experiment at the newly built NAL. It was also the first US/USSR collaboration in particle physics as well as the first experiment that can be confidently characterized as megascience. The experimental data were interpreted as an indication of the pomeron, a quasiparticle that had been named after the Soviet theorist I. Pomeranchuk. The idea of the experiment can be traced back to the Rochester conference held in 1970 in Kiev where two American and Soviet physicists met to develop it and later acquainted NAL director Robert Wilson with it. Wilson enthusiastically set the stage for the experiment at NAL. Involving a gas-jet target built at the Dubna machine shop of Joint Institute for Nuclear Research and brought to Batavia, Illinois, the experiment established cooperation between the US and the Soviets in the spirit of their contemporary Apollo-Soyuz space program, thus breaking the ice of the Cold War from within high-energy physics. In this talk based on the Fermilab Archives and interviews, we discuss the financial and administrative obstacles raised by Soviet officials that the Russian collaborators had to overcome, interinstitutional tensions among the Soviets that accompanied the collaboration, NAL culture as well as the roles of scientists in megascience as ambassadors of peace.

**4:42PM P47.00012 ABSTRACT WITHDRAWN —**

**4:54PM P47.00013 The Japanese aerial attack on Hanford Engineer Works** , CHARLES W. CLARK, Joint Quantum Institute — The day before the Pearl Harbor attack, December 6, 1941, the University of Chicago Metallurgical Laboratory was given four goals: design a plutonium (Pu) bomb; produce Pu by irradiation of uranium (U); extract Pu from the irradiated U; complete this in time to be militarily significant.<sup>1</sup> A year later the first controlled nuclear chain reaction was attained in Chicago Pile 1 (CP-1). In January 1943, Hanford, WA was chosen as the site of the Pu factory.<sup>2</sup> Neutron irradiation of <sup>238</sup>U was to be used to make <sup>239</sup>Pu. This was done by a larger version of CP-1, Hanford Reactor B, which went critical in September 1944. By July 1945 it had made enough Pu for two bombs: one used at the Trinity test in July; the other at Nagasaki, Japan in August. I focus on an ironic sidelight to this story: disruption of hydroelectric power to Reactor B by a Japanese fire balloon attack on March 10, 1945. This activated the costly coal-fired emergency backup plant to keep the reactor coolant water flowing, thwarting disaster and vindicating the conservative design of Hanford Engineer Works.

<sup>1</sup> *Management of the Hanford Engineer Works in World War II*, H. Thayer (ASCE Press 1996)

<sup>2</sup> *Made in Hanford: The Bomb that Changed the World*, H. Williams (Washington State U. Press 2011)

## Wednesday, March 16, 2016 2:30PM - 5:30PM —

**Session P48 GQI: Quantum Control in Superconducting Circuits** 349 - Alexander Korotkov, University of California, Riverside

**2:30PM P48.00001 Quantum Control of Cavity Resonators, Part I: Control Algorithms** , PHILIP REINHOLD, REINIER HEERES, NISSIM OFEK, KATRINA SLIWA, Yale University, MICHAEL HATRIDGE, University of Pittsburgh, STEFAN KRASTANOV, LIANG JIANG, LUIGI FRUNZIO, MICHEL DEVORET, ROBERT SCHOELKOPF, Yale University — Harmonic oscillators are linear systems with equally spaced energy levels, which makes them hard to control. We have previously explored a constructive control approach mediated by a far off-resonantly coupled two-level ancilla. Here we present an extension to that method which relies on optimal control algorithms to allow much more efficient quantum control of a combined resonator ancilla system. We show that full control of the resonator is possible on a time-scale of order  $1/\chi$ , the dispersive shift. In practice this means that a unitary operation on the Hilbert space of our superconducting resonator truncated to 8 levels can be performed using a pulse of around a microsecond.

**2:42PM P48.00002 Quantum Control of Cavity Resonators, Part II: Experiment** , REINIER HEERES, PHILIP REINHOLD, NISSIM OFEK, KATRINA SLIWA, Yale University, MICHAEL HATRIDGE, University of Pittsburgh, STEFAN KRASTANOV, LIANG JIANG, LUIGI FRUNZIO, MICHEL DEVORET, ROBERT SCHOELKOPF, Yale University — Harmonic oscillators offer a large Hilbert space that can potentially be used to encode multiple bits of quantum information. The long lifetime of superconducting cavity resonators make them a suitable candidate to explore this direction. Due to the linearity of harmonic oscillators it is not directly obvious how to manipulate them. Here we show that pulses designed using optimal control methods allow us to manipulate the combined cavity – transmon system on a time-scale of order  $1/\chi$ , the dispersive shift; in practice pulses of about a microsecond long. Several example unitary operations addressing the first 8 levels of the resonator are described and characterized.

**2:54PM P48.00003 Optimal control of single flux quantum (SFQ) pulse sequences** , PER LIEBERMANN, FRANK WILHELM, Saarland University — Single flux quantum (SFQ) pulses are a natural candidate for on-chip control of superconducting qubits [1]. High accuracy quantum gates are accessible with quantum optimal control methods. We apply trains of SFQ pulses to operate single qubit gates, under the constraint of fixed amplitude and duration of each pulse. Timing of the control pulses is optimized using genetic algorithms and simulated annealing, decreasing the average fidelity error by several orders of magnitude. Furthermore we are able to reduce the gate time to the quantum speed limit. Leakage out of the qubit subspace as well as timing errors of the pulses are considered, exploring the robustness of our optimized sequence. This takes us one step further to a scalable quantum processor. [1] R. McDermott and M.G. Vavilov, Phys. Rev. Appl. 2, 014007 (2014)

**3:06PM P48.00004 Robust Control of a Two-Qubit Operation in 3D Circuit Quantum Electrodynamics** , JOSEPH ALLEN, ATI, University of Surrey, ROBERT KOSUT, SC Solutions, Inc., JAEWOO JOO, ERAN GINOSSAR, ATI, University of Surrey — Superconducting qubits have shown great improvement in coherence times with the introduction of 3D cavities. In order to control the qubits in 3D a microwave drive is usually coupled to the common mode of the cavity, which makes individual addressability a challenge and causes additional unwanted single and two-qubit dynamics when performing two qubit operations. Quantum information processing requires precise control of the system dynamics in the presence of potential uncertainties in the estimated system parameters. We use optimal control theory to develop pulse shapes that are able to implement an all-microwave two-qubit gate, while mitigating extra unwanted interaction terms, with  $\mathcal{F} = 0.9964$ . In addition we develop pulses which are robust to errors in the two qubit transition frequencies. This is demonstrated with experimentally relevant parameters and includes realistic constraints in the possible pulse shapes, presenting pulses that can be implemented in experiment.

**3:18PM P48.00005 Gradient Optimization for Analytic conTrols - GOAT** , ELIE ASSÉMAT, Saarland University, SHAI MACHNES, DAVID TANNOR, Weizmann Institute of Science, FRANK WILHELM-MAUCH, Saarland University — Quantum optimal control becomes a necessary step in a number of studies in the quantum realm. Recent experimental advances showed that superconducting qubits can be controlled with an impressive accuracy. However, most of the standard optimal control algorithms are not designed to manage such high accuracy. To tackle this issue, a novel quantum optimal control algorithm have been introduced: the Gradient Optimization for Analytic conTrols (GOAT). It avoids the piecewise constant approximation of the control pulse used by standard algorithms. This allows an efficient implementation of very high accuracy optimization. It also includes a novel method to compute the gradient that provides many advantages, e.g. the absence of backpropagation or the natural route to optimize the robustness of the control pulses. This talk will present the GOAT algorithm and a few applications to transmons systems.

**3:30PM P48.00006 Fast resonator reset in circuit QED using open quantum system optimal control** , SAMUEL BOUTIN, Département de Physique, Université de Sherbrooke, CHRISTIAN KRAGLUND ANDERSEN, Department of Physics and Astronomy, Aarhus University, JAYAMEENAKSHI VENKATRAMAN, Department of Physics, Indian Institute of Technology Kanpur, ALEXANDRE BLAIS, Département de Physique, Université de Sherbrooke and Canadian Institute for Advanced Research — Practical implementations of quantum information processing requires repetitive qubit readout. In circuit QED, where readout is performed using a resonator dispersively coupled to the qubits, the measurement repetition rate is limited by the resonator reset time. This reset is usually performed passively by waiting several resonator decay times. Alternatively, it was recently shown that a simple pulse sequence allows to decrease the reset time to twice the resonator decay time [1]. In this work, we show how to further optimize the ring-down pulse sequence by using optimal control theory for open quantum systems. Using a new implementation of the open GRAPE algorithm that is well suited to large Hilbert spaces, we find active resonator reset procedures that are faster than a single resonator decay time. Simple quantum speed limits for this kind of active reset processes will be discussed. [1] McClure et al., arXiv 1503.01456

**3:42PM P48.00007 ABSTRACT WITHDRAWN —**

**3:54PM P48.00008 Analysis of non-adiabatic effects in circuit QED measurement of a transmon** , ERIC MLINAR, MOSTAFA KHEZRI, University of California, Riverside, JUSTIN DRESSEL, Chapman University, ALEXANDER N. KOROTKOV, University of California, Riverside — In a circuit QED setup with a transmon qubit dispersively coupled to a driven resonator, we investigate whether rapid resonator ringup will cause nonadiabatic effects that disturb the qubit state. We show that only unrealistically fast high-power pulses will produce significant deviations from adiabatic behavior, while typically the qubit-resonator dynamics is well described by coherent evolution in the joint eigenbasis. Nevertheless, even in typical parameter regimes we show that the qubit nonlinearity still produces a dynamical shearing effect that squeezes the state of the resonator field.

**4:06PM P48.00009 A method of extracting operating parameters of a quantum circuit** , EYOB A. SETE, MAXWELL BLOCK, MICHAEL SCHEER, CRIS ZANOCI, MEHRNOOSH VAHIDPOUR, DANE THOMPSON, CHAD RIGETTI, Rigetti Quantum Computing, Berkeley, CA — Rigorous simulation-driven design methods are an essential component of traditional integrated circuit design. We adapt these techniques to the design and development of superconducting quantum integrated circuits by combining classical finite element analysis in the microwave domain with Brune circuit synthesis by Solgun [PhD thesis 2014] and BKD Hamiltonian analysis by Burkard et al. [Phys. Rev. B **69**, 064503 (2004)]. Using the Hamiltonian of the quantum circuit, constructed using the synthesized equivalent linear circuit and the nonlinear Josephson junctions' contributions, we extract operating parameters of the quantum circuit such as resonance coupling strength, dispersive shift, qubit anharmonicity, and decoherence rates for single- and multi-port quantum circuits. This approach has been experimentally validated and allows the closed-loop iterative simulation-driven development of quantum information processing devices.

**4:18PM P48.00010 Critical fluctuations near excitation threshold of a quantum parametric oscillator** , M. I. DYKMAN, Michigan State University, Y. NAKAMURA, The University of Tokyo and CEMS RIKEN, Z. R. LIN, CEMS RIKEN — A weakly damped parametrically driven oscillator has several vibrational states already for weak driving. These are stable and unstable states with twice the modulation period and also the steady state. At the critical point all states merge. We show that this leads to anomalously strong quantum fluctuations. These fluctuations are similar whether the friction, in the classical picture, is linear or nonlinear. The critical region is  $\propto [\hbar(2\bar{n} + 1)]^{1/3}$  along the field frequency axis and  $\propto [\hbar(2\bar{n} + 1)]^{2/3}$  along the field amplitude axis, where  $\bar{n}$  is the Planck number. The correlation time scales as  $[\hbar(2\bar{n} + 1)]^{-2/3}$ . The number of photons for  $\bar{n} = 0$  scales as  $\hbar^{-2/3}$ . It is determined by the oscillator nonlinearity and decay rate. Above the threshold, quantum fluctuations induce transitions between the period-two states over the quasienergy barrier. We find the effective quantum activation energies for such transitions and their scaling with the difference of the driving amplitude from its critical value. We also present the results of relevant experimental observations obtained with a circuit QED system.

**4:30PM P48.00011 Fluctuations of a parametric oscillator: from the semiclassical to a strongly quantum regime** , YAXING ZHANG, MARK DYKMAN, Michigan State University — A semiclassical parametric oscillator has two dynamically stable vibrational states with equal amplitudes and with phases differing by  $\pi$ . The rate of switching between these states is exponentially small, and the oscillator displays fluctuations with the reciprocal correlation time given by this rate. It also displays critical slowing down near the excitation threshold. The parameter of the “quantumness” is the ratio of the nonequidistance  $\hbar V$  of the oscillator energy levels due to the nonlinearity and the level width  $\hbar\Gamma$  due to decay. In the strongly-quantum regime where  $V/\Gamma \gg 1$  and driving is not too strong, the picture of coexisting vibrational states with opposite phases does not apply. An insight into the transition from the semiclassical to strongly-quantum regime can be gained by studying the quasienergy spectrum and the decay of quantum fluctuations. An analogue of the critical slowing down in the strongly-quantum regime is a sharp increase of the fluctuation correlation time that occurs at a hypersurface in the oscillator parameter space. We find that the quasienergy spectrum and the ratio of the level spacing to their width also sensitively depend on the parameters, in particular on  $V/\Gamma$ .

**4:42PM P48.00012 Robust tomography of microwave resonator arrays for quantum simulation with light** , AMAN LACHAPPELLE, JOHN C OWENS, RUICHAO MA, JONATHAN SIMON, DAVID SCHUSTER, Univ of Chicago — We are interested in using a bottom-up approach to create topologically non-trivial states of light via Hamiltonian engineering in coupled microwave cavities. Characterization and reduction of disorder is paramount to realizing and studying idealized many-body Hamiltonians. Our tight-binding lattices are made of arrays of evanescently coupled three-dimensional microwave resonators. From the spectroscopic response measured at specific lattice sites, we develop methods to fully map out the underlying tight-binding Hamiltonian, including onsite energies, nearest-neighbor couplings and the local dissipation on all sites. We show that for a 1D system, one reflection measurement off of the site at the end of the chain is sufficient, while for 2D only measurements along one edge of the system is sufficient for complete tomography of the lattice Hamiltonian. The transmission between neighboring sites also reveals the phase of the tunnel coupling, thereby allow direct measurement of the flux in lattices with time-reversal breaking synthetic gauge fields. These methods can be readily applied to many other physical systems for the characterization of quantum processes or the validation of quantum simulators.

**4:54PM P48.00013 Analysis of qubit dynamics under strong resonant pulses using Floquet theory**, CHUNQING DENG, FEIRUO SHEN, JEAN-LUC ORGIAZZI, University of Waterloo, SAHEL ASHHAB, Qatar Foundation, ADRIAN LUPASCU, University of Waterloo — Resonant driving is the most common way of implementing single-qubit gates in various quantum systems. Most of the experiments and optimization of such gates are performed in the weak-driving regime, where the qubit dynamics is relatively slow and well described using the rotating wave approximation. However, the implementation of qubit gates with strong driving, which in principle promises a higher speed, has not been studied extensively. In this work, we consider the dynamics of a qubit driven by strong resonant pulses in the framework of Floquet theory. We analyze the role of pulse shaping in the dynamics, as determined by nonadiabatic transitions between the Floquet states. By suppressing the nonadiabatic transitions, we show that high-fidelity single-qubit operations can be achieved in very short times. This work provides the theoretical basis for optimizing strong pulses for single-qubit gates. These results are particularly relevant for the implementation of single-qubit gates in superconducting qubits, where strong driving with shaped pulses has been demonstrated experimentally.

**5:06PM P48.00014 Flexible, low-latency architecture for qubit control and measurement in circuit QED.**, WOUTER VLOTHUIZEN, D. DEURLOO, QuTech, Delft University of Technology and Netherlands Organisation for Applied Scientific Research (TNO), Delft, The Netherlands, J. DE STERKE, Topic Embedded Systems, Delft, The Netherlands, R. VERMEULEN, R.N. SCHOUTEN, LEO DICARLO, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, Delft, The Netherlands — Increasing qubit numbers in circuit QED requires an extensible architecture for digital waveform generation of qubit control and measurement signals. For quantum error correction, the ability to select from a number of predetermined waveforms based on measurement results will become paramount. We present a room-temperature architecture with very low latency from measurement to waveform output. This modular FPGA-based system can generate both baseband and RF modulated signals using DACs clocked at 1 GHz. A backplane that interconnects several modules allows exchange of (measurement) information between modules and maintains deterministic timing across those modules. We replace the typical line based sequencer used in arbitrary waveform generators by a user programmable processor that treats waveforms and measurements as instructions added to a conventional CPU architecture. This allows for flexible coding of triggering, repetitions, delays and interactions between measurement and signal generation. We acknowledge funding from the Dutch Research Organization (NWO), an ERC Synergy Grant, and European project SCALEQIT.

**5:18PM P48.00015 Fock State Generator**, SHAVINDRA PREMARATNE, Department of Physics, University of Maryland; Laboratory for Physical Sciences, F.C. WELLSTOOD, JQI, CNAM, Department of Physics, University of Maryland, B.S. PALMER, Department of Physics, University of Maryland; Laboratory for Physical Sciences — Using a single junction Al/AIO<sub>x</sub>/Al transmon qubit coupled to a superconducting Al cavity (at a temperature 15 mK), we have used a Raman technique to produce a single Fock state in the cavity. The technique requires 3 microwave tones to drive the system from the ground state of the cavity/qubit system. We achieve an experimental fidelity of the final Fock state of around 90%, limited by thermal photons in the cavity and by decay during the operation time. Using this technique, we have also generated an arbitrary superposition of Fock states and a superposition of qubit and cavity states. Results, simulations and applications of this technique will be discussed.

## Wednesday, March 16, 2016 2:30PM - 5:18PM –

**Session P50 DAMOP: Quenched Atomic Systems and Thermalization** Hilton Baltimore Holiday Ballroom  
1 - Mohammad Maghrebi, Joint Quantum Institute, University of Maryland

**2:30PM P50.00001 Prethermalization and exponentially slow energy absorption in periodically driven many-body systems**, DMITRY ABANIN, WEN WEI HO, University of Geneva, Switzerland, WOJCIECH DE ROECK, KU Leuven, Belgium, FRANCOIS HUVENEERS, Universit Paris-Dauphine, France — We establish some general dynamical properties of lattice many-body systems that are subject to a high-frequency periodic driving. We prove that such systems have a quasi-conserved extensive quantity  $H_*$ , which plays the role of an effective static Hamiltonian. The dynamics of the system (e.g., evolution of any local observable) is well-approximated by the evolution with the Hamiltonian  $H_*$  up to time  $\tau_*$ , which is exponentially long in the driving frequency. We further show that the energy absorption rate is exponentially small in the driving frequency. In cases where  $H_*$  is ergodic, the driven system prethermalizes to a thermal state described by  $H_*$  at intermediate times  $t < \tau_*$ , eventually heating up to an infinite-temperature state at times  $t \sim \tau_*$ . Our results indicate that rapidly driven many-body systems generically exhibit prethermalization and very slow heating. We briefly discuss implications for cold atoms experiments which realize topological states by periodic driving.

**2:42PM P50.00002 Universal aspects of thermalization after a quantum quench**, JAMES R. GARRISON, University of California, Santa Barbara, TARUN GROVER, Kavli Institute for Theoretical Physics — A very fundamental problem in quantum statistical mechanics involves whether—and how—an isolated quantum system will thermalize at long times. The Eigenstate Thermalization Hypothesis (ETH) posits that when thermalization occurs, it occurs at the level of each individual energy eigenstate. In recent work [1], we examined an isolated quantum system that obeys ETH and identified the precise class of operators for which ETH is satisfied. Here, we use similar techniques to study the more general case of a time-evolved system after a quantum quench. Given a “typical” initial state, we investigate the class of operators that thermalize and the associated time scales, and remark on the similarities and differences compared with a single eigenstate at finite energy density. Possible experimental implications will be discussed. [1] J. R. Garrison and T. Grover, arXiv:1503.00729.

**2:54PM P50.00003 Short- and long-time dynamics of isolated many-body quantum systems<sup>1</sup>**, MARCO TAVORA, Yeshiva University, JONATHAN TORRES-HERRERA, Universidad Autonoma de Puebla, Mexico, LEA FERREIRA DOS SANTOS, Yeshiva University — We show our results for the relaxation process of isolated interacting quantum spin chains in the integrable and chaotic regimes. The dynamics of the survival probability (the probability for finding the system still in its initial state at later times) and of few-body observables are analyzed. Different time scales are considered. While the short-time evolution is determined by the shape of the weighted energy distribution of the initial state, the long-time behavior depends on the bounds of the spectrum. Both numerical and analytical results are presented as well as comparisons with existing rigorous mathematical derivations. We consider initial states that can be prepared in experiments with cold atoms in optical lattices.

<sup>1</sup>NSF Grant No. DMR-1147430.

**3:06PM P50.00004 Temperature of a small quantum system as an internal property**, JIAOZI WANG, WENGE WANG, Univ of Sci & Tech of China — Equilibration of small quantum systems is a topic of current interest both theoretically and experimentally. In this work, we study the extent to which a temperature can be assigned to a small quantum (chaotic) system as an internal property, but not as a property of any large environment. Specifically, we study a total system, which is composed of an Ising chain in a nonhomogeneous transverse field and an additional spin coupled to one of the spins in the chain. The additional spin can be used as a probe to detect local temperature of the chain. The total system lies in a pure state under unitary evolution and initial state of the chain is prepared in a typical state within an energy shell. Our numerical simulations show that the reduced density matrix of the probe spin approaches canonical states with similar temperatures at different locations of the chain beyond a relaxation time, and the results are close to the theoretical prediction given by the statistical mechanics in the thermodynamic limit, namely  $\beta = \frac{\partial \ln \rho(E)}{\partial E}$  with  $\rho(E)$  being the density of states. We also study effects due to finite size of the chain, including the dependence on initial state of the probe and difference of numerically-obtain temperature from theoretical results.

**3:18PM P50.00005 Temporal fluctuations after a quantum quench: Many-particle dephasing**, FLORIAN MARQUARDT, University of Erlangen-Nuremberg, THOMAS KIENDL, Free University Berlin — After a quantum quench, the expectation values of observables continue to fluctuate in time. In the thermodynamic limit, one expects such fluctuations to decrease to zero, in order for standard statistical physics to hold. However, it is a challenge to determine analytically how the fluctuations decay as a function of system size. So far, there have been analytical predictions for integrable models (which are, naturally, somewhat special), analytical bounds for arbitrary systems, and numerical results for moderate-size systems. We have discovered a dynamical regime where the decrease of fluctuations is driven by many-particle dephasing, instead of a redistribution of occupation numbers. On the basis of this insight, we are able to provide exact analytical expressions for a model with weak integrability breaking (transverse Ising chain with additional terms). These predictions explicitly show how fluctuations are exponentially suppressed with system size.

**3:30PM P50.00006 Persistent Hall response after a quantum quench in Dirac systems**, JUSTIN WILSON, JUSTIN SONG, GIL REFAEL, Caltech — The geometry and topology of quantum states play a central role in producing novel types of responses, such as the quantum anomalous Hall effect. These have featured prominently in topological materials in equilibrium as well as driven systems in the steady state. Here we unveil how quantum geometry yields radically new types of responses in systems far from equilibrium such as that realized in a quantum quench. To illustrate this, we consider quenches of two-band systems with spin-orbit coupling (e.g. Dirac systems). We find that quenching a time-reversal broken gap gives a Hall-type response that persists even at long times. Intimately tied to the quantum geometry of the underlying Hilbert space, the unconventional persistent Hall response yield clear signatures in quench protocols that can be implemented in cold atoms set-ups.

**3:42PM P50.00007 Quantum Quenches in Arrays of Coupled Luttinger Liquids<sup>1</sup>**, ANDREW JAMES, ANDREW HALLAM, University College London, ROBERT KONIK, Brookhaven National Laboratory, ANDREW GREEN, University College London — Cold atom realisations of one dimensional interacting bosonic models are typically formed as large arrays of decoupled tubes. A low energy description of the individual tubes (including the Lieb-Liniger case) is provided by Luttinger liquid theory. Using matrix product state methods combined with integrability, we study the time evolution of an infinite array of coupled Luttinger Liquids, after a quantum quench in which *interchain* tunnelling is switched on to form a 2D system. We extract the time dependence of the density, bosonic modes, the Loschmidt echo and the entanglement entropy and consider possible implications for phase transitions in the coupled chain system. Our results are compared to perturbation theory and contrasted with simulations for coupled arrays of massive chains.

<sup>1</sup>EPSRC Grant No. EP/L010623/1 and DOE Contract No. DEAC02-98CH10886

**3:54PM P50.00008 Melting of a spin domain wall in the context of recent experiments with ultracold atoms**, LEV VIDMAR, Penn State University, DEEPAK IYER, Bucknell University, MARCOS RIGOL, Penn State University — When a one-dimensional spin domain wall of the form  $|\uparrow \dots \uparrow \uparrow \downarrow \downarrow \dots \downarrow \rangle$  is melting, transverse spin correlations in the XX model exhibit a power-law decay in the melted region. This model can be mapped to hard-core bosons via Jordan-Wigner transformation. For hard-core bosons, these emerging power-law correlations correspond to singularities in the quasimomentum distribution at finite quasimomenta  $\pm \pi/2$ , resulting in a dynamical quasicondensation with the emerging phase order different from the ground-state order. This phenomenon has been recently observed experimentally with ultracold bosons in optical lattices [1]. Here we study the emergence of correlations in melting domain walls for hard-core bosons, spinless fermions and the Fermi-Hubbard model at infinite onsite repulsion. In all cases, the density dynamics exhibit identical ballistic expansion, while the correlations show strikingly different features. References: [1] Vidmar et al, PRL 115, 175301 (2015)

**4:06PM P50.00009 Spatio-temporal correlations after a quantum quench in the Bose-Hubbard model<sup>1</sup>**, MATTHEW FITZPATRICK, MALCOLM KENNETT, Simon Fraser University — The quench dynamics of the Bose-Hubbard model (BHM) has received considerable attention in recent years. Theoretically, it has proven challenging to study spatio-temporal correlations in the BHM in dimensions higher than one. We use the Schwinger-Keldysh technique and a strong-coupling expansion to develop a two-particle irreducible formalism that allows the study of spatio-temporal correlations in both the superfluid (SF) and Mott-insulating (MI) regimes during a quantum quench for dimensions higher than one. In this talk, we focus on quenches from the SF to the MI regime and present our numerical results for the evolution of two-time correlation functions. We relate our results to recent cold-atom experiments.

<sup>1</sup>This work was supported by NSERC.

**4:18PM P50.00010 Entanglement dynamics after a quantum quench in the O(N) model<sup>1</sup>**, YONAH LEMONIK, ADITI MITRA, New York University — The entanglement properties of quenched quantum systems is an active area of study, however results in dimensions other than  $d = 1$  are generally lacking. We remedy this by investigating the entanglement properties after a critical quench in the bosonic O(N) model in  $d = 3$ , comparing our results to the free massless theory. We find that the evolution of the entanglement entropy for the free and interacting systems is nearly identical, as expected from a "quasi-particle" picture. However, the low-lying entanglement spectrum is controlled by the different non-equilibrium critical exponents of these two systems. Therefore we demonstrate that these critical exponents can be extracted by studying purely the entanglement in the system.

<sup>1</sup>This work was supported by NSF-DMR 1303177.

**4:30PM P50.00011 Quench dynamics of 1D spin-imbalanced Fermi-Hubbard model<sup>1</sup>**, XIAO YIN, LEO RADZIHOVSKY, University of Colorado at Boulder — We study a non-equilibrium dynamics of a 1D spin-imbalanced Fermi-Hubbard model following a quantum quench of on-site interaction, using bosonization and exact analysis. By focusing on the evolution of singlet-, triplet-, density and magnetization correlation functions, we find that the evolution and the final state display a strong dependence on the initial state. Thus, we demonstrate that such quantum quench may be used as a new approach to identify and probe the 1D gapless analogue of the elusive FFLO state.

<sup>1</sup>supported by NSF through DMR-1001240 and by Simons Investigator award from Simons

**4:42PM P50.00012 Quenched dynamics of superconducting Dirac fermions on honeycomb lattice**, MING LU, X. C. XIE<sup>1</sup>, International Center for Quantum Materials, School of Physics, Peking University, X.C. XIE'S GROUP TEAM — We study the BCS pairing dynamics for the superconducting Dirac fermions on honeycomb lattice after a sudden quench of pairing strength. We observe two distinct phases, one is the synchronized phase with undamped oscillations of pairing amplitude; the other phase has the pairing amplitude oscillates from positive to negative. The exact phase transition point is given by investigating the integrability of the system. Different from the previous work on normal superconducting fermions, which has three distinct phases, our results show the absence of the Landau damped phase and over damped phase. Moreover, we present a linear analysis in the weakly quenched regime, showing that in a rather long time scale, the dynamics can be approximated as the periodic oscillation with  $2\Delta_\infty$  angular frequency along with the logarithmic decay of the pairing amplitude, in contrast of the  $t^{-1/2}$  decay for the normal fermions, namely the Landau damped phase.

<sup>1</sup>The presenter's advisor

**4:54PM P50.00013 Preparation of Bose Einstein condensates in realistic trapping potentials for precision atom interferometry**, KATERINE POSSO TRUJILLO, ERNST M. RASEL, NACEUR GAALOUL, Univ Hannover, QUANTUS TEAM — Preparation of Bose Einstein condensates in realistic trapping potentials for precision atom interferometry. Theoretical studies of the ground state and the dynamical properties of Bose Einstein condensates (BECs) are typically realized by considering the ensemble as being initially trapped by a harmonic potential. Dramatic discrepancies were found by comparing numerical results of the long-time expansion of BECs after being released from the harmonic trap, and measurements of the free evolution and delta-kick cooling (DKC) of a <sup>87</sup>Rb BEC on large timescales of up to 2 s in micro-gravity (micro-g) environment such as those performed in the QUANTUS project from our group [1]. The modification in the dynamics of a <sup>87</sup>Rb BEC with the application of DKC by using experimentally implemented trapping geometries and the effect of gravity have been studied. Three different configurations have been considered: atom chip-based potential, dipole trap and the time-averaged orbiting potential. Such discrepancies may be crucial in high precision atom interferometry experiments in micro-g and zero-g platforms in which the implementation of DKC is mandatory to achieve the long-expansion times required. [1] H. Mntinga et al., Phys. Rev. Lett. vol. 110 093602 (2013).

**5:06PM P50.00014 Memory effects in noninteracting isolated systems from dynamical geometry transformations in ultracold quantum gases**, CHEN-YEN LAI, CHIN-CHUN CHIEN, Univ of California - Merced — Memory effects have been of broad interest and particularly relevant in condensate matter systems where dynamical properties depend on history. Here we explore possibilities of observing memory effects in simple isolated quantum systems undergoing geometry transformations. By transforming into lattices supporting flat-bands consisting of localized states, memory effects could be observed in ultracold atoms in optical lattices due to different time scales of localized and mobile atoms. As an optical lattice is continuously transformed from a triangular lattice into a kagome or square lattice, the system reaches a non-thermal quasi-steady state. In the absence of interactions and dissipations, the emergence of steady states are highly nontrivial and crucial in identifying memory effects unambiguously. Moreover, when the lattices transform from a triangular lattice into a kagome lattice with a flat band, history-dependent density distributions even in noninteracting systems can be observed in fermionic as well as bosonic systems. Rapid growth of cold atom technology and possibilities of various mechanisms for inducing memory effect promise interesting applications of novel quantum devices utilizing memory effect, especially in the thriving field of atomtronics. (arXiv:1510.08978)

## Wednesday, March 16, 2016 2:30PM - 5:30PM –

Session P51 FIAP: Fractional QHE: Level Mixing & Transitions Hilton Baltimore Holiday Ballroom 2 - John Cumings, University of Maryland

**2:30PM P51.00001 Heterostructure Symmetry and the Orientation of the Quantum Hall Nematic Phases<sup>1</sup>**, J.P. EISENSTEIN, J. POLLANEN, K.B. COOPER<sup>2</sup>, S. BRANDSEN, Institute for Quantum Information and Matter and Dept. of Physics, Caltech, Pasadena, CA, L.N. PFEIFFER, K.W. WEST, Dept. of Electrical Engineering, Princeton University, Princeton, NJ — The native symmetry-breaking potential which consistently orients the quantum Hall nematic phases in high mobility 2D electron systems relative to the host semiconductor crystal axes remains unknown. Here we report an extensive set of measurements examining the role of the structural symmetries of the potential confining the 2D system in determining the orientation of the nematics [1]. In single quantum well samples we find that neither the local symmetry of the confinement potential nor the depth of the 2D electron system beneath the sample surface dictates the orientation of the nematic. In contrast, for 2D electrons confined at a single heterointerface between GaAs and AlGaAs, the nematic orientation does depend on the depth of the 2D electron system beneath the sample surface. We relate these results to various theoretical models of the symmetry-breaking potential. [1] J. Pollanen et al., Phys. Rev B 92, 115410 (2015).

<sup>1</sup>Supported by the Institute for Quantum Information and Matter, a NSF Physics Frontiers Center (NSF Grant PHY-1125565) and the Gordon and Betty Moore Foundation via grant GBMF-12500028 and EPiQS Grant GBMF4420, and by NSF MRSEC Grant DMR-1420541.

<sup>2</sup>now at Jet Propulsion Laboratory, Pasadena, CA

**2:42PM P51.00002 Nematic quantum phase transition of composite Fermi liquids in half-filled Landau levels and their geometric response**, YIZHI YOU, University of Illinois at Urbana-Champaign, GIL YOUNG CHO, Korea Advanced Institute of Science and Technology, EDUARDO FRADKIN, University of Illinois at Urbana-Champaign — We present a theory of isotropic-nematic quantum phase transition in the composite Fermi liquid arising in the half-filled Landau levels. We show that the quantum phase transition is triggered by the attractive quadrupolar interaction. By performing flux attachment, system turns into a composite Fermi liquid. The nematic order parameters act as the dynamical metric interplaying with the underlying topology, the Chern-Simons theory. Here both the fluctuations of the gauge field and the nematic order parameter can soften the Fermi surface and thus the fermions form a non-Fermi liquid. The effective field theory for the isotropic-nematic phase transition has  $z = 3$  dynamical exponent due to the Landau damping due to the finite density of the fermions. We show that there is a Berry phase term of the nematic order parameter, which can be interpreted as the Hall viscosity of the dynamical metric. We also find the Wen-Zee-like term, which effectively dresses the nematic vortex with the electric charge. Both of the terms are originated from the time reversal breaking fluctuation of the Chern-Simons gauge fields. This indicates the fluctuations of the gauge fields modify the Hall viscosity and orbital spin of the compressible half-filled Landau level.

**2:54PM P51.00003 Phase Transition between Fermionic IQHE and Bosonic FQHE Via Feshbach Resonance**, SHUAN-FAN LIOU, KUN YANG, National High Magnetic Field Laboratory and Florida State Univ, ZI-XIANG HU, Chongqing University, China — We study an integer quantum Hall system with two species of fermions with total Landau filling factor two (or one per kind of fermions) on disk geometry. Via Feshbach resonance fermions interact with each other such that two different species of fermions become a boson as coupling strength increases. Through exact diagonalization method, we see that fermions undergo a phase transition from fermionic integer quantum Hall phase to bosonic fractional quantum Hall phase with  $\nu = \frac{1}{2}$ . Besides, it seems to be a second order phase transition by investigating the expectation value of particle number of bosons.

**3:06PM P51.00004 The effect of Landau level mixing on spin polarization of composite fermions: a non-perturbative study**, YUHE ZHANG, JAINENDRA K. JAIN, Department of Physics, 104 Davey Lab, Pennsylvania State University, University Park, PA 16802, USA — The spin polarization transitions enable precise tests of the fractional quantum Hall (FQH) theory. Possible factors responsible for the deviations between theories and experiments include Landau level (LL) mixing and finite quantum well width. Previous works generally treat LL mixing perturbatively. Following [1], we perform a fixed-phase diffusion Monte Carlo study to solve the many-body Schrodinger equation within the approximation of fixing the phase of the wave function. We calculate the critical Zeeman energy ( $E_z$ ) needed to fully spin polarize several FQH states, and find that  $E_z$  depends less sensitively on LL mixing than previously thought. We also take into account the effect of finite quantum well width by using an effective two-dimensional interaction based on the realistic charge distribution. We compare our results with experiments and make further predictions. [1] G. Ortiz, D. M. Ceperley, and R.M. Martin, Phys. Rev. Lett. 71, 2777 (1993).

**3:18PM P51.00005 Competing states for the fractional quantum Hall effect in the 1/3-filled second Landau level**, JAE-SEUNG JEONG, Institute for Basic Science:Center for Correlated Electron Systems, Department of Physics & Astronomy, Seoul National University, Seoul 08826, Korea, HANTAO LU, Center for Interdisciplinary Studies & Key Laboratory for Magnetism and Magnetic Materials of the MoE, Lanzhou University, Lanzhou 730000, China, KENJI HASHIMOTO, Max Planck Institute for Mathematics Vivatsgasse 7, 53111 Bonn, Germany, SUK BUM CHUNG, Institute for Basic Science : Center for Correlated Electron Systems, Department of Physics & Astronomy, Seoul National University, Seoul 08826, Korea, KWON PARK, School of Physics, Korea Institute for Advanced Study, Seoul 130-722, Korea — We study the nature of the fractional quantum Hall state in the 1/3-filled second Landau level at filling factor 7/3 via exact diagonalization. We show a series of transitions in the energy spectrum from a Laughlin-type spectrum, to an intermediate compressible spectrum, to a reentrant incompressible spectrum, and to a compressible spectrum with decrease of the Haldane pseudopotential. To search for a trial state describing the 7/3 state, we compute the overlap of the exact 7/3 ground state with various competing states including the Laughlin state, the particle-hole conjugate of the  $Z_4$  parafermion state, the fermionic Haffnian state, the antisymmetrized product state of two composite fermion seas (CFSs) at 1/6 filling, and the antisymmetrized correlated state of two CFSs at 1/4 filling, which are obtained as an antisymmetrized projection of the bilayer quantum Hall states. Specifically, we prove that the fermionic Haffnian state is equivalent to the antisymmetrized projection of the Halperin (551) state.

**3:30PM P51.00006 SU(3) and SU(4) singlet quantum Hall states at  $\nu = 2/3^1$** , FENGCHENG WU, Department of Physics, University of Texas at Austin, INTI SODEMANN, Department of Physics, Massachusetts Institute of Technology, ALLAN H. MACDONALD, Department of Physics, University of Texas at Austin, THIERRY JOLICOEUR, Laboratoire de Physique Théorique et Modèles statistiques, CNRS and Université Paris-Sud — We report on an exact diagonalization study of fractional quantum Hall states at a filling factor  $\nu = 2/3$  in a system with a four-fold degenerate  $n=0$  Landau level and SU(4) symmetric Coulomb interactions. Our investigation reveals previously unidentified SU(3) and SU(4) singlet ground states which appear at flux quantum shift 2 when a spherical geometry is employed, and lie outside the established composite-fermion or multicomponent Halperin state patterns. We will present the pair correlation functions of these states, and describe similar singlets at another filling factor 2/5. Strategies to construct trial wave functions will be discussed.

<sup>1</sup>F. Wu, I. Sodemann, A. H. MacDonald and Th. Jolicoeur, Phys. Rev. Lett. 115, 166805 (2015)

**3:42PM P51.00007 Adiabatic Transport of Geometric Singularities in the Quantum Hall Effect**, MICHAEL LASKIN, YU HUNG CHU, University of Chicago, TANKUT CAN, SUNY Stonybrook, PAUL WIEGMANN, University of Chicago — We present a framework for studying the fractional Quantum Hall Effect (FQHE) on singular surfaces - in particular surfaces with multiple geometric singularities. It is now known that, aside from the Hall conductance and viscosity, there exists a third universal transport coefficient of the FQHE - the gravitational anomaly. This coefficient is difficult to measure since it usually appears as a higher order correction to observable quantities, such as the particle density. Singular surfaces are the first setting where the gravitational anomaly appears as a leading order effect. These surfaces are therefore ideal for studying geometric response and the gravitational anomaly within the FQHE. We expand the generating functional in the large  $N$  limit on such surfaces. From there, we braid the conical singularities of the surface and find a remarkable result - the gravitational anomaly determines the braiding statistics of the transported conical singularities.

**3:54PM P51.00008 Quantum Hall State on Singular Surfaces**, YU HUNG CHIU, Univ of Chicago, TANKUT CAN, Simons center for Geometry and Physics, Stony Brook University, MICHAEL LASKIN, PAUL B. WIEGMANN, Univ of Chicago — We propose a framework to study the response towards geometry with FQHE state on singular surfaces. Such study on singular surface provides a path to measure the gravitational anomaly, the third universal transport coefficient of FQHE, in leading order. The large  $N$  expansion of generating functional is computed via two independent methods: a Ward Identity and a field theory approach. Meanwhile the second moment of the density is also obtained via Ward Identity. We observe that the generating functional on singular surfaces can be viewed as vertex operators at the cone tips. Divergence in the Liouville functional due to singularities is, as expected, a source for the modification, but not the sole source. From both methods, we are able to obtain the charge and conformal dimension  $h_\alpha$  of such a vertex operator. The talk will concentrate on the one cone result obtained via both approaches.

**4:06PM P51.00009 12/5 and 13/5 fractional quantum Hall states and Landau level mixing**, KIRYL PAKROUSKI, Theoretische Physik, ETH Zurich, Zurich 8093, Switzerland, MICHAEL PETERSON, Physics & Astronomy, California State University, Long Beach, CA, US, YANG-LE WU, Joint Quantum Institute and Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, Maryland 20742, US, MATTHIAS TROYER, Theoretische Physik, ETH Zurich, Zurich 8093, Switzerland — We use exact diagonalization to study the way Landau level mixing breaks the particle-hole symmetry between the 12/5 and 13/5 fractional quantum Hall states in GaAs. We discuss the possible relationship between our observations and the absence of the 13/5 state in experiment.

**4:18PM P51.00010 Exactly Solvable Model for Impurity Scattering at the Edge of the  $\nu = 2/3$  FQH State**, CHRIS HEINRICH, MICHAEL LEVIN, University of Chicago — We present an exactly solvable model for impurity scattering on the edge of a  $\nu = 2/3$  FQH state that is valid in the strong scattering limit. For this model we obtain exact mode expansions for the charge density and current operators, as well as the exact low energy spectrum. Importantly, we find that the low energy theory of the model consists of decoupled and counterpropagating charge and neutral modes, agreeing with the earlier work of Kane, Fisher, and Polchinski. Unlike the previous derivation, which relied on perturbative renormalization group arguments, our approach allows us to derive the emergence of decoupled charge and neutral modes from a microscopic model which is initially far from the decoupled fixed point.

**4:30PM P51.00011 Fragile Fractional Quantum Hall States in the Lowest and the Second Landau Level**, GABOR CSATHY, ETHAN KLEINBAUM, Purdue University, ASHWANI KUMAR, Monmouth College, NODAR SAMKHARADZE, Purdue University, LOREN PFEIFFER, KEN WEST, Princeton University — Ultra-low temperature measurements of the two-dimensional electron gas have revealed some of the most fragile fractional quantum Hall states. In these experiments electron thermalization was achieved using a He-3 immersion cell and the temperature of the bath is monitored using a quartz tuning fork viscometer. We will review the recently discovered fractional quantum Hall state at filling factor  $\nu = 3 + 1/3$  observed in the second Landau level and those at the filling factor  $\nu = 4/11$  and  $5/13$  in the lowest Landau level. The work at Purdue was supported by NSF DMR 1207375 and 1505866 grants. The work at Princeton University was funded by the Gordon and Betty Moore Foundation through the EPiQS initiative Grant GBMF4420, and by the National Science Foundation MRSEC Grant DMR-1420541.

**4:42PM P51.00012 Band geometry of higher Landau levels<sup>1</sup>**, RAHUL ROY, FENNER HARPER, THOMAS JACKSON, University of California, Los Angeles — A set of recent results have shown that the quantum geometry of bands as encoded in quantities such as the mean fluctuations of the Berry curvature and the quantum metric provide a useful way of analyzing the stability of FQHE phases in Chern bands. These quantum geometric quantities measure the closeness of Chern bands to the lowest Landau level. Here, we find a more complete set of criteria for the stability of FQHE phases which incorporate a distance measure to an arbitrary Landau level.

<sup>1</sup>Supported by the NSF under CAREER DMR-1455368 and the Alfred P. Sloan foundation

**4:54PM P51.00013 Fractional Chiral metal from the wire construction**, ADOLFO GRUSHIN, Univ of California - Berkeley, TOBIAS MENG, Technical University Dresden, KIRILL SHTENGEL, Univ of California - Riverside, JENS BARDARSON, Max Planck Institute for the Physics of Complex Systems — In this work we use the wire construction to build integer and fractional phases of the 4+1 dimensional quantum Hall effect by coupling 3+1 dimensional Weyl semimetals in an extra dimension. In the presence of an external magnetic field, each Weyl species reduces to a (degenerate) chiral wire, the zeroth Landau level, which, upon coupling, delivers a consistent response to an external electromagnetic field in terms of a 4+1 dimensional Chern Simons field theory. Going one step beyond, we show that the theory at the boundary is gapless and explicitly write the quantum field theory that represents and defines this novel state of matter, the fractional chiral metal. We end by discussing the construction in the absence of external magnetic fields.

**5:06PM P51.00014 Mapping a fractional quantum Hall state to a fractional Chern insulator**, YINHAN ZHANG, JUNREN SHI, Peking University — We establish a variational principle for properly mapping a fractional quantum Hall (FQH) state to a fractional Chern insulator (FCI). We find that the mapping has a gauge freedom which could generate a class of FCI ground state wave functions appropriate for different forms of interactions. Therefore, the gauge should be fixed by a variational principle that minimizes the interaction energy of the FCI model. For a soft and isotropic electron-electron interaction, the principle leads to a gauge coinciding with that for maximally localized two-dimensional projected Wannier functions of a Landau level.

**5:18PM P51.00015 Suppression of interference in quantum Hall Mach-Zehnder geometry by upstream neutral modes**, YUVAL GEFEN, The Weizmann Institute of Science, Israel, MOSHE GOLDSTEIN, Tel Aviv University, Israel — Mach-Zehnder interferometry has been suggested as a probe for anyonic quasiparticles in fractional quantum Hall states. However, all experimental attempts to measure such an interference signal have failed to date, despite the high visibility of interference fringes in the integer quantum Hall case. In our work we have studied the relation between this null result and another recent surprising experimental finding, namely the detection of upstream neutral modes in virtually all fractional quantum Hall states (including, e.g., filling  $1/3$ ), not only in hole-like filling factors (such as  $2/3$ ). We have found that the excitation of upstream modes makes the interference visibility in the Mach-Zehnder geometry decay exponentially with the total length of the interferometer arms, even when the lengths are exactly equal. We also suggest ways to overcome this suppression.

**Wednesday, March 16, 2016 2:30PM - 5:30PM –**  
**Session P52 DAMOP FIAP: Optomechanics and Hybrid Systems III: Fundamental Methods and Applications** Hilton Baltimore Holiday Ballroom 3 - Chen-lung Hung, Purdue University

**2:30PM P52.00001 A general framework for analyzing pulsed optomechanical systems**, BASSAM HELOU, BELINDA PANG, HAIXING MIAO, YANBEI CHEN, Caltech — One difficulty in understanding driven optomechanical systems comes from keeping track of the continuum of input and output optical modes. Can we formulate a simpler description? In the case of optical pulses of finite duration, the answer is yes. The dynamics of the joint optical and mechanical system can be summarized by a finite number of generalized modes! On the other hand, the analysis of the entanglement structure between the mechanics and optics is more involved, but could be approximated by a simple and bounded structure. Our work has immediate applications to the quantum engineering of optomechanical setups. We rigorously justify the formalism used in proposals for arbitrary Fock state preparation, extend the proposals to more realistic setups, and propose additional state preparation and state transfer protocols.

**2:42PM P52.00002 Quench dynamics in optomechanical arrays**, SADEGH RAEISI, VITTORIO PEANO, FLORIAN MARQUARDT, University of erlangen-nuremberg — Optomechanical arrays are a novel quantum system that provide a promising tool for exploring many-body physics. The tunability of optomechanical arrays can be exploited for studying the non-equilibrium dynamics. Despite the technological challenges, experimental implementation of simple one-dimensional systems seems feasible in the next few years. Here we focus on the non-equilibrium dynamics of one-dimensional optomechanical arrays and investigate the quench dynamics in these systems. In particular, we study the topological properties and phases of these one-dimensional optomechanical arrays.

**2:54PM P52.00003 Correlated anomalous phase diffusion of sideband-excited phonons in an electromechanical resonator**, XIAOSHI DONG, FENGPEI SUN, JIE ZOU, Hong Kong University of Science and Technology, MARK DYKMAN, Michigan State University, HOBUN CHAN, Hong Kong University of Science and Technology — We study the phase fluctuations of self-sustained oscillations induced by dynamical backaction in a micromechanical resonator. The resonator has two vibrational modes with strongly differing frequencies and decay rates. The high-frequency mode acts as a phonon cavity mode, playing a similar role as photon modes in optomechanical systems. When sufficiently strong pumping is applied at the blue-detuned sideband of the cavity, the dynamical backaction leads to a parametric instability accompanied by self-sustained oscillations. We find that self-sustained oscillations are induced not only in the low frequency mechanical mode, but also in the high frequency cavity mode. The nonlinear nature of the backaction leads to hysteresis of this self-sustained oscillations. In each mode, the phase undergoes anomalous diffusion, where the mean square phase change in time follows a superlinear power law. The exponent of this power law is determined by the  $1/f$ -type intrinsic frequency noise of the resonator. Remarkably, the phase fluctuation of the two modes show near perfect anti-correlation, our findings show that self-sustained oscillations induced by dynamical backaction offer new opportunities of phase manipulation and investigation of fundamental properties of resonating.

**3:06PM P52.00004 Topological energy transfer in an optomechanical system with an exceptional point<sup>1</sup>** , HAITAN XU, DAVID MASON, LUYAO JIANG, JACK HARRIS, Yale University — We have measured an exceptional point in a cryogenic cavity optomechanical system, and have studied its topological properties. An exceptional point is a topological defect in the spectrum of a pair of coupled oscillators at which the system's two complex eigenvalues coalesce. We monitored the evolution of two mechanical oscillators while using a laser to encircle the exceptional point, thereby realizing topological energy transfer between mechanical modes. Moreover, by reversing the encircling direction, we observe the breakdown of the adiabatic theorem and show that the energy transfer possesses a diode-like asymmetry.

<sup>1</sup>This work is supported by AFOSR Grant FA9550-15-1-0270.

**3:18PM P52.00005 Optomechanical synchronization phenomena in the presence of (quantum) noise** , TALITHA WEISS, ANDREAS KRONWALD, STEFAN WALTER, FLORIAN MARQUARDT, Institute for Theoretical Physics, FAU Erlangen-Nuremberg — Synchronization is a phenomenon that appears in various natural and man-made systems. Optomechanical limit-cycle oscillators can synchronize when they are coupled to each other or to an external periodic force. Classically, in the absence of noise, different synchronization regimes can be identified. Notably, optomechanical systems tend to synchronize either in-phase or anti-phase. We investigate how the synchronization behaviour is affected in the presence of the fundamental quantum noise (arXiv:1507.06190). We find a regime where fluctuations drive transitions between the classical synchronization states and explore the quantum-to-classical crossover. Finally, we compare the effects of quantum noise to the effects of thermal noise.

**3:30PM P52.00006 Stochastic dynamics and phase-field roughening in optomechanical oscillator arrays** , ROLAND LAUTER, University of Erlangen-Nuremberg, ADITI MITRA, New York University, FLORIAN MARQUARDT, University of Erlangen-Nuremberg — We consider arrays of coupled optomechanical systems, each of which consists of a laser-driven optical mode interacting with a mechanical (vibrational) mode. For sufficiently strong laser driving, the mechanical modes can settle into stable finite-amplitude oscillations on a limit cycle. We study the collective classical nonlinear dynamics of the phases of these oscillators, which is effectively described by an extension of the well-known Kuramoto model. In this extended model, we study the effect of noise on the dynamics in the case of homogeneous-phase initial conditions. We analytically establish a connection to the physics of surface growth as described by the Kardar-Parisi-Zhang model. Simulations of one-dimensional arrays of our model indeed show roughening of the phase field and universal scaling of the phase-field width. In contrast to the continuum Kardar-Parisi-Zhang model, our model is a genuine lattice model. We discuss interesting effects due to this difference, including crossover timescales and the role of instabilities of the roughening process.

**3:42PM P52.00007 Topological Transport of Light and Sound** , CHRISTIAN BRENDL, VITTORIO PEANO, MICHAEL SCHMIDT, FLORIAN MARQUARDT, FAU Erlangen-Nuremberg — Since they exploit global features of a materials band structure, topological states of matter are particularly robust. Having already been observed for electrons, atoms, and photons, it is an outstanding challenge to create a Chern insulator of sound waves in the solid state. In this work, we propose an implementation based on cavity optomechanics in a photonic crystal. We demonstrate the feasibility of our proposal by means of an effective lattice model as well as first principle simulations. The topological properties of the sound waves can be wholly tuned in situ by adjusting the amplitude and frequency of a driving laser that controls the optomechanical interaction between light and sound. The resulting chiral, topologically protected phonon transport can be probed completely optically.

**3:54PM P52.00008 ORIGIN AND IMPLICATIONS OF  $A^2$  -LIKE CONTRIBUTION IN THE QUANTIZATION OF CIRCUIT-QED SYSTEMS** , MOHAMMAD MOEIN MALEKAKHLAGH, HAKAN TURECI, Princeton Univ — It is known that the electromagnetic modal structure of a cavity is modified by placing an atom into it. In cavity QED, this phenomenon manifests itself through the appearance of the  $A^2$ -contribution, a gauge-dependent diamagnetic term. Despite the negligible effect in the case of atomic cavity QED systems, in recent superconducting circuit realizations [1] these corrections may be observable and have qualitative implications. In this talk [2], we revisit the canonical quantization of a circuit QED system consisting of a single superconducting transmon qubit coupled to a multimode superconducting microwave resonator. We introduce a new set of modes that properly satisfies current conservation in the entire circuit and discuss how in terms of this set of modes, light-matter coupling can deviate drastically from the previous theories in the literature. Finally, we present a sum rule for the dipole transition matrix elements of a multi-level transmon qubit which provides an upper bound for the possible light-matter coupling strengths. [1] Neereja M. Sundaresan, Yanbing Liu, Darius Sadri, Laszlo J. Szocs, Devin L. Underwood, Moein Malekakhlagh, Hakan E. Tureci, Andrew A. Houck, Phys. Rev. X 5, 021035 [2] Moein Malekakhlagh and Hakan E. Tureci, arXiv:1506.02773 (2015)

**4:06PM P52.00009 Dynamical Gauge Fields in Optomechanics** , STEFAN WALTER, FLORIAN MARQUARDT, University of Erlangen-Nürnberg — Artificial gauge fields for neutral particles such as photons, recently attracted a lot of attention in various fields ranging from photonic crystals to ultracold atoms in optical lattices to optomechanical arrays. Here we point out that, among all implementations of gauge fields, the optomechanical setting allows for the most natural extension where the gauge field becomes dynamical. The mechanical oscillation phases determine the effective artificial magnetic field for the photons, and once these phases are allowed to evolve, they respond to the flow of photons in the structure. We discuss a simple three-site model where we identify four different regimes of the gauge-field dynamics. Furthermore, we extend the discussion to a two-dimensional lattice. Our proposed scheme could for instance be implemented using optomechanical crystals.

**4:18PM P52.00010 Topologically Reconfigurable Atomic Lattice Quantum Metamaterial.** , PANKAJ JHA, MICHAEL MREJEN, JEONGMIN KIM, CHIHUI WU, YUAN WANG, Univ of California - Berkeley, YURI ROSTOVTSSEV, Univ of North Texas, Denton, XIANG ZHANG, Univ of California - Berkeley — Metamaterials have attracted unprecedented attention owing to their exceptional light-matter interaction properties. However, harnessing metamaterial at single photon or few photon excitations is still a long way to go due to several critical challenges such as optical loss, defects to name a few. Here we introduce and theoretically demonstrate a novel platform toward quantum metamaterial, immune to aforementioned challenges, with ultra-cold neutral atoms trapped in an artificial crystal of light. Such periodic atomic density grating – an atomic lattice – exhibits extreme anisotropic optical response where it behaves like a metal in one direction but dielectric along orthogonal directions. We harness the interacting dark resonance physics to eliminate the absorption loss and demonstrate an all-optical and ultra-fast control over the photonic topological transition from a close to an open topology at the same frequency. Such atomic lattice quantum metamaterial enables dynamic manipulation of the decay rate of a quantum emitter by more than an order of magnitude. Our proposal brings together two important contemporary realm of science – cold atom physics and metamaterial for applications in both fundamental and applied science. Atomic lattice quantum metamaterial may provide new opportunities, at single or few photon level, for quantum sensing, quantum information processing with metamaterials.

**4:30PM P52.00011 Optomechanical Quantum Correlation Thermometry** , T. P. PURDY, Joint Quantum Institute/NIST, K. E. GRUTTER, M. I. DAVANCO, K. SRINIVASAN, Center for Nanoscale Science and Technology/NIST, J. M. TAYLOR, Joint Quantum Institute/NIST; Joint Center for Quantum Information and Computer Science/UMD — We present an optomechanical approach for producing accurate thermometry over a wide temperature range using quantum Brownian motion. Optical measurements induce quantum correlations in an optomechanical system when quantum-limited intensity fluctuations of a probe laser drive mechanical motion. The size of the correlations in the weak probe limit are dictated by the scale of individual phonons. We have recently measured optomechanical quantum correlations in the cross correlation spectrum between the amplitude and phase fluctuations of a single probe laser interacting with a silicon nitride optomechanical crystal. These correlations are independent of thermally-induced Brownian motion. However, Brownian motion does simultaneously produce much larger correlation signals between other optical quadratures. A comparison of the size of thermally-induced correlations to quantum correlations allows us to absolutely calibrate Brownian motion thermometry to the mechanical energy quantization scale.

**4:42PM P52.00012 Energy decay measurements in graphene-based mechanical resonators** , PETER WEBER, JOHANNES GÜTTINGER, ADRIEN NOURY, JOEL MOSER, ADRIAN BACHTOLD, ICFO - Institut de Ciències Fotoniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels (Barcelona), Spain — Shrinking nanomechanical resonators has led to new record sensitivities in mass and force detection and has provided novel insights into the rich physics of mechanical nonlinearities. However, the high sensitivity and enhanced nonlinearities in ultra small resonators pose new challenges for the detection of motion. This has so far prevented a more detailed investigation of the energy decay, which is the key figure of merit for most technological and scientific applications. Here we present a method to carry out time-resolved energy decay measurements of few-layer graphene resonators. In the high vibration amplitude regime, we observe a strong deviation from previous energy decay measurements. Contrary to expectations, the exponential decay rate decreases abruptly at a few threshold amplitudes. At the lowest measured vibrational amplitude, the energy decay rate is weakest, corresponding to quality factors that can surpass 1 million.

**4:54PM P52.00013 Demonstration of the reversed dissipation regime in cavity electro-mechanics** , A.K. FEOFANOV, L.D. TOTH, N.R. BERNIER, T.J. KIPPENBERG, Ecole polytechnique federale de Lausanne — Cavity optomechanical phenomena, such as cooling, amplification or optomechanically induced transparency, emerge due to a strong imbalance in the dissipation rates of the parametrically coupled electromagnetic and mechanical resonators. Here we explore experimentally for the first time the reversed dissipation regime where the mechanical energy relaxation rate exceeds the energy decay rate of the electromagnetic cavity. We demonstrate optomechanically induced modifications of the microwave cavity resonance frequency and decay rate as well as mechanically-induced amplification of the electromagnetic mode and self-sustained oscillations (maser action) with high spectral purity of emitted microwave tone.

**5:06PM P52.00014 Ground state cooling of a nanomechanical resonator using electron transport in hybrid systems.**<sup>1</sup> , GIANLUCA RASTELLI, PASCAL STADLER, WOLFGANG BELZIG, University of Konstanz — A still open challenge in nanoelectromechanical systems is the achievement of the quantum regime via active cooling and using electron transport. I will discuss active ground state cooling in a bottom-up device, viz. a carbon nanotube quantum dot suspended between two electric nano-contacts, and for two different coherent transport regimes: (i) spin-polarized current between two ferromagnets and (ii) sub-gap Andreev current between a superconductor and a normal metal. I will show that efficient ground state cooling of the resonator can be achieved for realistic parameters of the system and varying the transport parameters, e.g. gate voltage, magnetic field, etc. Finally I will discuss the signatures in the current-voltage characteristics of the non-equilibrium state of the nanoresonator.

<sup>1</sup>Zukunftskolleg of the University of Konstanz; DFG through SFB 767 and BE 3803/5.

**5:18PM P52.00015 Laser cooling of a harmonic oscillator's bath with optomechanics** , XUNNONG XU, Joint Quantum Institute, University of Maryland/National Institute of Standards and Technology, College Park, Maryland 20742, USA, JACOB TAYLOR<sup>1</sup>, Joint Quantum Institute, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA — Thermal noise reduction in mechanical systems is a topic both of fundamental interest for studying quantum physics at the macroscopic level and for application of interest, such as building high sensitivity mechanics based sensors. Similar to laser cooling of neutral atoms and trapped ions, the cooling of mechanical motion by radiation pressure can take single mechanical modes to their ground state. Conventional optomechanical cooling is able to introduce additional damping channel to mechanical motion, while keeping its thermal noise at the same level, and as a consequence, the effective temperature of the mechanical mode is lowered. However, the ratio of temperature to quality factor remains roughly constant, preventing dramatic advances in quantum sensing using this approach. Here we propose an efficient scheme for reducing the thermal load on a mechanical resonator while improving its quality factor. The mechanical mode of interest is assumed to be weakly coupled to its heat bath but strongly coupled to a second mechanical mode, which is cooled by radiation pressure coupling to a red detuned cavity field. We also identify a realistic optomechanical design that has the potential to realize this novel cooling scheme.

<sup>1</sup>Joint Center for Quantum Information and Computer Science, University of Maryland, College Park, MD 20742, USA

**Wednesday, March 16, 2016 2:30PM - 5:18PM –**  
**Session P53 DFD GSOFD DBIO: Swimming, Migration and Porous Media Flows** Hilton Baltimore  
Holiday Ballroom 4 -

**2:30PM P53.00001 The intestine is a blender** , PATRICIA YANG, MORGAN LAMARCA, VICTORIA KRAVETS, DAVID HU, Georgia Institute of Technology — According to the U.S. Department of Health and Human Services, digestive disease affects 60 to 70 million people and costs over 140 billion annually. Despite the significance of the gastrointestinal tract to human health, the physics of digestion remains poorly understood. In this study, we ask a simple question: what sets the frequency of intestinal contractions? We measure the frequency of intestinal contractions in rats, as a function of distance down the intestine. We find that intestines contract radially ten times faster than longitudinally. This motion promotes mixing and, in turn, absorption of food products by the intestinal wall. We calculate viscous dissipation in the intestinal fluid to rationalize the relationship between frequency of intestinal contraction and the viscosity of the intestinal contents. Our findings may help to understand the evolution of the intestine as an ideal mixer.

### 2:42PM P53.00002 Confinement of Single Microswimmers in Circular Microfluidic Chambers

, TANYA OSTAPENKO, THOMAS BOEDDEKER, CHRISTIAN KREIS, FABIAN SCHWARZENDAHL, MARCO G. MAZZA, OLIVER BAEUMCHEN, Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Goettingen, Germany — The characteristics of active fluids, such as suspensions of biological microswimmers, may not only originate from the mutual interactions between the constituents, but also from interactions with interfaces and confining walls. In fact, the natural habitats of many living organisms are complex geometric environments, rather than bulk situations. The influence of interfaces on the dynamics was recognized as an important factor, and there are differences in the way that pusher-type swimmers (e.g. *E. coli*) and puller-type swimmers (e.g. *C. reinhardtii*) behave close to flat interfaces. Using experiments and simulations, we report on the dynamics of single puller-type swimmers in 2D circular microfluidic chambers. We find that the radial probability distribution of trajectories displays a characteristic wall hugging effect, where swimmers remain trapped at a concave interface for decreasing chamber size. For trajectories in the vicinity of the concave wall, an alignment of the local swimming direction with the local wall tangent is observed. In contrast, the swimmers tend to scatter off convex interfaces with short interaction times. Based on geometric arguments involving the swimmer's persistence length, we explain this entrapment effect at concave interfaces.

### 2:54PM P53.00003 Mirror-symmetry breakings in human sperm rheotaxis

, NORBERT STOOP, Massachusetts Inst of Tech-MIT, ANTON BUKATIN, IGOR KUKHTEVICH, Russian Academy of Sciences, St. Petersburg Academic University, JOERN DUNKEL, Massachusetts Inst of Tech-MIT, VASILY KANTSLER, University of Warwick — Rheotaxis, the directed response to fluid velocity gradients, has been shown to facilitate stable upstream-swimming of mammalian sperm cells along solid surfaces, suggesting a robust mechanism for long-distance navigation during fertilization. However, the dynamics by which a human sperm orients itself w.r.t. ambient flows is poorly understood. Here, we combine microfluidic experiments with mathematical modeling and 3D flagellar beat reconstruction to quantify the response of individual sperm cells in time-varying flow fields. Single-cell tracking reveals two kinematically distinct swimming states that entail opposite turning behaviors under flow reversal. We constrain an effective 2D model for the turning dynamics through systematic large-scale parameter scans, and find good quantitative agreement with experiments. We present comprehensive 3D data demonstrating the rolling dynamics of freely swimming sperm cells around their longitudinal axis. Contrary to current beliefs, this analysis uncovers ambidextrous flagellar waveforms and shows that the cells turning direction is not defined by the rolling direction. Instead, the different rheotactic turning behaviors are linked to a broken mirror-symmetry in the midpiece section, likely arising from a buckling instability.

### 3:06PM P53.00004 Microorganism billiards in closed plane curves

, MADISON KRIEGER, Brown University — Recent experiments and numerical simulations have demonstrated that many species of microorganisms reflect specularly from a solid surface — due to steric and hydrodynamic interactions with the wall, their outgoing angle is fixed and independent of the angle of incidence. Motivated by these results, we discuss theory and computation of the “aspecular billiard”, a modification of the classical billiard in which the outgoing angle is constant. We restrict our attention to closed plane curves, focusing on three canonical examples: the ellipse, the Bunimovich stadium, and the Sinai billiard. These systems can have a rich array of orbits, and the Lyapunov exponent is shown to be dependent on the billiard geometry and the outgoing angle. We apply these results to the design of tunable passive sorting mechanisms.

### 3:18PM P53.00005 *Helicobacter pylori* displays spiral trajectories while swimming like a corkscrew in solutions.<sup>1</sup>

, MAIRA A. CONSTANTINO, JOSEPH M. HARDCASTLE, RAMA BANSIL, Boston University, MEHDI JABBARZADEH, HENRY C. FU, University of Nevada at Reno — *Helicobacter pylori* is a helical shaped bacterium that causes gastritis, ulcers and gastric cancer in humans and other animals. In order to colonize the harsh acidic environment of the stomach *H. pylori* has evolved a unique biochemical mechanism to go across the viscoelastic gel-like gastric mucus layer. Many studies have been conducted on the swimming of *H. pylori* in viscous media. However a yet unanswered question is if the helical cell shape influences bacterial swimming dynamics or confers any advantage when swimming in viscous solution. We will present measurements of *H. pylori* trajectories displaying corkscrew motion while swimming in solution obtained by tracking single cells using 2-dimensional phase contrast imaging at high magnification and fast frame rates and simultaneously imaging their shape. We observe a linear relationship between swimming speed and rotation rate. The experimental trajectories show good agreement with trajectories calculated using a regularized Stokeslet method to model the low Reynolds number swimming behavior.

<sup>1</sup>Supported by NSF PHY 1410798 (PI: RB)

### 3:30PM P53.00006 Investigating wake patterns and propulsive frequencies of a flat plate under pitching motion.

, JOSEPH MOUBOGHA MOUBOGHA<sup>1</sup>, JACQUES ANDRE ASTOLFI<sup>2</sup>, French Naval Academy Institute - IRENav — Fundamental mechanisms of swimming are explored using a simple geometry device - flat plate - in pure-pitching motion in a hydrodynamic tunnel. The experiments are carried out at different Reynolds numbers based on the plate length  $c$ . Pitching motion is generated for reduced frequencies  $k$  between 0 and 2 and for an angular amplitude of 10 deg. Velocity fields are obtained in the wake of the plate using Particle Image Velocimetry and measurements of drag coefficients are estimated from mean velocity profiles. This study confirms the occurrence of a threshold oscillation frequency beyond which the plate enters a propulsive regime and the wake features organized structures. In this case an inversion of the typical Karman vortex street is observed. The evolution of mean transverse velocity profiles in the wake of the plate shows that the usual wake profile with velocity deficit - plate with drag - can be transformed into a jet - plate with thrust - above a certain reduced frequency.

<sup>1</sup>PhD Student Mechanical Engineering Departement

<sup>2</sup>Associate professor Mechanical Engineering Departement Tel +33(0)2 98 23 40 17 fax: +33(0)2 98 23 38 57

### 3:42PM P53.00007 Continuous-flow Electrokinetic Particle Separation in a Bifurcating Microchannel.

, DI LI, XINYU LU, XIANGCHUN XUAN, Clemson University — Separating particles from a heterogeneous mixture is important and necessary in many engineering and biomedical applications. Electrokinetic flow-based continuous particle separation has so far been realized primarily by the use of particle dielectrophoresis induced in constricted and/or curved microchannels. We demonstrate in this talk that particles can be continuously separated by size when passing through a bifurcating microchannel. This sheathless label-free separation relies on the wall-induced electrical lift force that acts to focus particles to the center of the main-branch and deflect them to size-dependent flow paths in the two side-branches. We also develop a numerical model to predict and understand this separation.

**3:54PM P53.00008 Predator-prey model for the self-organization of stochastic oscillators in dual populations**<sup>1</sup>, SARA MORADI, Universit Libre de Bruxelles, 1050 Brussels, Belgium, JOHAN ANDERSON, Department of Earth and Space Sciences, Chalmers University of Technology, SE-412 96 Gteborg, Sweden, OZGUR D. GRCAN, Ecole Polytechnique, CNRS UMR7648, LPP, F-91128, Palaiseau, France — A predator-prey model of dual populations with stochastic oscillators is presented. A linear cross-coupling between the two populations is introduced that follows the coupling between the motions of a Wilberforce pendulum in two dimensions: one in the longitudinal and the other in torsional plain. Within each population a Kuramoto type competition between the phases is assumed. Thus, the synchronization state of the whole system is controlled by these two types of competitions. The results of the numerical simulations show that by adding the linear cross-coupling interactions predator-prey oscillations between the two populations appear which results in self-regulation of the system by a transfer of synchrony between the two populations. The model represents several important features of the dynamical interplay between the drift wave and zonal flow turbulence in magnetically confined plasmas, and a novel interpretation of the coupled dynamics of drift wave-zonal flow turbulence using synchronization of stochastic oscillator is discussed.

<sup>1</sup>Sara Moradi has benefited from a mobility grant funded by the Belgian Federal Science Policy Office and the MSCA of the European Commission (FP7-PEOPLE-COFUND-2008 n 246540).

**4:06PM P53.00009 Exploring the Spatiotemporal Dynamics of Covariant Lyapunov Vectors for Chaotic Convection**<sup>1</sup>, MU XU, MARK PAUL, Virginia Tech — Covariant Lyapunov vectors provide access to fundamental features of chaos in high-dimensional systems that are driven far-from-equilibrium. We explore the spatiotemporal dynamics of covariant Lyapunov vectors for chaotic Rayleigh-Bénard convection to provide new physical insights. We use the covariant Lyapunov vectors to quantify the transition from hyperbolic to non-hyperbolic dynamics, to determine the degree of Oseledec splitting exhibited by the dynamics, and to shed light upon upon the tangled nature of the Lyapunov vectors. In this talk, we will explore the spatiotemporal dynamics of the Lyapunov vectors and their relation with the chaotic pattern dynamics of the flow field. Our results suggest that the Lyapunov vectors contain two distinct spatiotemporal features consisting of highly localized regions near defect structures and a spatially distributed checkerboard pattern. We will explore the connection between these features and the ideas of physical and spurious modes that may compose the dynamics.

<sup>1</sup>This research was funded by NSF grant no. DMS-1125234.

**4:18PM P53.00010 Lattice-Boltzmann Simulation of Tablet Disintegration**, JIAOLONG JIANG, NING SUN, DILIP GERSAPPE, Department of Materials Science and Engineering, Stony Brook University, Stony Brook, NY, 11794, USA — Using the lattice-Boltzmann method, we developed a 2D model to study the tablet disintegration involving the swelling and wicking mechanisms. The surface area and disintegration profile of each component were obtained by tracking the tablet structure in the simulation. Compared to pure wicking, the total surface area is larger for swelling and wicking, which indicates that the swelling force breaks the neighboring bonds. The disintegration profiles show that the tablet disintegrates faster than pure wicking, and there are more wetted active pharmaceutical ingredient particles distributed on smaller clusters. Our results indicate how the porosity would affect the disintegration process by changing the wetting area of the tablet as well as by changing the swelling force propagation.

**4:30PM P53.00011 The role of the capillary force in the liquid distribution in porous media**, BOJAN MARKICEVIC, Pall Corp — The dynamics of the liquid spreading in porous media occupied by gas is investigated numerically using the capillary network models. In the numerical solution, the flow at the free interface is fully resolved from the force balance at each pore along the interface allowing for local flows to fill or empty the pores. The flow is transient and the interface shape is determined at each time step. The liquid/solid interactions are investigated for whole range from fully wetting to fully non-wetting cases, and the spread of neutral fluid is also solved. For the neutral fluid, the interface irregularity are caused by pore varying volume with the interface of specific thickness separating fully saturated and gas occupied parts of porous medium. For the capillary interactions present, the interface thickness increases and due to the gas entrapment by spreading liquid, the saturation profiles develop in the direction of the liquid flow. The profiles depend on the capillary force as liquid spreads along the paths consisting of smaller pores for wetting, and larger pores for non-wetting interactions. Finally, the influence of the capillary force is counteracted by viscous force, where for faster flows, the saturation profiles vanish and the interface of limited thickness develops.

**4:42PM P53.00012 Numerical modeling and simulation of flow through porous fabric surface**, ZHENG GAO, XIAOLIN LI, Stony Brook University — We designed a numerical scheme to model the permeability of the fabric surface in an incompressible fluid by coupling the projection method with the Ghost Fluid Method in the front tracking framework. The pressure jump condition is obtained by adding a source term to the Poisson's equation in the projection step without modifications on its coefficients. The numerical results suggest that this approach has the ability to reproduce the relationship between pressure drop and relative velocity observed in the experiments. We use this algorithm to study the effects of porosity on the drag force and stability of parachutes during its inflation and deceleration.

**4:54PM P53.00013 A Numerical Study of Shear Flow in Partially Vegetated Open Channels**, JINGFANG QU, SUNY, Stony Brook, S CHEN, North Carolina State University, JIE YU, XIAOLIN LI, SUNY, Stony Brook — Shear flow at the interface between a porous layer and an open conduit is a problem of fundamental importance to problems ranging from natural to engineered flows. Such shear flows are known to be unstable, inducing waves and coherent vortices via Kelvin-Helmholtz instability. These coherent flow structures can strongly enhance the exchange of scalar variables and vector variable such as momentum in and out of the canopy, hence playing an important role in controlling environmental quality of these system. We developed a numerical model using finite difference method for flow in open channel occupied by a vegetation canopy. We apply the method to simulate the shear flow and compare with the experimental study by White and Nepf in 2007. Preliminary comparisons with the experimental data show good agreements.

**5:06PM P53.00014 Finite Amplitude Analysis of Mixed Convection in a Vertical Annulus Filled with Porous Medium.**, PREMANANDA BERA<sup>1</sup>, MOUMITA BHOWMIK, Indian Institute of Technology Roorkee — Using the weakly nonlinear stability analysis, we have investigated the stability of stably stratified mixed convective flow in a vertical annulus filled with fluid saturated metallic foam with porosity 0.97. Since the curvature parameter ( $C$ ) plays a vital role to describe the geometry, therefore special attention has been given to understand the effect of  $C$  on the flow by considering three different values of  $C$  (0.001, 0.6, and 10). The nonlinear results are presented for the fluid as water (Prandtl number ( $Pr$ ) equal to 7) and a fixed Reynolds number  $Re$  equal to 500. In the entire weakly nonlinear analysis, only super critical bifurcation has been predicted at and beyond the critical Rayleigh number ( $Ra$ ). The equilibrium amplitude ( $|A|$ ) increases beyond the critical point and decreases on reducing the gap between the concentric cylinders. Due to nonlinear interaction, a substantial enhancement in heat transfer rate is also observed from the basic state beyond the bifurcation point, i.e. Nusselt number predicted by nonlinear analysis is much more than those predicted by fully developed basic state.

<sup>1</sup>He is an expert person in Hydrodynamics stability and also in many areas of computational fluid dynamics.

**Wednesday, March 16, 2016 2:30PM - 5:18PM –**

**Session P54 GERA DPOLY FIAP: Organic Systems for Photovoltaics, Including Perovskites**

Hilton Baltimore Holiday Ballroom 5 -

**2:30PM P54.00001 Ovshinsky Sustainable Energy Fellowship: Excitronics for Transparent Photovoltaics**, RICHARD LUNT, Michigan State University — Room-temperature excitonic materials offer new opportunities for low-cost photovoltaic (PV) systems and provide prospects for unique solar harvesting science and applications. In the first part of this talk, I will introduce our pioneering work on developing transparent PVs that are creating a new paradigm for seamless solar harvesting around buildings, automobiles, and mobile electronics. These devices are enabled by the manipulation of excitonic semiconductor materials with selective harvesting in the nearinfrared and ultraviolet components of the solar spectrum. I will describe key photophysical properties, outline the thermodynamic and practical limits to these new classes of materials and devices, and briefly discuss their commercial impact for a range of applications. In the second part, I will describe the development of a new series organic salts that allow tunable photoresponse from 900nm to 1600nm, an unprecedented range for smallmolecule semiconductors. These organic salts also enable precise tuning of frontier orbital levels and heterojunction interface gaps through anion alloying that result in voltages near the thermodynamic limit. This design strategy can further enable rapid development of efficient and lowcost multijunction devices (both opaque and transparent) with complimentary response across the solar spectrum.

**3:06PM P54.00002 The role of molecular layer mixing on the thermal conductance of organic-inorganic heterojunctions**, SHUBHADITYA MAJUMDAR, ALAN J.H. MCGAUGHEY, JONATHAN A. MALEN, Carnegie Mellon University — The role of interfacial properties in affecting energy transport characteristics is an extensive area of research. Hybrid materials composed of organic-inorganic heterojunctions are gaining popularity as alternatives to conventional semiconductors for various energy-generation devices, thus requiring detailed study of their interfacial properties – especially thermal transport. Previous works have isolated the organic-inorganic interface thermal properties using self-assembled monolayer (SAM) junctions between two inorganic substrates and characterized them based on interfacial bonding strength, vibrational mismatch and molecule length. Here, we investigate the effect of having a mixed SAM layer on the thermal conductance of the SAM junction. The mixed SAM layers either have molecules of the same length but different end groups (thiols and methyl) or different lengths. This creates a modifiable bonding environment at one interface either through a varying ratio of strong and weakly bonded end groups or a decreasing surface coverage of the molecule. Both these scenarios are investigated to study the cooperative nature of the molecules/interface bonds and their effect on the heat transport across the junction. We follow a combined experimental and computational approach in our investigation – we fabricate the SAM junctions (alkanethiols between two gold substrates) and measure their thermal conductance using Frequency Domain Thermoreflectance, and use molecular dynamics simulations to get a deeper understanding of the role of intermolecular cross talk.

**3:18PM P54.00003 MOVED TO X33.011 –**

**3:30PM P54.00004 Switchable Solar Window Devices Based on Polymer Dispersed Liquid Crystals<sup>1</sup>**, JOSEPH MURRAY, DAKANG MA, JEREMY MUNDAY, University of Maryland — Windows are an interesting target for photovoltaics due to the potential for large area of deployment and because glass is already a ubiquitous component of solar cell devices. Many demonstrations of solar windows in recent years have used photovoltaic devices which are semitransparent in the visible region. Much research has focused on enhancing device absorption in the UV and IR ranges as a means to circumvent the basic tradeoff between efficiency and transparency to visible light. Use of switchable solar window is a less investigated alternative approach; these windows utilize the visible spectrum but can toggle between high transparency and high efficiency as needed. We present a novel switchable solar window device based on Polymer Dispersed Liquid Crystals (PDLC). By applying an electric field to the PDLC layer, the device can be switched from an opaque, light diffusing, efficient photovoltaic cell to a clear, transparent window. In the off state (i.e. scattering state), these devices have the added benefits of increased reflectivity for reduced lighting and cooling costs and haze for privacy. Further, we demonstrate that these windows have the potential for self-powering due to the very low power required to maintain the on, or high transparency, state.

<sup>1</sup>Support From: University of Maryland and Maryland Nano-center and its Fablab

**3:42PM P54.00005 Discovery of Novel Perovskites for Solar Thermochemical Water Splitting from High-Throughput First-Principles Calculations**, ANTOINE EMERY, CHRIS WOLVERTON, Northwestern Univ — Among the several possible routes of hydrogen synthesis, thermochemical water splitting (TWS) cycles is a promising method for large scale production of hydrogen. The choice of metal oxide used in a TWS cycle is critical since it governs the rate and efficiency of the gas splitting process. In this work, we present a high-throughput density functional theory (HT-DFT) study of  $\text{ABO}_3$  perovskite compounds to screen for thermodynamically favorable two-step thermochemical water splitting materials. We demonstrate the use of two screens, based on thermodynamic stability and oxygen vacancy formation energy, on 5,329 different compositions to predict 139 stable potential candidate materials for water splitting applications. Several of these compounds have not been experimentally explored yet and present promising avenues for further research. Additionally, the large dataset of compounds and stability in our possession allowed us to revisit the structural maps for perovskites. This study shows the benefit of using first-principles calculations to efficiently screen an exhaustively large number of compounds at once. It provides a baseline for further studies involving more detailed exploration of a restricted number of those compounds.

**3:54PM P54.00006 Super-ion inspired colorful hybrid perovskite solar cells.**, HONG FANG, PURU JENA, Virginia Commonwealth Univ — Organic-inorganic hybrid perovskites, with the general formula  $\text{AMX}_3$  (A=cation; M=metal; X=halogen), have emerged as a new generation of efficient yet inexpensive photovoltaic cells. These materials show record high conversion efficiency as solar cells and have excellent light-emission properties that can also be used in other optoelectronic devices. They can be processed easily from solution with optic band gaps, tunable from visible to infrared regions and are considered to be “the next big thing in photovoltaics”. However, several important issues such as the relationship between their photoexcitation properties and the chemical structures, their stability under ambient conditions, as well as the possibility to invent their environment-friendly analogues remain unsolved. In this work, our aim is not only to gain a fundamental understanding of the structure-property relationship of organic-inorganic hybrid perovskites, but also to rationally design a new class of hybrid perovskites that have desired electronic band gaps for solar cell applications. This is accomplished by using super-ions that can mimic the properties of elementary alkali and halogen ions as building blocks. These super-ions include superalkalis –  $\text{CH}_3\text{NH}_3^+$ ,  $\text{HC}(\text{NH}_2)_2^+$ , and  $\text{Li}_3\text{O}^+$  as cations and hyperhalogens –  $\text{Ge}(\text{BH}_4)_3^-$  and  $\text{Sn}(\text{BH}_4)_3^-$  as anions. The results are compared with perovskites composed of  $\text{GeCl}_3^-$ ,  $\text{GeBr}_3^-$ ,  $\text{GeI}_3^-$ ,  $\text{SnCl}_3^-$ ,  $\text{SnBr}_3^-$ , and  $\text{SnI}_3^-$  superhalogen anions. We develop a strategy to assemble these super-ions to form environment-friendly solar cells with adjustable band gaps (covering the visible range and beyond) and with improved resistance to moisture.

2Department of Chemistry, University of California at Berkeley, Berkeley, California 94720, USA

3Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

4Kavli Energy Nanosciences Institute at the University of California, Berkeley, and the Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

**4:06PM P54.00007 High efficiency graded band gap perovskite solar cells**, ONUR ERGEN, SALLY DEMAIO-TURNER, THANG THOAN PHAM, MARK TIAN ZHI TAN, JONGMIN YUK, ALEX ZETTL, University of California at Berkeley — We report high efficiency graded band gap perovskite solar cells with very large current output and high power conversion efficiencies (PCE) by using simultaneously mixed halides ( $\text{CH}_3\text{NH}_3\text{SnI}_3$  and  $\text{CH}_3\text{NH}_3\text{PbI}_{3-x}\text{Br}_x$ ) perovskite absorber layers. An analysis of the experimental data yields a high fill factor (FF) of ~75% and high short circuit current density ( $J_{\text{sc}}$ ) of up to 46.2 mA/cm<sup>2</sup>. These devices provide the highest current output aiming above 20% PCE.

**4:18PM P54.00008 Efficient organic-inorganic hybrid perovskites and doped metal oxide heterojunction solar cells.**, XIAOJUAN FAN, Marshall University — Organic-Inorganic hybrid perovskite  $\text{CH}_3\text{NH}_3\text{PbI}_3$  has recently attracted much attention for its high efficient solar energy conversion. This semiconducting pigment with a direct bandgap of 1.55 eV has made it an interesting optical and electronic material over the whole visible solar emission spectrum. The role of hole conducting has been found in this semiconductor that allows perovskite solar cell (PSC) to be formed by  $\text{CH}_3\text{NH}_3\text{PbI}_3/\text{TiO}_2$  heterojunctions that use  $\text{TiO}_2$  as scaffold, and carbon as a back contact. We will report a double layer metal doped  $\text{TiO}_2/\text{Al}_2\text{O}_3$  mesoporous scaffold covered by the p-type semiconducting pigment to form a high efficient PSC through solution method.  $\text{TiO}_2$  and  $\text{Al}_2\text{O}_3$  are both large band gap semiconductors that affect conducting and recombination rate in solar cells. One improvement work is doping other metal elements in  $\text{TiO}_2$  to raise the mobility while extend the recombination time. It has suggested that optimal amounts of doped metals such as Cu, Co, Mn can suppress the reduction of  $\text{Ti}^{4+}$  resulting better transportation.  $\text{TiO}_2$  thin films doped with metals are subjected to the EPR analysis and the results will be correlated with measurements of electronic-optical properties.

**4:30PM P54.00009 Modeling morphology dependence of the power generation in bulk heterojunction organic photovoltaics**, TIMOTHY SCHLITTENHARDT, SELMAN HERSHFIELD, Univ of Florida - Gainesville — Bulk heterojunctions are mixtures of differently doped organic semiconducting materials that provide for a highly interconnected and complex morphology. A three dimensional simulation is conducted of these systems, where the junctions are modeled by diodes with a given j-V characteristic and the transport within a particular material is treated as ohmic. The current and potential profile are calculated throughout the sample with an iterative method that allows us to readily treat systems with  $10^4$  sites for a full range of applied voltage biases. Visualizations of the current flow and voltage profile are given. It is found that power is not generated uniformly throughout the sample, but is concentrated near the edges. As has been observed experimentally, this leads to an optimal thickness for power generation. A simple analytical model is presented which reproduces and provides understanding of our simulation results.

**4:42PM P54.00010 Reliable thermal processing of organic perovskite films deposited on ZnO**, ALEX ZAKHIDOV, CHRIS MANSPEAKER, DMITRY LYASHENKO, Texas State University, ALEX ZAKHIDOV TEAM — Zinc oxide (ZnO) is a promising semiconducting material to serve as an electron transport layer (ETL) for solar cell devices based on organo-halide lead perovskites. ZnO ETL for perovskite photovoltaics has a combination of attractive electronic and optical properties: i) the electron affinity of ZnO is well aligned with valence band edge of the  $\text{CH}_3\text{NH}_3\text{PbI}_3$ , ii) electron mobility of ZnO is  $>1 \text{ cm}^2/(\text{Vs})$ , which is a few orders of magnitude higher than that of  $\text{TiO}_2$  (another popular choice of ETL for perovskite photovoltaic devices), and iii) ZnO has a large of band gap of 3.3 eV, which ensures optical transparency and large barrier for the hole injection. Moreover, ZnO nanostructures can be printed on flexible substrates at room temperatures in cost effective manner. However, it was recently found that organic perovskites deposited on ZnO are unstable and readily decompose at  $>90^\circ\text{C}$ . In this work, we further investigate the mechanism of decomposition of  $\text{CH}_3\text{NH}_3\text{PbI}_3$  film deposited on ZnO and reveal the role of the solvent in the film during the annealing process. We also develop a restricted volume solvent annealing (RVSA) process for post annealing of the perovskite film on ZnO without decomposition. We demonstrate that RVSA enables reliable perovskite solar cell fabrication.

**4:54PM P54.00011 Charge Generation Dynamics in Efficient All-Polymer Solar Cells: Influence of Polymer Packing and Morphology**, BHOJ GAUTAM, North Carolina State University, CHANGYEON LEE, Korea Advanced Institute of Science and Technology (KAIST), ROBERT YOUNTS, North Carolina State University, WONHO LEE, Korea Advanced Institute of Science and Technology (KAIST), EVGENY DANILOV, North Carolina State University, BUMJOON KIM, Korea Advanced Institute of Science and Technology (KAIST), KENAN GUNDOGDU, North Carolina State University — All-polymer solar cells exhibit rapid progress in power conversion efficiency (PCE) from 2 to 7.7% over the last few years. While this improvement is primarily attributed to efficient charge transport and balanced mobility between the carriers, not much is known about the charge generation dynamics in these systems. Here we measured exciton relaxation and charge separation dynamics using ultrafast spectroscopy in polymer/polymer blends with different molecular packing and morphology. These measurements indicate that preferential face on configuration with intermixed nanomorphology increases the charge generation efficiency. In fact there is a direct quantitative correlation between the free charge population in the ultrafast time scales and the external quantum efficiency, suggesting not only the transport but also charge generation is key for the design of high performance all polymer solar cells.

**5:06PM P54.00012 Phonon Mode Transformation across the Orthorhombic-Tetragonal Phase Transition in a Lead-Iodide Perovskite  $\text{CH}_3\text{NH}_3\text{PbI}_3$ : a Terahertz Time-Domain Spectroscopy Approach**<sup>1</sup>, ELBERT E. M. CHIA, Nanyang Tech Univ, CHAN LA-O-VORAKIAT, King Mongkuts University of Technology Thonburi, JEANNETTE KADRO, TEDDY SALIM, DAMING ZHAO, Nanyang Tech Univ, TOWFIQ AHMED, Los Alamos National Laboratory, YENG MING LAM, Nanyang Tech Univ, JIAN-XIN ZHU, Los Alamos National Laboratory, RUDOLPH MARCUS<sup>2</sup>, California Institute of Technology, MARIA-ELISABETH MICHEL-BEYERLE, Nanyang Tech Univ — Using terahertz time-domain spectroscopy (THz-TDS), we study the temperature-dependent phonon modes of the organometallic lead iodide perovskite  $\text{CH}_3\text{NH}_3\text{PbI}_3$  thin film across the terahertz (0.5-3 THz) and temperature (20-300 K) ranges. These modes are related to the vibration of the Pb-I bonds. We found that two phonon modes in the tetragonal phase at room temperature split into four modes in the low-temperature orthorhombic phase. By use of the Lorentz model fitting, we analyze the critical behavior of this phase transition.

<sup>1</sup>King Mongkuts University of Technology Thonburi (Grant No. SCI58-003), Singapore MOE Tier 1 (RG13/12, RG123/14), ONR, ARO, NTU Biophysics Center, LANL LDRD, LANL CINT.

<sup>2</sup>Nanyang Tech Univ

**Wednesday, March 16, 2016 2:30PM - 5:30PM —**  
**Session P55 DBIO DFD GSOFT: Active Fluids in Living Matter: Collective Cell Motility** Hilton  
Baltimore Holiday Ballroom 6 - Yuhai Tu, IBM, Inc.

**2:30PM P55.00001 Collective dynamics of cell migration and cell rearrangements** , ALEXANDRE KABLA, University of Cambridge — Understanding multicellular processes such as embryo development or cancer metastasis requires to decipher the contributions of local cell autonomous behaviours and long range interactions with the tissue environment. A key question in this context concerns the emergence of large scale coordination in cell behaviours, a requirement for collective cell migration or convergent extension. I will present a few examples where physical and mechanical aspects play a significant role in driving tissue scale dynamics.

1. Geometrical confinement is one of the key external factors influencing large scale coordination during collective migration. Using a combination of in vitro experiments and numerical simulations, we show that the velocity correlation length, measured in unconfined conditions, provides a convenient length scale to predict the dynamic response under confinement. The same length scale can also be used to quantify the influence range of directional cues within the cell population.
2. Heterogeneity within motile cell populations is frequently associated with an increase in their invasive capability and appears to play an important role during cancer metastasis. Using in silico experiments, we studied the way cell invasion is influenced by both the degree of cell coordination and the amount of variability in the motile force of the invading cells. Results suggest that mechanical heterogeneity dramatically enhances the invasion rate through an emerging cooperative process between the stronger and weaker cells, accounting for a number of observed invasion phenotypes.
3. Effective convergent extension requires on a consistent orientation of cell intercalation at the tissue scale, most often in relation with planar cell polarity mechanisms to define the primary axes of deformation. Using a novel modelling approach for cells mechanical interactions, we studied the dynamics of substrate free motile cell populations. Ongoing work shows in particular that nematic order emerges from interacting cells without the need for biochemical cues setting tissue polarity.

**3:06PM P55.00002 Multicellular Streaming in Solid Tumours** , JOSEF KAS, Leipzig University — As early as 400 BCE, the Roman medical encyclopaedist Celsus recognized that solid tumours are stiffer than surrounding tissue. However, cancer cell lines are softer, and softer cells facilitate invasion. This paradox raises several questions: Does softness emerge from adaptation to mechanical and chemical cues in the external microenvironment, or are soft cells already present inside a primary solid tumour? If the latter, how can a more rigid tissue contain more soft cells? Here we show that in primary tumour samples from patients with mammary and cervix carcinomas, cells do exhibit a broad distribution of rigidities, with a higher fraction of softer and more contractile cells compared to normal tissue. Mechanical modelling based on patient data reveals that, surprisingly, tumours with a significant fraction of very soft cells can still remain rigid. Moreover, in tissues with the observed distributions of cell stiffnesses, softer cells spontaneously self-organize into lines or streams, possibly facilitating cancer metastasis.

**3:42PM P55.00003 Active unjamming of confluent cell layers**<sup>1</sup> , M CRISTINA MARCHETTI, Syracuse University — Cell motion inside dense tissues governs many biological processes, including embryonic development and cancer metastasis, and recent experiments suggest that these tissues exhibit collective glassy behavior. Motivated by these observations, we have studied a model of dense tissues that combines self-propelled particle models and vertex models of confluent cell layers. In this model, referred to as self-propelled Voronoi (SPV), cells are described as polygons in a Voronoi tessellation with directed noisy cell motility and interactions governed by a shape energy that incorporates the effects of cell volume incompressibility, contractility and cell-cell adhesion. Using this model, we have demonstrated a new density-independent solid-liquid transition in confluent tissues controlled by cell motility and a cell-shape parameter measuring the interplay of cortical tension and cell-cell adhesion. An important insight of this work is that the rigidity and dynamics of cell layers depends sensitively on cell shape. We have also used the SPV model to test a new method developed by our group to determine cellular forces and tissue stresses from experimentally accessible cell shapes and traction forces, hence providing the spatio-temporal distribution of stresses in motile dense tissues.

<sup>1</sup>This work was done with Dapeng Bi, Lisa Manning and Xingbo Yang. MCM was supported by NSF-DMR-1305184 and by the Simons Foundation.

**4:18PM P55.00004 Modeling collective cell motility**<sup>1</sup> , WOUTER-JAN RAPPEL, Univ of California - San Diego — Eukaryotic cells often move in groups, a critical aspect of many biological and medical processes including wound healing, morphogenesis and cancer metastasis. Modeling can provide useful insights into the fundamental mechanisms of collective cell motility. Constructing models that incorporate the physical properties of the cells, however, is challenging. Here, I discuss our efforts to build a comprehensive cell motility model that includes cell membrane properties, cell-substrate interactions, cell polarity, and cell-cell interaction. The model will be applied to a variety of systems, including motion on micropatterned substrates and the migration of border cells in *Drosophila*.

<sup>1</sup>This work was supported by NIH Grant No. P01 GM078586 and NSF Grant No. 1068869

**4:54PM P55.00005 Water Dynamics in Living Cells and Tumor Cell Migration in Confined Microenvironments** , SEAN SUN, Johns Hopkins University — More than 70% of the total mass in living cells is water. In most biological scenarios water serves as a passive medium responsible for solvation and proper functioning of proteins. However, it has been long recognized that there are situations where dynamic transport of water in cells is important. First, cells actively transport water in order to maintain its volume, and because cell volume directly influences cell shape and internal hydrostatic pressure, it is a critical aspect of cell mechanics. Furthermore, cell volume is coupled to protein synthesis which ultimately determines the cell size. Therefore water transport and cell volume dynamics ultimately impact cell growth and division. Second, epithelial cells in organs such as the eye and kidney actively transport water across the cell membrane and the epithelial layer. Indeed, water channels such as aquaporins increase water permeability of the membrane and facilitate this transport. Recent, we have shown that in confined microenvironments, active transport of water is responsible for actin-independent cell movement in confined spaces, especially for cancer cells. These results suggest that cells actively control its water content. The active regulation of water content is a crucial aspect of cell dynamics. We will discuss a theoretical model of cell pressure/volume control. Implications of this model for active cell dynamics in multi-cellular epithelial sheets will be discussed.

**Wednesday, March 16, 2016 5:00PM - 6:00PM —**  
Session Q2 APS: NSBP Meetup Hilton Baltimore Johnson A -

**5:00PM Q2.00001 NSHP/NSBP Meetup —**

**Wednesday, March 16, 2016 5:45PM - 6:45PM —**  
Session Q3 APS: NSHP Meetup Hilton Baltimore Johnson B -

**5:45PM Q3.00001 NSHP meetup —**

## **Wednesday, March 16, 2016 5:45PM - 6:45PM —**

**Session Q4 GMAG: GMAG Jobs Mixer** Hilton Baltimore Pickersgill -

**5:45PM Q4.00001 GMAG Jobs Mixer** — This event is open to the members of the magnetism community, especially postdocs and students, who are interested in jobs in industry, national labs, and academia, or have a job opportunity to offer. Refreshments will be served

## **Wednesday, March 16, 2016 7:00PM - 8:30PM —**

**Session Q5 APS: Diversity Networking Session** Hilton Baltimore Peale -

**7:00PM Q5.00001 Diversity Networking Session** — Please join us to network with your colleagues and to learn about APS Diversity Initiatives and the work of the APS Committees on women, Minorities, and LGBT issues

## **Wednesday, March 16, 2016 5:45PM - 6:45PM —**

**Session Q16 GSCCM: GSCCM Business Meeting** 315 -

**5:45PM Q16.00001 GSCCM BUSINESS MEETING** —

## **Wednesday, March 16, 2016 5:45PM - 6:45PM —**

**Session Q37 GSOF: GSOF Business Meeting** 340 -

**5:45PM Q37.00001 GSOF BUSINESS MEETING** —

## **Wednesday, March 16, 2016 5:45PM - 6:45PM —**

**Session Q50 Joint Task Force on Undergraduate Physics Programs** Hilton Baltimore Holiday Ballroom

1 -

**5:45PM Q50.00001 Joint Task Force on Undergraduate Physics Programs** — This session will focus on the guidelines and recommendations being developed by the APS/AAPT Joint Task Force on Undergraduate Physics Programs. J-TUPP is studying how undergraduate physics programs might better prepare physics majors for diverse careers. The guidelines and recommendations will focus on curricular content, flexible tracks, pedagogical methods, research experiences and internships, the development of professional skills, and enhanced advising and mentoring for all physics majors.

## **Wednesday, March 16, 2016 6:00PM - 8:00PM —**

**Session Q51 FOEP: Outreach Happy Hour and FOEP Business Meeting** Pratt Street Ale House Restaurant - Rebecca Thompson, APS

**6:00PM Q51.00001 Outreach Happy Hour and FOEP Business Meeting** , BECKY THOMPSON, APS — Come meet others doing public outreach and learn more about the Forum on Outreach and Engaging the Public. Outreach mini grant awardees and applicants are particularly encouraged to attend

## **Wednesday, March 16, 2016 9:00PM - 10:30PM —**

**Session Q56 APS: Rock-n-Roll Physics Sing-a-Long** Hilton Baltimore Holiday Ballroom 6 -

**9:00PM Q56.00001 Rock 'n' Roll Physics Sing-Along** — Like to learn new favorites? Wish you had some snappy songs that teach physics? Just want to sing and laugh or listen and laugh? Join us for an evening of fun physics tunes set to familiar rock, blues, and swing tunes. Light refreshments will be served.

## **Wednesday, March 16, 2016 8:00PM - 10:00PM —**

**Session Q55 FHP FOEP: A Staged Reading of the Play: No No Nobel** Hilton Baltimore Key Ballroom

9 -

**8:00PM Q55.00001 A Staged Reading of the Play: No No Nobel** — A Staged Reading of the Play: No No Nobel In Biology, what discovery is considered the most important breakthrough of the 20th century? In Chemistry, what pattern development enabled chemists and physicists to understand the nature of and ultimately the atomic physics of the elements? In Physics, what experiment and theory in nuclear physics led to the most important journalistic story of the 20th century? In Cosmology, what theory was developed that enabled the understanding of the now named Big Bang theory and the evolution of the universe? In Science Education, what graduate student made a most important observation and ultimately the identification of a remnant of a supernova explosion? Join us for a dramatic staged reading of No No Nobel and find out what unifies all the above questions. The playwright is the science historian David Cassidy and the staged reading is performed by the Baltimore Improv Group [www.bigimprov.org](http://www.bigimprov.org) . After the performance, the playwright, the director Mike Harris and the actors will be available for a talk-back audience discussion. Produced by Brian Schwartz, Brooklyn College and the Graduate Center of the City University of New York

**Thursday, March 17, 2016 8:00AM - 11:00AM –**

**Session R1 DCMP: 3D Dirac Materials** Ballroom I - Ady Stern, Weizmann Institute of Science

**8:00AM R1.00001 Weyl Semimetal Phase in Noncentrosymmetric Transition-Metal Monophosphides**, XI DAI, Institute of Physics, CAS — Based on first-principle calculations, we show that a family of nonmagnetic materials including TaAs, TaP, NbAs, and NbP are Weyl semimetals (WSM) without inversion centers. We find twelve pairs of Weyl points in the whole Brillouin zone (BZ) for each of them. In the absence of spin-orbit coupling (SOC), band inversions in mirror-invariant planes lead to gapless nodal rings in the energy-momentum dispersion. The strong SOC in these materials then opens full gaps in the mirror planes, generating nonzero mirror Chern numbers and Weyl points off the mirror planes. The transport properties obtained by the Boltzmann equation combined with the semiclassical treatments of the unique electronic structure in these materials will also be discussed in comparison with the most recent experimental data.

**8:36AM R1.00002 Chirality transfer dynamics in quantum orbits in the Dirac semi-metal  $\text{Cd}_3\text{As}_2$** , PHILIP MOLL, UC Berkeley — No abstract available.

**9:12AM R1.00003 Evidence for the chiral anomaly in the Dirac semimetal  $\text{Na}_3\text{Bi}$** <sup>1</sup>, JUN XIONG, Princeton University — Chiral symmetry describes the conservation of handedness of massless chiral fermions in high-energy physics. Such symmetry can be broken by the coexistence of electric ( $\vec{E}$ ) and magnetic ( $\vec{B}$ ) fields, known as the chiral (Adler-Bell-Jackiw) anomaly. This anomaly describes an axial current pumped between left-handed and right-handed Weyl fermions. In condensed matter physics, the recent development in both theory and experiments has confirmed the existence of Weyl nodes in the Dirac and Weyl semimetals. Generated by the  $\vec{E} \cdot \vec{B}$  term, the axial current could induce negative magnetoresistance in the Dirac and Weyl semimetals. Here we report the observation of a large, negative longitudinal magnetoresistance in the Dirac semimetal  $\text{Na}_3\text{Bi}$ . By rotating both the direction of  $\vec{E}$  and  $\vec{B}$ , we found that the small deviation of  $\vec{E}$  from  $\vec{B}$  greatly suppresses the observed negative magnetoresistance. We will discuss its consistency with the predicted chiral anomaly effect in the Dirac/Weyl semimetal.

<sup>1</sup>Supported by Army Research Office grant ARO W911NF-11-1-0379, a MURI award for topological insulators (ARO W911NF-12-1-0461), and the Gordon and Betty Moore Foundations EPiQS Initiative through grant GBMF4539.

**9:48AM R1.00004 Experimental realization of new topological phases of matter beyond topological insulators**, MADHAB NEUPANE, Department of Physics, University of Central Florida, Orlando, Florida 32816, USA — A three-dimensional (3D)  $\text{Z}_2$  topological insulator (TI) is a crystalline solid, which is an insulator in the bulk but features spin-polarized Dirac electron states on its surface. In 2007, the first 3D TI was discovered in a bismuth-based compound. The discovery of the first TI tremendously accelerated research into phases of matter characterized by non-trivial topological invariants. Not only did the 3D  $\text{Z}_2$  TI itself attract great research interest, it also inspired the prediction of a range of new topological phases of matter. The primary examples are the topological Kondo insulator, the topological 3D Dirac and Weyl semimetals, the topological crystalline insulator, topological nodal line semimetal and the topological superconductor. Each of these phases was predicted to exhibit surface states with unique properties protected by a non-trivial topological invariant. In this talk, I will discuss the experimental realization of these new phases of matter in real materials by momentum and time-resolved photoemission spectroscopy. Special attention will be given to the experimental discovery of Dirac semimetal phase in  $\text{Cd}_3\text{As}_2$  and topological nodal-line phase in  $\text{PbTaSe}_2$ . The unusual properties of the protected topological surface states can lead to potential future applications in spintronics and quantum information, which hold promise to revolutionize our electronics and energy industries. *This work is supported by start-up funds from University of Central Florida (MN) and Los Alamos National Laboratory LDRD program. The work at Princeton and Princeton-led ARPES measurements are supported by the Gordon and Betty Moore Foundations EPiQS Initiative through grant GBMF4547 (Hasan) and by U.S. Department of Energy DE-FG-02-05ER46200.*

**10:24AM R1.00005 Time-reversal symmetry breaking type II Weyl state in  $\text{YbMnBi}_2$** , SERGEY BORISENKO, IFW-Dresden, Germany — Detection of Dirac, Majorana and Weyl fermions in real materials may significantly strengthen the bridge between high-energy and condensed-matter physics. While the presence of Dirac fermions is well established in graphene and topological insulators, Majorana particles have been reported recently and evidence for Weyl fermions in non-centrosymmetric crystals has been found only a couple of months ago, the "magnetic" Weyl fermions are still elusive despite numerous theoretical predictions and intense experimental search. In order to detect a time-reversal symmetry breaking Weyl state we designed two materials with Fermi velocities superior to that of graphene and I will present the experimental evidence of realization of such a state in one of them,  $\text{YbMnBi}_2$ . We model the time reversal symmetry breaking observed by magnetization measurements by a canted antiferromagnetic state and find a number of Weyl points both above and below the Fermi level. Using angle-resolved photoemission, we directly observe these latter Weyl points and a hallmark of the exotic state – the arc of the surface states which connects these points. Our results not only provide a fundamental link between the two areas of physics, but also demonstrate the practical way to design novel materials with exotic properties.

**Thursday, March 17, 2016 8:00AM - 10:24AM –**

**Session R2 DCMP GMAG: Advances in Collective Effects in Organic Semiconductors** Ballroom II - Michael Flatte, University of Iowa

**8:00AM R2.00001 Electrical detection of proton-spin motion in a polymer device at room temperature<sup>1</sup>**, CHRISTOPH BOEHME, Department of Physics and Astronomy, University of Utah — With the emergence of spintronics concepts based on organic semiconductors there has been renewed interest in the role of both, electron as well as nuclear spin states for the magneto-optoelectronic properties of these materials. In spite of decades of research on these molecular systems, there is still much need for an understanding of some of the fundamental properties of spin-controlled charge carrier transport and recombination processes [1]. This presentation focuses on mechanisms that allow proton spin states to influence electronic transition rates in organic semiconductors. Remarkably, even at low-magnetic field conditions and room temperature, nuclear spin states with energy splittings orders of magnitude below thermal energies are able to influence observables like magnetoresistance and fluorescence [2]. While proton spins couple to charge carrier spins via hyperfine interaction, there has been considerable debate about the nature of the electronic processes that are highly susceptible to these weak hyperfine fields. Here, experiments are presented which show how the magnetic resonant manipulation of electron and nuclear spin states in a  $\pi$ -conjugated polymer device causes changes of the device current [3]. The experiments confirm the extraordinary sensitivity of electronic transitions to very weak magnetic field changes and underscore the potential significance of spin-selection rules for highly sensitive absolute magnetic fields sensor concepts [4]. However, the relevance of these magnetic-field sensitive spin-dependent electron transitions is not just limited to semiconductor materials but also radical pair chemistry [5] and even avian magnetoreceptors [6]. [1] C. Boehme, J. M. Lupton, *Nat. Nanotechn.* **8**, 9 (2013); [2] S.-Y. Lee et al., *JACS* **133**, 072019 (2011); [3] H. Malissa et al., *Science* **345**, 1487 (2014); [4] W. J. Baker et al., *Nature Commun.* **3**, 898 (2012); [5] U.E. Steiner and T. Ulrich, *Chem. Rev.* **89**, 51-147 (1989); [6] T. Ritz, et al., *Nature* **429**, 17780 (2004).

<sup>1</sup>This work was supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award #DE-SC0000909. The Utah NSF - MRSEC program #DMR 1121252 is acknowledged for instrumentation support.

**8:36AM R2.00002 Active control of magnetoresistance of organic spin valves using ferroelectricity**, JIAN SHEN, Fudan Univ — Organic spintronic devices have been appealing because of the long spin lifetime of the charge carriers in the organic materials and their low cost, flexibility and chemical diversity. In previous studies, the control of resistance of organic spin valves is generally achieved by the alignment of the magnetization directions of the two ferromagnetic electrodes, generating magnetoresistance. Here we employ a new knob to tune the resistance of organic spin valves by adding a thin ferroelectric interfacial layer between the ferromagnetic electrode and the organic spacer: the magnetoresistance of the spin valve depends strongly on the history of the bias voltage, which is correlated with the polarization of the ferroelectric layer; the magnetoresistance even changes sign when the electric polarization of the ferroelectric layer is reversed. These findings enable active control of resistance using both electric and magnetic fields, opening up possibility for multi-state organic spin valves.

**9:12AM R2.00003 Organic magnetoelectroluminescence for room temperature transduction between magnetic and optical information**, MARKUS WOHLGENANT, University of Iowa — No abstract available.

**9:48AM R2.00004 New Directions for Organic Spintronics: Novel Materials and Emergent Phenomena<sup>1</sup>**, EZEKIEL JOHNSTON-HALPERIN, Department of Physics, The Ohio State University — Organic and organic-based materials are attractive candidates for applications in magnetoelectronics and spintronics due to their low cost, ease of fabrication, and low spin-orbit coupling (and consequently long spin lifetimes). However, in comparison to the case for inorganic systems, robust intrinsic magnetic ordering in this class of materials is exceedingly rare and as a result the potential of these materials has yet to be fully realized. Here we present a series of recent breakthroughs in the synthesis, encapsulation, and measurement of organic-based magnets that lay the foundation for all organic magnetoelectronic and spintronic devices. We will discuss advances in encapsulation strategies that allow lifetimes of up to 1 month in air for functional magnetoelectronic devices, the use of ligand substitution to generate a library of related magnetic materials, the growth of all-organic and hybrid organic/inorganic magnetic heterostructures, and measurements of the magnetization dynamics that reveal ferromagnetic resonance (FMR) linewidths of  $\sim 1$  G, comparable to or narrower than corresponding measurements in yttrium iron garnet (YIG). These results establish the validity of organic-based magnets for applications in next-generation magnetoelectronics and provide unique leverage on long-standing challenges in the field of organic spintronics. For example, organic magnetic heterostructures promise to provide an exciting opportunity to explore exchange, dynamic spin injection, and spin transport in all-organic spintronic devices.

<sup>1</sup>This work was supported in part by NSF DMR-1507775 and the Center for Emergent Materials (an NSFMRSEC; Award Number DMR-1420451) at The Ohio State University.

**Thursday, March 17, 2016 8:00AM - 11:00AM —**  
**Session R3 DCMP GSOFT GSNP: Glass and Jamming Transitions** Ballroom III - Sydney Nagel, University of Chicago

**8:00AM R3.00001 The Gardner Transition: A new approach for understanding low-temperature glasses**, PATRICK CHARBONNEAU, Duke University — Recent theoretical advances in the mean-field theory of glasses predict the existence deep in the glass phase of a novel phase transition, a so-called Gardner transition. This transition signals the emergence of a complex free energy landscape composed of a marginally stable hierarchy of sub-basins within a broad glass metabasin. It is thus the onset of marked changes in thermal and transport properties of glasses, and ultimately leads to the unusual critical behavior at jamming. The Gardner transition itself is immediately related to a diverging (i) characteristic relaxation time, (ii) caging susceptibility and (iii) correlation length of the caging heterogeneity as well as aging, even in well-thermalized glasses. We have detected some of these signatures both in a mean-field model and in standard hard-sphere glass formers. We find the results to quantitatively agree with theory in the former and qualitatively so in the latter, which suggest that the transition should be detectable in a wide array of numerical and experimental systems. Interestingly, although the Gardner transitions is primarily associated with structural glass formers, we also find features of the transition in crystals of polydisperse particles once the landscape becomes rough.

**8:36AM R3.00002 Scaling theory for the jamming transition<sup>1</sup>**, ANDREA J. LIU, University of Pennsylvania, Department of Physics and Astronomy — The existence of a critical jamming transition, which marks the onset of rigidity in athermal packings of spheres, suggests that universal physics underlies the origin and nature of rigidity in disordered solids ranging from glasses to foams and granular materials. The jamming transition was originally proposed as a zero-temperature critical point in a non-equilibrium phase diagram in packing density and shear stress. Many studies have documented critical phenomena near the jamming transition, including power-law scaling, diverging length scales and scaling collapse, and theories have been developed to understand these phenomena. However, a number of confusing features have precluded a unified critical scaling analysis of the transition. Here we resolve these issues to present a scaling ansatz for the jamming critical point in terms of density and shear stress. The theory predicts new exponents that we verify with numerical simulations.

<sup>1</sup>work done with C. P. Goodrich and J. P. Sethna and supported by DOE DE-FG02-05ER46199

**9:12AM R3.00003 Frustration by Shape-Designed Local Polymorphism: A Near-Equilibrium Colloidal Glass of Hard Kites**, THOMAS MASON, University of California- Los Angeles — We study glass formation in uniform Brownian dispersions of hard colloidal polygonal platelets having the shape of 72-degree achiral kites, fabricated using optical stepper lithography. These kites are confined to a plane through roughness-controlled depletion attractions, and they diffuse in two-dimensions as we very slowly raise the particle density in the system. Although the densest packing of these kites is a crystalline lattice that fully tiles the plane, remarkably, we observe that the kites do not crystallize even for such quasi-static osmotic compression. By contrast, we have previously shown that such slow compression does cause crystallization of Brownian systems of other convex 2D lithographic shapes, such as squares and rhombs. Instead, the system of kites forms a disordered glass that undergoes an ergodic to non-ergodic transition, both in a rotational and a translational sense, while remaining near-equilibrium, as we measure by video particle tracking. We show that the high diversity of few-particle local polymorphic configurations (LPCs) of kites, related to our choice of angles and lengths in the designed shape, is responsible for suppressing long range spatial order and consequently favors glass formation instead. The prevalence and diversity of 5-particle LPCs, such as the pentagonal star, frustrate crystallization because these pentagonal LPCs are topologically different than the one 4-particle LPC that corresponds to the space-filling crystal. We anticipate that this mechanism of glass formation through shape-dependent frustration by diverse and incommensurate LPCs will also be relevant for molecular systems in three dimensions.

**9:48AM R3.00004 Solution of the dynamics of high-dimensional liquids**, JORGE KURCHAN<sup>1</sup>, LPS-ENS 24 rue Lhomond, 75231 Paris — The dynamics of a liquid composed of particles with spherically symmetric potentials has been solved exactly in limit of high dimensions  $d$ . The calculation is long but straightforward. At high density, an ergodicity-breaking glass transition is found. This computation allows one to assess the validity of approximation schemes such as Mode-Coupling Theory. As a by-product, because our calculation is, if not rigorous, elementary, an improvement in the bound for sphere packings in large dimensions is now at hand.

<sup>1</sup>work with: Thibaud Maimbourg and Francesco Zamponi

**10:24AM R3.00005 Spinodals with Disorder: from Avalanches in Random Magnets to Glassy Dynamics**, GIULIO BIROLI, IPHT CEA Saclay and LPS ENS Paris — We revisit the phenomenon of spinodals in the presence of quenched disorder and develop a complete theory for it. We focus on the spinodal of an Ising model in a quenched random field (RFIM), which has many applications in many areas from materials to social science. By working at zero temperature in the quasi-statically driven RFIM, thermal fluctuations are eliminated and one can give a rigorous content to the notion of spinodal. We show that the spinodal transition is due to the depinning and the subsequent expansion of rare droplets. We work out the critical behavior, which, in any finite dimension, is very different from the mean-field one: the characteristic length diverges exponentially and the thermodynamic quantities display very mild non-analyticities much like in a Griffith phenomenon. Thanks to the recently established connection between the spinodal of the RFIM and glassy dynamics, our results allow us to conclusively assess the physical content and the status of the dynamical transition predicted by the mean-field theory of glass-forming liquids.

**Thursday, March 17, 2016 8:00AM - 11:00AM —**

**Session R4 DPOLY: Where Electrostatics Counts: Assembly and Dynamics of Ionic Polymers**  
Ballroom IV - Svetlana Sukhishvili, Stevens Institute of Technology

**8:00AM R4.00001 Funny and Functional Physics: PEC Nanoparticles**, MARTIEN COHEN STUART, Physical Chemistry & Soft Matter, Wageningen University, Netherlands — When the tendency of polyelectrolyte complexes to phase separate is judiciously combined with appropriate concepts from the realms of polymer physics and supramolecular chemistry, a wealth of novel self-assembled nanoparticles with original properties can be prepared. This presentation discusses how a high degree of complexity and functionality arises spontaneously, in the form of equilibrium structures, and how these structures can be understood from physical principles. Some promising applications are mentioned as well.

**8:36AM R4.00002 Quantifying Contributions to Transport in Ionic Polymers Across Multiple Length Scales**, LOUIS MADSEN, Virginia Tech — Self-organized polymer membranes conduct mobile species (ions, water, alcohols, etc.) according to a hierarchy of structural motifs that span sub-nm to  $>10\ \mu\text{m}$  in length scale. In order to comprehensively understand such materials, our group combines multiple types of NMR dynamics and transport measurements (spectroscopy, diffusometry, relaxometry, imaging) with structural information from scattering and microscopy as well as with theories of porous media,<sup>1</sup> electrolytic transport, and oriented matter.<sup>2</sup> In this presentation, I will discuss quantitative separation of the phenomena that govern transport in polymer membranes, from intermolecular interactions ( $\leq 2\ \text{nm}$ ),<sup>3</sup> to locally ordered polymer nanochannels (a few to 10s of nm),<sup>2</sup> to larger polymer domain structures (10s of nm and larger).<sup>1</sup> Using this multi-scale information, we seek to give informed feedback on the design of polymer membranes for use in, *e.g.*, efficient batteries, fuel cells, and mechanical actuators. **References:**

1. J. Hou, J. Li, D. Mountz, M. Hull, and L. A. Madsen. *Journal of Membrane Science* **448**, 292-298 (2013).
2. J. Li, J. K. Park, R. B. Moore, and L. A. Madsen. *Nature Materials* **10**, 507-511 (2011).
3. M. D. Lingwood, Z. Zhang, B. E. Kidd, K. B. McCreary, J. Hou, and L. A. Madsen. *Chemical Communications* **49**, 4283 - 4285 (2013).

**9:12AM R4.00003 Nonequilibrium Simulations of Ion Dynamics in Ionomer Melts**, AMALIE FRISCHKNECHT, Sandia National Laboratories — Ionomers, polymers containing a small fraction of covalently bound ionic groups, are of interest as possible electrolytes in batteries. However, to date ionomers do not have sufficiently high conductivities for practical application, most likely because the ions tend to form aggregates, leading to slow ion transport. To build a better understanding of the relationships among ionomer chemistry, morphology, and ion transport, we have performed a series of molecular dynamics simulations and connected aspects of these simulations with experiment. In previous work using both atomistic and coarse-grained models, we showed that precise ionomers (with a fixed spacing between ionic groups along the polymer backbone) exhibit a range of ionic aggregate morphologies, from discrete clusters to percolated aggregates. In this talk I will describe recent simulations of our coarse-grained ionomer melts in an applied electric field. From a constant applied field, we are able to extract the ion mobilities and hence conductivities. We find that ionomers with percolated ionic aggregate morphologies have higher ion mobilities and hence higher conductivities. Application of an oscillating electric field enables us to calculate the frequency-dependent conductivity of the model ionomer melts. The real part of the conductivity has a high frequency peak associated with plasma oscillations, and a very broad low frequency peak associated with ion motions in ionic aggregates. I will end with comments on the connections to atomistic simulations and to experimental probes of ion dynamics.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

**9:48AM R4.00004 Electrostatic Assembly of Polymers and Nanoparticles at Liquid-Liquid Interfaces.**<sup>1</sup>, DAVID HOAGLAND, Univ. of Massachusetts Amherst — The electrostatic attraction between charged solutes on opposite sides of the interface between immiscible liquids offers an efficient route to the self-assembly of two-dimensional films. As implemented by us, a hydrophobic polymer with amine end(s) or block(s) is presented in an oil phase, and a negatively charged nanoparticle is presented in an aqueous phase; both solutes are insoluble in the opposite phase but efficiently driven to the liquid-liquid interface by mutual electrostatic attraction to the solute in the opposite phase. Depending on experimental conditions (salt concentration, pH, solute concentrations, etc.), a continuous, nanoscopically thin composite film builds at the oil-water interface over the timescale of minutes, often accompanied by a dramatic reduction of interfacial tension akin to that observed for a surfactant. Film formation and properties by the new route will be discussed, as principally probed through pendant drop interfacial tensiometry and pendant drop interfacial rheometry. Components of model system are toluene-dissolved amine end-capped polystyrene and water-dispersed acid-treated carbon nanotubes or citrate-treated gold nanospheres. Film structures are complicated, as are crucial electrostatic interactions near the interface. With amine end-capped polystyrene partnered with acid-treated carbon nanotubes, high pH (above 5) and high polystyrene molecular weight (above 5000 g/mol) strongly hinder film formation. These films, which are liquid-like, show two viscoelastic relaxations, a fast relaxation (about 10 s) associated with polystyrene chain rearrangements (slightly impacted by carbon nanotube association) and a slow relaxation (about 20 min) associated with polystyrene adsorption/desorption; at intermediate times (or frequencies), the two-dimensional storage and loss moduli follow approximately the same power law dependences.

<sup>1</sup>Support by NSF through the Univ. of Massachusetts MRSEC

**10:24AM R4.00005 Polymerized Ionic Liquids: Promising Class of Polymer Electrolytes**, ALEXEI SOKOLOV, University of Tennessee, and Oak Ridge National Laboratory — Use of polymer electrolytes instead of traditional liquid electrolytes offers an elegant solution to many problems in current battery technology. However, a major obstacle in use of polymer electrolytes is their low ionic conductivity and low transference number (percentage of charge transported by the desired ion). Polymerized ionic liquids (PolyILs), a relatively new class of polymer electrolytes, are essentially single ion conductors and provide simple solution for the increase of the transference number. However, their ionic conductivity at ambient conditions remains low. Our earlier studies demonstrated that only *strong decoupling of ionic conductivity from segmental dynamics* can lead to a 'superionic' behavior of a polymer and might provide sufficiently high conductivity [1,2]. Based on this concept, we overview recent developments in the field of polymerized ionic liquids, with the emphasis on the polymer specific decoupling of ionic conductivity from segmental dynamics. The latter is well illustrated by the comparison of ionic liquids with their polymerized analogs [3,4]. Ways to further improvement of ionic conductivity in PolyILs, and their possible limitations are discussed at the end.

1. Y. Wang, et al., **Phys. Rev. Letters** **108**, 088303 (2012).

2. Y. Wang, et al., **Polymer** **55**, 4067 (2014).

3. J. R. Sangoro, et al., **Soft Matter** **10**, 3536 (2014).

4. F. Fan, et al., **Macromolecules** **48**, 4461 (2015).

## Thursday, March 17, 2016 8:00AM - 11:00AM –

**Session R5 DMP: Disorder and Substitution Studies in Fe-based Superconductors** 301 - Johnpierre Paglione, University of Maryland

**8:00AM R5.00001 Effect of electron irradiation on  $(\text{Ba}_{1-x}\text{K}_x)\text{Fe}_2\text{As}_2$  from London penetration depth measurements**, KYUIL CHO, S. TEKNOWIJOYO, M. A. TANATAR, Y. LIU, T. A. LOGRASSO, R. PROZOROV, Ames Laboratory and Iowa State University, USA, M. KONCZYKOWSKI, Ecole Polytechnique, France, S. MAITI, P. HIRSCHFELD, University of Florida, USA, V. MISHRA, Oak Ridge National Laboratory, USA — The effects of artificial disorder induced by 2.5 MeV electron irradiation on superconducting properties of single crystals of  $(\text{Ba}_{1-x}\text{K}_x)\text{Fe}_2\text{As}_2$  (fifteen different compositions covering a wide interval of  $0.20 \leq x \leq 1.0$ ) was systematically studied by tunnel-diode resonator measurements of the in-plane London penetration depth,  $\lambda(T)$ , down to 50 mK before and after irradiation. Upon electron irradiation (with total doses up to  $2 \times 10^{19} \text{ e}^-/\text{cm}^2$ ), the increase of resistivity at  $T_c$ ,  $\Delta\rho(T = T_c)$  and the decrease of  $\Delta T_c/T_{c0}$  was largest at heavily over-doped compositions. A non-exponential behavior in samples with  $x \geq 0.8$  was found from the low-temperature variation of  $\lambda(T)$  suggesting a change in the superconducting gap structure or peculiarities of (inter-, intra-) band scattering and pairing. We will discuss possible scenarios to connect a fully gapped state at the optimal doping ( $x \approx 0.40$ ) with the apparent nodal behavior in the heavily over-doped region ( $x \geq 0.8$ ).

The work performed in Ames Lab and Iowa State University was supported by the U.S. DOE, OS, MSED under contract DE-AC02-07CH11358. The work performed in University of Florida was supported by NSF-DMR-1005625.

**8:12AM R5.00002 A shift of the phase diagram in  $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$  by controlled disorder**, YUTA MIZUKAMI, KOHEI MATSUURA, University of Tokyo, MARCIN KONCZYKOWSKI, Ecole Polytechnique, TATSUYA WATASHIGE, SHIGERU KASAHARA, YUJI MATSUDA, Kyoto University, TAKASADA SHIBAUCHI, University of Tokyo — The relationship between unconventional superconductivity and quantum critical point (QCP) is one of the most important issues in strongly correlated electron systems. A systematic study on the impurity scattering is performed in iron-based superconductor  $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ , in which clear evidence for QCP has recently been presented[1]. We introduce point defects into  $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$  by electron irradiation, which has less effects on lattice constant and carrier density compared to the chemical substitution of atoms[2]. Here, we report on the changes of the magnetic and superconducting transition temperatures with electron irradiation in a wide range of substitution, from which we discuss the effect of impurity scattering on superconducting dome and QCP. [1]T. Shibauchi *et al.*, Annu. Rev. Condens. Matter Phys. **5**, 113 (2014). [2]Y. Mizukami *et al.*, Nat. Commun. **5**, 5657 (2014).

**8:24AM R5.00003 Robustness of quantum critical pairing against disorder in iron-based superconductors**<sup>1</sup>, JIAN KANG, RAFAEL FERNANDES, School of Physics and Astronomy, University of Minnesota — Several experiments in iron pnictides and cuprates reveal a superconducting (SC) state remarkably robust against non-magnetic disorder at least when compared to the simple extension of the Abrikosov-Gorkov formalism to dirty unconventional superconductors. Motivated by the fact that most of these SC states appear in proximity to a magnetic instability, here we study the impact of non-magnetic disorder on the SC state promoted by quantum critical magnetic fluctuations. We go beyond the weak coupling approach by applying a variational formalism of the Eliashberg equations of the spin-fermion model, taking into account the effects of disorder on both fermionic and bosonic degrees of freedom. We find that the reduced fermionic coherent spectral weight near the magnetic quantum critical point strongly decreases the suppression rate of  $T_c$  by weak disorder, as compared to the Abrikosov-Gor'kov universal value. Furthermore, because the bosons promoting the Cooper pairs emerge as collective modes of the fermions, they are also impacted by disorder, giving rise to an additional reduction of the suppression rate of  $T_c$  by weak disorder. Our results qualitatively agree with experiments, shedding new light on why unconventional superconductors are robust against disorder.

<sup>1</sup>This work is supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under award number DE-SC0012336.

**8:36AM R5.00004 Numerical Studies of Doped Iron Pnictides<sup>1</sup>**, CHRISTOPHER BISHOP, SHUHUA LIANG, ADRIANA MOREO, ELBIO DAGOTTO, Univ of Tennessee, Knoxville — The phase diagram of electron-doped pnictides is studied varying the temperature, electronic density, and isotropic disorder strength and dilution via numerical studies of a three-orbital spin-fermion model with lattice degrees of freedom [1]. Doping introduces disorder but in theoretical studies the effect of the randomly located dopants is difficult to address. Numerically the effects of electronic doping, regulated by a chemical potential, and impurity disorder at randomly selected sites can be independently controlled. It was found that the reduction with doping of the Neel and the structural transition temperatures, and the stabilization of a nematic state, is mainly controlled by the magnetic dilution due to the disorder. Fermi surface changes due to doping affect only slightly both critical temperatures. Our findings are compatible with neutron scattering and STM results, unveiling a patchy network of locally magnetically ordered anisotropic clusters, despite the isotropic disorder. The fragile tendency to nematicity intrinsic of translational invariant electronic systems needs to be supplemented by disorder and dilution to stabilize the robust nematic phase experimentally found in electron-doped 122 pnictides. [1] S. Liang et al., Phys. Rev. B 92, 104512 (2015).

<sup>1</sup> National Science Foundation Grant No. DMR-1404375

**8:48AM R5.00005 Mechanically - induced disorder in  $\text{CaFe}_2\text{As}_2$ : a  $^{57}\text{Fe}$  Mössbauer study<sup>1</sup>**, XIAOMING MA, Ames Laboratory/ Iowa State University and Lanzhou University, China, SHENG RAN, PAUL C. CANFIELD, SERGEY L. BUD'KO, Ames Laboratory/Iowa State University —  $^{57}\text{Fe}$  Mössbauer spectroscopy was used to study an extremely pressure and strain sensitive compound,  $\text{CaFe}_2\text{As}_2$ , with different degrees of strain introduced by grinding and annealing. At the base temperature, in the antiferromagnetic/orthorhombic phase, compared to a sharp sextet Mössbauer spectrum of single crystal  $\text{CaFe}_2\text{As}_2$ , which is taken as an un-strained sample, an obviously broadened sextet and an extra doublet were observed for ground  $\text{CaFe}_2\text{As}_2$  powders with different degrees of strain. The Mössbauer results suggest that the magnetic phase transition of  $\text{CaFe}_2\text{As}_2$  can be inhomogeneously suppressed by the grinding induced strain to such an extent that the antiferromagnetic order in parts of the grains forming the powdered sample remain absent all the way down to 4.6 K. However, strain has almost no effect on the temperature dependent hyperfine magnetic field in the grains with magnetic order. The quadrupole shift in the magnetic phase approaches zero with increasing degrees of strain, indicating that the strain reduces the average lattice asymmetry at Fe atom position.

<sup>1</sup>Supported by US DOE under the Contract No. DE-AC02-07CH11358 and by the China Scholarship Council

**9:00AM R5.00006 Effects of Tilted Columnar Defects on  $J_c$  Behavior in  $(\text{Ba},\text{K})\text{Fe}_2\text{As}_2$** , TSUYOSHI TAMEGAI, AKIYOSHI PARK, KENGO OHARA, SUNSENG PYON, The University of Tokyo, TADASHI KAMBARA, RIKEN, HISASHI KITAMURA, National Institute of Radiological Sciences — Iron-based superconductors have very promising characteristics to be used for practical applications at high fields. We have already demonstrated a remarkable enhancement of  $J_c$  in  $(\text{Ba},\text{K})\text{Fe}_2\text{As}_2$  by irradiating swift particles [1,2]. In order to further enhance  $J_c$ , we introduced columnar defects at an angle from the  $c$ -axis. We found a novel non-monotonic field dependence of  $J_c$  as well as its enhancement in such samples at relatively high temperatures. Origins of these anomalous  $J_c$  behavior and the degree of  $J_c$  enhancement with the tilted columnar defects will be discussed. [1] T. Taen et al., Supercond. Sci. Technol. 28, 085003 (2015). [2] F. Ohtake et al., Physica C518, 47 (2015).

**9:12AM R5.00007 Magnetic penetration depth in disordered iron-based superconductors<sup>1</sup>**, ALEX LEVCHENKO, University of Wisconsin-Madison, MAXIM DZERO, Kent State University, MAXIM KHODAS, Hebrew University of Jerusalem, ALEX KLIRONOMOS, American Physical Society, MAXIM VAVILOV, University of Wisconsin-Madison — We study the effect of disorder on the London penetration depth in iron-based superconductors. The theory is based on a two-band model with quasi-two-dimensional Fermi surfaces, which allows for the coexistence region in the phase diagram between magnetic and superconducting states in the presence of intraband and interband scattering. Within the quasiclassical approximation we derive and solve Eilenberger's equations, which include a weak external magnetic field, and provide analytical expressions for the penetration depth in the various limiting cases. A complete numerical analysis of the doping and temperature dependence of the London penetration depth reveals the crucial effect of disorder scattering, which is especially pronounced in the coexistence phase. The experimental implications of our results are discussed.

<sup>1</sup>NSF-DMR-1401908, NSF-DMR-1506547, NSF-DMR-0955500, BSF-2014107

**9:24AM R5.00008 The study of vortex state across the phase diagram in single crystals of  $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$  using current voltage characteristics.<sup>1</sup>**, X. Y. HUANG, Y. P. SINGH, D. J. HANEY, S. ZHANG, Kent State University, H. H. WEN, Nanjing University, T. HU, Shanghai Institute of Microsystem and Information Technology, M. DZERO, C. C. ALMASAN, Kent State University — Utilizing the current voltage (I-V) characteristic measurement, we investigate the vortex state of  $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$  single crystals across a wide doping range: under-doped ( $x = 0.042$  and  $0.056$ ), near optimally-doped ( $x = 0.06$  and  $0.072$ ), and the over-doped ( $x = 0.1$ ). We compare the nature of the I-V characteristic curves obtained in our measurements with those of conventional type II superconductors. Using our data we could find a direct relationship between the critical current and flux-flow resistivity over the whole doping range studied. The implications of the comparison between the I-V curves of a conventional type II superconductor and  $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$  will be discussed. We will also comment on the observed relationship between the critical current and the flux-flow resistivity for the  $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$  crystals studied.

<sup>1</sup>This work has been supported by the US NSF (Grant Nos. DMR-1506547 and DMR-1505826) at KSU. M.D. also acknowledges financial support from KSU and MPI-PKS.

**9:36AM R5.00009 The role of magnetism and disorder in superconductivity of gold-doped  $\text{BaFe}_2\text{As}_2$  crystals<sup>1</sup>**, LI LI, HUIBO CAO, MIAOFANG CHI, ATHENA S. SEFAT, Oak Ridge National Lab — We present bulk magnetic and transport properties, and find structural and magnetic transitions, in order to construct the detailed T-x phase diagram for  $\text{Ba}(\text{Fe}_{1-x}\text{Au}_x)_2\text{As}_2$  single crystals [1]. The Au substitution into the FeAs-planes is only possible up to a small amount of ~3%, probably due to the large size of gold. We find that 5d is more effective in reducing magnetism in  $\text{BaFe}_2\text{As}_2$  than its counter 3d Cu, and this relates to superconductivity. In this talk, we reveal more comprehensive neutron diffraction data in order to clarify some of the inferred  $T_N$ ,  $T_S$  points in our literature report [1]. New transmission electron microscopy results will be presented that sheds light on the role of chemical disorder for preventing high  $T_c$  in these crystals. [1] L. Li et al., Phys. Rev. B 92, 094504 (2015).

<sup>1</sup>The work (LL, AS) is supported by the U.S. DOE, Office of Science, BES. The work (HC) at ORNLs HFIR, and the work (MC) at CNMS are sponsored by the Scientific User Facilities Division.

**9:48AM R5.00010 Defect-induced Superconductivity up to 49 K in  $(\text{Ca}_{1-x}\text{R}_x)\text{Fe}_2\text{As}_2$** , L.Z. DENG, B. LV, K. ZHAO, F. Y. WEI, Y. Y. XUE, Z. WU, Texas Center for Superconductivity at the University of Houston, C.W. CHU, Texas Center for Superconductivity at the University of Houston; Lawrence Berkeley National Laboratory, Berkeley, California — To explore the origin of the unusual non-bulk superconductivity with a  $T_c$  up to 49 K reported in the rare-earth-doped  $\text{CaFe}_2\text{As}_2$ , the chemical composition, magnetization, specific heat, resistivity and low temperature annealing effect are systematically investigated on nominal  $(\text{Ca}_{1-x}\text{R}_x)\text{Fe}_2\text{As}_2$  single crystals with different  $x$ 's and  $\text{R} = \text{La}, \text{Ce}, \text{Pr}$  and  $\text{Nd}$ . All display a doping independent  $T_c$  once superconductivity is induced, a doping dependent low field superconducting volume fraction  $f$ , and a large magnetic anisotropy  $\eta$  in the superconducting state, suggesting a rather inhomogeneous superconducting state in an otherwise chemically "homogeneous" superconductor. The wavelength dispersive spectroscopy, specific heat and magnetization measurements show the presence of defects which form superparamagnetic clusters for  $\text{R} = \text{Ce}, \text{Pr}$  and  $\text{Nd}$ , but not for  $\text{La}$  and display both inter and intra-cluster interactions, implying that defects are locally self-organized. Low temperature annealing reduces only the residual strain in the samples without varying  $x$  and suppresses  $f$  profoundly; however, the  $T_c$  was unaffected. The above observations are consistent with the interface-enhanced superconductivity recently proposed and also demonstrates the crucial role of defects in the occurrence of the unusually high  $T_c \sim 49$  K in  $(\text{Ca}_{1-x}\text{R}_x)\text{Fe}_2\text{As}_2$ .

**10:00AM R5.00011 Optical spectroscopy of superconducting Pt-doped  $\text{BaFe}_2\text{As}_2$** <sup>1</sup>, ZHEN XING, M. QAZILBASH, Department of Physics, College of William and Mary, SHANTA SAHA, J. PAGLIONE, Center for Nanophysics and Advanced Materials, Department of Physics, University of Maryland, College Park — Substitution of iron with platinum in  $\text{BaFe}_2\text{As}_2$  leads to suppression of the antiferromagnetic and structural transitions, and the occurrence of bulk superconductivity with superconducting transition temperature ( $T_c$ ) around 20 K. In this work, we perform optical spectroscopy study of a  $\text{BaFe}_{1.9}\text{Pt}_{0.1}\text{As}_2$  single crystal. The  $ab$ -plane optical conductivity has been obtained by performing cryogenic infrared reflectance spectroscopy and spectroscopic ellipsometry both above and below  $T_c$ . Below  $T_c$ , bulk superconductivity is directly observed as perfect reflectance in the far infrared data. We model the optical conductivity in the superconducting state using Mattis-Bardeen formalism and find that the data is best fit with two energy gaps. We also analyze the optical conductivity in the normal state and discuss the nature of charge transport.

<sup>1</sup>This work was supported by NASA / Virginia Space Grant Consortium.

**10:12AM R5.00012 Effects of single- and multi-substituted Zn ions in doped-122 type iron-based superconductors**, YUANYUAN ZHAO, BO LI, Department of Physics and Texas Center for Superconductivity, University of Houston, Houston, Texas 77204, USA, WEI LI, State Key Laboratory of Functional Materials for Informatics and Shanghai Center for Superconductivity, Shanghai Institute of Microsystem and Informat, HONG-YI CHEN, National Taiwan Normal University, Department of Physics, Taipei 116, Taiwan, KEVIN E. BASSLER, C. S. TING, Department of Physics and Texas Center for Superconductivity, University of Houston, Houston, Texas 77204, USA — Recent experiments on Zn-substituted 122-type iron-based superconductors at electron- and hole- doped region provide us with a testing ground to understand the effect of Zn impurities in the system. Here, our first-principle calculations of the electronic structure reveal the Zn 4s-orbital is partially occupied, suggesting the effect of Zn 4s-orbital could not be neglected. We focus on Zn 4s-orbital instead of its 3d-orbital. Through self-consistent lattice Bogoliubov-de Gennes (BdG) calculation on a two-orbital model, our results qualitatively agree with the experimental measurements.

**10:24AM R5.00013 From Kondo behavior to high temperature superconductivity in  $\text{Sr}(\text{Ni}_{1-x}\text{Fe}_x)_2\text{As}_2$** , NICHOLAS WAKEHAM, Los Alamos National Laboratory, NI NI, UCLA, Department of Physics and Astronomy, ERIC BAUER, JOE THOMPSON, FILIP RONNING, Los Alamos National Laboratory —  $\text{SrFe}_2\text{As}_2$  has an antiferromagnetic groundstate at ambient pressure that can be suppressed by chemical doping or pressure to produce unconventional superconductivity.  $\text{SrNi}_2\text{As}_2$  is a non-magnetic conventional superconductor with  $T_c$  of 0.6 K. It has been shown that in  $\text{Sr}(\text{Ni}_{1-x}\text{Fe}_x)_2\text{As}_2$  there is a dome of superconductivity between  $x = 0.95$  and  $x = 0.9$ . However, little is known about this doping series for small  $x$  values. We will present the study of the thermodynamic and transport properties of the doping series of  $\text{Sr}(\text{Ni}_{(1-x)}\text{Fe}_x)_2\text{As}_2$  for  $x \leq 0.6$ . In the dilute Fe limit ( $x \leq 0.01$ ) we find strong evidence for single-ion Kondo behaviour. As the concentration of Fe is increased, Fe-Fe interaction effects become significant and the Kondo scale increases. For  $0.2 \leq x \leq 0.6$  magnetic susceptibility measurements show the presence of a spin glass transition. The presence of Kondo behaviour in  $\text{Sr}(\text{Ni}_{(1-x)}\text{Fe}_x)_2\text{As}_2$  indicates the formation of local moments interacting with conduction electrons. Therefore, we will address the relevance of this result to the discussion of the itineracy of the magnetism in  $\text{SrFe}_2\text{As}_2$ , as well as the observed enhancement of the effective mass seen in many pnictide compounds.

**10:36AM R5.00014 Weak-coupling superconductivity in a strongly correlated iron pnictide**<sup>1</sup>, ALIAKSEI CHARNUKHA, Univ of California - San Diego — Iron-based superconductors have been found to exhibit an intimate interplay of orbital, spin, and lattice degrees of freedom, dramatically affecting their low-energy electronic properties, including superconductivity. Albeit the precise pairing mechanism remains unidentified, several candidate interactions have been suggested to mediate the superconducting pairing, both in the orbital and in the spin channel. Here, we employ optical spectroscopy (OS), angle-resolved photoemission spectroscopy, ab initio band-structure, and Eliashberg calculations to show that nearly optimally doped  $\text{NaFe}_{0.978}\text{Co}_{0.022}\text{As}$  exhibits some of the strongest orbitally selective electronic correlations in the family of iron pnictides. Unexpectedly, we find that the mass enhancement of itinerant charge carriers in the strongly correlated band is dramatically reduced near the  $\Gamma$  point and attribute this effect to orbital mixing induced by pronounced spin-orbit coupling. Embracing the true band structure allows us to describe all low-energy electronic properties obtained in our experiments with remarkable consistency and demonstrate that superconductivity in this material is rather weak and mediated by spin fluctuations.

<sup>1</sup>A. Charnukha acknowledges financial support by the Alexander von Humboldt foundation.

**10:48AM R5.00015 In situ characterization of pulsed-laser-deposition grown Co doped  $\text{BaFe}_2\text{As}_2$  on  $\text{SrTiO}_3$  (001)**, SUNWOUK YI, SUNGMIN KIM, MINJUN LEE, HANHO LEE, HOYEON JEON, YONGCHAN YOO, INHAE ZOH, CHAO ZHANG, MYUNGCHUL OH, YOUNG KUK, Department of Physics and Astronomy, Seoul National University, Republic of Korea — We report epitaxial growth of  $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$  (BFCA) thin films on  $\text{SrTiO}_3$  (001) substrates using pulsed laser deposition (PLD) technique under ultrahigh vacuum. The growth was performed using a pellet with the optimal Co concentration  $x=0.08$ . The temperature dependent conductivity of BFCA films was compared with those in the pellet form. The crystallinity was monitored with reflection high-energy electron diffraction during the growth and low energy electron diffraction (LEED) patterns. Optimal growth condition was obtained at the substrate temperature of  $700 \pm 20^\circ$ . The grown sample was immediately transferred to measure the topography and spectroscopy using a scanning tunneling microscope. LEED/STM result reveals modulation of  $\sqrt{2} \times \sqrt{2}$  surface reconstruction on the top plane and STM result shows the same structure. The average sizes of terraces were  $\approx 10\text{nm}$  with a homogeneous electronic structure. The geometric and electronic structure of BFCA films will be reported.

**Thursday, March 17, 2016 8:00AM - 11:00AM –**

**Session R6 GMAG DMP: Frustrated Magnetism: Triangular Lattice Magnets** 302 - Collin Broholm, Johns Hopkins University

**8:00AM R6.00001 Frustrated quantum magnetism in the 6H-perovskites**, JEFFREY QUILLIAM, University of Sherbrooke — I will review the recent state of research on the 6H-perovskites,  $\text{Ba}_3\text{MA}_2\text{O}_9$ , a large class of materials that can accommodate many different magnetic ions on ostensibly triangular lattices. This class of materials has given rise to several important discoveries in recent years, including quantum spin liquids, a quantum spin-orbital liquid and the first perfectly triangular spin-1/2 antiferromagnet. Many of these materials also provide an interesting interplay of magnetic, orbital and charge degrees of freedom. Others suffer from high levels of site disorder, which leads to interesting physics, at least in the case of the spin-orbital liquid candidate  $\text{Ba}_3\text{CuSb}_2\text{O}_9$ . I will primarily discuss our recent work on the materials  $\text{Ba}_3\text{MSb}_2\text{O}_9$ , where  $\text{M} = \text{Cu}, \text{Ni}$  and  $\text{Co}$  using the techniques of nuclear magnetic resonance (NMR), muon spin rotation ( $\mu\text{SR}$ ) and ultrasound velocity measurements.

**8:36AM R6.00002 Spin glassy behaviors and isolated spin dimers in  $\text{BaCr}_{9p}\text{Ga}_{12-9p}\text{O}_{19}$** , JUNJIE YANG, ANJANA SAMARAKOON, KYUN WOO HONG, SEUNG-HUN LEE, Department of Physics, University of Virginia, Charlottesville, VA 22903, USA, JOHN R. D. COPLEY, QINGZHEN HUANG, NIST Center for Neutron Research, Gaithersburg, Maryland 20899, USA, TAKU J SATO, IMRAM, Tohoku University, Katahira, Sendai 980-8577, Japan — Theoretical results suggested that quantum fluctuations may induce glassy states (spin jam states) in defect-free spin systems. Recently our experimental results indicated the existence of spin jam states in  $\text{SrCr}_p\text{Ga}_{12-9p}\text{O}_{19}$  (SCGO( $p$ )) in which the  $\text{Cr}^{3+}$  ions form two-dimensional (2D) triangular lattice of bi-pyramids. Here we report a isostructural new system  $\text{BaCr}_{9p}\text{Ga}_{12-9p}\text{O}_{19}$  (BCGO( $p$ )) with  $0.4 < p < 0.9$ . Neutron diffraction results show that BCGO( $p$ ) is isostructural as SCGO( $p$ ) but with a larger lattice indicating that BCGO( $p$ ) is more 2D. BCGO( $p$ ) exhibits similar glassy behaviors as SCGO( $p$ ) but with higher freezing temperature. Very high Curie-Weiss temperature and frustration index were also observed in BCGO( $p$ ) suggesting that BCGO( $p$ ) is one of the most frustrating system. Inelastic neutron scattering results show that BCGO( $p$ ) has dispersionless magnetic excitations at an energy of 16.5(1) meV arising from  $4f_{vi}-4f_{vi}$  spin dimers. These spin dimers are adjacent spins in neighboring triangular lattice planes which separate the 2D interacting triangular lattice of bi-pyramids. These results indicate that BCGO( $p$ ) is a new good candidate for studying spin jam states.

**8:48AM R6.00003 Muon spin rotation study of spin dimers on a triangular lattice in  $\text{Ba}_3\text{MRu}_2\text{O}_9$** , DJAMEL ZIAT, AIM VERRIER, Graduate student, JEFFREY QUILLIAM, Professor, ADAM ACZEL, RYAN SINCLAIR, QIANG CHEN, HAIDONG ZHOU, PhD — The family of hexagonal perovskites,  $\text{Ba}_3\text{MA}_2\text{O}_9$  has recently been proven to be fertile ground for the discovery of new, exotic magnetic phases, including several quantum spin liquid candidates. The 6H-perovskites can also accommodate spin dimers on a triangular lattice, as in the ruthenate materials  $\text{Ba}_3\text{MRu}_2\text{O}_9$ . We will present measurements on materials containing  $\text{M}^{3+}$  ( $\text{M} = \text{Y}, \text{La}, \text{Lu}, \text{In}$ ), which give rise to mixed valence  $\text{Ru}^{4.5+}$  ions wherein the orbital and charge degrees of freedom must also be considered. In particular, muon spin rotation (SR) experiments, have allowed us to probe the nature of the magnetically ordered ground state of these materials at low temperatures.

**9:00AM R6.00004 Magnetic Correlations in the Triangular Antiferromagnet  $\text{TbInO}_3$** , GABRIELE SALA, McMaster University, LUCY CLARK, University of St Andrews, DALINI MAHARAJ, McMaster University, MATTHEW B. STONE, Oak Ridge National Laboratory, KEVIN S. KNIGHT, ISIS Neutron Facility, SANG-WOOK CHEONG, Rutgers University, BRUCE D. GAULIN, McMaster University —  $\text{TbInO}_3$  crystallizes with a hexagonal  $P6_3cm$  structure in which layers of edge-sharing triangles of magnetic  $\text{Tb}^{3+}$  ions are separated by non-magnetic  $[\text{InO}_5]^{7-}$  units.  $\text{TbInO}_3$ , therefore, realizes an excellent opportunity to explore the behavior of a two-dimensional magnetic triangular lattice, a canonical model of geometric frustration. Here we present our study of a polycrystalline sample of  $\text{TbInO}_3$ . Our high resolution powder neutron diffraction data (HRPD, ISIS) of  $\text{TbInO}_3$  confirm that the triangular layers of  $\text{Tb}^{3+}$  remain undistorted to at least 0.46 K. Magnetic susceptibility data follow Curie-Weiss behavior over a wide range of  $T$  with  $\theta = -17.19(3)$  K indicating the dominance of antiferromagnetic correlations. The susceptibility data also show an absence of conventional long-range spin order down to at least 0.55 K, reflecting the frustrated nature of  $\text{TbInO}_3$ . Elastic magnetic diffuse neutron scattering (SEQUOIA, SNS) is observed below  $\sim 15$  K, due to the presence of static two-dimensional spin correlations. The spectrum of crystal field excitations in  $\text{TbInO}_3$  appears to have an exotic form due to the existence of two crystallographically distinct  $\text{Tb}^{3+}$  sites and leads to a strong Ising anisotropy of the spin symmetry.

**9:12AM R6.00005 ABSTRACT WITHDRAWN —**

**9:24AM R6.00006 A spin-orbit coupled triangular lattice quantum spin liquid in  $\text{YbMgGaO}_4$ : a semiclassical study**, YAO-DONG LI, Department of Computer Sciences, Fudan University, GANG CHEN<sup>1</sup>, Department of Physics, State Key Laboratory of Surface Physics, Fudan University; Perimeter Institute for Theoretical Physics — Recently  $\text{YbMgGaO}_4$  is proposed to be the first strong spin-orbit coupled quantum spin liquid candidate system that contains odd number of electron per unit cell with effective spin 1/2 local moments. In this talk we analyze the classical phase diagram of the most generic model that describes the Yb effective spin 1/2 local moments on the triangular lattice. We show the frustration is strong near the phase boundary between the 120 degree state and the stripe ordered phase. Further, we study the quantum fluctuation of the spin momentum by the linear spin wave theory and find that the magnetic order is destroyed in the strongly frustrated regimes of the phase diagram. Our result is compatible with the experimental results that suggest a quantum spin liquid ground state.

<sup>1</sup> Collaborative Innovative Center of Advanced Microstructures, Fudan University

**9:36AM R6.00007 Magnetic Ground State of the Ideal Triangular-Lattice Antiferromagnets Tuned by the Inter-layer Interactions<sup>1</sup>**, JIE MA, University of Tennessee, M MATSUDA, Oak Ridge National Laboratory, Y. KAMIYA, RIKEN, Z. L. DUN, University of Tennessee, C. DELA CRUZ, Oak Ridge National Laboratory, C. D. BATISTA, Los Alamos National Laboratory, Y. QIU, N BUTCH, J. R. D. COPLEY, NIST, H. D. ZHOU, University of Tennessee — Neutron inelastic scattering and diffraction techniques have been applied to investigate both structures and spin wave excitations of the tri-perovskite  $\text{Ba}_3\text{MM}'_2\text{O}_9$ , which is antiferromagnetic with the equilateral-triangular lattice M layers. Although the magnetic structure of the system is non-collinear 120 in ab-plane, the c-axis canting appears by increasing the spin momentum from  $S(\text{Co}^{2+}) = 1/2$  to  $S(\text{Mn}^{2+}) = 5/2$ . Our measurements clearly show that the magnetic ground state and excitations could be modified by the inter-layer interaction, which is strongly interfered by the type and staggering method of the nonmagnetic  $\text{M}'\text{O}_6$  clusters. In addition, the lattice-related quantum phenomena were discussed, such as the temperature-dependent acoustic mode in  $\text{Ba}_3\text{NiNb}_2\text{O}_9$ , and the pressure-effect on the magnetic dynamics of the Fermi-liquid-like ground state,  $\text{Ba}_3\text{NiSb}_2\text{O}_9(6\text{H-B})$ .

<sup>1</sup> Magnetic Ground State of the Ideal Triangular-Lattice Antiferromagnets Tuned by the Inter-layer Interactions

**9:48AM R6.00008 An indirect RIXS study of roton excitation in triangular lattice antiferromagnet**, TRINANJAN DATTA, Georgia Regents University, CHENG LUO, DAO-XIN YAO, Sun Yat-Sen University — The antiferromagnetic triangular lattice is characterized by the presence of roton excitations. We propose that the K-edge indirect resonant inelastic x-ray scattering (RIXS) spectrum of a triangular lattice antiferromagnet can serve as a novel spectroscopic tool to detect the presence of roton excitations. By considering self-energy corrections to the spin-wave spectrum and magnon decay rates in its ordered coplanar three-sublattice 120 degree magnetic state, we find that a single-peak RIXS spectrum forms at the roton momentum, Luo et. al. Phys. Rev. B 92, 035109 (2015). The single peak feature is in sharp contrast to the other high symmetry points where the RIXS spectrum splits into a multipeak structure. It is this contrast which can be utilized as an experimental signature to detect the presence of rotons. We also investigate the effect of XXZ spin anisotropy, orthorhombic spatial anisotropy, and DM interaction in the triangular lattice and find that the roton peak is affected.

**10:00AM R6.00009 2D Heisenberg Triangular Antiferromagnet in  $\text{Ba}_3\text{CoSb}_2\text{O}_9$** , ALUN BIFFIN, Laboratory for Neutron Scattering, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland, FRANZ DEMMEL, HELEN WALKER, ISIS Facility, Didcot, Oxfordshire, OX11 0QX, U.K., MICHAEL HAYWARD, Department of Chemistry, Inorganic Chemistry Laboratory, University of Oxford, South Parks Road, Oxford OX1 3QR, United Kingdom, RADU COLDEA, Clarendon Laboratory, University of Oxford, Parks Road, Oxford OX1 3PU, U.K. — We present inelastic neutron scattering (INS) experiments on the triangular antiferromagnet (TAF)  $\text{Ba}_3\text{CoSb}_2\text{O}_9$ . High energy INS measurements allowed the crystal field levels of  $\text{Co}^{2+}$  ions to be resolved, and subsequently the terms relevant to its single ion Hamiltonian to be derived with the conclusion that the ions have a  $J_{\text{eff}} = 1/2$  doublet as their groundstate with relatively weak local trigonal distortion of  $\text{CoO}_6$  octahedra. The result is a system which is a rare realisation of the canonical spin 1/2 Heisenberg TAF. Following this, low energy, high-resolution INS experiments have been performed which reveal the spin wave excitations emanating from the  $120^\circ$  ordered phase below  $T_N = 3.8\text{K}$ . However, as will be seen, linear spin wave calculations are not sufficient to describe all the features of the data, and these anomalies hint at quantum dynamics beyond linear spin wave theory within this realisation of the canonical  $S=1/2$  TAF system.

**10:12AM R6.00010 Quantum phase transitions in triangular lattice Heisenberg antiferromagnet in a magnetic field**, MENGXING YE, ANDREY CHUBUKOV, Univ of Minnesota - Twin Cities — We present the zero temperature phase diagram of a large  $S$  Heisenberg anti-ferromagnet on a frustrated triangular lattice with the nearest neighbor ( $J_1$ ) and the next nearest neighbor ( $J_2$ ) interactions, in a magnetic field. We show that the classical model has an accidental degeneracy for all  $J_2/J_1$  and all fields below the saturation field, which gives rise to the extended manifold of the ground state spin configurations. Quantum fluctuations, however, lift this degeneracy. For small  $J_2/J_1$ , they select one of three different co-planar states, depending on the field value. We argue that above some critical ratio of  $J_2/J_1$ , which weakly depends on a magnetic field, these fluctuations select the stripe phase. We analyze in detail the mechanism of the selection of the stripe phase and explore the nature of the quantum phase transition in a magnetic field between the ordered phases as  $J_2/J_1$  passes through a critical value.

**10:24AM R6.00011 Neutron diffraction study of low dimensional magnetic system: single crystal  $\alpha\text{-NaMnO}_2$** , REBECCA DALLY, Boston College, STEPHEN WILSON, University of California, Santa Barbara, JEFFREY LYNN, ROBIN CHISNELL, LELAND HARRIGER, NIST Center for Neutron Research, MICHAEL GRAF, Boston College —  $\alpha\text{-NaMnO}_2$  contains complex, low dimensional interactions and is magnetically frustrated due to the triangular arrangement of  $\text{Mn}^{3+}$  ( $S=2$ ,  $t_{2g}^3 e_g^1$ ) atoms in the crystal. Nearest neighbor Mn atoms lie along the  $b$ -axis in a chain; these chains span the  $ab$ -plane, where a mean-field approach to the interchain exchange predicts the cancellation of interactions, giving rise to quasi-1D behavior. Here we will present the results of our recent single crystal neutron diffraction measurements of correlated spin behavior in this  $\text{Na}_x\text{MnO}_2$ . A complex evolution of the ordering wave vector, spin anisotropy, and dimensionality is observed as the system approaches the antiferromagnetic phase transition. The implications for the inherent dimensionality of this system and its coupling to the lattice will be discussed.

**10:36AM R6.00012 Giant magnon-phonon coupling in  $\text{LiCrO}_2$** , SNDOR TTH, Paul Scherrer Institut, Laboratory for Neutron Scattering and Imaging, KATHARINA ROLFS, Paul Scherrer Institut, Laboratory for Scientific Developments and Novel Materials, BJRN WEHINGER, University of Geneva, Department of Quantum Matter Physics, TURAN BIROL, Rutgers University Department of Physics and Astronomy, UWE STUHR, Paul Scherrer Institut, Laboratory for Neutron Scattering and Imaging, BJRN FK, Institut Laue Langevin, KENTA KIMURA, Osaka University, Department of Materials Engineering Science, HIROSHI TAKATSU, Tokyo Metropolitan University, Department of Physics, CHRISTIAN REGG, Paul Scherrer Institut, Laboratory for Neutron Scattering and Imaging — The study of low dimensional and frustrated quantum magnets has been a central problem in condensed matter physics over the past decades. The main feature of frustrated magnets is the macroscopic degeneracy of the ground state that can be lifted by weak additional effects such as quantum fluctuations. This can lead to new exotic ground states without long-range order and novel excitations. Here we present an example,  $\text{LiCrO}_2$ , where frustration (and electronic properties) leads to strong coupling between magnons and phonons in a triangular lattice antiferromagnet. This coupling leads to a novel magnon dispersion with a roton minima at the zone boundary [1]. We show direct evidence using inelastic neutron and X-ray scattering that the roton is the direct result of the magnon-phonon coupling. Furthermore the discovered effect could shed light on the underlying physics of other  $\text{Cr}^{3+}$  compounds with strange properties, such as the observed flat magnetic modes in the pyrochlore lattice antiferromagnet  $\text{MgCr}_2\text{O}_4$ . [1] S. Toth, et al., PRL 109, 127203 (2012).

**10:48AM R6.00013 Nanosized helical magnetic domains in strongly frustrated  $\text{Fe}_3\text{PO}_4\text{O}_3$** <sup>1</sup>, MITCHELL BORDELON, KATE ROSS, GREG TERHO, JAMES NEILSON, Colorado State University — Non-centrosymmetric  $\text{Fe}_3\text{PO}_4\text{O}_3$  (space group  $R\bar{3}m$ ) contains triangular motifs of  $\text{Fe}^{3+}$  ions coupled by strong antiferromagnetic interactions ( $|\Theta_{CW}| > 900\text{K}$ ). Neutron powder diffraction below  $T_N = 163\text{K}$  reveals the formation of an ordered helical incommensurate magnetic structure, with helical axis in the hexagonal  $ab$  plane and modulation length of  $\sim 100$ . The magnetic structure forms needle-like correlation volumes perpendicular to the  $ab$  plane that extend at least to 900 along the  $c$ -axis, but are confined to  $\sim 70$  in the  $ab$  plane. The refined magnetic moment, supported by magnetization measurements of a magnetically diluted series ( $\text{Fe}_{3-x}\text{Ga}_x\text{PO}_4\text{O}_3$ ), indicates a reduced  $\text{Fe}^{3+}$  moment, suggesting metal-ligand charge transfer. High-resolution synchrotron X-ray diffraction reveals no lattice symmetry change below  $T_N$ . Absence of long-range in-plane order below  $T_N$  signifies the formation of a high density of defects in the magnetic structure. The defect-rich helical magnetic phase in  $\text{Fe}_3\text{PO}_4\text{O}_3$  offers insight into the stabilization of topological spin textures in antiferromagnets.

<sup>1</sup>Partial support from NSERC of Canada.

**Thursday, March 17, 2016 8:00AM - 9:24AM —**

**Session R7 FEd: Physics Education Student Retention** 303 - Michael Falk, Johns Hopkins University

**8:00AM R7.00001 From Start to Finish: Retention of Physics Undergraduates** , DONNA HAMMER, TIM UHER, University of Maryland — The University of Maryland Physics Department's NSF Scholarships in Science Technology, Engineering and Mathematics (S-STEM) project is a unique program that aims to reduce the attrition of students that occurs in the "pre-major-to-major" gap – i.e., students who begin at the university intending to study physics, but do not graduate with a physics degree. To increase the retention of admitted students, the UMD S-STEM program is designed to provide student with financial assistance, a strong sense of community, academic support, and career planning. We will discuss how the program has been integrated into the curriculum and culture of the physics department, and focus on developing key components of the program: a nurturing environment, dedicated mentorship, early research experience, and professional development.

**8:12AM R7.00002 GRAD-MAP: A Joint Physics and Astronomy Diversity Initiative at the University of Maryland<sup>1</sup>** , PETER MEGSON, NEIL ANDERSON, KATIE JAMESON, LORA PRICE, GARETH ROBERG-CLARK, ZEEVE ROGOSZINKSI, KYLE SHEPPARD, CORBIN TAYLOR, TIM UHER, ASHLEE WILKINS, DONNA HAMMER, University of Maryland — Graduate Resources for Advancing Diversity with Maryland's Astronomy and Physics (GRAD-MAP), builds connections between UMD and mid-Atlantic HBCUs, Minority-Serving Institutions, and community colleges, and uses seminars, forums, and workshops to foster a diverse community of undergraduates prepared to succeed in graduate school, and is now in its third year. GRAD-MAP launched with a three-pronged approach: 1) Collaborative Seminars, 2) A Winter Workshop, and 3) A Spring Symposium. This program allows GRAD-MAP to do more than just increase the numbers of minority students participating in astronomy and physics research (or, worse, simply shuffle around students who already are or would be); it is committed to identifying students who are otherwise underserved or overlooked by the traditional academic pipeline, not only to get them on the path to be successful undergraduate researchers and eventual graduate applicants, but also to make the climate of academic physics and astronomy more inclusive to them and all other underrepresented minority students. We will describe the key elements of our program, and highlight successes and lessons learned; GRAD-MAP can serve as a model for other universities committed to diversity and inclusion.

<sup>1</sup>Supported by NSF PIRE and CAREER programs, Maryland Space Grant Consortium, and UMD Departments of Physics and Astronomy

**8:24AM R7.00003 Explaining the Gender Gap: Comparing Undergraduate and Graduate/Faculty Beliefs about Talent Required for Success in Academic Fields** , KIMBERLYN BAILEY, AMPALAVANAR NANTHAKUMAR, SCOTT PRESTON, CAROLINA C. ILIE, State University of New York at Oswego — Recent research has proposed that the gender gap in academia is caused by differing perceptions of how much talent is needed to succeed in various fields. It was found that, across the STEM/non-STEM divide, the more that graduate students and faculty see success in their own field as requiring as requiring talent, the fewer women participate in that field. This research examines whether undergraduate students share these attitudes. If these attitudes trickle down to the undergraduate population to influence students to choose different fields of study, then undergraduate beliefs should reflect those of graduate students and faculty. Using a large survey of undergraduates across the country, this study aims to characterize undergraduate attitudes and to determine variables that explain the differences between the attitudes of these two populations. Our findings suggest that the two populations have similar beliefs, but that undergraduate beliefs are strongly influenced by information about the gender ratio in each field and that this strong influence greatly differs between STEM and non-STEM fields. These findings seek to help direct future research to ask the right questions and propose plausible hypotheses about gender the imbalance in academia.

**8:36AM R7.00004 Perception, Attitude and Instructional Preferences on Physics in High School Students: An Exploration in an International Setting** , MINI NARAYANAN, ABDUL GAFOOR, Department of Education, Calicut University, India — Questionnaire survey explored perception, attitude and instructional preferences with respect to gender and nationality in high school students of India and USA, a sample of 1101 Indian and 458 US students. Descriptive Statistics techniques were adopted for analysis. Male and female students in USA were at the high and low ends of the spectrum, respectively, in perception and attitude. Preference on instructional strategies was found to be independent of nationality, exposed strategies, opting science, class size and facilities. Responses from both countries indicate preference for an integrated instructional strategy that has strong teacher involvement in a student-centered framework. A thoughtful and properly designed instructional strategy could provide sufficient elements in modifying students' epistemological beliefs. Understanding the nature and process of physics along with a better learning outcome is usually not possible by administering student-centered or teacher-centered strategies alone in their purest form. This study provides adequate support in obtaining two equally significant but contrasting goals in Physics Education Research, to gain conceptual development with increased interest and attainment in learners, through integration.

**8:48AM R7.00005 Examining the Needs and Dispositions of Sumter School District High School Students with Regards to Studying Physics, Part 1** , JESSICA KOHLER, University of South Carolina Sumter — Out of a total student population of 4740 in the Sumter School District (SSD) in Sumter, SC, only 167 were enrolled in a physics course in Spring 2015. That was 3.52% of the total student population in the district. As advised by Lori Smith, Coordinator of Science and Fine Arts of SSD, enrollment in physics courses was insufficient. Since physics is the basis of all sciences and a prerequisite for engineering courses, not having enrolled and succeeded in a physics course during high school could impede a students success in such majors during college. This project aimed to examine the needs and dispositions of high school students in SSD with regards to studying physics by exploring the reasons behind their decisions to enroll or not enroll in a physics course during their high school careers. The project also found out how they believe their physics classes could be improved. This was achieved by conducting an electronic survey among voluntary participants from the seniors. A quantitative analysis of the results is presented. These results are intended to help to improve the physics program in SSD as well as shape The University of South Carolina Sumters outreach efforts in the local high schools to encourage students to enroll in college physics courses.

"Examining the Needs and Dispositions of Sumter School District High School Students with Regards to Studying Physics, Part 1",

"Examining the Needs and Dispositions of Sumter School District High School Students with Regards to Studying Physics, Part 2"

and

"Examining the Needs and Dispositions of Sumter School District High School Students with Regards to Studying Physics, Part 3"

**9:00AM R7.00006 Examining the Needs and Dispositions of Sumter School District High School Students with Regards to Studying Physics, Part 4**

Out of a total student population of 4740 in the Sumter School District (SSD) in Sumter, SC, only 167 were enrolled in a physics course in Spring 2015. That was 3.52% of the total student population in the district. As advised by Lori Smith, Coordinator of Science and Fine Arts of SSD, enrollment in physics courses was insufficient. Since physics is the basis of all sciences and a prerequisite for engineering courses, not having enrolled and succeeded in a physics course during high school could impede a students success in such majors during college. This project aimed to examine the needs and dispositions of high school students in SSD with regards to studying physics by exploring the reasons behind their decisions to enroll or not enroll in a physics course during their high school careers. The project also found out how they believe their physics classes could be improved. This was achieved by conducting an electronic survey among voluntary participants from the seniors. A quantitative analysis of the results is presented. These results are intended to help to improve the physics program in SSD as well as shape The University of South Carolina Sumters outreach efforts in the local high schools to encourage students to enroll in college physics courses.

in this consecutive order. Please also schedule us for the latest time possible on Friday, 3/18/2015.

**9:12AM R7.00007 Examining the Needs and Dispositions of Sumter School District High School Students with Regards to Studying Physics, Part 3** , HUI-YIING CHANG, University of South Carolina Sumter — Out of a total student population of 4740 in the Sumter School District (SSD) in Sumter, SC, only 167 were enrolled in a physics course in Spring 2015. That was 3.52% of the total student population in the district. As advised by Lori Smith, Coordinator of Science and Fine Arts of SSD, enrollment in physics courses was insufficient. Since physics is the basis of all sciences and a prerequisite for engineering courses, not having enrolled and succeeded in a physics course during high school could impede a students success in such majors during college. This project aimed to examine the needs and dispositions of high school students in SSD with regards to studying physics by exploring the reasons behind their decisions to enroll or not enroll in a physics course during their high school careers. The project also found out how they believe their physics classes could be improved. This was achieved by conducting an electronic survey among voluntary participants from the seniors. A quantitative analysis of the results is presented. These results are intended to help to improve the physics program in SSD as well as shape The University of South Carolina Sumters outreach efforts in the local high schools to encourage students to enroll in college physics courses.

**Thursday, March 17, 2016 8:00AM - 11:00AM —**  
**Session R8 DMP: Hybrid Organic Inorganic Perovskite Photovoltaics** 304 - Dali Sun, University of Utah

**8:00AM R8.00001 Understanding the Unique Properties of Organometal Trihalide Perovskite with Single Crystals<sup>1</sup>** , JINSONG HUANG, University of Nebraska Lincoln — Organometal Trihalide Perovskite has been discovered to be all-round optoelectronic materials many types of electronic devices. The understanding of this family of materials is however limited yet due to the complicated grain structures in polycrystalline films which are generally used in most of the devices. In this contribution, I will present our recent progress in understanding the fundamental properties, including optoelectronic properties and electromechanical properties, using the high quality organometal trihalide perovskite single crystals. I will report the crystallographic orientation dependent charge transport and collection, surface and bulk charge recombination process, and direction measuring of carrier diffusion length using the lasing induced photocurrent scanning. The polarity of the organometal trihalide perovskite crystals will also be examined.

<sup>1</sup>We thank financial support from SunShot Initiative at Department of Energy under Award DE-EE0006709, and from National Science Foundation Grant DMR-1505535 and Grant DMR-1420645, and from Office of Naval Research under award N00014-15-1-2713.

**8:36AM R8.00002 High Performance Tandem Perovskite/Polymer Solar Cells<sup>1</sup>** , YAO LIU, MONOJIT BAG, ZACHARIAH PAGE, LAWRENCE RENNA, PAUL KIM, JAEWON CHOI, TODD EMRICK, D. VENKATARAMAN, THOMAS RUSSELL<sup>2</sup>, UMASS — Combining perovskites with other inorganic materials, such as copper indium gallium diselenide (CIGS) or silicon, is enabling significant improvement in solar cell device performance. Here, we demonstrate a highly efficient hybrid tandem solar cell fabricated through a facile solution deposition approach to give a perovskite front sub-cell and a polymer:fullerene blend back sub-cell. This methodology eliminates the adverse effects of thermal annealing during perovskite fabrication on polymer solar cells. The record tandem solar cell efficiency of 15.96% is 40% greater than the corresponding perovskite-based single junction device and 65% greater than the polymer-based single junction device, while mitigating deleterious hysteresis effects often associated with perovskite solar cells. The hybrid tandem devices demonstrate the synergistic effects arising from the combination of perovskite and polymer-based materials for solar cells.

<sup>1</sup>This work was supported by the Department of Energy-supported Energy Frontier Research Center at the University of Massachusetts (DE-SC0001087). The authors acknowledge the W.M. Keck Electron Microscopy

<sup>2</sup>corresponding author

**8:48AM R8.00003 Nanoimprinted Perovskite Solar Cells With Enhanced Photocurrent** , ROSS HAROLDSON, BALASUBRAMANIAM BALACHANDRAN, YIXIN REN, ANVAR ZAKHIDOV, WENCHUANG HU, Univ of Texas - Dallas, UTD NANOIM-PRINT TEAM — We have developed a new method of Nanoimprint Lithography (NIL) to shape the morphology of organolead trihalide perovskite. With this hot stamping process we created ordered gratings or other micro or nanostructures of perovskite resembling 2D photonic crystals on the scale of 200 to 600 nm from a starting small grain spin-coated film of the same scale. With this new method of nanoimprinting, we demonstrate that perovskite PV device performance can be improved and controlled. Initial results comparing flat vs. NIL-PV structure devices show dramatic increase in photocurrent as well as better crystallinity. The origin of Isc enhancement is explained in terms of better morphology and larger grains, resulting in longer diffusion length of carriers, while better light absorption by photonic crystal nanopatterns cannot be excluded.

**9:00AM R8.00004 Designing lead-free and stable perovskite materials for photovoltaic applications.** , YIYANG SUN, SHENGBAI ZHANG, Department of Physics, Rensselaer Polytechnic Institute — A critical barrier for large-scale deployment of the current perovskite solar materials is the use of Pb to achieve high power conversion efficiency. While this appears to be a technical issue, there are more fundamental reasons behind. The current research has mainly focused on the replacement of Pb by other elements, in particular, Sn. However, in halide perovskites (i.e., I-II-VI<sub>3</sub> composition), Sn is in its less stable 2+ state. The formation of more stable 4+ centers in the Sn(II)-based materials under ambient conditions makes the device efficiency very low. Worse, there might be no other elements across the Periodic Table that can replace Pb while maintaining the desirable properties, such as band gap. Out-of-the-box ideas are therefore called for to stimulate the research in this field. In this talk, two approaches are proposed based on state-of-the-art first-principles calculations. Through a screening of chalcogenide perovskite materials, CaTiS<sub>3</sub>, BaZrS<sub>3</sub>, CaZrSe<sub>3</sub>, and CaHfSe<sub>3</sub> have been predicted to have suitable band gaps for making solar cells. Among these materials, BaZrS<sub>3</sub> have been synthesized experimentally. Another proposed approach is to introduce dual anions (i.e., splitting the anion sites) that allow the composition to satisfy charge neutrality, while replacing Pb by more environmentally benign elements. One of the candidate materials is CH<sub>3</sub>NH<sub>3</sub>BiS<sub>2</sub>, which is predicted to have band gap around 1.4 eV and high optical absorption.

**9:12AM R8.00005 Light induced polaron formation in perovskite solar cell devices** , AMANDA NEUKIRCH, WANYI NIE, JEAN-CHRISTOPHE BLANCON, LANL, KANNATASSEN APPAVOO, BNL, HSINHAN TSAI, LANL, MANISH CHHOWALLA, Rutgers University, MUHAMMAD ALAM, Purdue University, MATTHEW SFEIR, BNL, CLAUDINE KATAN, ISCR, JACKY EVEN, FOTON, JARED CROCHET, GAUTAM GUPTA, ADITYA MOHITE, SERGEI TRETIKOV, LANL — The need for a low-cost, clean, and abundant source of energy has generated large amounts of research in solution processed solar cell materials. The lead halide perovskite has rapidly developed as a serious candidate for the active layer of photovoltaic devices. The efficiencies of devices made with this material have increased from 3.5% to over 20% in around 5 years. Despite the remarkable progress associated with perovskite materials, there are still fundamental questions regarding their lack of photo-stability over prolonged solar irradiation that need to be addressed. Recent experiments on photo-degradation under constant illumination have found fast self-healing by resting the device in the dark for less than 1 minute. Density functional theory and symmetry analysis show that localized charge states couple to local structural lattice distortions and methyl ammonium quasistatic configurations. Once translational symmetry is lost, additional bonding configurations become symmetry allowed, triggering localized charges in the vicinity over time under constant illumination, thus seeding the formation of macroscopic charged domains and preventing efficient charge extraction. Here we present an in-depth study of polaron formation and binding energy at the atomistic level.

### 9:24AM R8.00006 Electric polarization of $CH_3NH_3PbI_3$ and enhancement by Cl substitution<sup>1</sup>

, WEN-LI YAN, Beihang University, University of Utah, GUANG-HONG LU, Beihang University, FENG LIU, University of Utah — As a prototype of organic-inorganic hybrid perovskite,  $CH_3NH_3PbI_3$  has attracted extensive attention recently due to its applications in high power-conversion-efficiency solar cells. In comparison with its inorganic perovskite counterparts such as  $CsPbI_3$ , the organic cation  $CH_3NH_3^+$  is expected to play multiple important roles in distorting crystal structures and thus band structures as well as creating local electrically polarized domains to help separate charge carriers. Using first-principles method and berry phase theory, the electric polarization vectors of  $CH_3NH_3PbI_3$  have been calculated. The off-center displacement of Pb within the  $PbI_6$  octahedral is shown to introduce major intrinsic polarization, with additional contributions from off-center displacement of  $CH_3NH_3^+$  within  $PbI_3$  cage and charge polarization within the organic cation. With chlorine substitution of iodine, the electronegativity difference between halogen and Pb becomes larger, and the lattice distortion and hence the electric polarization increases, which provides a possible mechanism to further assist charge carrier separation in solar cell devices. This is consistent with enhanced photovoltaics properties of  $CH_3NH_3PbI_{3-x}Cl_x$  found in recent experiments.

<sup>1</sup>This work is supported by China Scholarship Council (Grant No. 201306020117) and US DOE-BES (Grant No. DE-FG02-04ER46148).

### 9:36AM R8.00007 Hybrid organic-inorganic halide perovskites: Electronic structure, dielectric properties, native defects, and the role of $ns^2$ ions

, MAOHUA DU, Oak Ridge National Laboratory, DONGWEN YANG, College of Materials Science and Engineering, Jilin University, China, HONGLIANG SHI, Oak Ridge National Laboratory, LIJUN ZHANG, College of Materials Science and Engineering, Jilin University, China —  $CH_3NH_3PbI_3$  possesses an interesting combination of properties, i.e., efficient carrier transport, high density of defects (which are nevertheless benign in terms of carrier trapping), large static dielectric constant, and significant ion migration. These properties have important effects on the solar cell performance and are unusual for a photovoltaic material. However, they are not unique; they have been reported for other halides. In the talk, we discuss the underlying physics behind these material properties in  $CH_3NH_3PbI_3$  and other halide electronic materials. The large static dielectric constant resulting from the presence of the  $ns^2$  ions and the molecular dipoles is related to the high defect concentration, defect tolerance, and the defect diffusion. We will also show the calculations of the defect and impurity diffusion and discuss their impact on the solar cell performance.

### 9:48AM R8.00008 Quasiparticle band gap of organic-inorganic hybrid perovskites: Crystal structure, spin-orbit coupling, and self-energy effects<sup>1</sup>

, WEIWEI GAO, State Univ of NY - Buffalo, XIANG GAO, Beijing Computational Science Research Center, TESFAYE ABTEW, State Univ of NY - Buffalo, YIYANG SUN, SHENGBAI ZHANG, Rensselaer Polytechnic Institute, PEIHONG ZHANG, State Univ of NY - Buffalo — The quasiparticle band gaps of organic-inorganic hybrid perovskites are often determined (and can be controlled) by various factors, complicating predictive materials optimization. Here we report a comprehensive investigation on the band gap formation mechanism in  $CH_3NH_3PbI_3$  by decoupling various contributing factors which ultimately determine their electronic structure and quasiparticle band gap. Four major factors, namely, quasiparticle self-energy, spin-orbit coupling, volume (lattice constant) effects, and structural distortions due to the presence of organic molecules, and their influences on the quasiparticle band structure of organometal hybrid perovskites are illustrated. We find that although methylammonium cations do not contribute directly to the electronic states near band edges, they play an important role in defining the band gap through a lattice distortion mechanism and by controlling the overall lattice constants (thus the chemical bonding of the optically active  $PbI_3^-$ ). The spin-orbit coupling effects drastically reduce the electron and hole effective masses in these systems, which is beneficial for high carrier mobilities and small exciton binding energies.

<sup>1</sup>This work is supported by the National Natural Science Foundation of China (Grant No. 11328401), NSF (Grant No. DMR-0946404 and DMR-1506669), and the SUNY Networks of Excellence.

### 10:00AM R8.00009 Light-induced defects in hybrid lead halide perovskite

, ONISE SHARIA, WILLIAM SCHNEIDER, University of Notre Dame — One of the main challenges facing organohalide perovskites for solar application is stability. Solar cells must last decades to be economically viable alternatives to traditional energy sources. While some causes of instability can be avoided through engineering, light-induced defects can be fundamentally limiting factor for practical application of the material. Light creates large numbers of electron and hole pairs that can contribute to degradation processes. Using *ab initio* theoretical methods, we systematically explore first steps of light induced defect formation in methyl ammonium lead iodide,  $MAPbI_3$ . In particular, we study charged and neutral Frenkel pair formation involving Pb and I atoms. We find that most of the defects, except negatively charged Pb Frenkel pairs, are reversible, and thus most do not lead to degradation. Negative Pb defects create a mid-gap state and localize the conduction band electron. A minimum energy path study shows that, once the first defect is created, Pb atoms migrate relatively fast. The defects have two detrimental effects on the material. First, they create charge traps below the conduction band. Second, they can lead to degradation of the material by forming Pb clusters.

### 10:12AM R8.00010 Ab initio study of the polarization dependence of the optoelectronic properties of hybrid halide perovskites

, LINN LEPPERT, SEBASTIAN E. REYES-LILLO, Molecular Foundry, Lawrence Berkeley National Lab; Department of Physics, University of California Berkeley, JEFFREY B. NEATON, Molecular Foundry, Lawrence Berkeley National Lab; Department of Physics, University of California Berkeley; Kavli Energy NanoSciences Institute, NEATON TEAM — With efficiencies as high as 20%, hybrid organic-inorganic halide perovskites have garnered much of the photovoltaic community's attention. In light of recent experimental results [1], we investigate the coupling mechanism between polarization and optoelectronic properties of methylammonium (MA) lead iodide,  $(CH_3NH_3)PbI_3$ , and related halide perovskites. In particular, we study the conditions that promote a combined effect of strong spin-orbit coupling and inversion symmetry breaking and that lead to a sizable Rashba/Dresselhaus effect. Using density functional theory calculations, we elucidate the emergence of Rashba/Dresselhaus splitting associated with local distortions and long-range coherent alignment of MA moieties in the material. We examine the extent to which the magnitude of the splitting, as well as other important electronic and optical properties [1], can be altered by increasing the macroscopic polarization. This opens avenues for manipulation of optoelectronic properties by an external electric field and/or chemical substitution of the MA molecule.

[1] S.Y. Leblebici, L. Leppert, et al, Facet-dependent photovoltaic efficiency variations in single perovskite grains, submitted (2015).

### 10:24AM R8.00011 Degradation of Co-evaporated Perovskite Thin Films<sup>1</sup>

, CONGCONG WANG, Univ of Rochester, YOUZHEN LI, XUEMEI XU, Central South University, CHENGCONG WANG, Univ of Rochester, FANGYAN XIE, Sun Yat-Sen University, YONGLI GAO, Univ of Rochester — Methylammonium lead halide perovskites have been developed as highly promising materials to fabricate efficient solar cells in the past few years. We have investigated degradation of co-evaporated  $CH_3NH_3PbI_3$  films using x-ray photoelectron spectroscopy (XPS), small angle x-ray diffraction (XRD), and atomic force microscopy (AFM). The  $CH_3NH_3PbI_3$  films have an excellent atomic ratio and crystal structure. The films were exposed to oxygen, air and water, respectively. The results indicate that  $CH_3NH_3PbI_3$  film is not sensitive to oxygen and dry air. The XPS results of  $H_2O$  exposure are similar to those of ambient exposure except for the higher intensity of C and O. The XRD results indicate that the perovskite turned to  $PbI_2$  after ambient exposure. The AFM measurements reveal that the morphology of the film changed drastically from smooth to rough by ambient exposure. The experiment indicated that  $H_2O$  plays a dominated role in the degradation of  $CH_3NH_3PbI_3$  films. The degradation can be characterized by almost complete removal of N, substantial reduction of I, residual of  $PbI_2$ , C, O, and I compounds on the surface.

<sup>1</sup>The authors thank the supports from National Science Foundation and National Natural Science Foundation of China.

**10:36AM R8.00012 Use of Nanoconfinement to Control Metal-Halide Perovskite Crystallization and Stability**, SANGCHUL LEE, JOSHUA FELDMAN, STEPHANIE LEE, Department of Chemical Engineering and Materials Science, Stevens Institute of Technology — We present a systematic study of the effect of nanoconfinement on the crystallization of methylammonium lead halide (MAPbI<sub>3</sub>) perovskite crystallization. MAPbI<sub>3</sub> was spin coated onto anodized aluminum oxide (AAO) templates with uniaxially-aligned pores ranging from 20 – 200 nm in diameter and examined using 2-D X-ray diffraction and scanning electron microscopy. X-ray diffraction patterns revealed the presence of a transient precursor phase that converts to the MAPbI<sub>3</sub> crystal structure upon thermal annealing. The orientation of the precursor phase and conversion rate to the MAPbI<sub>3</sub> crystal structure were found to depend on the pore size of the AAO template. The stability of MAPbI<sub>3</sub> in air also depends on the extent of nanoconfinement. When deposited on flat SiO<sub>2</sub> surfaces, MAPbI<sub>3</sub> degraded into PbI<sub>2</sub> and MA after 21 days. When deposited in AAO templates exhibiting 20-nm pore sizes, however, MAPbI<sub>3</sub> crystals were stable for longer than 16 days. These findings suggest that nanoconfinement of MAPbI<sub>3</sub> crystals may be a promising strategy for improving the stability of perovskite-based solar cells.

**10:48AM R8.00013 Structural Effects on the Bandstructure of Methylammonium Lead Iodide**, MARCO BERNARDI, California Institute of Technology, BRADFORD A BARKER, DEREK VIGIL-FOWLER, JEFFREY B NEATON, STEVEN G LOUIE, University of California at Berkeley, LOUIE TEAM — Metal-organic halide perovskites possess peculiar physical properties. The carrier diffusion length in methylammonium lead iodide (MAPbI) exceeds 1  $\mu\text{m}$ , but this unusually high value for a solution-processed material is poorly understood. We developed first-principles calculations of carrier lifetimes and diffusion lengths in semiconductors, which require accurate knowledge of the bandstructure. In this talk, we show that in MAPbI the structure strongly affects the bandstructure and band edges, and that density functional theory (DFT) is unable to predict the room temperature tetragonal structure due to the polymorphism of MAPbI. The Rashba splitting induced by the spin-orbit interaction, and the DFT band gap and effective masses, all depend strongly on the chosen structure, a point that previous work failed to address. Working with multiple stochastic realizations of large unit cells with random methylammonium orientations, we compute average effective masses and show that the effective mass depends linearly on the band gap. The average Rashba coefficient we find is an order of magnitude smaller than previously reported, and the band edges are almost parabolic. Our structures possess the correct symmetry and are free of the spurious Pb off-centering assumed in previous work. We identify the correct starting point for GW bandstructure calculations and to compute the carrier lifetime and diffusion length.

**Thursday, March 17, 2016 8:00AM - 11:00AM –**  
**Session R11 GMAG DMP FIAP: Spin-Hall IV** 307 - Igor Barsukov, UC Irvine

**8:00AM R11.00001 Magnonic charge-pumping and spin-orbit torques in conducting ferromagnets**, ARNE BRATAAS, Norwegian University of Science and Technology — In conducting ferromagnets, the spin-transfer torque and spin-motive force are known to exhibit a reciprocal relationship. Recent works on ferromagnets with strong spin-orbit coupling have revealed a rich complexity of the interaction between itinerant charge carriers and magnetization. As a result, currents can also induce magnetization excitations via spin-orbit torques, sometimes in more efficient ways than via spin-transfer torques. The reciprocal phenomenon of spin-orbit torques is magnonic charge-pumping. We will discuss how the material symmetry governs spin-orbit torques and magnonic charge-pumping. We will also relate magnonic charge pumping and spin-orbit torques via the Onsager reciprocal relations. Finally, we will give examples for important classes of systems including isotropic ferromagnets with nonuniform magnetization.

**8:36AM R11.00002 The Spin Hall Effect in Rare Earth Thin Films**, NEAL REYNOLDS, JONATHAN GIBBONS, JOHN HERON, Physics Department Cornell University, DARRELL SCHLOM, Materials Science and Engineering Cornell University, DANIEL RALPH, Physics Department Cornell University — The spin Hall effect results in a spin current which flows transverse to an applied electric field in non-magnetic materials. We report measurements of the strength of the spin Hall effect in a series of lanthanide rare earth materials in order to determine whether the large spin and orbital moments in f-electron materials might enhance the spin Hall effect. To ensure trustworthy results, we compare the results of several complementary measurement techniques: off-resonant electrical and optical second harmonic detection of current-induced magnetic tilting, spin-torque ferromagnetic resonance, and spin pumping. We compare the results to ab-initio calculations of the intrinsic Berry curvature contribution to spin Hall effect.

**8:48AM R11.00003 Towards brain-inspired computing with spin-torque nano-oscillators**, JULIE GROLLIER, JACOB TORREJON, MATHIEU RIOU, CNRS/Thales, Palaiseau, France, VINCENT CROS, CNRS/Thales lab, DAMIEN QUERLIOZ, Institut d'Electronique Fondamentale, Orsay, France, SUMITO TSUNEGI, AKIO FUKUSHIMA, HITOSHI KUBOTA, SHINJI YUASA, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan, GURU KHALSA, MARK D. STILES, National Institute of Science and Technology (NIST), Gaithersburg, USA — The brain displays many features typical of non-linear dynamical networks, such as synchronization or chaotic behaviour. These observations have inspired a whole class of models that harness the power of complex non-linear dynamical networks for computing. In this framework, neurons are modeled as non-linear oscillators, and synapses as the coupling between oscillators. These abstract models are very good at processing waveforms for pattern recognition or at generating precise time sequences useful for robotic motion. However there are very few hardware implementations of these systems, because large numbers of interacting non-linear oscillators are indeed. In this talk, I will show that coupled spin-torque nano-oscillators are very promising for realizing cognitive computing at the nanometer and nanosecond scale, and will present our first results in this direction.

**9:00AM R11.00004 Oscillatory spin transport in spin Hall multilayers**, IGOR BARSUKOV, University of California, Irvine, A. M. GONALVES, P. SOLEDADE, C. A. C. PASSOS, M. COSTA, CBPF, Rio de Janeiro, Brazil, N. M. SOUZA-NETO, LNLS, Campinas, Brazil, F. GARCIA, CBPF, Rio de Janeiro, Brazil, H. K. LEE, A. SMITH, University of California, Irvine, O. TRETIAKOV, Tohoku University, Sendai, Japan, I. N. KRIVOROTOV, University of California, Irvine, L. C. SAMPAIO, CBPF, Rio de Janeiro, Brazil — We study multilayers of sputtered Pt/(d)Cu/Py as a function of the Cu thickness  $d$  using ferromagnetic resonance (FMR). The FMR linewidth reveals a linear dependence on the frequency with negligible inhomogeneous contribution. The Gilbert damping falls smoothly with increasing  $d$ , but presents a strong superimposed oscillation with a period of  $\sim 1.5\text{nm}$ . We attribute this behavior to RKKY-like spin transport in the confinement of the Cu layer. The induced perpendicular anisotropy due to the proximity effect shows a similar behavior. We evaluate the induced magnetic moment on Pt using x-ray magnetic circular dichroism and find that it decreases with increasing Cu thickness smoothly. Again, we see oscillations of the magnetic moment and show that the oscillatory spin transport affects proximity induced magnetism in Pt. We extend our study to multilayer systems with increased oxidation levels and with out-of-plane crystal texture, in order to investigate the effects of disorder and electron's k-vectors that are responsible for the oscillatory spin transport.

**9:12AM R11.00005 Magnon emission and radiation induced by spin-polarized current.**<sup>1</sup>, ANDREI ZHOLUD, RYAN FREEMAN, RONGXING CAO, SERGEI URAZHIDIN, Emory University — The spin-torque effect due to spin injection into ferromagnets can affect their effective dynamical damping, and modify the magnon populations. The latter leads to the onset of nonlinear damping that can prevent spontaneous current-induced magnetization oscillations. It has been argued that these nonlinear processes can be eliminated by the radiation of magnons excited by local spin injection in extended magnetic films. To test these effects, studies of the effects of spin injection on the magnon populations in nanoscale spin valves and magnetic point contacts. Measurements of the giant magnetoresistance show a significant resistance component that is antisymmetric in current, and linearly dependent on temperature  $T$ . This component is significantly larger for the nanopatterned ferromagnets than for point contacts. We interpret our observations in terms of stimulated generation of magnons by the spin current, and their radiation in point contacts. 1. V.E. Demidov, S. Urazhdin, H. Ulrichs, V. Tiberkevich, A. Slavin, D. Baither, G. Schmitz, and S. O. Demokritov, *Nature Mater.*, **11**, 1028-1031 (2012)

<sup>1</sup>supported by NSF ECCS-1305586, ECCS-1509794

**9:24AM R11.00006 Electric probe for spin transition and fluctuation**, ZHIYONG QIU, Tohoku University, JIA LI, University of California at Berkeley, DAZHI HOU, Tohoku University, ELKE ARENHOLZ, ALPHA T. NDIAYE, ALI TAN, Lawrence Berkeley National Laboratory, KEN-ICHI UCHIDA, KOJI SATO, Tohoku University, YAROSLOV TSERKOVNIAK, University of California, Z. Q. QIU, University of California at Berkeley, EIJI SAITOH, Tohoku University — Spin fluctuation and transition have always been one of central topics of magnetism and condensed matter science. To probe them, neutron scatterings have been used as powerful tools. A part of neutrons injected into a sample is scattered by spin fluctuation inside the sample. This process transcribes the spin fluctuation onto scattering intensity, which is commonly represented by dynamical magnetic susceptibility of the sample and is maximized at magnetic phase transitions. Importantly, a neutron carries spin without electric charge, and it thus can bring spin into a sample without being disturbed by electric energy: an advantage of neutrons, although large facilities such as a nuclear reactor is necessary. Here we show that spin pumping, frequently used in nanoscale spintronic devices, provides a desktop micro probe for spin fluctuation and transition; not only a neutron beam, spin current is also a flux of spin without an electric charge and its transport reflects spin fluctuation in a sample. We demonstrate detection of anti-ferromagnetic transition in ultra-thin CoO films via frequency dependent spin-current transmission measurements.

**9:36AM R11.00007 Electrical manipulation of a ferromagnet by an antiferromagnet**, V TSHITOYAN, C CICCARELLI, Cavendish Laboratory, University of Cambridge, UK, A P MIHAL, M ALI, School of Physics and Astronomy, University of Leeds, UK, A C IRVINE, Cavendish Laboratory, University of Cambridge, UK, T A MOORE, School of Physics and Astronomy, University of Leeds, UK, T JUNGWIRTH, Institute of Physics ASCR, Prague, CZ and School of Physics and Astronomy, University of Nottingham, UK, A J FERGUSON, Cavendish Laboratory, University of Cambridge, UK — Several recent studies of antiferromagnetic (AFM) spintronics have focused on transmission and detection of spin-currents in AFMs. Efficient spin transmission through AFMs was inferred from experiments in FM/AFM/NM (normal metal) structures. Measurements in FM/AFM bilayers have demonstrated that a metallic AFM can also act as an efficient ISHE detector of the spin-current, with spin-Hall angles comparable to heavy NMs. Here we demonstrate that an antiferromagnet can be employed for a highly efficient electrical manipulation of a ferromagnet. We use an all-electrical excitation and detection technique of ferromagnetic resonance in a NiFe/IrMn bilayer. We observe antidamping-like spin torque acting on the NiFe generated by the in-plane current driven through the IrMn antiferromagnet. A large enhancement of the torque, characterized by an effective spin-Hall angle exceeding most heavy transition metals, correlates with the presence of the exchange-bias field at the NiFe/IrMn interface. It highlights that, in addition to strong spin-orbit coupling, the AFM order in IrMn governs the observed phenomenon.

**9:48AM R11.00008 Spin pumping and inverse spin Hall effects in heavy metal/antiferromagnet/Permalloy trilayers**<sup>1</sup>, HILAL SAGLAM, WEI ZHANG, M. BENJAMIN JUNGFLISCH, WANJUN JIANG, JOHN E. PEARSON, AXEL HOFFMANN, Argonne National Laboratory — Recent work shows efficient spin transfer via spin waves in insulating antiferromagnets (AFMs) [1], suggesting that AFMs can play a more active role in the manipulation of ferromagnets. We use spin pumping and inverse spin Hall effect experiments on heavy metal (Pt and W)/AFMs/Py (Ni<sub>80</sub>Fe<sub>20</sub>) trilayer structures, to examine the possible spin transfer phenomenon in metallic AFMs, *i.e.*, FeMn and PdMn. Previous work has studied electronic effects of the spin transport in these materials, yielding short spin diffusion length on the order of 1 nm [2]. However, the work did not examine whether besides diffusive spin transport by the conduction electrons, there are additional spin transport contributions from spin wave excitations [1]. We clearly observe spin transport from the Py spin reservoir to the heavy metal layer through the sandwiched AFMs with thicknesses well above the previously measured spin diffusion lengths, indicating that spin transport by spin waves may lead to non-negligible contributions. [1] H. Wang, et al., *Phys. Rev. Lett.* **113**, 097202 (2014). [2] W. Zhang et al., *Phys. Rev. Lett.* **113**, 196602 (2014).

<sup>1</sup>This work was supported by US DOE, OS, Materials Sciences and Engineering Division. Lithographic patterning was carried out at the CNM, which is supported by DOE, OS under contract no. DE-AC02-06CH11357.

**10:00AM R11.00009 Phase-sensitive inductive detection of ac currents due to spin-pumping/inverse spin Hall effect in unpatterned Permalloy/Pt bilayers**, THOMAS SILVA, NIST, HANS NEMBACH, University of Colorado, JUSTIN SHAW, NIST, ALEXY KARENOWSKA, Oxford University, MATHIAS WEILER, WMI — We present a new method to measure the ac inverse spin Hall effect at GHz frequencies. Unlike previous methods [1-3], our does not rely on any patterning or electrical contacts. We utilize phase-sensitive, broad-band, perpendicular-field ferromagnetic resonance to detect the ac current by the inverse spin Hall effect (ISHE) in Py/Pt bilayers. The ISHE component of the signal is non-linear in the excitation frequency; while the inductive FMR response scales linearly with frequency, the ISHE signal scales quadratically because the ISHE current itself is proportional to  $dm/dt$ . This differential gain affords us detection of previously unreported higher order contributions to the ISHE signal. We compare FMR measurements with a control samples that do not include the high spin-orbit layer, *e.g.* Pt. Data sets with and without Pt are normalized by the complex Polder susceptibility, which nullifies any effects due to differences in line-width and anisotropy. The complex ratio of the normalized inductive amplitudes is analyzed with a simple model that considers how the ac currents generated by the ISHE couple inductively back into the excitations waveguide. The linear ISHE signal agrees with previous reported values. The nonlinear ISHE signal is 3-4 orders of magnitude weaker, but is easily detected over the frequency range of 5-45 GHz. [1] M. Weiler, et al., *PRL* **113**, 157204 (2014), [2] C. Hahn, et al., *PRL* **111**, 217204 (2013) [3] D. Wei, et al., *Nat. Comm.* **5**, (2014)

**10:12AM R11.00010 Extrinsic Spin Hall effect of AuW alloys**, PIOTR LACZKOWSKI, JUAN CARLOS ROJAS-SANCHEZ, UMPHY CNRS-Thales - 1-Avenue Augustin Fresnel - 91767 PALAISEAU, WILLIAMS SAVERO-TORRES, INAC-SP2M, CEA-Universit Joseph Fourier, F-38054 Grenoble, France, NICOLAS REYREN, CYRIL DERANLOT, JEAN-MARIE GEORGE, HENRI JAFFRES, UMPHY CNRS-Thales - 1-Avenue Augustin Fresnel - 91767 PALAISEAU, CYRIL BEIGN, LUCIEN NOTIN, INAC-SP2M, CEA-Universit Joseph Fourier, F-38054 Grenoble, France, SOPHIE COLLIN, UMPHY CNRS-Thales - 1-Avenue Augustin Fresnel - 91767 PALAISEAU, ALAIN MARTY, JEAN-PHILIPPE ATTAN, LAURENT VILA, INAC-SP2M, CEA-Universit Joseph Fourier, F-38054 Grenoble, France, FREDERIC PETROFF, ALBERT FERT, UMPHY CNRS-Thales - 1-Avenue Augustin Fresnel - 91767 PALAISEAU, UMPHY CNRS-THALES PALAISEAU TEAM, CEA-SP2M-INAC GRENOBLE TEAM — The spin Hall effect (SHE) allows a reciprocal conversion between charge and spin currents using spin orbit interactions. Large Spin Hall angle have been reported in transition metals (Pt, W, Beta-Ta) and in alloys made of heavy metals [1]. We will report on SHA in AuW alloys [2] exhibiting a non-monotonic relation with W content. In this regime, it suggests a skew-scattering to side-jump dominant contribution to the spin Hall resistivity, thus allowing precise tuning of SHA vs. W content. We will present experiments by using Lateral Spin Valves with refined spin-absorption model adapted to strong spin-orbit interactions. By using complementary FMR/Spin-Pumping techniques, we demonstrate very large SHA of the order of 15 % at rather high W concentration in rather good agreement with the previous method. [1] *PRL* **109**, 156602 (2012), *PRB* **89**, 054401 (2014), [2] P. Laczkowski *et al.*, *APL* **104**, 142403 (2014).

**10:24AM R11.00011 Chiral damping in magnetic domain walls dynamics** , EMILIE JUÉ, SPINTEC - Grenoble, now: NIST - Boulder — Domain wall (DW) motion in materials with structural inversion asymmetry (SIA) and high spin-orbit coupling has attracted much interest in the recent years due to the discovery of unexpected physical mechanisms. Especially, it has been shown that the DW dynamics in such materials can be explained by chiral DWs with (partly or fully) Néel structure, whose stability derives from an interfacial Dzyaloshinskii-Moriya interaction (DMI) [1]. In this work, we show that DMI is not the only effect inducing chiral dynamics and demonstrate the existence of a chiral damping. This result is supported by the study of the asymmetry induced by an in-plane magnetic field on field induced domain wall motion in perpendicularly magnetized asymmetric Pt/Co/Pt trilayers. Using time reversal properties, we show that this asymmetry cannot be attributed to an effective field but originates from a purely dissipative mechanism. The observation of chiral damping, not only enriches the spectrum of physical phenomena engendered by the SIA, but since it can coexist with DMI it is essential for conceiving DW and skyrmion devices. [1] A. Thiaville, et al., EPL 100, 57002 (2012)

**Thursday, March 17, 2016 8:00AM - 10:30AM –**  
**Session R12 DCOMP: Recent Computational Advances in the Understanding of Complex Oxides** 308 - James Rondinelli, Northwestern University

**8:00AM R12.00001 The role of Coulomb correlations in complex oxides** , SILKE BIERMANN, cole Polytechnique — No abstract available.

**8:30AM R12.00002 Strong correlations in new multiferroics** , DANIEL PUGGIONI, Northwestern University — No abstract available.

**9:00AM R12.00003 Hybrid functionals for simulating complex oxides** , CESARE FRANCHINI, University of Vienna — Hybrid functionals are a class of exchange-correlation (XC) functionals in density functional theory (DFT) that are constructed by a suitable mixing of local/semi-local XC functionals (LDA/GGA) with a certain portion of the exact Hartree-Fock exchange. After being used for years in the chemistry community for studying molecular properties, hybrid functionals are being increasingly widely used for solid state problems, for which standard LDA/GGA approximations provide a defective description. In particular, hybrid functionals appear to account well for the complicated coupling between lattice, charge and spin degrees of freedom in transition metal oxides, a class of materials that has recently attracted a lot of interest due to its technological relevance (all-oxides electronics), the large spectrum of functionalities, and the many challenging issues related to strong electronic correlation [1,2]. The purpose of this talk is to present the essential ideas and physical picture of hybrid functionals and to present a map of recent applications to complex oxides aiming to cover an ample spectra of cases (*sp*, *3d*, *4d* and *5d* compounds) and to discuss an extended array of physical phenomena including: metal-to-insulator transitions, electron localization, bandgap prediction, polarons, multiferroism, and spin-orbit coupling. [1] C. Franchini, J. Phys. Condens. Matter 26, 253202 (2014). [2] J. G. He and C. Franchini, Phys. Rev. B 86, 235117 (2012).

**9:30AM R12.00004 Electron-electron interactions and lattice distortions in the perovskite titanates** , LARS BJAALIE, University of California, Santa Barbara — A two-dimensional electron gas (2DEG) with the unprecedented high density of  $3 \times 10^{14}$  (corresponding to 1/2 electron per interface unit cell area) can be formed at the interface between  $\text{SrTiO}_3$  and a rare-earth titanate ( $\text{RTiO}_3$ ). The 2DEG resides in the  $\text{SrTiO}_3$ , and arises from a polar discontinuity at the interface. The formation of this 2DEG has led us to study these perovskite titanates in detail. Some of these compounds are Mott insulators, where a Mott-Hubbard gap opens up between partially filled Ti *3d* bands. This talk focuses on the importance of the interplay between electron-electron interactions and lattice distortions in these complex oxides, which we study with density functional theory using a hybrid functional, capable of correctly describing electron localization and Mott-insulating behavior. These effects are crucial to understanding the metal-to-insulator transition as a function of electron density. Indeed, very thin  $\text{SrTiO}_3$  layers inserted in  $\text{GdTiO}_3$  show insulating behavior, in contrast to the metallic character of thicker layers in which the electrons form a 2DEG. The same physics is observed in bulk  $\text{SrTiO}_3$  when doped with 1/2 electron per Ti atom <sup>1</sup>. Charge localization and lattice distortions also govern the formation of small hole polarons in the rare-earth titanates. We demonstrate that these polarons impact the optical absorption measurements commonly used to determine the value of the Mott-Hubbard gap <sup>2</sup>. Work performed in collaboration with Anderson Janotti, Burak Himmetoglu, and Chris G. Van de Walle, and supported by NSF and ARO.

<sup>1</sup>L. Bjaalie, A. Janotti, B. Himmetoglu, and C. G. Van de Walle, Phys. Rev. B. 90, 195117 (2014).

<sup>2</sup>L. Bjaalie, D. G. Ouellette, P. Moetakef, T. A. Cain, A. Janotti, B. Himmetoglu, S. J. Allen, S. Stemmer and C. G. Van de Walle, Appl. Phys. Lett. 106, 232103 (2015).

**10:00AM R12.00005 Transport Properties of Complex Oxides: New Ideas and Insights from Theory and Simulation** , NICOLE BENEDEK, Cornell University — Complex oxides are one of the largest and most technologically important materials families. The  $\text{ABO}_3$  perovskite oxides in particular display an unparalleled variety of physical properties. The microscopic origin of these properties (how they arise from the structure of the material) is often complicated, but in many systems previous research has identified simple guidelines or 'rules of thumb' that link structure and chemistry to the physics of interest. For example, the tolerance factor is a simple empirical measure that relates the composition of a perovskite to its tendency to adopt a distorted structure. First-principles calculations have shown that the tendency towards ferroelectricity increases systematically as the tolerance factor of the perovskite decreases. Can we uncover a similar set of simple guidelines to yield new insights into the ionic and thermal transport properties of perovskites? I will discuss recent research from my group on the link between crystal structure and chemistry, soft phonons and ionic transport in a family of layered perovskite oxides, the  $\text{Ln}_2\text{NiO}_{4+\delta}$  Ruddlesden-Popper phases. In particular, we show how the lattice dynamical properties of these materials (their tendency to undergo certain structural distortions) can be correlated with oxide ion transport properties. Ultimately, we seek new ways to understand the microscopic origins of complex transport processes and to develop first-principles-based design rules for new materials based on our understanding.

**Thursday, March 17, 2016 8:00AM - 11:00AM –**  
**Session R13 DAMOP: Atomtronics** 309 - Mark Edwards, Georgia Southern University

**8:00AM R13.00001 Magnon optics and thermodynamics in a degenerate spinor Bose gas** , DAN STAMPER-KURN, Univ of California - Berkeley — At low temperature, spinor Bose gases form magnetically ordered superfluids. Like other magnetic materials, such a fluid supports magnons, the Nambu-Goldstone bosons corresponding to the spontaneous breaking of rotational symmetry. We have developed methods to produce and detect such excitations in a  $^{87}\text{Rb}$   $F = 1$  spinor Bose gas. I will discuss precise measurements of the magnon recoil energy using coherent magnon interferometry, the use of thermalized magnons to measure and lower the temperature of quantum gases, and the phenomenon of magnon condensation in a quantum gas.

**8:36AM R13.00002 Atomtronics with Ultracold Bose Gases** , HERWIG OTT, University of Kaiserslautern — Neutral atom systems can exhibit similar transport properties like solid state devices. For instance, a neutral atom current is induced by a difference in chemical potential very much in the same way as a voltage drives an electric current. Employing Bose-Einstein condensed atomic gases allows observing superfluid transport phenomena, thus drawing connections to superconductivity. With help of light fields, the atomic current can additionally be guided in engineered potential landscapes in which one can also incorporate tunneling junctions. Eventually, the different components and elements can be integrated in atomtronic circuits which shed light on fundamental transport properties of many-body quantum systems. In this talk, I will present two fundamental atomtronic devices. The first is the observation of negative differential conductivity, which occurs at a multimode tunneling junction for ultracold atoms [1]. The second is the appearance of a DC Josephson current in a biased tunneling junction [2], which features bistable transport characteristics. I will discuss the prospects of these basic elements for more complex atomtronic circuits. References [1] R. Labouvie, B. Santra, S. Heun, S. Wimberger, and H. Ott “Negative Differential Conductivity in an Interacting Quantum Gas” Phys. Rev. Lett. 115, 050601 (2015). [2] R. Labouvie, B. Santra, Simon Heun, and H. Ott “Nonequilibrium steady states in a driven-dissipative superfluid” arXiv:1507.05007

**9:12AM R13.00003 Dynamics of quantum impurities in many-body systems of ultracold atoms** , EUGENE DEMLER, Harvard University — Recent theoretical and experimental progress in the study of dynamics of quantum impurities in ensembles of ultracold atoms will be reviewed. Examples include RF spectroscopy of Bose and Fermi polarons, interferometric measurements of ultrafast dynamics of impurities in an atomic Fermi sea, exploring crossover from few- to many-body dynamics in Rydberg excitations. New directions including realizations of Kondo type models and Shiba states in Fermi superfluids will be discussed.

**9:48AM R13.00004 Transport dynamics and dissipation in polariton ring condensates and cold atoms** , ANDREW DALEY, Univ of Strathclyde — Recent progress in experiments has opened new contexts in which to observe and explore out-of-equilibrium quantum transport dynamics. On the side of cold atoms, significant advances are made possible by the ability to control and measure atomic dynamics time-dependently, as well as to explore the effects of strong interactions. This is especially true in recent experiments with quantum gas microscopes, which now provide single-site and single atom measurement and control. At the same time, new methods for control and longer coherence times have been realised in condensates of exciton polaritons. This has enabled the development of ring geometries for these systems, and corresponding quantised circulation. I will discuss our recent theoretical work looking at the interplay between coherent dynamics and dissipation in these systems. For polaritons in a ring trap, half-quantum vortices are allowed in which there is a phase rotation of  $\pi$  and a corresponding polarisation vector rotation of  $\pi$  around the ring. The observed half-quantum state in current experiments is novel, in that the handedness of the spin flips from one side of the ring to the other side in addition to the rotation of the linear polarization component. This type of state is not possible for vortices in a simply connected geometry, and we investigate how the interplay between the polariton production and dissipation can give rise to this state in a ring trap. I will also discuss the transport dynamics of cold atoms in tilted optical lattices, in the presence of decoherence from sources including spontaneous emissions.

**10:24AM R13.00005 Driving transitions between quantized flow states in an atomtronic circuit** , STEPHEN ECKEL, Joint Quantum Institute (NIST/UMD) — Superfluidity, or flow without resistance, is a macroscopic quantum effect that is present in a multitude of systems, including liquid helium, superconductors, and ultra-cold atomic gases. In superconductors, flow without resistance has led to the development of a number of useful devices. Here, I will present our work studying a superfluid analog to the rf-superconducting interference device (SQUID). Our atomtronic analog is formed in a ring-shaped Bose-Einstein condensate (BEC) of sodium atoms. Ring condensates are unique in that they can support persistent currents that are quantized. We drive transitions between persistent current states using a rotating perturbation, or weak link. Here, rotation acts as the analog to magnetic field in superconductors. In our system, a current (as viewed in the frame co-rotating with the perturbation) develops to oppose any change in rotation. If the rotation rate is sufficiently large, the critical current of the superfluid is exceeded in the weak link region, causing a transition to a state of larger persistent current. The strength of the perturbation tunes the critical rotation rates. Like the rf-SQUID, the transitions show hysteresis rotation rates that increase the quantized current are different from those that decrease the current. The size of the hysteresis loop allows us to explore the microscopic mechanisms responsible for the transitions. In a more recent experiment, we have observed the time it takes for the first persistent current state to decay in the presence of a stationary perturbation. The measured timescales depend strongly on temperature, but in a way that suggests that other physical effects, like quantum coherence, could also play a role in the transitions between current states.

**Thursday, March 17, 2016 8:00AM - 11:00AM —**  
**Session R14 GSNP GSOF: Geometry and Mechanics of Folded Filaments, Writhing Ribbons and Braided Bundles** 310 - Gregory Grason, Univeristy of Massachusetts-Amherst

**8:00AM R14.00001 Collective Behavior of Hair, and Ponytail Shape and Dynamics.**<sup>1</sup> , ROBIN BALL, Dept of Physics, University of Warwick — I will discuss how we can build a mathematical model of the behaviour of a bundle of hair, comparing the results with experimental studies of the shape and dynamics of human ponytails. We treat the individual fibers as elastic filaments with random intrinsic curvature, in which the balance of bending elasticity, gravity, orientational disorder and inertia is recast as a differential equation for the envelope of the fibre bundle. The static elements of this work were first reported in R.E. Goldstein, P.B. Warren and R.C. Ball, Physical Review Letters 108, 078101 (2012). The compressibility of the bundle enters through an equation of state whose empirical form is shown to arise from a Confined Helix Model, in which the constraint of the surrounding hair is on a given fibre is represented as a confining cylinder. Using this model we find the ponytail shape is well fit with only one adjustable parameter, which is the degree to which the confining cylinders over fill space. The dynamics of driven vertical ponytail motion is well reproduced provided we introduce some damping, and we find the level of damping required is consistent with that arising from viscous drag of the lateral motion of the hair fibres through the interstitial air. Most of our match with experiment is achieved by approximating the fibre density of the ponytail to be uniform across its cross-section, and to vary only length-wise. However we show that detail near the exit from a confining clamp (aka hairband) is only captured by computing the full cross-sectional variation.

<sup>1</sup>The work reported is joint with RE Goldstein (Cambridge UK) and PB Warren (Unilever Research).

**8:36AM R14.00002 Equilibrium theory for braided elastic filaments** , GERT VAN DER HEIJDEN, University College London — Motivated by supercoiling of DNA and other filamentous structures, we formulate a theory for equilibria of 2-braids, i.e., structures formed by two elastic rods winding around each other in continuous contact and subject to a local interstrand interaction. Unlike in previous work no assumption is made on the shape of the contact curve. Rather, this shape is found as part of the solution. The theory is developed in terms of a moving frame of directors attached to one of the strands with one of the directors pointing to the position of the other strand. The constant-distance constraint is automatically satisfied by the introduction of what we call braid strains. The price we pay is that the potential energy involves arclength derivatives of these strains, thus giving rise to a second-order variational problem. The Euler-Lagrange equations for this problem give balance equations for the overall braid force and moment referred to the moving frame as well as differential equations that can be interpreted as effective constitutive relations encoding the effect that the second strand has on the first as the braid deforms under the action of end loads. Simple analytical cases are discussed first and used as starting solutions in parameter continuation studies to compute classes of both open and closed (linked or knotted) braid solutions.

### 9:12AM R14.00003 Deformation and transport of micro-fibers and helices in viscous flows ,

ANKE LINDNER, PMMH-ESPCI, Paris, France — Fluid-structure interactions between flexible objects and viscous flows are, to a large extent, governed by the shape of the flexible object. Using microfabrication methods, we obtain complex “particles” in fiber and helix form with perfect control not only over the material properties, but also the particle geometry. We then perform an experimental study on the deformation and transport of these particles in microfluidic flows. Fibers are shown to drift laterally in confined flows due to the transport anisotropy of the elongated object. When these fibers interact with lateral walls, complex dynamics are observed, such as fiber oscillation. Fiber flexibility modifies these dynamics. Flexible microhelices are easily stretched by a viscous flow and we characterize the overall shape as a function of the frictional properties. The deformation of these helices is well-described by non-linear finite extensibility. Due to the non-uniform distribution of the pitch of a helix subject to viscous drag, linear and nonlinear behavior is identified along the contour length of a single helix. When a polymer solution is used for the viscous flow, an interesting multiscale problem arises and the typical polymer size needs to be compared not only to the global size of the helix, but also to the dimensions of the ribbon.

### 9:48AM R14.00004 Wrinkles, loops, and topological defects in twisted ribbons , JULIEN CHOPIN,

ESPCI ParisTech — Nature abounds with elastic ribbon like shapes including double-stranded semiflexible polymers, graphene and metal oxide nanoribbons which are examples of elongated elastic structures with a strongly anisotropic cross-section. Due to this specific geometry, it is far from trivial to anticipate if a ribbon should be considered as a flat flexible filament or a narrow thin plate. We thus perform an experiment in which a thin elastic ribbon is loaded using a twisting and traction device coupled with a micro X-ray computed tomography machine allowing a full 3D shape reconstruction. A wealth of morphological behaviors can be observed including wrinkled helicoids, curled and looped configurations, and faceted ribbons. In this talk, I will show that most morphologies can be understood using a far-from-threshold approach and simple scaling arguments. Further, we find that the various shapes can be organized in a phase diagram using the twist, the tension, and the geometry of the ribbon as control parameters. Finally, I will discuss the spontaneous formation of topological defects with negatively-signed Gaussian charge at large twist and small but finite stretch.

### 10:24AM R14.00005 to be determined by you , ETIENNE VOUGA, UT Austin — No abstract available.

## Thursday, March 17, 2016 8:00AM - 11:00AM —

Session R15 DMP: 2D Materials: Superconductivity and Correlations I 314 - Jie Shan, Penn State University

### 8:00AM R15.00001 Universal increase in the superconducting critical temperature of two-dimensional semiconductors at low doping by the electron-electron interaction<sup>1</sup> , MATTEO CALANDRA,

CNRS — In two-dimensional multivalley semiconductors, at low doping, even a moderate electron-electron interaction enhances the response to any perturbation inducing a valley polarization. If the valley polarization is due to the electron-phonon coupling, the electron-electron interaction results in an enhancement of the superconducting critical temperature. By performing first-principles calculations beyond density functional theory, we prove that this effect accounts for the unconventional doping dependence of the superconducting transition temperature ( $T_c$ ) and of the magnetic susceptibility measured in  $\text{LiZrNCl}$ . Finally, we discuss what are the conditions for a maximal  $T_c$  enhancement in weakly doped two-dimensional semiconductors. References: M. Calandra, P. Zoccante and F. Mauri, Pys. Rev. Lett. 114, 077001 (2015) B. Pamuk, J. Baima, R. Dovesi, M. Calandra and F. Mauri, in preparation.

<sup>1</sup>We acknowledge support from Agence National Recherche and Graphene Flagship

### 8:36AM R15.00002 Superconducting phases of monolayer transition-metal dichalcogenides<sup>1</sup> ,

EVAN SOSENKO, VIVEK AJI, Univ of California - Riverside — Layered group-VI dichalcogenides, e.g.,  $\text{MoS}_2$ , are two dimensional materials that engender novel coupled spin and valley physics. Characterized by strong spin-orbit coupling and inversion symmetry breaking, they give rise to novel phenomena such as the spin Hall and valley Hall effect. In this talk, I focus on the intrinsic and substrate induced superconducting phases expected in this new class of materials. We will discuss the nature of the quasiparticles resulting from valley discriminating, pair breaking processes, and the effect of the BCS phase on the nature of opto-electronic coupling and nontrivial Berry curvature associated with the bands near each valley.

<sup>1</sup>We would like to acknowledge support from ARO W911NF1510079.

### 8:48AM R15.00003 Two Dimensional Ising Superconductivity in Gated $\text{MoS}_2$ , NOAH

Univ of Sci & Tech, JIANMING LU, Zernike Institute for Advanced Materials, KAM TUEN LAW, Hong Kong Univ of Sci & Tech, OLIVIERO ZERNIKE, Zernike Institute for Advanced Materials, INGE LEERMAKERS, ULRICH ZEITLER, Radboud University, JIANTING YE, Zernike Institute for Advanced Materials — The Zeeman effect, which is usually considered to be detrimental to superconductivity, can surprisingly protect the superconducting state in layered transition metal dichalcogenide. This effective Zeeman field, which is originated from intrinsic spin orbit coupling induced by broken inversion symmetry, can reach nearly a hundred Tesla in magnitude. It strongly pins the spin orientation of the electrons to the out-of-plane direction, protecting superconductivity from being destroyed by an in-plane external magnetic field. In magnetotransport experiments of ionic-gate  $\text{MoS}_2$  transistors, we prepare individual superconducting state with different carrier doping, we indeed observe a spin-protected superconductivity by measuring the critical field  $B_{c2}$  far beyond the Pauli paramagnetic limit. The gating-enhanced  $B_{c2}$  is more than an order of magnitude larger compared to the phases where the effective Zeeman field is weakened by interlayer coupling. Our study gives the first experimental evidence of an Ising superconductivity where the spins of the pairing electrons are strongly pinned by an effective Zeeman field.

### 9:00AM R15.00004 Disorder-enhanced superconductivity in Li intercalated $\text{ZrNCl}$ , YUJI NAKA-

GAWA, YU SAITO, The University of Tokyo, WU SHI, University of California at Berkeley, YUICHI KASAHARA, Kyoto University, YOSHIHIRO IWASA, The University of Tokyo — Electrolyte gating, as represented by electric-double-layer transistor (EDLT), possesses various functionalities; forming of  $p-n$  junction, electrostatic control of phase transitions, electrochemical etching and intercalation. These different functions, namely, electrostatic function or electrochemical function, strongly depends on the geometry of the device and the temperature in which a gate voltage is applied, and are considerably useful to unveil hidden intrinsic properties of a system. In this talk, we report a study on the transport properties in Li intercalated  $\text{ZrNCl}$ , which exhibits a maximum transition temperature of 15.2 K in lightly doped regime near the superconductor-insulator transition point. By the application of gate voltages in an EDLT configuration, we succeeded in *in-situ* resistance measurement in the electrochemical intercalation process, and thereby superconductivity in a single crystal. We found that superconductivity in Li intercalated  $\text{ZrNCl}$  changed from 2D to anisotropic 3D. Furthermore, enhancement of  $T_c$  in the lightly doped regime is accompanied by the increase of disorder and superconducting fluctuation. These results suggest that superconductivity of  $\text{ZrNCl}$  in the lightly doped regime is enhanced by disorder.

**9:12AM R15.00005 Magnetic response and pair-breaking effect in superconducting transition metal dichalcogenides<sup>1</sup>**, JUNHUA ZHANG, EVAN SOSENKO, VIVEK AJI, University of California, Riverside — The low-energy physics of monolayer transition metal group-VI dichalcogenides is significantly affected by the strong spin-orbit interaction in company with inversion symmetry breaking. As a result, the superconducting state in this system exhibits different physical behaviors compared to the conventional superconductors. Motivated by this, we study in detail the effects of the in-plane magnetic field and the non-magnetic disorder on this superconducting state. In particular, we discuss the unusual magnetic response and the pair-breaking effect in this system and their indication to experiments.

<sup>1</sup>We acknowledge support from ARO W911NF1510079.

**9:24AM R15.00006 Numerical study of giant nonlocal resistance in 2D spin orbital coupling system**, ZIBO WANG, Peking University, HUA JIANG, Soochow University, XINCHEG XIE, Peking University — Recent experiments find the signal of giant nonlocal resistance  $R_{NL}$  in H-shaped graphene sample due to the Spin/Valley Hall Effect. Interestingly, compared with the local resistance  $R_L$ ,  $R_{NL}$  decreases much more quickly when the Fermi energy deviates from the Dirac point, which does not satisfy the classical relation:  $R_{NL} \propto R_L^3$ . In this work, we simulate such transport phenomenon in H-shaped graphene based on the non-equilibrium Green function method. Near the Dirac point, there does exist a large nonlocal resistance signal, which exhibits much sharper than the local one. Moreover, we investigate the relationship between  $R_L$  and  $R_{NL}$ , which can be affected by spin-orbital coupling strength, Fermi energy, sample size, etc. At last, we discuss the possible mechanism that leads to the deviation of  $R_{NL}$  from classical  $R_{NL} \propto R_L^3$ .

**9:36AM R15.00007 Thermoelectric Powerfactor and Density of States in 2D MoS<sub>2</sub>**, KEDAR HIPPAL-GAONKAR, Institute of Materials Research and Engineering, YING WANG, YU YE, HANYU ZHU, YUAN WANG, JOEL MOORE, XIANG ZHANG, University of California, Berkeley — Efficient thermoelectric devices require high voltage generation from a temperature gradient and a large electrical conductivity, while maintaining a low thermal conductivity. For a given thermal conductivity and temperature, thermoelectric powerfactor is determined by the electronic structure of the material. Low dimensionality (1D and 2D) opens new routes to high powerfactor due to unique density of states (DOS) of confined electrons and holes. Emerging 2D transition metal dichalcogenide (TMDC) semiconductors represent a new class of thermoelectric materials not only because of their discretized density of states, but also due to their large effective masses and high carrier mobilities. We report a measured powerfactor of MoS<sub>2</sub> as large as  $8.5 \text{ mWm}^{-1}\text{K}^{-2}$  at room temperature, which is amongst the highest among all thermoelectric materials and we show that the powerfactor scales with mobility for 1L and 2L samples. Moreover, measurement of thermoelectric properties of monolayer MoS<sub>2</sub> allows us to determine the confined 2D DOS near the conduction band edge and in the insulating state, which cannot be measured by electrical conductivity alone. The demonstrated record high electronically tunable powerfactor in 2D TMDCs holds promise for efficient thermoelectric energy conversion.

**9:48AM R15.00008 Thermoelectric Transport Measurements of Graphene on hBN<sup>1</sup>**, JUNXI DUAN, Department of Physics and Astronomy, Department of Mechanical Engineering, XIAOMING WANG, Department of Mechanical Engineering, GUOHONG LI, XINYUAN LAI, Department of Physics and Astronomy, MONA ZEBARJADI, Department of Mechanical Engineering, Rutgers University, EVA Y. ANDREI, Department of Physics and Astronomy, Rutgers University — The unique electronic transport properties of graphene, arising from massless charge carriers whose sign and density can be tuned by gating, have been studied extensively. Much less work was devoted to graphene's thermal properties. Unlike electrical transport which depends on total carrier density, the thermopower is determined by the net charge transferred and not by the carrier density. This leads to profound differences between the two phenomena. For example, when the Fermi level is close to the Dirac point (DP) where electron-hole (e-h) puddles are populated symmetrically, the electron and hole contributions to the thermopower cancel out. In contrast, their contributions to the electrical current add up. We studied the thermoelectric properties of high quality graphene supported on an hBN substrate, where the e-h puddle regime is significantly reduced compared to that on SiO<sub>2</sub> substrates, which allows closer access to the DP. At room temperature we find that the maximum Seebeck coefficient close to the DP reaches up to twice the values on SiO<sub>2</sub> substrates. Upon cooling down to 77K it decreases in a non-linear fashion with temperature. We will discuss possible origins of this behavior.

<sup>1</sup>Work Supported by DOE-FG02-99ER45742, NSF DMR 1207108 and FA9550-14-1-0316

**10:00AM R15.00009 Gate-induced Gap in Bilayer Graphene Suppressed by Coulomb Repulsion**, YU-ZHONG ZHANG, JIN-RONG XU, ZE-YI SONG, Tongji Univ, HAI-QING LIN, Beijing Computational Science Research Center — We investigate the effect of on-site Coulomb repulsion  $U$  on the band gap of the electrically gated bilayer graphene by employing coherent potential approximation in the paramagnetic state, based on an ionic two-layer Hubbard model. We find that, while either the on-site Coulomb repulsion  $U$  or the external perpendicular electric field  $E$  alone will favor a gapped state in the bilayer graphene, competition between them will surprisingly lead to a suppression of the gap amplitude. Our results can be applied to understand the discrepancies of gap size reported from optical and transport measurements, as well as the puzzling features observed in angular resolved photoemission spectroscopic study.

**10:12AM R15.00010 A comparative study of the tunable spin-orbit coupling in graphene proximity coupled to topological insulators**, ZHUONAN LIN, Wuhan University, WEI QIN, JIANG ZENG, ICQD, HFNL, University of Science and Technology of China, WEI CHEN, ICQD, HFNL, University of Science and Technology of China and Harvard University, PING CUI, ICQD, HFNL, University of Science and Technology of China, JUN-HYUNG CHO, Hanyang University, ZHENYU ZHANG, ICQD, HFNL, University of Science and Technology of China — We present a comparative study of the electronic properties of the heterostructures consisting of a graphene sheet proximity coupled to the surfaces of three-dimensional topological insulators (TIs). Using density functional theory method, we first calculate the band structures of a single-layer graphene on the Bi<sub>2</sub>Te<sub>3</sub> thin film. Counterintuitively, the spin-orbit coupling (SOC) can be barely induced in the graphene even though the intrinsic SOC strength of Bi<sub>2</sub>Te<sub>3</sub> is stronger than that of Sb<sub>2</sub>Te<sub>3</sub>, which can readily introduce a giant SOC interaction into the graphene through proximity effect. In order to understand this exotic phenomenon, we next investigate the differences of the work functions and the charge transfers between the graphene and the TI substrates. It is found that the proximity-induced SOC in the graphene sheet can be enhanced by reducing the work function difference. These findings provide a simple work-function criterion for searching realistic materials that can be utilized as substrates to induce a large SOC gap in the graphene. Our criterion extends the possibilities of experimental realization of quantum spin Hall state in graphene.

**10:24AM R15.00011 Odd frequency pairing of interacting Majorana fermions<sup>1</sup>**, ZHOUSHEN HUANG, Los Alamos National Laboratory, USA, PETER WOELFLE, Karlsruhe Institute of Technology, Germany, ALEXANDAR BALATSKY, Los Alamos National Laboratory, USA — Majorana fermions are rising as a promising key component in quantum computation. While the prevalent approach is to use a quadratic (i.e. non-interacting) Majorana Hamiltonian, when expressed in terms of Dirac fermions, generically the Hamiltonian involves interaction terms. Here we focus on the possible pair correlations in a simple model system. We study a model of Majorana fermions coupled to a boson mode and show that the anomalous correlator between different Majorana fermions, located at opposite ends of a topological wire, exhibits odd frequency behavior. It is stabilized when the coupling strength  $g$  is above a critical value  $g_c$ . We use both, conventional diagrammatic theory and a functional integral approach, to derive the gap equation, the critical temperature, the gap function, the critical coupling, and a Ginzburg-Landau theory allowing to discuss a possible subleading admixture of even-frequency pairing.

<sup>1</sup>Work supported by USDOE DE-AC52-06NA25396 E304, Knut and Alice Wallenberg Foundation, and ERC DM-321031

**10:36AM R15.00012 Indirect bonding mechanism for proximity-induced giant spin-orbit coupling in graphene-topological insulator van der Waals heterostructure<sup>1</sup>**, SHIVANI RAJPUT, YAOYI LI, MICHAEL WEINERT, LIAN LI, Univ of Wisconsin, Milwaukee — We demonstrate proximity-induced spin-orbit coupling in graphene/topological insulator van der Waals (vdW) heterostructures fabricated by transferring chemical vapor deposited graphene onto Bi<sub>2</sub>Se<sub>3</sub> film grown by molecular beam epitaxy. Using scanning tunneling microscopy/spectroscopy, we observe a spin-orbit splitting of the graphene Dirac states up to 80 meV, with a spatial variation of 20 meV due to the inherent lack of epitaxial relation in the graphene/Bi<sub>2</sub>Se<sub>3</sub> vdW junction. Density functional theory calculations further reveal that this giant spin-orbit splitting of the graphene bands is a consequence of the orthogonalization requirement on the overlapping wave functions, rather than simple direct bonding at the interface. This revelation of an indirect bonding mechanism of the proximity effect will facilitate more effective engineering of desired properties in vdW heterostructures.

<sup>1</sup>This work is supported by the U.S. Department of Energy under Award DE-FG02-07ER46228.

**10:48AM R15.00013 Magnetic field induced suppression of the forward bias current in Bi<sub>2</sub>Se<sub>3</sub>/Si Schottky barrier diodes<sup>1</sup>**, HAOMING JIN, ARTHUR HEBARD, University of Florida — Schottky diodes formed by van der Waals bonding between freshly cleaved flakes of the topological insulator Bi<sub>2</sub>Se<sub>3</sub> and doped silicon substrates show electrical characteristics in good agreement with thermionic emission theory. The motivation is to use magnetic fields to modulate the conductance of the topologically protected conducting surface state. This surface state in close proximity to the semiconductor surface may play an important role in determining the nature of the Schottky barrier. Current-voltage (I-V) and capacitance-voltage (C-V) characteristics were obtained for temperatures in the range 50-300 K and magnetic fields, both perpendicular and parallel to the interface, as high as 7 T. The I-V curve shows more than 6 decades linearity on semi-logarithmic plots, allowing extraction of parameters such as ideality ( $\eta$ ), zero-voltage Schottky barrier height (SBH), and series resistance ( $R_s$ ). In forward bias we observe a field-induced decrease in current which becomes increasingly more pronounced at higher voltages and lower temperature, and is found to be correlated with changes in  $R_s$  rather than other barrier parameters. A comparison of changes in  $R_s$  in both field direction will be made with magnetoresistance in Bi<sub>2</sub>Se<sub>3</sub> transport measurement.

<sup>1</sup>The work is supported by NSF through DMR 1305783

## Thursday, March 17, 2016 8:00AM - 11:00AM – Session R16 DCMP DMP: Transport in Transition Metal Dichalcogenides 315 -

**8:00AM R16.00001 Memristive Phenomena in Polycrystalline Single Layer MoS<sub>2</sub>**, VINOD SANGWAN, DEEP JARIWALA, IN-SOO KIM, KAN-SHENG CHEN, TOBIN MARKS, LINCOLN LAUHON, MARK HERSAM, Northwestern University, HERSAM LABORATORY TEAM — Recently, a new class of layered two-dimensional semiconductors has shown promise for various electronic applications. In particular, single layer transition metal dichalcogenides (e.g. MoS<sub>2</sub>) present a host of attractive features such as high electrical conductivity, tunable band-gap, and strong light-matter interaction. However, available growth methods produce large-area polycrystalline films with grain-boundaries and point defects that can be detrimental in conventional electronic devices. In contrast, we have developed unconventional device structures that exploit these defects for useful electronic functions.[1] In particular, we observe grain-boundary mediated memristive phenomena in single layer MoS<sub>2</sub> transistors. Memristor current-voltage characteristics depend strongly on the topology of grain-boundaries in MoS<sub>2</sub>. A grain boundary directly connecting metal electrodes produces thermally assisted switching with dynamic negative differential resistance, whereas a grain boundary bisecting the channel shows non-filamentary soft-switching. In addition, devices with intersecting grain boundaries in the channel show bipolar resistive switching with high on/off ratios up to  $\sim 10^3$ . [1] Furthermore, the gate electrode in the field-effect geometry can be used to control the absolute resistance of the on and off states. Complementary electrostatic force microscopy, photoluminescence, and Raman microscopy reveal the role of sulfur vacancies in the switching mechanism. *References: 1. Sangwan et al., Nature Nanotechnology, 10 403-406 (2015)*

**8:12AM R16.00002 Transport measurements on monolayer and few-layer WSe<sub>2</sub>**, TAUNO PALOMAKI, WENJIN ZHAO, JOE FINNEY, ZAIYAO FEI, PAUL NGUYEN, FRANK MCKAY, DAVID COBDEN, University of Washington — The behavior of the electrical contacts often dominates transport measurements in mono and few-layer transition metal dichalcogenide (TMD) devices. Creating good contacts for some TMDs is particularly challenging since the fabrication procedure should prevent the TMD from oxidizing or chemically interacting with the contacts. In this talk, we discuss our progress on creating mono and few-layer WSe<sub>2</sub> devices with both good electrical contacts and minimal effects from the substrate, polymer contamination, oxidation and other chemistry. For example, we have developed a technique for encapsulating metallic contacts and WSe<sub>2</sub> flakes together in hexagonal boron nitride with multiple gates to separate and control the contributions from the channel and the Schottky barriers at the contacts. Research supported in part by Samsung GRO grant US 040814

**8:24AM R16.00003 Negative to Positive Crossover of Magnetoresistance in WS<sub>2</sub> nanoflakes with Ohmic Contact**, YANGWEI ZHANG, HONGLIE NING, YANAN LI, YANZHAO LIU, JIAN WANG<sup>1</sup>, — We report studies on the transport measurements of WS<sub>2</sub> nanoflakes including contact optimization and magnetoresistance measurement. We find that the platinum electrodes deposited by focused ion beam (FIB) technology on WS<sub>2</sub> exhibit an ohmic contact, which provides a pathway to solve the dilemma of Shottky barrier for WS<sub>2</sub> devices. A temperature-modulated negative-to-positive crossover of magnetoresistance (MR) is also observed, replenishing the existing data which mainly emphasizes field effect transistor (FET) related transport. Our work may stimulate further studies and potential electronic and optoelectronic applications on transition-metal dichalcogenides.

1

**8:36AM R16.00004 Shubnikov-de Haas oscillations of high mobility holes in monolayer and bilayer WSe<sub>2</sub>: spin-valley locking, effective mass, and inter-layer coupling<sup>1</sup>**, BABAK FALLAHAZAD, HEMA CHANDRA PRAKASH MOVVA, KYOUNGHWAN KIM, STEFANO LARENTIS, Univ of Texas, Austin, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, 1-1 Namiki Tsukuba, Ibaraki 305-0044, Japan, SANJAY K. BANERJEE, EMANUEL TUTUC, Univ of Texas, Austin — We study the magnetotransport properties of high mobility holes in monolayer and bilayer WSe<sub>2</sub>, measured in dual-gated samples with top and bottom hexagonal boron-nitride dielectrics, and using platinum bottom contacts. Thanks to the Pt high work-function combined with the a high hole density induced electrostatically by an applied top gate bias, the contacts remain ohmic down to low (1.5 K) temperatures. The samples display well defined Shubnikov-de Haas (SdH) oscillations, and quantum Hall states (QHS) in high magnetic fields. In both mono and bilayer WSe<sub>2</sub>, the SdH oscillations and the QHSs occur predominantly at even filling factors, evincing a two-fold Landau level degeneracy consistent with spin-valley locking. The Fourier transform analysis of the SdH oscillations in dual-gated bilayer WSe<sub>2</sub> reveal the presence of two subbands, each localized in the top or the bottom layer, as well as negative compressibility. From the temperature dependence of the SdH oscillation amplitude we determine a hole effective mass of 0.45m<sub>0</sub> for both mono and bilayer WSe<sub>2</sub>. The top and bottom layer densities can be independently tuned using the top and bottom gates, respectively, evincing a weak interlayer coupling.

<sup>1</sup>This work has been supported by NRI-SWAN and Intel corporation.

**8:48AM R16.00005 The suppression of the large magnetoresistance in thin WTe<sub>2</sub>.** , JIE SHEN, JOHN WOODS, JUDY CHA, Yale Univ — The layered nature of WTe<sub>2</sub> suggests the possibility of making a single layer WTe<sub>2</sub> memory device that exploits the recently observed large magnetoresistance. Presently, the origin of the magnetoresistance is attributed to the charge balance between the electron and hole carriers, yet the exact underlying physical mechanism is unclear. Here we show a systematic suppression of the large magnetoresistance, as well as turn-on temperature, with decreasing thickness of WTe<sub>2</sub>. We attribute the thickness-dependent transport properties to undesirable parasitic effects that become dominant in thin films of WTe<sub>2</sub>. Our results highlight the increasing importance of characterizing the parasitic effects for 2D layered materials in a single- to a few-layer thick limit. Finally, our observations support the hypothesis that the origin of the large magnetoresistance may be due to the charge balance between the electron and the hole carriers.

**9:00AM R16.00006 Landau levels and Shubnikov-de Haas oscillations in monolayer transition metal dichalcogenide semiconductors** , ANDOR KORMANYOS, University of Konstanz, PETER RAKYTA, Budapest University of Technology and Economics, GUIDO BURKARD, University of Konstanz — We study the Landau level (LL) spectrum using a multi-band  $\mathbf{k} \cdot \mathbf{p}$  theory in monolayer transition metal dichalcogenide semiconductors [1]. We find that in a wide magnetic field range the LL can be characterized by a harmonic oscillator spectrum and a linear-in-magnetic field term which describes the valley degeneracy breaking. The effect of the non-parabolicity of the band-dispersion on the LL spectrum is also discussed. Motivated by recent magnetotransport experiments, we use the self-consistent Born approximation and the Kubo formalism to calculate the Shubnikov-de Haas oscillations of the longitudinal conductivity. We investigate how the doping level, the spin-splitting of the bands and the broken valley degeneracy of the LLs affect the magnetoconductance oscillations. We consider monolayer MoS<sub>2</sub> and WSe<sub>2</sub> as concrete examples and compare the results of numerical calculations and an analytical formula which is valid in the semiclassical regime. Finally, we briefly analyze the recent experimental results [Cui et al., Nat. Nanotechnol. 10 534 (2015)] using the theoretical approach we have developed. [1] New J. Phys. 17, 103006 (2015).

**9:12AM R16.00007 Anisotropic Electron transport and device applications of atomically thin ReS<sub>2</sub>** , ERFU LIU, YAJUN FU, YAOJIA WANG, YANQING FENG, HUIMEI LIU, XIANGANG WAN, WEI ZHOU, BAIGENG WANG, JUNWEN ZENG, Nanjing University, CHING-HWA HO, YING-SHENG HUANG, National Taiwan University of Science and Technology, HONGTAO YUAN, HAROLD Y. HWANG, YI CUI, Stanford University, DINGYU XING, FENG MIAO, Nanjing University — Semiconducting two-dimensional transition metal dichalcogenides are emerging as top candidates for post-silicon electronics. While most of them exhibit isotropic behavior, lowering the lattice symmetry could induce anisotropic properties, which are both scientifically interesting and potentially useful. In this talk, we will present atomically thin rhenium disulfide (ReS<sub>2</sub>) flakes with unique distorted 1T structure, which exhibit in-plane anisotropic properties. We first fabricated mono- and few-layer ReS<sub>2</sub> field effect transistors, which exhibit competitive performance with large current on/off ratios ( $\sim 10^7$ ) and low subthreshold swings (100 mV dec<sup>-1</sup>). The observed anisotropic ratio along two principle axes reaches up to 3.1. Furthermore, we successfully demonstrated an integrated digital inverter with good performance by utilizing two ReS<sub>2</sub> anisotropic field effect transistors, suggesting the promising implementation of large-scale two-dimensional logic circuits. Recent results on ultra-high responsivity (as high as 88,600 A W<sup>-1</sup>) phototransistors based on few-layer ReS<sub>2</sub> will also be discussed. Our results underscore the unique properties of two-dimensional semiconducting materials with low crystal symmetry for future electronic and optoelectronic applications.

**9:24AM R16.00008 Hidden symmetry and enhanced Rudermann-Kittel-Kasuya-Yosida interaction in P-N junctions of two-dimensional materials<sup>1</sup>** , WEN YANG, SHUHUI ZHANG, 1Beijing Computational Science Research Center, Beijing 100094, China, JIAJI ZHU, Institute for quantum information and spintronics, College of Science, Chongqing University of Posts and Telecommunications, Chongqing 400065, China, KAI CHANG, SKLSM, Institute of Semiconductors, Chinese Academy of Sciences, P.O. Box 912, Beijing 100083, China — Correlation between magnetic atoms (spins) in non-magnetic two-dimensional (2D) systems and materials is one of the central issues in condensed matter physics. Engineering this correlation relies heavily on the carrier-mediated Rudermann-Kittel-Kasuya-Yosida (RKKY) interaction. However, tailoring and direct detection of spin-spin correlation has been limited to spins separated by a few nanometers due to the rapid  $1/R^2$  decay of RKKY interaction with inter-spin distance R. Here we reveal a hidden symmetry – absent from the Hamiltonian – in planar P-N junctions, which could qualitatively change the spatial scaling of various response functions in a wide range of 2D systems and materials. In particular, it allows RKKY interaction to attain  $1/R$  decay, the slowest decay in extended systems. This dramatically enhances RKKY interaction and enables long-range correlation between distant spins, with applications in nanoscale magnetism, spintronics, and solid-state quantum computation.

<sup>1</sup>This work was supported by the MOST (Grant No. 2015CB921503, and No. 2014CB848700) and NSFC (Grant No. 11434010, No. 11274036, No. 11322542, and No. 11404043).

**9:36AM R16.00009 Measurements of Schottky barrier heights formed from metals and 2D transition metal dichalcogenides** , CHANGSIK KIM, INYONG MOON, Sungkyunkwan university Advanced Institute of Nano-Technology (SAINT), SEUNGGEOL NAM, YEONCHOO CHO, HYEON-JIN SHIN, SEONGJUN PARK, Device & System Research Center, Samsung Advanced Institute of Technology (SAIT), WON JONG YOO, Sungkyunkwan university Advanced Institute of Nano-Technology (SAINT) — Schottky barrier height (SBH) is an important parameter that needs to be considered for designing electronic devices. However, for two dimensional (2D) materials based devices, SBH control is limited by 2D structure induced quantum confinement and 2D surface induced Fermi level pinning. In this work, we explore differences in measuring SBH between 2D and 3D materials. Recently, low temperature I-V measurement has been reported to extract SBH based on thermionic emission equation for Schottky diode. However, 2D devices are not real Schottky diode in that both source and drain metal electrodes make Schottky contact. According to our experimental results, SBH extracted from linear slope of  $\ln(I/T^{3/2})$  against  $1/T$  show widely diverse values, dependent on applied voltage bias and tested temperature which affect carrier transport including tunneling or thermionic emission across the metal-2D material interface. In this work, we wish to demonstrate the method to determine SBH and Fermi level pinning which are attributed to 2D transition metal dichalcogenides, differently from conventional 3D materials. .

**9:48AM R16.00010 Fermi Level Pinning at the Interface of Molybdenum Based Chalcogenides and Metals** , INYONG MOON, CHANGSIK KIM, Samsung-SKKU Graphene Center, SKKU Advanced Institute of Nano-Technology, Sungkyunkwan University, 2066, Seobu-ro, Jangan-gu, Suwon-si, Korea, SEUNGGEOL NAM, YEONCHOO CHO, HYEON-JIN SHIN, SEONGJUN PARK, Device & System Research Center, Samsung Advanced Institute of Technology (SAIT), 130 Samsung-ro, Yeongtong-gu, Suwon-si, Gyeonggi-do 443-803, Korea, WON JONG YOO, Samsung-SKKU Graphene Center, SKKU Advanced Institute of Nano-Technology, Sungkyunkwan University, 2066, Seobu-ro, Jangan-gu, Suwon-si, Korea — MoS<sub>2</sub> and MoTe<sub>2</sub> as the layered two dimensional materials have a sizable band gap suitable for future semiconductor application. However, their Schottky/ohmic contact engineering is found difficult to perform when varying contact metals due to Fermi level pinning at their metal interface. In this work, we investigate Schottky barrier heights at the interfaces formed between mono- or bi-layer MoS<sub>2</sub>, MoTe<sub>2</sub> and Ti, Cr, Au, Pd. By varying temperature in the range from 200 to 500 K, we obtained their current – voltage and hysteresis characteristics so as to determine accurate Schottky barrier heights. It is found that the Pd contact with MoS<sub>2</sub> and MoTe<sub>2</sub> shows the most pronounced Fermi level pinning; -0.8 and -1.2 eV respectively. Furthermore, the pinned energy level is found to be located near the conduction band edge for MoS<sub>2</sub> whereas it is near the intrinsic level for MoTe<sub>2</sub>. These results are found to be crucial to understand the Fermi level pinning mechanism of two dimensional materials, which can be used for developing future MoS<sub>2</sub> and MoTe<sub>2</sub> based transistor devices.

**10:00AM R16.00011 Weak Fermi Level Pinning Effect in Schottky Junction of  $\alpha$ -MoTe<sub>2</sub>**, SHU NAKAHARAI, MAHITO YAMAMOTO, Natl Inst for Materials Sci, KEIJI UENO, Saitama Univ, KAZUHIITO TSUKAGOSHI, Natl Inst for Materials Sci — Difficulty in hole injection from metal contacts to transition metal dichalcogenide (TMDC) semiconductors has been one of the most serious issues in the application of these 2D materials to future nanoelectronics, which is caused by the strong Fermi level pinning effect in the metal/TMDC Schottky junction. In this work, we found that the holes can be injected efficiently from a large work function metal of Pt to  $\alpha$ -molybdenum ditelluride ( $\alpha$ -MoTe<sub>2</sub>; 2H-type), a TMDC semiconductor. The Schottky barrier height for holes at the Pt/ $\alpha$ -MoTe<sub>2</sub> interface was extracted to be 40 meV by the temperature dependence of back-gate modulated currents under the flat band condition at the junction, while the Schottky barrier for electrons in the junction with a small work function metal of Ti was found to be 50 meV. Considering the difference in the work functions of Pt and Ti, the Fermi level pinning effect in  $\alpha$ -MoTe<sub>2</sub> was found to be much weaker than that in other TMDC semiconductors such as MoS<sub>2</sub>. These results open a way to the realization of complementary type circuits in the 2D materials for future low-power consumption electronics. This work was supported by JSPS KAKENHI Grant Numbers 15K06006, 25107004.

**10:12AM R16.00012 Experimental determination of the massive Dirac-fermion parameters in MoS<sub>2</sub>, MoSe<sub>2</sub>, WS<sub>2</sub>, and WSe<sub>2</sub>**, BEOM SEO KIM, Seoul Natl Univ, JUN-WON RHIM, Max Planck Institute, BEOMYOUNG KIM, Pohang Univ of Science and Technology, CHANGYOUNG KIM, Seoul Natl Univ, SEUNG RYONG PARK, Incheon Natl Univ — The physics associated with group 6 transition metal dichalcogenides (TMDs) MX<sub>2</sub> (M = Mo, W; X = S, Se) is one of the most intriguing issues in condensed matter physics. These materials have several interesting aspects, especially the direct to indirect band gap transition and spin-orbit interaction (SOI) induced spin band splitting at the K point. Recently, one reported a minimal band model, called massive Dirac-fermion model, for K point of the monolayer MX<sub>2</sub> Brillouin zone. There are several parameters in this model obtained by calculations, not by experiment, until now. Here we report the parametric studies on MX<sub>2</sub> using angle resolved photoemission spectroscopy (ARPES). We factor out the massive Dirac-Fermion parameters from the bulk MX<sub>2</sub>, not monolayer. For confirming the accurate experimental values, we performed the photon energy dependence experiment to find the exact  $\Gamma$  point and in-situ potassium-dosing experiment were performed for each MX<sub>2</sub>.

**10:24AM R16.00013 Electrical transport properties of ReS<sub>2</sub> with polymer electrolyte gating in the high-doping limit**, DMITRY OVCHINNIKOV, ADRIEN ALLAIN, DIEGO PASQUIER, DUMITRU DUMCENCO, Ecole Polytech Fed de Lausanne, CHING-HWA HO, YING-SHENG HUANG, National Taiwan University of Science and Technology, OLEG YAZYEV, ANDRAS KIS, Ecole Polytech Fed de Lausanne — Two-dimensional (2D) materials have emerged as promising candidates for future electronic applications. Among them, transition metal dichalcogenides (TMDs) demonstrate not only potential as ultrathin transistor channel material, but also intriguing spin and valley physics, which in principle could allow new types of devices and circuits. Here we report on the first study of two-dimensional anisotropic ReS<sub>2</sub> at high doping levels, enabled by polymer electrolyte gating. Significantly increasing the doping level using electrolyte instead of standard solid gate, we measured an unusual modulation of the conductivity at high carrier densities in monolayer ReS<sub>2</sub>. In the case of thicker flakes, the effect is milder and an insulator-metal-insulator sequence with increasing doping is observed. Transport measurements provide the evidence of major influence of ionic disorder. Furthermore, we discuss possible band structure effects.

**10:36AM R16.00014 Tempo-spatially resolved dynamics of electrons and holes in bilayer MoS<sub>2</sub>-WS<sub>2</sub>**<sup>1</sup>, J.M. GALICIA-HERNANDEZ, University of Puebla, Puebla 72550, Mexico and University of Central Florida, Orlando, FL 32816, V. TURKOWSKI, University of Central Florida, Orlando, FL 32816, G. HERNANDEZ-COCOLETZI, University of Puebla, Puebla 72550, Mexico, T.S. RAHMAN, University of Central Florida, Orlando, FL 32816 — We have performed a Density-Matrix Time-Dependent Density-Functional Theory analysis of the response of bilayer MoS<sub>2</sub>-WS<sub>2</sub> to external laser-pulse perturbations. Time-resolved study of the dynamics of electrons and holes, including formation and dissociation of strongly-bound intra- and inter-layer excitonic states, shows that the experimentally observed [1] ultrafast inter-layer MoS<sub>2</sub> to WS<sub>2</sub> migration of holes may be attributed to unusually large delocalization of the hole state which extends far into the inter-layer region. We also argue that the velocity of the hole transfer may be further enhanced by its interaction with transfer phonon modes. We analyze other possible consequences of the hole delocalization in the system, including reduction of the effects of the electron-electron and hole-hole repulsion in the trions and biexcitons as compared to that in the monolayers. [1] X. Hong et al., Nature Nano 9, 682 (2014).

<sup>1</sup>Work supported in part by DOE Grant No. DOE-DE-FG02-07ER46354 and by CONACYT Scholarship No. 23210 (J.M.G.H.).

**10:48AM R16.00015 Giant Photocurrent Generation at Topological Singularities in Graphene Superlattices**, SANFENG WU, University of Washington, LEI WANG, Columbia University, YOU LAI, NHMFL, WENYU SHAN, Carnegie Mellon University, GRANT AIVAZIAN, University of Washington, XIAN ZHANG, Columbia University, TAKASHI TANIGUCHI, KENJI WATANABE, NIMS, DI XIAO, Carnegie Mellon University, CORY DEAN, JAMES HONE, Columbia University, ZHIQIANG LI, NHMFL, XIAODONG XU, University of Washington — The energy spectrum of graphene away from the Dirac point contains topological critical points where Van Hove singularities (VHSs) appear and are predicted to host fascinating phenomena. However, the required extreme doping has prevented the experimental access to these VHSs. Alternatively, the formation of Moiré superlattices in twisted graphene bilayers or graphene on hexagonal boron-nitride (hBN) heterostructures generates electronic mini-bands that mimic graphene's energy spectrum but with reduced energy scale, providing a remarkable opportunity to study a variety of physics previously inaccessible. Here we reveal that the formation of saddle point VHSs in the mini-bands of graphene/hBN superlattice enables anomalously enhanced photocurrent generation through a photo-Nernst effect at low magnetic fields. We establish that this enhancement is unambiguously linked to the electronic topological transition at VHSs. The obtained zero-bias photocurrent is giant, with a photoresponsivity as high as about 0.3 ampere per watt, corresponding to an external quantum efficiency exceeding 50%.

**Thursday, March 17, 2016 8:00AM - 11:00AM —**

**Session R17 DMP: 2D Semiconductor Physics I** 316 - John Schaibley, University of Washington

**8:00AM R17.00001 2D semiconductor optoelectronics**, KOSTYA NOVOSELOV, University of Manchester — The advent of graphene and related 2D materials has recently led to a new technology: heterostructures based on these atomically thin crystals. The paradigm proved itself extremely versatile and led to rapid demonstration of tunnelling diodes with negative differential resistance, tunnelling transistors, photovoltaic devices, etc. By taking the complexity and functionality of such van der Waals heterostructures to the next level we introduce quantum wells engineered with one atomic plane precision. Light emission from such quantum wells, quantum dots and polaritonic effects will be discussed.

**8:36AM R17.00002 Tuning the trion photoluminescence polarization in monolayer WS<sub>2</sub>**<sup>1</sup>, A.T. HANBICKI, K.M. MCCREARY, M. CURRIE, Naval Research Laboratory, G. KIOSEOGLOU, University of Crete, C.S. HELLBERG, A.L. FRIEDMAN, B.T. JONKER, Naval Research Laboratory — Monolayer transition metal dichalcogenides (TMDs) such as MoS<sub>2</sub> or WS<sub>2</sub> are semiconductors with degenerate, yet inequivalent k-points labeled K and K' that define the direct gap. The valence band maximum in each valley has only one spin state of opposite sense for K and K'. Consequently, one can selectively populate each valley independently with circularly polarized light, and determine the valley populations via the polarization of emitted light. Optical emission is dominated by neutral and charged exciton (trion) features, and changes in emitted polarization provide insight into the fundamental processes of intervalley scattering. We prepare single-layer WS<sub>2</sub> films such that the photoluminescence is from the negatively charged trion and observe a room temperature optical polarization in excess of 40

<sup>1</sup>This work was supported by core programs at NRL and the NRL Nanoscience Institute, and by the Air Force Office of Scientific Research AOARD 14IOA018-134141.

**8:48AM R17.00003 High circular polarization in a MoSe<sub>2</sub> light-emitting transistor**, MASARU ONGA, YIJIN ZHANG, RYUJI SUZUKI, YOSHIHIRO IWASA, Quantum-Phase Electronics Center (QPEC) and Department of Applied Physics, The University of Tokyo — The exclusive coupling between the valley degree of freedom and the optical helicity is a unique phenomenon in transition metal dichalcogenides (TMDs), and thus the circularly polarized luminescence is one of the main research topics in these materials. MoSe<sub>2</sub>, however, is known to exhibit exceptionally low polarization in photoluminescence (PL). Here, we report electroluminescence (EL) properties of MoSe<sub>2</sub> demonstrating electrical switching of the optical helicity in the same manner as WSe<sub>2</sub> [1]. More importantly, the observed polarization in EL is one order of magnitude higher than that in PL. The present results reveal that the mechanism of EL polarization possesses the intrinsic robustness against intervalley scattering. [1] Y. J. Zhang, et.al., Science 344, 725 (2014).

**9:00AM R17.00004 Single Quantum Emitters in Monolayer Tungsten Diselenide**, GENEVIEVE CLARK, JOHN SCHABLEY, JASON ROSS, University of Washington, YU-MING HE, YU HE, University of Science and Technology of China, WANG YAO, The University of Hong Kong, CHAOYANG LU, JIANWEI PAN, University of Science and Technology of China, XIAODONG XU, University of Washington — Single quantum emitters are essential for developing photonic quantum technologies, providing single photon sources as well as stationary quantum bits. While they have been realized in a variety of solid state systems including single quantum dots and color centers in diamond, their three dimensional bulk matrix will be difficult to integrate with emerging nanoscale devices. We present single quantum emitters in a two-dimensional semiconductor, in the form of excitons localized to defects within atomically thin Tungsten Diselenide monolayers. These localized excitons show strong photoluminescence with 130 eV emission lines from two non-degenerate, cross-polarized transitions. Second-order correlation measurements show strong photon anti-bunching, establishing that these localized excitons are single photon emitters. Magneto-optical measurements reveal an exciton g-factor of 8.7, significantly larger than that of delocalized excitons. In addition to potential advantages such as efficient photon extraction and in-situ control of local environment, the two-dimensional matrix can be incorporated into more complex van-der-Waals heterostructure devices. This enables external control of emitters in the semiconductor, while integrating seamlessly with nanoscale device architectures.

**9:12AM R17.00005 Quantum confined stark effect of single photon emitters in atomically thin semiconductors**, CHITRALEMA CHAKRABORTY, Materials Science, University of Rochester, KENNETH GOODFELLOW, SAJAL DHARA, NICK VAMIVAKAS, The Institute of Optics, University of Rochester — The optical properties of semiconducting monolayer materials have been widely studied since the isolation of monolayer transition metal dichalcogenides (TMDCs). They have rich opto-electronic properties owing to their large direct bandgap, the interplay between the spin and the valley degree of freedom of charge carriers, and the recently discovered localized excitonic states giving rise to single photon emission. We study quantum confined Stark shift from these localized emitters present on the edges of monolayer tungsten diselenide. We employ a vertically stacked van der Waal's heterostructure to fabricate a field effect device using hexagonal boron nitride as the tunnel barrier on either side of the TMDC and few layer graphene as top and bottom electrical contacts. We report the Stark shift of different defect centers to have linear or both linear and quadratic behavior with electric field. Further, evaluation of the spectral shift in the photoluminescence signal as a function of the applied voltage enables us to extract the polarizability as well as information on the dipole moment of an individual defect center.

**9:24AM R17.00006 Optical studies of dual gated WSe<sub>2</sub> transistors**, ZEFANG WANG, JIE SHAN, KIN FAI MAK, Penn State University — Recent advances in the development of atomically thin layers of transition metal dichalcogenides (TMDs) have opened up new possibilities for the exploration of novel 2D physics as well as materials for applications. The atomic thickness of these materials allows effective control of their optical and electronic properties by electrostatic gates. In this work, we fabricate dual-gate transistors of monolayer WSe<sub>2</sub> and investigate the optical and electronic properties as a function of doping and fields by the absorption and photoluminescence spectroscopy. The combination of the top and bottom gates allows us to independently vary the electric field and doping density in the monolayer over a large range. As a function of doping density, we observe the evolution of the electronic excitations from locally bound excitons, to excitons and charged excitons, to the Fermi edge singularity. We will discuss the effects of external fields on these excitations and the effects of strong Coulomb interactions in 2D semiconductors.

**9:36AM R17.00007 Photocurrent measurements in Coupled Quantum Well van der Waals Heterostructures made of 2D Transition Metal Dichalcogenides.**, ANDREW JOE, LUIS JAUREGUI, ALEX HIGH, ALAN DIBOS, ELGIN GULPINAR, KATERYNA PISTUNOVA, HONGKUN PARK, PHILIP KIM, Harvard University, Physics Department — , Luis A. Jauregui, Alex A. High, Alan Dibos, Elgin Gulpinar, Kateryna Pistunova, Hongkun Park, Philip Kim Harvard University, Physics Department -abstract- Single layer transition metal dichalcogenides (TMDC) are 2-dimensional (2D) semiconductors van der Waals (vdW) characterized by a direct optical bandgap in the visible wavelength (~2 eV). Characterization of the band alignment between TMDC and the barrier is important for the fabrication of tunneling devices. Here, we fabricate coupled quantum well (CQW) heterostructures made of 2D TMDCs with hexagonal Boron nitride (hBN) as an atomically thin barrier and gate dielectric and with top and bottom metal (or graphite) as gate electrodes. We observe a clear dependence of the photo-generated current with varying hBN thickness, electrode workfunctions, electric field, laser excitation power, excitation wavelength, and temperature. We will discuss the implication of photocurrent in relation to quantum transport process across the vdW interfaces.

**9:48AM R17.00008 Multi-terminal Monolayer WSe<sub>2</sub> devices**, WENJIN ZHAO, TAUNO PALOMAKI, JOE FINNEY, ZAIYAO FEI, PAUL NGUYEN, Univ of Washington, FRANK MCKAY, Retired, DAVID COBDEN, Univ of Washington — Two-dimensional transition-metal dichalcogenide (TMD) semiconductors are promising materials for next-generation electronic and optoelectronic devices. WSe<sub>2</sub> in particular has shown excellent optical properties, but it has proven difficult to make reliable electrical contacts to this material. We use a new chemical vapor deposition technique to grow monolayer single crystal WSe<sub>2</sub> reliably on a large scale with edges up to 15 microns long. We then fabricate these crystals into multi-terminal devices encapsulated in boron nitride using dry transfer techniques. We achieve sufficiently good electrical contacts reproducibly to allow comprehensive study of the intrinsic optical and electrical properties of gated WSe<sub>2</sub> monolayers as a function of temperature and magnetic field.

**10:00AM R17.00009 Gate-defined Single Electron Transistor in a Graphene-MoS<sub>2</sub> van der Waals Heterostructure**, KE WANG, Department of Physics, Harvard University, Cambridge, MA 02138, USA, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, Namiki 1-1, Tsukuba, Ibaraki 305-0044, Japan, PHILIP KIM, Department of Physics, Harvard University, Cambridge, MA 02138, USA — We report experimental demonstration of fabrication of laterally confined single electron transistor (SET) on MoS<sub>2</sub> transition metal dichalcogenide (TMDC) semiconductor. A few atomic layers of MoS<sub>2</sub> single crystals are encapsulated in hBN layers in order to improve mobility of 2-dimensional (2D) electron channel. Graphene layers are employed to provide Ohmic contact to the TMDC channels. The laterally confined quantum dots are formed by electrostatically depleting the near-by 2D channel employing local gate fabricated by electron lithography. Typical SET transport signatures such as gate-tunable Coulomb blockade have been observed. We have demonstrated the quantum confinement can be sensitively tuned to adjust the dot-reservoir coupling. The work paves way for more complicated device structure such as valley-spin filter and vertically coupled quantum dots in Coulomb drag devices.

**10:12AM R17.00010 Probing interlayer interactions in WS<sub>2</sub>-graphene van der Waals heterostructures**, TING FUNG CHUNG, LONG YUAN, LIBAI HUANG, YONG P. CHEN, Purdue University — Two-dimensional crystals based van der Waals coupled heterostructures are of interest owing to their potential applications for flexible and transparent electronics and optoelectronics. The interaction between the 2D layered crystals at the interfaces of these heterostructures is crucial in determining the overall performance and is strongly affected by contamination and interfacial strain. We have fabricated heterostructures consisting of atomically thin exfoliated WS<sub>2</sub> and chemical-vapor-deposited (CVD) graphene, and studied the interaction and coupling between the WS<sub>2</sub> and graphene using atomic force microscopy (AFM), Raman spectroscopy and femtosecond transient absorption measurement (TAM). Information from Raman-active phonon modes allows us to estimate charge doping in graphene and interfacial strain on the crystals. Spatial imaging probed by TAM can be correlated to the heterostructure surface morphology measured by AFM and Raman maps of graphene and WS<sub>2</sub>, showing how the interlayer coupling alters exciton decay dynamics quantitatively.

**10:24AM R17.00011 Coherently stacked MoS<sub>2</sub>/WSe<sub>2</sub> heterostructures: Moiré pattern and its effect on interlayer couplings**, CHENDONG ZHANG, UT at Austin, MING-YANG LI, Academia Sinica; KAUST, CHIH-PIAO CHUU, Academia Sinica, MEI-YIN CHOU, Academia Sinica; Georgia Institute of Technology; NTU, Taiwan, LAIN-JONG LI, KAUST, CHIH-KANG SHIH, UT at Austin — Vertically stacked heterojunctions (HJs) of transition metal dichalcogenides (TMDs) have been proposed as fundamental building blocks for several novel electronic and photonic devices. Although such HJs can be easily achieved by sequential transferring of different TMDs, this approach is not scalable, and the orientation relationship between the layers is difficult to control. A much more desirable approach is to directly grow one kind of TMD on top of the other. In addition to being a scalable platform, the epitaxial approach also results in a well-defined orientation relationship. A very important question to ask is “What is the role of the interlayer coupling on the electronic structures of such a bilayer stack?” By using scanning tunneling microscopy/spectroscopy (STM/S) and first-principles calculations, we investigate the MoS<sub>2</sub>/WSe<sub>2</sub> vertical heterojunctions formed by direct epitaxial growth. The different lateral lattice constants between MoS<sub>2</sub> and WSe<sub>2</sub> lead to the formation of a well-ordered Moiré pattern with a superlattice constant of ~8.5 nm. This superlattice reflects the variation of the lateral alignment between the MoS<sub>2</sub> and WSe<sub>2</sub> lattices. STS shows very large variations of interlayer coupling, as a function of the lateral alignment. More interestingly, depending on the location in the BZ, the interlayer coupling has very different consequences on the electronic structures.

**10:36AM R17.00012 Interface exciton at lateral heterojunction of monolayer semiconductors<sup>1</sup>**, KA WAI LAU, The Univ of Hong Kong, ZHIRUI GONG, Shenzhen University, HONGYI YU, WANG YAO, The Univ of Hong Kong — Heterostructures based on 2D transition metal dichalcogenides (TMDs) have attracted extensive research interest recently due to the appealing physical properties of TMDs and new geometries for forming heterostructures. One such heterostructure is the lateral heterojunctions seamlessly formed in a monolayer crystal between two different types of TMDs, e.g. WSe<sub>2</sub> and MoSe<sub>2</sub>. Such heterojunction exhibits a type II band alignment, with electrons (holes) having lower energy on the MoSe<sub>2</sub> (WSe<sub>2</sub>) region. Here we present the study of an interface exciton at the 1D lateral junction of monolayer TMDs. With the distance dependent screening, we find that the interface exciton can have strong binding even though the electron-hole separation is much larger compare to the 2D excitons in TMDs. Neutral excitons are studied using two different approaches: the solution based on a real-space tight binding model, and the perturbation expansion in a hydrogen-like basis in an effective mass model. We have also used the latter method to study charged excitons at a MoSe<sub>2</sub>-WSe<sub>2</sub>-MoSe<sub>2</sub> nanoscale junction.

<sup>1</sup>The work is supported by the Research Grant Council of Hong Kong (HKU705513P, HKU9/CRF/13G), the Croucher Foundation, and the HKU OYRA.

**10:48AM R17.00013 Indirect Band Gap Emission by Hot Electron Injection in Metal/MoS<sub>2</sub> and Metal/WSe<sub>2</sub> Heterojunctions**, ZHEN LI, University of Southern California, GOUTHAM EZHILARASU, College of Engineering Guindy, Anna University, IOANNIS CHATZAKIS, ROHAN DHALL, CHUN-CHUNG CHEN, STEPHEN CRONIN, University of Southern California — Transition metal dichalcogenides (TMDCs), such as MoS<sub>2</sub> and WSe<sub>2</sub>, are free of dangling bonds, therefore make more ‘ideal’ Schottky junctions than bulk semiconductors, which produce recombination centers at the interface with metals, inhibiting charge transfer. Here, we observe a more than 10X enhancement in the indirect band gap PL of TMDCs deposited on various metals, while the direct band gap emission remains unchanged. We believe the main mechanism of light emission arises from photoexcited hot electrons in the metal that are injected into the conduction band of MoS<sub>2</sub> and WSe<sub>2</sub>, and subsequently recombine radiatively with minority holes. Since the conduction band at the K-point is 0.5eV higher than at the  $\Sigma$ -point, a lower Schottky barrier of the  $\Sigma$ -point band makes electron injection more favorable. Also, the  $\Sigma$  band consists of the sulfur  $p_z$  orbital, which overlaps more significantly with the electron wavefunctions in the metal. This enhancement only occurs for thick flakes, and is absent in monolayer and few-layer flakes. Here, the flake thickness must exceed the depletion width of the Schottky junction, in order for efficient radiative recombination to occur in the TMDC. The intensity of this indirect peak decreases at low temperatures. Reference: DOI: 10.1021/acs.nanolett.5b00885

**Thursday, March 17, 2016 8:00AM - 10:12AM —**

**Session R18 GMAG DMP FIAP: Spintransport Phenomena II** 317 - See-Hun Yang, IBM Almaden

**8:00AM R18.00001 Magnetic and electron-transport properties of spin-gapless semiconducting CoFeCrAl films.<sup>1</sup>**, DAVID SELLMYER, YUNLONG JIN, University of Nebraska Lincoln, PARASHU KHAREL, South Dakota State University, SHAH VALLOPPILLY, TOM GEORGE, BALAMURUGAN BALASUBRAMANIAN, RALPH SKOMSKI, University of Nebraska Lincoln — Recently, spin-gapless semiconductors (SGS) with a semiconducting or insulating gap in one spin channel and zero gap in the other at the Fermi level have attracted much attention due to their new functionalities such as voltage-tunable spin polarization, the ability to switch between spin-polarized n-type and p-type conduction, high spin polarization and carrier mobility. For the development of spintronic devices utilizing SGS, it is necessary to have a better understanding of the magnetic and transport properties of the thin films of these materials. In this study, the structural, magnetic, and electron-transport properties of a SGS material CoFeCrAl in the thin film geometry have been investigated. CoFeCrAl films were grown on atomically flat SiO<sub>2</sub> substrates using magnetron sputtering. The Curie temperature was measured to be 550 K very close to the value reported for bulk CoFeCrAl. Electron-transport measurements on the oriented films revealed a negative temperature coefficient of resistivity, small anomalous Hall conductivity and linear field dependence of magnetoresistance, which are transport signatures of SGS. The effect of elemental compositions and structural ordering on the SGS properties of the CoFeCrAl films will be discussed.

<sup>1</sup>Research supported by NSF (Y. J.), DoE (B. B., D. J. S), ARO (T. A. G., S. R. V.), SDSU (P. K.), and NRI (Facilities)

**8:12AM R18.00002 Theory of spin relaxation at metallic interfaces<sup>1</sup>**, K. D. BELASHCHENKO, ALEXEY A. KOVALEV, University of Nebraska-Lincoln, MARK VAN SCHILFGAARDE, King's College London — Spin-flip scattering at metallic interfaces affects transport phenomena in nanostructures, such as magnetoresistance, spin injection, spin pumping, and spin torques. It has been characterized for many material combinations by an empirical parameter  $\delta$ , which is obtained by matching magnetoresistance data for multilayers to the Valet-Fert model [J. Bass and W. P. Pratt, J. Phys.: Condens. Matter **19**, 183201 (2007)]. However, the relation of the parameter  $\delta$  to the scattering properties of the interface remains unclear. Here we establish this relation using the scattering theory approach and confirm it using a generalization of the magnetoelectronic circuit theory, which includes interfacial spin relaxation. The results of first-principles calculations of spin-flip scattering at the Cu/Pd and Cu/Pt interfaces are found to be in reasonable agreement with experimental data.

<sup>1</sup>Supported by NSF Grant DMR-1308751.

**8:24AM R18.00003 Spin relaxation through Kondo scattering in Cu/Py lateral spin valves.**, J. T. BATLEY, M. C. ROSAOND, M. ALI, E. H. LINFIELD, G. BURNELL, B. J. HICKEY, University of Leeds — Within non-magnetic metals it is reasonable to expect the Elliot-Yafet mechanism to govern spin-relaxation and thus the temperature dependence of the spin diffusion length might be inversely proportional to resistivity. However, in lateral spin valves, measurements have found that at low temperatures the spin diffusion length unexpectedly decreases. We have fabricated lateral spin valves from Cu with different concentrations of magnetic impurities. Through temperature dependent charge and spin transport measurements we present clear evidence linking the presence of the Kondo effect within Cu to the suppression of the spin diffusion length below 30 K. We have calculated the spin-relaxation rate and isolated the contribution from magnetic impurities. At very low temperatures electron-electron interactions play a more prominent role in the Kondo effect. Well below the Kondo temperature a strong-coupling regime exists, where the moments become screened and the magnetic dephasing rate is reduced. We also investigate the effect of this low temperature regime ( $>1$  K) on a pure spin current. This work shows the dominant role of Kondo scattering, even in low concentrations of order 1 ppm, within pure spin transport.

**8:36AM R18.00004 Electronic structure and magnetocrystalline anisotropy of the Bi<sub>2</sub>Se<sub>3</sub> topological insulator/ferromagnet interface**, JIA ZHANG, Physics and Astronomy, University of Nebraska, Lincoln, Nebraska 68588, USA, JULIAN P. VELEV, Department of Physics, University of Puerto Rico, San Juan, Puerto Rico 00931, USA, EVGENY Y. TSYMBAL, Physics and Astronomy, University of Nebraska, Lincoln — Interesting spin-dependent phenomena are expected to emerge when a topological insulator is interfaced with a magnetic material. In this work the magnetic properties of the interface between a topological insulator Bi<sub>2</sub>Se<sub>3</sub> and ferromagnetic metals (FM) fcc (111) Ni and Co are investigated by first-principles calculations. Different interface terminations are considered, and the most stable interface termination is identified to be an interface Ni (Co) atom located atop the hollow site of the interfacial Se monolayer. We find that the proximity effect induces a small magnetic moment on the interface Se atom (0.028  $\mu_B$  for Ni and 0.023  $\mu_B$  for Co). The surface state in Bi<sub>2</sub>Se<sub>3</sub> disappears due to the strong interface hybridization between FM and Bi<sub>2</sub>Se<sub>3</sub> and metal induced gap states appear in the bandgap region of Bi<sub>2</sub>Se<sub>3</sub>. We find that both the Bi<sub>2</sub>Se<sub>3</sub>/Ni(111) and Bi<sub>2</sub>Se<sub>3</sub>/Co(111) interfaces exhibit an in-plane easy axis with the magnetic anisotropy energy of around 2 erg/cm<sup>2</sup> per interface. An interesting feature resulting from our calculations is a non-collinear k-dependent spin texture at the interface which may have important consequences for the spin-dependent transport properties, such as the spin transfer torque.

**8:48AM R18.00005 Observation of thermal spin transfer torque via ferromagnetic resonance in magnetic tunnel junctions<sup>1</sup>**, ZHAOHUI ZHANG, LIHUI BAI, CAN-MING HU, Department of Physics and Astronomy, University of Manitoba, XIAOBIN CHEN, HONG GUO, Centre for the Physics of Materials and Department of Physics, McGill University, XIAOLONG FAN, DESHENG XUE, The Key Lab for Magnetism and Magnetic Materials of Ministry of Education, Lanzhou University, DIMITRI HOUSSEMEDDINE, Everspin Technologies — The temperature gradient driven spin-transfer torque, called the thermal spin-transfer torque (TSTT) attracts people's attention since it has potential in magnetization switching by utilizing wasted heat as well as in the study of spin transportation. We observed the effects of TSTT on magnetic tunnel junction (MTJ) via analysis of the ferromagnetic resonance (FMR) spectra. We used an external laser beam to heat the MTJ in order to establish a temperature gradient effectively. A TSTT was driven by the temperature gradient and applied to the magnetization of the free FM layer of the MTJ. By measuring and analyzing the FMR spectra, after excluding the effects caused by the temperature rise, we conclude that the FMR line-shape change is a result of the TSTT generated by a temperature gradient via laser heating. The most interesting result is that the angular dependence of the TSTT and DC-bias spin-transfer torque are very different. A modified or new theory may be needed to explain this in the future.

<sup>1</sup>NSERC, CFI, URGF, CSC, Faculty of Graduate Studies of University of Manitoba, UMGSA, Faculty of Science of University of Manitoba

**9:00AM R18.00006 Intrinsic Gilbert Damping in Metallic Ferromagnets in Ballistic Regime and the Effect of Inelastic Electron Scattering from Magnetic Moments: A Time Dependent Keldysh Green Function Approach**, FARZAD MAHFOUZI, NICHOLAS KIOUSSIS, California State University, Northridge — Gilbert damping in metallic ferromagnets is mainly governed by the exchange coupling between the electrons and the magnetic degree of freedom, where the time dependent evolution of the magnetization leads to the excitation of electrons and loss of energy as a result of flow of spin and charge currents. However, it turns out that when the magnetization evolves slowly in time, in the presence of spin-orbit interaction (SOI), the resonant electronic excitations has a major contribution to the damping which leads to infinite result in ballistic regime. In this work we consider the inelastic spin-flip scattering of electrons from the magnetic moments and show that in the presence of SOI it leads to the relaxation of the excited electrons. We show that in the case of clean crystal systems such scattering leads to a linear dependence of the Gilbert on the SOI strength and in the limit of diffusive systems we get the Gilbert damping expression obtained from Kambersky's Fermi breathing approach. This research was supported by NSF-PREM Grant No. DMR-1205734

**9:12AM R18.00007 Carbon Tetragons as Definitive Spin Switches in Narrow Zigzag Graphene Nanoribbons<sup>1</sup>**, ZHENYU ZHANG, PING CUI, QIANG ZHANG, HONGBIN ZHU, XIAOXIA LI, WEIYI WANG, QUNXIANG LI, CHANGGAN ZENG, University of Science and Technology of China — Precise spatial control of the spin propagation channels is of fundamental and practical importance in future graphene-based spintronic devices. Here we use first-principles calculations to show that when narrow zigzag graphene nanoribbons are connected to form junctions or superlattices, properly placed square-shaped carbon tetragons not only serve as effective bundles of the two incoming spin edge channels, but also act as definitive topological spin switches for the two outgoing channels. The nanoribbon segments are largely drawn from different acene molecules. We further show that such spin switches can lift the degeneracy between the two spin propagation channels, which enables tunability of different magnetic states upon charge doping. Preliminary experimental supports for the realization of such tetragons connecting nanoribbon segments are also presented.

<sup>1</sup>Supported by MOST, CAS, and NNSF of China.

**9:24AM R18.00008 Spin Transport and Giant Electroresistance in Ferromagnetic Graphene Vertical Heterostructures<sup>1</sup>**, HEE CHUL PARK, Center for Theoretical Physics of Complex Systems, IBS, NOJOON MYUNG, Department of Material Science and Engineering, University of Ioannina, SEUNG JOO LEE, Quantum-functional Semiconductor Research Center, Dongguk University — We investigate spin transport through ferromagnetic graphene vertical heterostructures where a sandwiched tunneling layer is either a normal or ferroelectric insulator. We show that the spin-polarization of the tunneling current is electrically controlled via gate voltages. We also demonstrate that the tunneling current of Dirac fermions can be prohibited when the spin configuration of ferromagnetic graphene sheets is opposite. Giant electroresistance can thus be developed by using the proposed heterostructure in this study. The effects of temperature on spin transport and the giant electroresistance ratio are also investigated. Our findings discover the prospect of manipulating the spin transport properties in vertical heterostructures through electric fields via gate and bias electrodes.

<sup>1</sup>The research leading to these results has received funding from the European Union Seventh Framework Programme under grant agreement No604391 Graphene Flagship, Project Code (IBS-R024-D1), and the NRF grant funded by MSIP(No. 2014-066298).

**9:36AM R18.00009 Spin relaxation mechanism in graphene spin valves with Al<sub>2</sub>O<sub>3</sub> and MgO tunnel barriers<sup>1</sup>**, WALID AMAMOU, ZHISHENG LIN, JEREMIAH VAN BAREN, JING SHI, UC Riverside, ROLAND KAWAKAMI, Ohio State University — Contact induced spin relaxation in graphene lateral spin valves is one of major limiting factors for obtaining long spin lifetimes in graphene. There are various spin relaxation mechanisms, including spin absorption, interfacial spin scattering, and fringe field effects, which may account for the observed short spin lifetimes. One possible solution is to introduce a tunnel barrier between graphene and the ferromagnetic electrode, which should reduce contact induced spin relaxation and allow for longer spin lifetimes. We study the spin relaxation mechanisms in our graphene spin valves with two different types of tunnel barriers, aluminum oxide and MgO/TiO<sub>2</sub> using the standard non-local measurement geometry. To extract the spin lifetime from Hanle spin precession data, we perform fits based on Bloch equation models that include the effects of spin absorption into the magnetic contacts. We observe a strong dependence of the extracted spin lifetime on the resistance-area (RA) product of the contacts. To understand the role of spin absorption, we compare these results to fits obtained using Hanle models that do not take spin absorption into account. Analysis shows that spin absorption might not be the dominant source of contact induced spin relaxation for graphene spin valves with sputtered Al<sub>2</sub>O<sub>3</sub> and MgO/TiO<sub>2</sub> barriers. Interfacial spin-flip scattering or spin dephasing resulting from local magnetostatic fields due to contact roughness are likely to be more important.

<sup>1</sup>C-SPIN, ONR

**9:48AM R18.00010 Spin fluctuations in 3d paramagnetic metals**, ALEKSANDER WYSOCKI, ANDREY KUTEPOV, VLADIMIR ANTROPOV, Ames Laboratory, U.S. Department of Energy, Ames, Iowa 50011, USA — Spin fluctuations (SFs) in 3d paramagnetic metals were investigated using the linear response formalism within the time dependent density functional theory. An efficient scheme of frequency integration using the Matsubara technique has been implemented and tested. The SFs spectrum in 3d paramagnets is analyzed in real and reciprocal spaces as a function of frequency and temperature. For all materials the SFs are characterized by the coexistence of low and high energy branches which originate from different regions of the Brillouin zone. The low-energy ones can be measured by neutron scattering experiments while the high-energy SFs appear to be more localized. Further, we studied the nature of square of fluctuating magnetic moment in these materials. This work was supported, in part, by the Critical Materials Institute, an Energy Innovation Hub funded by the U.S. Department of Energy (DOE), and by the Office of Basic Energy Science, Division of Materials Science and Engineering. The research was performed at Ames Laboratory, which is operated for the U.S. DOE by Iowa State University under contract # DE-AC02-07CH11358.

**10:00AM R18.00011 ABSTRACT WITHDRAWN —**

**Thursday, March 17, 2016 8:00AM - 11:00AM —**

**Session R19 GMAG DMP: Magnetic Bulk Materials** 318 - James Lee, Lawrence Berkeley Laboratory

**8:00AM R19.00001 Field induced spin density and spiral phases in a layered antiferromagnet<sup>1</sup>**, MATTHEW STONE, MARK LUMSDEN, VASILE GARLEA, Quantum Condensed Matter Division, Oak Ridge National Laboratory, BEATRICE GRENIER, ERIC RESSOUCHE, INAC-SPSMS, CEA & Universite Grenoble Alpes, ERIC SAMULON, IAN FISHER, Department of Applied Physics and Geballe Laboratory for Advanced Materials Stanford University, LISA DEBEER-SCHMITT, Chemical & Engineering Materials Division, Oak Ridge National Laboratory, ALEXANDER HRISTOV, Department of Applied Physics and Geballe Laboratory for Advanced Materials Stanford University, JORGE GAVILANO, Paul Scherrer Institute, Villigen, Switzerland — We will present neutron scattering measurements examining the low-field ordered magnetic phases of the  $S = 1$  dimerized antiferromagnet Ba<sub>3</sub>Mn<sub>2</sub>O<sub>8</sub>. We have found that for magnetic both spin density wave order with incommensurate wave vectors and a higher field spiral phase with incommensurate wave vectors only along the  $[hh0]$  direction. For both field induced ordered phases, the magnetic moments are lying in the plane perpendicular to the field direction. The nature of these two transitions is fundamentally different: the low-field transition is a second order transition to a spin-density wave ground state, while the one at higher field, toward the spiral phase, is of first order. More recent SANS measurements of the magnetic phases with  $H \parallel c$  will be presented if available at the time of the meeting.

<sup>1</sup>A portion of this research at ORNL was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. DOE. Work at Stanford supported by the NSF

**8:12AM R19.00002 Incommensurate Spin Density Wave state in metamagnetic Fe<sub>3</sub>Ga<sub>4</sub>**, YAN WU, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, HUIBO CAO, ANTONIO DOS SANTOS, Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, GREG MCCANDLESS, JULIA CHAN, Department of Chemistry, University of Texas at Dallas, Richardson, TX 75080, AMAR KARKI, RONGYING JIN, JOHN DITUSA, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803 — Fe<sub>3</sub>Ga<sub>4</sub> displays a rich competition between magnetic states without structural transitions: a ferromagnetic(FM) ground state transitions to an antiferromagnetic(AFM) intermediate state above 68 K followed by a reemergence of the FM state above room temperature(T). The reentrance of the FM state hints of a coupling of the magnetic degrees of freedom to other modes. To explore the nature of the magnetic states, we have performed extensive single crystal neutron diffraction measurements over a wide range of T and pressure. These measurements revealed two very different magnetic states with the low T FM state having magnetic moments along the c-axis while we discovered that the AFM state is in an incommensurate spin density wave(SDW) order with moments mostly along the a-axis. However, there is still considerable non-collinear and non-coplanar contributions along the b- and c-axial directions. This non-coplanar moment is likely to be the origin of the very large anomalous Hall effect(HE) including a substantial topological HE that we discovered in Fe<sub>3</sub>Ga<sub>4</sub>. Study of the effect of hydrostatic pressure indicates a reduction of the T<sub>c</sub> and a destabilization of the SDW phase.

**8:24AM R19.00003 Increased operational temperature of Cr<sub>2</sub>O<sub>3</sub>-based spintronic devices<sup>1</sup>**, MICHAEL STREET, WILL ECHTENKAMP, TAKASHI KOMESU, SHI CAO, University of Nebraska-Lincoln, JIAN WANG, University of Saskatchewan, PETER DOWBEN, CHRISTIAN BINEK, University of Nebraska-Lincoln — Spintronic devices have been considered a promising path to revolutionizing the current data storage and memory technologies. This work is an effort to utilize voltage-controlled boundary magnetization of the magnetoelectric chromia (Cr<sub>2</sub>O<sub>3</sub>) to be implemented into a spintronic device. The electric switchable boundary magnetization of chromia can be used to voltage-control the magnetic states of an adjacent ferromagnetic layer. For this technique to be utilized in a spintronic device, the antiferromagnetic ordering temperature of chromia must be enhanced above the bulk value of  $T_N = 307\text{K}$ . Previously, based on first principle calculations, boron doped chromia thin films were fabricated via pulsed laser deposition showing boundary magnetization at elevated temperatures. Measurements of the boundary magnetization were also corroborated by spin polarized inverse photoemission spectroscopy. Exchange bias of B-doped chromia was also investigated using magneto-optical Kerr effect, showing an increased blocking temperature from 307K. Further boundary magnetization measurements and spin polarized inverse photoemission measurements indicate the surface magnetization to an in-plane orientation from the standard perpendicular orientation.

<sup>1</sup>This project was supported by the SRC through CNFD, an SRC-NRI Center under Task ID (2398.001) and by C-SPIN, part of STARnet, sponsored by MARCO and DARPA (No. SRC 2381.001)

**8:36AM R19.00004 "Switching" of Magnetic Anisotropy in Magnets with Strong Spin-Orbit Coupling**, HIROAKI ISHIZUKA, LEON BALENTS, Univ of California - Santa Barbara — Motivated by recent studies on heavy-element magnetic oxides, we theoretically study a spin model on a fcc lattice with bond-dependent anisotropic interactions. Strong spin-orbit coupling in heavy elements often gives rise to bond-dependent anisotropic interactions in magnetic compounds. Such anisotropic interactions are known to induce peculiar magnetic behavior such as quantum spin-liquid and order-by-disorder. In this study, we investigate magnetic anisotropy of a fcc lattice antiferromagnet with bond-dependent interactions. We show that, in this model, the magnetic anisotropy is induced by fluctuations in both high-temperature paramagnetic and low-temperature magnetically-ordered phases. Furthermore, they show strong temperature dependence and switching of the magnetic anisotropy as the temperature decreases;  $j_{111}$  direction is favored in high-temperature above magnetic transition, while  $j_{100}$  or  $j_{110}$  is favored in the ordered phase, depending on the parameter. This is in contrast to the magnetic anisotropy induced by crystal field, which is independent of temperature. Observation of this temperature dependent anisotropy may provide a way to experimentally determine the anisotropic interaction in heavy-element magnets.

**8:48AM R19.00005 Lattice Dynamics and Magnetoelastic Coupling in a Frustrated Shape Memory Alloy**, PAUL STONAH, MIKE MANLEY, Oak Ridge National Lab, NICK BRUNO, IBRAHIM KARAMAN, RAYMUNDO ARROYAVE, Texas AM University, NAVDEEP SINGH, University of Houston, ELIOT SPECHT, DOUG ABERNATHY, SONGXUE CHI, XIAOPING WANG, Oak Ridge National Lab, CRYSTAL FABRICATION TEAM, SCATTERING EXPERIMENTS TEAM, THEORY TEAM — Magnetocaloric (MC) materials present an avenue for chemical-free, solid state refrigeration through cooling via adiabatic demagnetization. We have used inelastic neutron scattering to measure the lattice dynamics in the MC shape memory alloy Ni<sub>45</sub>Co<sub>5</sub>Mn<sub>36.6</sub>In<sub>13.4</sub>. In this presentation, we present the results of inelastic neutron scattering near the Curie temperature. We find that there is an unaccounted-for change in phonon entropy of 0.22 kJ atom<sup>-1</sup> (26 J kg<sup>-1</sup> K<sup>-1</sup>), which we attribute to phonon-magnon coupling. We identify an anomalous softening of the TA[100] phonon mode. We also present the results of diffuse neutron and X-ray diffraction experiments and provide an interpretation on the implied local order.

**9:00AM R19.00006 Magnetotransport anisotropy in microstructures of Yb<sub>2</sub>Pt<sub>2</sub>Pb**, TONI HELM, PHILIP J.W. MOLL, NoneMax-Planck-Institute for Chemical Physics of Solids, Dresden, Germany — The Yb<sup>3+</sup> moments in Yb<sub>2</sub>Pt<sub>2</sub>Pb (YPP) form a strongly frustrated Shastry-Sutherland lattice (SSL) [1]. Below 2 K, a dimerized antiferromagnetic order consisting of two AF sublattices has been recently identified by neutron diffraction [2]. Unlike other quantum magnets, YPP is a highly conductive metal and the large Sommerfeld coefficient  $\Gamma \sim 300$  mJ/molK<sup>2</sup> suggests hybridization of the Yb-4f states with the conduction band [3]. This opens the possibility to search for signatures of the metamagnetism associated with the plateaus at fractions of the saturation magnetization, a characteristic of SSL systems. To study the influence of YPPs rich magnetic structure on the anisotropic charge transport, we fabricated micron-sized transport devices from single crystalline YPP by Focused Ion Beam etching. This technique enables thickness and length dependent magnetotransport measurements along the most relevant lattice directions. [1] M. S. Kim et al. PRB 77,144425 (2008) [2] W. Müller et al. arXiv:1408.0209v1 (2014) [3] M. S. Kim, M. C. Aronson, PRL 110, 017201 (2013)

**9:12AM R19.00007 Magnetic anisotropy of rare-earth magnets calculated by SIC and OEP<sup>1</sup>**, HISAZUMI AKAI, ISSP, Univ of Tokyo, MASAKO OGURA, PGI, Juelich Research Center — We have pointed out in our previous study that the chemical bonding between N and Sm plays an important role in the magnetic anisotropy change of Sm<sub>2</sub>Fe<sub>17</sub> from in-plane to uniaxial ones caused by the introducing of N. This effect of N insertion was discussed in terms of change in the electronic structure calculated in the framework of LDA+SIC. The main issue here is whether the 4f states are dealt with properly in SIC. In the present study, we examine the applicability of SIC for the evaluation of the magnetic anisotropy of rare-earth (RE) magnets by comparing the results with various methods, in particular, the optimized effective potential (OEP) method. In this study, OEP is applied only on the RE sites. Admittedly, this is a drawback from the viewpoint of the consistent treatment of uncertainly inherent in the so-called KLI (Krieger-Li-Iafrate) constants. Putting this aside for the moment, we have calculated the electronic structure of RE magnets R<sub>2</sub>Fe<sub>17</sub>N<sub>x</sub> and RCo<sub>5</sub> (R=light RE), by OEP with exact-exchange (EXX) combined with Colle-Salvetti correlation. Our preliminary results have shown considerable differences between the SIC and OEP calculations. We will discuss the meaning of this discrepancy.

<sup>1</sup>This work was supported by the Elements Strategy Initiative Center for Magnetic Materials under the outsourcing project of MEXT and by a Grant-in-Aid for Scientific Research (No. 26400330) from MEXT.

**9:24AM R19.00008 Domain wall order and motion in Mn<sub>3</sub>O<sub>4</sub>**, ALEXANDER THALER, Oak Ridge National Lab, Oak Ridge, TN, ALEXANDER ZAKJEVSKII, BRIAN NGUYEN, YEWON GIM, Physics Illinois & Seitz MRL, University of Illinois, Urbana, IL, ADAM ACZEL, LISA DEBEER-SCHMITT, Oak Ridge National Lab, Oak Ridge, TN, S. LANCE COOPER, GREGORY MACDOUGALL, Physics Illinois & Seitz MRL, University of Illinois, Urbana, IL — Mn<sub>3</sub>O<sub>4</sub> is an orbitally ordered, magnetically frustrated spinel with strong spin-lattice coupling, which exhibits a series of low temperature magnetic and structural transitions. Transverse field  $\mu$ SR has shown that ordered and disordered volumes coexist within this material, while MFM measurements have further shown that the magnetic domain walls themselves order in specific crystallographic directions, with a typical length scale of 100's of nm. In order to directly study these phenomena, we have performed small angle neutron scattering (SANS) measurements at both zero and applied magnetic field. We will present the results of these measurements and discuss what they show as far as the formation of domains, as well as the motion of the domain walls. We will also discuss the effects of internal disorder on the behavior of the material. This work was sponsored by the National Science Foundation, under grant number DMR-1455264.

**9:36AM R19.00009 Nanoscale Magnetic Structure of Non-Joulian Magnets**, RAVINI CHANDRASENA, WEIBING YANG, Department of Physics, Temple University, ANDREAS SCHOLL, Advanced Light Source, LBNL, JAN MINAR, Department of Chemistry, Ludwig Maximilian University, PADRAIC SHAFER, ELKE ARENHOLZ, Advanced Light Source, LBNL, HUBERT EBERT, Department of Chemistry, Ludwig Maximilian University, ALEXANDER GRAY, Department of Physics, Temple University, HARSH DEEP CHOPRA, Mechanical Engineering Department, Temple University — Strain dependence of magnetic anisotropy energy produces Joule magnetostriction that is a volume conserving process, whereas sensitivity of isotropic exchange energy to interatomic distance is the cause of volume magnetostriction. In a typical magnet, Joule magnetostriction dominates as the volume fraction occupied by regions of uniform spin alignment (domains) is 2-4 orders of magnitude higher than that which is occupied by regions with magnetoelastic gradients (domain walls). Recently, 'giant' non-volume conserving or non-Joulian magnetostriction has been discovered in iron-gallium alloys. Here we show using high-resolution polarization-dependent photoelectron microscopy that non-Joulian magnetism arises from an unusual partition of the crystal into nm-scale lamellar domains and domain walls within highly periodic magnetic microcells. High-resolution x-ray circular dichroism measurements at the Fe and Ga L absorption edges further provide evidence of weak iron-induced magnetism on gallium atoms via negative exchange. The results are in excellent agreement with the state-of-the-art theoretical electronic-structure calculations.

**9:48AM R19.00010 Control over magnetic properties in bulk hybrid materials<sup>1</sup>**, CHRISTIAN URBAN, University of California San Diego, ADRIAN QUESADA, Instituto de Cerámica y Vidrio, CSIC, 28049, Madrid, Spain, THOMAS SAERBECK, Institut Laue-Langevin, 71 Av. Des Martyrs, 38000 Grenoble, France, MIGUEL ANGEL DE LA RUBIA, MIGUEL ANGEL GARCIA, JOSE FRANCISCO FERNANDEZ, Instituto de Cerámica y Vidrio, CSIC, 28049, Madrid, Spain, IVAN K. SCHULLER, University of California San Diego, UCSD COLLABORATION, INSTITUTO DE CERAMICA, MADRID COLLABORATION, INSTITUT LAUE-LANGEVIN, GRENoble COLLABORATION — We present control of coercivity and remanent magnetization of a bulk ferromagnetic material embedded in bulk vanadium sesquioxide (V<sub>2</sub>O<sub>3</sub>) by using a standard bulk synthesis procedure. The method generalizes the use of structural phase transitions of one material to control structural and magnetic properties of another. A structural phase transition (SPT) in the V<sub>2</sub>O<sub>3</sub> host material causes magnetic properties of Ni to change as function of temperature. The remanent magnetization and the coercivity are reversibly controlled by the SPT without additional external magnetic fields. The reversible tuning shown here opens the pathway for controlling the properties of a vast variety of magnetic hybrid bulk systems.

<sup>1</sup>This Work is supported by the Office of Basic Energy Science, U.S. Department of Energy, BES-DMS funded by the Department of Energys Office of Basic Energy Science, DMR under grant DE FG02 87ER-45332.

**10:00AM R19.00011 A Study of Phase Stability and Properties of TiO<sub>2</sub> Polymorphs with Diffusion Monte Carlo**, YE LUO, ANOUAR BENALI, Argonne National Laboratory, LUKE SHULENBURGER, Sandia National Laboratories, JARON KROGEL, Oak Ridge National Laboratory, OLLE HEINONEN, Argonne National Laboratory, PAUL KENT, Oak Ridge National Laboratory — In the past decades, many studies have focused on the fundamental properties of TiO<sub>2</sub> due to its important role in effectively converting solar energy such as in photovoltaic batteries and photocatalytic water splitting. TiO<sub>2</sub> presents many stable and metastable phases of which, Rutile Anatase and Brookite are the most studied. Using density functional theory (DFT), the energy ordering of these phases depends strongly on the scheme describing the electronic correlation, for instance GGA+U and Hybrid functionals, often tied to an empirical parameter for reproducibility with no guarantee of predictability. We present the first analysis of the polymorphic energy ordering and properties of three naturally existing phases Rutile, Anatase and Brookite, by performing the highly accurate ab initio calculation with fixed node diffusion Monte Carlo (DMC) implemented in QMCPACK[1]. [1] QMCPACK, <http://www.qmcpack.org>

**10:12AM R19.00012 On the Electronic and Magnetic Properties of the ionic superatomic solid Ni<sub>9</sub>Te<sub>6</sub>(PEt<sub>3</sub>)<sub>8</sub>C<sub>60</sub><sup>1</sup>**, VIKAS CHAUHAN, SANJUBALA SAHOO, SHIV KHANNA, Virginia Commonwealth University, PHYSICS DEPARTMENT VCU COLLABORATION — We have carried out first principles electronic structure studies to examine the atomic structure, stability, and electronic and magnetic properties of the recently synthesized Ni<sub>9</sub>Te<sub>6</sub>(PEt<sub>3</sub>)<sub>8</sub>C<sub>60</sub> ionic material consisting of Ni<sub>9</sub>Te<sub>6</sub>(PEt<sub>3</sub>)<sub>8</sub> superatoms and C<sub>60</sub>. It is shown that the PEt<sub>3</sub> ligands result in an internal coulomb well that lifts the quantum states of the Ni<sub>9</sub>Te<sub>6</sub> cluster lowering its ionization potential to 3.39 eV thus creating a superatomic alkali motif. The metallic core has a spin magnetic moment of 5.3  $\mu_B$  in agreement with experiment. The clusters are marked by low magnetic anisotropy energy (MAE) of 2.72 meV and a larger intra-exchange coupling exceeding 0.2 eV indicating that the observed paramagnetic behavior around 10K is due to superparamagnetic relaxations. The magnetic motifs separated by C<sub>60</sub> experience a weak superexchange that stabilizes a ferromagnetic ground state as observed around 2K. The calculated MAE is sensitive to the charged state that could account for the observed change in magnetic transition temperature with size of the ligands or anion.

<sup>1</sup>We gratefully acknowledge funding support from the Department of Energy under Award Number DE-SC0006420.

**10:24AM R19.00013 Submicron sized R<sub>2</sub>Fe<sub>14</sub>B particles fabricated by mechanochemical process<sup>1</sup>**, OZLEM KOYLU-ALKAN, Department of Physics and Astronomy, University of Delaware, Newark, DE, USA, JOSE MANUEL BARANDI-ARAN, BCMaterials, Technology Park of Biscay E-48160 Derio, Spain & Dept. Electricity & Electronics, Univ. Basque Country (UPV/EHU) E-48080 Bilbao, Spain, DANIEL SALAZAR, BCMaterials, Technology Park of Biscay E-48160 Derio, Spain, GEORGE C. HADJIPANAYIS, Department of Physics and Astronomy, University of Delaware, Newark, DE, USA, UNIV. OF DELAWARE TEAM, UNIV. BASQUE COUNTRY TEAM — In this work, we have synthesized submicron R<sub>2</sub>Fe<sub>14</sub>B particles by the mechanochemical process. Mechanical activation of oxides of rare earth, iron and boron was done by high energy ball milling in a CaO with a reduction agent (Ca). After a heat treatment at 900 C the powder was washed with water and glycerol solution to remove the dispersant and other non-magnetic phases. Magnetic measurements showed that the as-synthesized unwashed powders had coercivity values of 10.3 kOe, 12.8 kOe, and 24.6 kOe for R=Nd, Pr, and Dy, respectively. During washing, H<sub>2</sub> is released and absorbed by the 2:14:1 structure. After removing the H<sub>2</sub>, the submicron particles have coercivities of 3.3 kOe (Nd), 4.4 kOe (Pr) and 21.0 kOe (Dy) with average sizes 160 nm, 242 nm, and 107 nm, respectively. Fitting of high field M(H) measurements to the law of approach to saturation showed that the anisotropy constant of the Nd<sub>2</sub>Fe<sub>14</sub>B particles are 3.73x10<sup>7</sup> erg/cm<sup>3</sup> which is comparable to bulk. Work supported by DOE DE-FG02-04ERU4612 and Bizkaia Talent AYD-000-195.

<sup>1</sup>DOE DE-FG02-04ERU4612

**10:36AM R19.00014 First-principles study of intrinsic magnetic properties of hexagonal and orthorhombic  $(\text{Fe}_{1-x}\text{Co}_x)_2\text{P}$  alloys<sup>1</sup>**, IVAN ZHURAVLEV, University of Nebraska-Lincoln, V. P. ANTROPOV, Ames Laboratory, K. D. BELASHCHENKO, University of Nebraska-Lincoln —  $(\text{Fe}_{1-x}\text{Co}_x)_2\text{P}$  is a candidate rare-earth-free alloy for permanent-magnet applications, which is hexagonal (*h*) up to  $x \approx 0.12$  and orthorhombic (*o*) at larger  $x$ . The Curie temperature  $T_C$ , which is only 270 K in  $\text{Fe}_2\text{P}$ , raises sharply with  $x$ , peaking above 450 K in the *o*-phase [1]. The measurement [2] of magnetocrystalline anisotropy (MCA) in the *o*-phase is inconsistent with Mössbauer data suggesting a spin reorientation transition (SRT) at  $x \approx 0.3$  [1]. Here we report the results of *ab initio* calculations of the magnetization, mean-field  $T_C$ , and MCA in *h*- and *o*-phases as a function of  $x$ , addressing the role of unequal site occupation, which is confirmed by total-energy calculations. The trends in the magnetization are reproduced, as well as MCA in the *h*-phase, and so is the SRT near  $x \approx 0.3$  (at odds with the results of Ref. 2). The trends in the mean-field  $T_C$ , obtained using the disordered-local-moment method, agree with experimental data. [1] R. Fruchart *et al.*, J. Appl. Phys. 40, 1250 (1969). [2] T. Hokabe *et al.*, J. Phys. Soc. Japan 36, 1704 (1974).

<sup>1</sup>Work at UNL is supported by NSF Grant DMR-1308751.

**10:48AM R19.00015 Magnetic effects of H in Metals, the case of Iron<sup>1</sup>**, PATRICIO VARGAS, ANDREA LEN, JUAN MANUEL FLOREZ, Physics Department, USM, Valparaiso, Chile — A growing consensus on the possible role of hydrogen in future energy technology has incited worldwide efforts for the development of new hydrogen-storage materials and their application to rechargeable batteries and fuel cells. Meanwhile, research in the basic properties of metal-hydrogen systems has also been advanced. High-pressure experiments have unraveled new features of elemental hydrogen (phases of solid H<sub>2</sub> and metallization of liquid H<sub>2</sub> and superconductivity) as well as of many metal-hydrogen systems (superabundant vacancy formation, phase diagrams over wide  $p$ - $x$ - $T$  ranges). In this work we address the magnetic changes induced by interstitial hydrogen in Fe. From the point of view of the Slater Pauli Curve, Fe alloys  $(\text{Fe}(1-x)\text{M}_x)$  show an increase of the magnetization (but always less than pure Fe) due substitutional non magnetic impurities like  $\text{M} = \text{V}, \text{Cr}, \text{Ti}$ . For the magnetic impurity Cobalt, the Slater Pauli Curve reaches its maximum of about 2.5 Bohr magnetons per atom when  $x=0.4$ . For an interstitial impurity H, which adds one electron to the system, we observe an increasing of the magnetization too but less than the effect induced by the volume expansion. Therefore like the case of  $\text{NiH}_x$ , one of the effects of interstitial hydrogen on a ferromagnetic material is to fill the minority spin states.

<sup>1</sup>Authors acknowledge financial support from FONDECYT under contract 1130950 and DGIP contract 11.15.73

**Thursday, March 17, 2016 10:00AM - 11:00AM —**  
Session R20 APS: Update from DOE's Office of Science 319 -

**10:00AM R20.00001 Update from DOE's Office of Science**, CHERRY MURRAY, United States Department of Energy

**Thursday, March 17, 2016 8:00AM - 11:00AM —**

Session R21 GSCCM DCOMP DMP: Materials at Extremes: Dynamic Compression 320 - Jon Belof, Lawrence Livermore National Laboratory

**8:00AM R21.00001 Ultrafast X-ray Studies on the Dynamics of Structural Transitions**, ARIANNA GLEASON, LANL — Understanding the processes which dictate physical properties such as strength, elasticity, plasticity, and the kinetics of phase transformation/crystallization requires studies at the relevant length-scales (e.g., interatomic spacing and grain size) and time-scales (e.g., phonon period). Experiments performed at the Matter in Extreme Conditions end-station at the Linac Coherent Light Source, SLAC combine a laser-driven dynamic compression pump and X-ray free electron laser probe. To showcase some of the capabilities of this end-station, we present time-resolved structural and/or electronic transformations in a suite of materials over a pressure range of a few to tens of GPa, including: 1) quartz/fused silica, 2) water, 3) Fe-bearing pyroxene, 4) iron and 5) titanium.

**8:36AM R21.00002 Nanosecond homogeneous nucleation and crystal growth in shock-compressed  $\text{SiO}_2$** , YUAN SHEN, Stanford Univ, SHAI JESTER, TINGTING QI, EVAN REED, Stanford University — Understanding the kinetics of shock-compressed  $\text{SiO}_2$  is of great importance for mitigating optical damage for high-intensity lasers and for understanding meteoroid impacts. Experimental work has placed some thermodynamic bounds on the formation of high-pressure phases of this material, but the formation kinetics and underlying microscopic mechanisms are yet to be elucidated. Here, by employing multiscale molecular dynamics studies of shock-compressed fused silica and quartz, we find that silica transforms into a poor glass former that subsequently exhibits ultrafast crystallization within a few nanoseconds. We also find that, as a result of the formation of such an intermediate disordered phase, the transition between silica polymorphs obeys a homogeneous reconstructive nucleation and grain growth model. Moreover, we construct a quantitative model of nucleation and grain growth, and compare its predictions with stishovite grain sizes observed in laser-induced damage and meteoroid impact events.

**8:48AM R21.00003 Order parameter aided phase space exploration under extreme conditions<sup>1</sup>**, AMIT SAMANTA, SEBASTIAN HAMEL, ERIC SCHWEGLER, Lawrence Livermore National Laboratory — Efficient exploration of configuration space and identification of metastable structures in condensed phase systems are challenging from both computational as well as algorithmic perspectives. In this talk I will illustrate how we can extend the recently proposed order-parameter aided temperature accelerated sampling schemes to efficiently and systematically explore free energy surfaces, and search for metastable states and reaction pathways within the framework of density functional theory based molecular dynamics. I will illustrate how this sampling scheme can be used to explore the relevant parts of configuration space in prototypical materials, like  $\text{SiO}_2$  and identify the different metastable structures, transition pathways and phase boundaries.

<sup>1</sup>This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

**9:00AM R21.00004 Multi-frame X-ray Phase Contrast Imaging of Impact Experiments at the Advanced Photon Source** , BRIAN JENSEN, Los Alamos National Laboratory, ADAM IVERSON, CARL CARLSON, MATTHEW TEEL, NATIONAL SECURITY TECHNOLOGIES, BENJAMIN MORROW, DAVID FREDENBURG, Los Alamos National Laboratory — Recent advances in coupling synchrotron X-ray diagnostics to dynamic compression experiments are providing new information about the response of materials at extremes conditions. For example, propagation based X-ray Phase Contrast Imaging (PCI) which is sensitive to differences in density (or index of refraction) has been successfully used to study a wide range of phenomena including jet-formation in metals, crack nucleation and propagation, and detonator dynamics. These experimental results have relied, in part, on the development of a robust, optically multiplexed detector system that captures single X-ray bunch images with micrometer spatial resolution on the nanosecond time scale. In this work, the multi-frame PCI (MPCI) system is described along with experiment highlights that include the compression of an idealized system of spheres subjected to impact loading. Additional advances to the detector system will be presented that are designed to increase the efficiency of the detector system and to retrieve phase information from the X-ray images which is required for determining the density during dynamic loading. Experimental results, implications, and future work will be discussed.

**9:12AM R21.00005 The Challenge of Time-Dependent Control of Both Processing and Performance of Materials at the Mesoscale, and the MaRIE Project** , CRIS W. BARNES, Los Alamos National Laboratory — DOE and NNSA are recognizing a mission need for flexible and reduced-cost product-based solutions to materials through accelerated qualification, certification, and assessment. The science challenge lies between the nanoscale of materials and the integral device scale, at the middle or "mesoscale" where interfaces, defects, and microstructure determine the performance of the materials over the lifecycle of the intended use. Time-dependent control of the processing, structure and properties of materials at this scale lies at the heart of qualifying and certifying additive manufactured parts; experimental data of high fidelity and high resolution are necessary to discover the right physical mechanisms to model and to validate and calibrate those reduced-order models in codes on Exascale computers. The scientific requirements to do this are aided by a revolution in coherent imaging of non-periodic features that can be combined with scattering off periodic structures. This drives the need to require a coherent x-ray source, brilliant and high repetition rate, of sufficiently high energy to see into and through the mesoscale. The Matter-Radiation Interactions in Extremes (MaRIE) Project is a proposal to build such a very-high-energy X-ray Free Electron Laser.

**9:24AM R21.00006 The behavior of single-crystal silicon to dynamic loading using in-situ X-ray diffraction and phase contrast imaging<sup>1</sup>** , HAE JA LEE, ZHOU XING, ERIC GALTIER, BRICE ARNOLD, EDUARDO GRANADOS, SHAUGHNESSY B. BROWN, FRANZ TAVELLA, EMMA MCBRIDE, ALAN FRY, BOB NAGLER, SLAC National Accelerator Laboratory, ANDREAS SCHROPP, FRANK SEIBOTH, DIRK SAMBERG, CHRISTIAN SCHROER, DESY, ARIANNA E. GLEASON, Los Alamos National Laboratory, ANDREW HIGGINBOTHAM, University of York — Hydrostatic and uniaxial compression studies have revealed that crystalline silicon undergoes phase transitions from a cubic diamond structure to a variety of phases including orthorhombic Imma phase, body-centered tetragonal phase, and a hexagonal primitive phase [1, 2]. The dynamic response of silicon at high pressure, however, is not well understood. Phase contrast imaging has proven to be a powerful tool for probing density changes caused by the shock propagation into a material [3]. In order to characterize the elastic and phase transitions, we image shock waves in Si with high spatial resolution using the LCLS X-ray free electron laser and Matter in Extreme Conditions instrument. In this study, the long pulse optical laser with pseudo-flat top shape creates high pressures up to 60 GPa. We measure the crystal structure by observing X-ray diffraction orthogonal to the shock propagation direction over a range of pressures. We describe the capability of simultaneously performing phase contrast imaging and in situ X-ray diffraction during shock loading and discuss the dynamic response of Si in high-pressure phases. [1] Jamieson, Science, 139, 762 (1963); Hu et al. Phys. Rev. B 34, 4679 (1986) [2] McMahon and Nelmes, Phys. Rev. B 47, 8337 (1993); Moggi et al. Phys. Rev. B 89, 064104 (2014) [3] Nagler et al. J. Synchrotron Rad. 22 (2015); Schropp et al. Scientific Reports 5, 11089 (2015)

<sup>1</sup>Use of the Linac Coherent Light Source (LCLS), SLAC National Accelerator Laboratory, is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-76SF00515. The MEC instrument is supported by

**9:36AM R21.00007 Calculation of Si L<sub>2,3</sub>-edge Non-Resonant Inelastic X-ray Scattering Spectra of Compressed Silica Glass** , KEITH GILMORE, European Synchrotron Radiation Facility, JOHN TSE, University of Saskatchewan — Despite the abundance of silica in Earth's crust and its corresponding importance to geological processes, debate continues as to the local coordination of Si in silica at geological pressures. Recent *ab initio* molecular dynamics simulations [M. Wu et al., Sci. Rep. 2, 398 (2012)] predicted a change from 4-fold coordinated Si at ambient pressure to 6-fold coordination by 22 GPa. This was consistent with experimental non-resonant inelastic x-ray scattering (NRIXS) measurements at the O K-edge that also suggested a conversion to 6-fold coordination by 22 GPa [J. Lin et al., Phys. Rev. B 75, 012201 (2007)]. However, NRIXS measured at the Si L-edge found the spectra to be largely independent of pressure up to 74 GPa [H. Fukui et al., Phys. Rev. B 78, 12203 (2008)] indicating that 4-fold coordination is maintained. The discrepancy may potentially be due to low instrument resolution of the Si L-edge measurements. We present calculated Si L-edge NRIXS spectra at multiple pressures between ambient and 150 GPa and for several momentum transfer values. This allows us to identify spectral features that may be used to better distinguish 4-fold and 6-fold coordinated environments as experimental resolutions improve.

**9:48AM R21.00008 Probing off-Hugoniot states in Ta, Cu, and Al to 10 Mbar compression with magnetically driven liner implosions** , T.R. MATTSSON, R.W. LEMKE, D.H. DOLAN, D.G. DALTON, J.L. BROWN, G.R. ROBERTSON, M.D. KNUDSON, E. HARDING, A.E. MATTSSON, J.H. CARPENTER, R.R. DRAKE, K. COCHRANE, A.C. ROBINSON, Sandia National Laboratories, K. TOMLINSON, General Atomics, B.E. BLUE, Lawrence Livermore National Laboratory — We report on a technique for obtaining off-Hugoniot equation of state data on solid metals by a magnetically driven cylindrical liner implosion on Sandia's Z-machine (Z). The sample material is in an inner tube with an outer tube composed of Al that serves as the current carrying cathode. A shaped current pulse quasi-isentropically compresses the sample as it implodes. Photonic Doppler velocimetry measures the implosion velocity of the free inner surface of the sample material, and the explosion velocity of the return current anode free outer surface. The velocimetry measurements are used in conjunction with magnetohydrodynamic simulations and optimization to infer pressure and density in the sample. Results are presented for experiments on the Z-machine in which Ta, Cu, and Al samples were compressed to peak pressure 10 Mbar. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energys National Nuclear Security Administration under contract DE-AC04-94AL85000.

**10:00AM R21.00009 Spall Response of Tantalum at Extreme Strain-Rates** , ERIC HAHN, Univ of California - San Diego, TIM GERMANN, Los Alamos National Laboratory, MARC MEYERS, Univ of California - San Diego — Strain-rate and microstructure play a significant role in the ultimate mechanical response of materials. Using non-equilibrium molecular dynamics simulations, we characterize the ductile tensile failure of single and nanocrystalline tantalum over multiple orders of magnitude of strain-rate. This comparison is extended to over nine orders of magnitude including experimental results from recent laser shock campaigns. Spall strength primarily follows a power law dependence with strain-rate over this extensive range. In all cases, voids nucleate heterogeneously at pre-existing defects. Predictions based on traditional theory suggest that, as strain-rate increases, tensile strength should increase. Alternatively, as grain size decreases, tensile strength may decrease due to an increased propensity to fail at a growing volume fraction of grain boundaries. Strain-rate and grain size dictate void nucleation sites by changing the type and density of available defects: vacancies, dislocations, twins, and grain boundaries.

**10:12AM R21.00010 Sound velocity in shock compressed molybdenum obtained by ab initio molecular dynamics**, TYMOFIY LUKINOV, ANATOLY BELONOSHKO, Royal Inst of Tech, SERGEY SIMAK, Linkping University — The sound velocity of Mo along the Hugoniot adiabat is calculated from first principles using density-functional theory based molecular dynamics. These data are compared to the sound velocity as measured in recent experiments. The theoretical and experimental Hugoniot and sound velocities are in very good agreement up to pressures of 210 GPa and temperatures of 3700 K on the Hugoniot. However, above that point the experiment and theory diverge. This implies that Mo undergoes a phase transition at about the same point. Considering that the melting point of Mo is likely much higher at that pressure, the related change in the sound velocity in experiment can be ascribed to a solid-solid transition.

**10:24AM R21.00011 Atomistic Simulation of shock induced dislocation dynamics and evolution of different plasticity mechanisms in Single Crystal Copper**, ANUPAM NEOGI, NILANJAN MITRA, Indian Institute of Technology Kharagpur — Deformation and observation of different types of plasticity mechanisms of FCC metals (e.g. Copper) under shock loading of various intensities has been investigated by several groups of researchers around the globe through different types of experiments and/or atomistic simulations. However, there still exists lacuna in this well researched area. In this study the temporal details of dislocation dynamics are provided. Simulations also demonstrate different types of temporal evolution of different loops observed for single crystal Cu under different intensities of shock loading. Observance of formation of twins and their temporal evolution at higher intensities of shock loading are also demonstrated as part of this study. Comparisons of these NEMD simulations using EAM potential are discussed with regards to different experimental and simulation studies in literature.

**10:36AM R21.00012 Effects of porosity on shock-induced melting of honeycomb-shaped Cu nanofoams.**, FENG PENG ZHAO, Institute of Systems Engineering, CAEP — Metallic foams are of fundamental and applied interests in various areas, including structure engineering (e.g., lightweight structural members and energy absorbers), and shock physics (e.g., as laser ablaters involving shock-induced melting and vaporization). Honeycomb-shaped metallic foams consist of regular array of hexagonal cells in two dimensions and have extensive applications and represent a unique, simple yet useful model structure for exploring mechanisms and making quantitative assessment. We investigate shock-induced melting in honeycomb-shaped Cu nanofoams with extensive molecular dynamics simulations. A total of ten porosities ( $\phi$ ) are explored, ranging from 0 to 0.9 at an increment of 0.1. Upon shock compression, void collapse induces local melting followed by supercooling for sufficiently high porosity at low shock strengths. While superheating of solid remnants occurs for sufficiently strong shocks at  $\phi < 0.1$ . Both supercooling of melts and superheating of solid remnants are transient, and the equilibrated shock states eventually fall on the equilibrium melting curve for partial melting. However, phase equilibrium has not been achieved on the time scale of simulations in supercooled Cu liquid (from completely melted nanofoams). The temperatures for incipient and complete melting are related to porosity via a power law and approach the melting temperature at zero pressure as  $\phi$  tends to 1.

**10:48AM R21.00013 Dynamic Behaviors of Materials under Ramp Wave Loading on Compact Pulsed Power Generators**, JIANHENG ZHAO, BINQIANG LUO, GUIJI WANG, TAO CHONG, FULI TAN, CANG LIU, CHENGWEI SUN, Institute of fluid physics, CAEP — The technique using intense current to produce magnetic pressure provides a unique way to compress matter near isentropically to high density without obvious temperature increment, which is characterized as ramp wave loading, and firstly developed by Sandia in 1998. Firstly recent advances on compact pulsed power generators developed in our laboratory, such as CQ-4, CQ-3-MMAF and CQ-7 devices, are simply introduced here, which devoted to ramp wave loading from 50 GPa to 200 GPa, and to ultrahigh-velocity flyer launching up to 30 km/s. And then, we show our progress in data processing methods and experiments of isentropic compression conducted on these devices mentioned above. The suitability of Gruneisen EOS and Vinet EOS are validated by isentropic experiments of tantalum, and the parameters of SCG constitutive equation of aluminum and copper are modified to give better prediction under isentropic compression. Phase transition of bismuth and tin are investigated under different initial temperatures, parameters of Helmholtz free energy and characteristic relaxation time in kinetic phase transition equation are calibrated. Supported by NNSF of China under contract No.11327803 and 11176002

**Thursday, March 17, 2016 8:00AM - 10:48AM —**

**Session R22 DCMP: URu<sub>2</sub>Si<sub>2</sub> and Other Related Heavy Fermions** 321 - Adam Dioguardi, Los Alamos National Laboratory

**8:00AM R22.00001 Metamagnetism and Quantum Acoustic Oscillations in UPt<sub>3</sub>:**<sup>1</sup>, V. ULRICH, B SHIVARAM, Univ of Virginia — We present results of high resolution sound velocity measurements performed at the NHMFL, Tallahassee, in magnetic fields upto 33 T in a dilution refrigerator at temperatures down to 35 mK. For magnetic field parallel to the basal plane the observed quantum acoustic oscillations show a change in frequency as expected at the metamagnetic transition of 20 T. However, we find a similar abrupt change in frequency at 25 T for magnetic field parallel to the c-axis. The implications of this Fermi surface instability even though there is no metamagnetic transition in this orientation will be discussed.

<sup>1</sup>Work at the University of Virginia was supported through NSF DMR-0073456 and the NHMFL is supported by NSF and the State of Florida.

**8:12AM R22.00002 Antiferromagnetism and Hidden Order in Isoelectronic Doping of URu<sub>2</sub>Si<sub>2</sub>**, MURRAY WILSON, McMaster University, TRAVIS WILLIAMS, Oak Ridge National Laboratory, YIPENG CAI, ALANNAH HALLAS, TERESA MEDINA, TIMOTHY MUNSIE, McMaster University, SKY CHEUNG, LIAN LIU, BENJAMEN FRANDSEN, YASUTOMO UEMURA, Columbia University, GRAEME LUKE, McMaster University — URu<sub>2</sub>Si<sub>2</sub> has been studied for three decades to understand its unusual hidden order state. Doping of this compound on the Ru site usually causes the transition temperature to decrease and hidden order to transition to magnetic order. In contrast, the isoelectronic dopings Fe and Os cause a substantial increase in the transition temperature over a wide range of dopings, with Fe in particular mimicking applied hydrostatic pressure. However, until recently, the magnetic states of these dopings have not been well characterized. In the past year, neutron scattering results have been reported on Fe doping that show antiferromagnetism with moments that are twice as large as those measured for pure URu<sub>2</sub>Si<sub>2</sub> under pressure. In this talk we present an investigation of the magnetic properties of single crystal samples of URu<sub>2-x</sub>Fe<sub>x</sub>Si<sub>2</sub> and URu<sub>2-x</sub>Os<sub>x</sub>Si<sub>2</sub> by muon spin rotation ( $\mu$ SR) and susceptibility. Our  $\mu$ SR results demonstrate that both of these dopings show an antiferromagnetic ground state with internal fields comparable to pure URu<sub>2</sub>Si<sub>2</sub> under pressure. Interpretation of our data indicates that the evolution of magnetism with doping for both Fe and Os is driven by changes in hybridization.

**8:24AM R22.00003 Kondo bahavior in antiferromagnetic NpPdSn<sup>1</sup>**, K. SHRESTHA, Idaho National laboratory, K. PROKES, Helmholtz-Zentrum Berlin fr Materialien und Energie, Germany, J.-C. GRIVEAU, R. JARDIN, E. COLINEAU, R. CACIUFFO, R. ELOIRDI, European Commission, Institute for Transuranium Elements, Germany, K. GOFTRYK, Idaho National laboratory — Actinide-based intermetallics show a large variety of exotic physical phenomena mainly coming from 5f hybridization with both on-site and neighboring ligand states. Depending on the strength of these process unusual behaviors such as long-range magnetic order, Kondo effect, heavy-fermion ground state, valence fluctuations, and/or superconductivity have been observed. Here we report results of our extensive studies on NpPdSn. The compound crystalizes in hexagonal ZrNiAl-type of crystal structure and is studied by means of x-ray and neutron diffraction, magnetization, heat capacity, electrical resistivity, and thermoelectric power measurements, performed over a wide range of temperatures and applied magnetic fields. All the results revealed Kondo lattice behavior and antiferromagnetic ordering below 19 K. NpPdSn can be classified as a moderately enhanced heavy-fermion system, one of very few known amidst Np-based intermetallics.

<sup>1</sup>Work at Idaho National Laboratory was supported by the Department of Energy, Office of Basic Energy Sciences, Materials Sciences, and Engineering Division.

**8:36AM R22.00004 A Model for the Polar Kerr Effect in the Hidden-Order Phase of URu<sub>2</sub>Si<sub>2</sub>**, LANCE BOYER, VICTOR YAKOVENKO, Univ of Maryland-College Park — We propose an explanation for the recent experiment [1], where an optical polar Kerr effect (PKE) was observed in the otherwise non-magnetic hidden-order phase of URu<sub>2</sub>Si<sub>2</sub>. In this experiment, a sample was cooled through the hidden-order transition in a strong magnetic field, which was then turned off at low temperature, and the PKE was then observed and measured on warm-up in the absence of magnetic field. We propose an explanation within the framework of a previously developed Ginzburg-Landau theory [2] for a complex order parameter, whose real and imaginary parts correspond to the hidden-order and magnetic states. The former corresponds to the hexadecapole operator as seen in experiment [3], while the latter has ferromagnetic and antiferromagnetic components of z-axis magnetization in a bilayer of URu<sub>2</sub>Si<sub>2</sub>. Exploring the energy landscape for the three competing states, we find to a metastable ferromagnetic local minimum induced by an external magnetic field and preserved after the field has been turned off, which can explain the observed PKE.

[1] E. Schemm et al., PRB, 91, 140506 (2015)

[2] K. Haule and G. Kotliar, EPL, 89, 57006 (2010)

[3] H. Kung et al., Science, 347, 1259729 (2015)

**8:48AM R22.00005 <sup>31</sup>P NMR Study of of URu<sub>2</sub>Si<sub>2-x</sub>P<sub>x</sub>**, KENT SHIRER, Univ of California - Davis, ANDREW GALLAGHER, RYAN BAUMBACH, National High Magnetic Field Laboratory, NICHOLAS CURRO, Univ of California - Davis — We report initial <sup>31</sup>P nuclear magnetic resonance measurements in single crystals of URu<sub>2</sub>Si<sub>2-x</sub>P<sub>x</sub> in the antiferromagnetic and paramagnetic phases. We compare these results with the undoped compound both at ambient pressure and under pressure.

**9:00AM R22.00006 Lifshitz transition in high magnetic fields in UPt<sub>2</sub>Si<sub>2</sub>: Magnetoresistivity, Hall effect, magnetostriction and Fermi surface**, S. SULLOW, D. SCHULZE GRACHTRUP, N. STEINKI, Institute of Physics of Condensed Matter, TU Braunschweig, D-38106 Braunschweig, Germany, Z. CAKIR, G. ZWICKNAGL, Institute of Mathematical Physics, TU Braunschweig, D-38106 Braunschweig, Germany, I. SHEIKIN, Laboratoire National des Champs Magnetiques Intenses, F-38042 Grenoble, France, M. JAIME, National High Magnetic Field Laboratory, Los Alamos National Lab., Los Alamos, NM, USA, J. A. MYDOSH, Kamerlingh Onnes Laboratory, Leiden University, 2300RA Leiden, The Netherlands — We have measured the magnetoresistivity and Hall effect of single crystalline UPt<sub>2</sub>Si<sub>2</sub> in DC magnetic fields up to 35 T at temperatures down to 50 mK. Moreover, we have carried out magnetostriction measurements in pulsed magnetic fields up to 55 T for temperatures down to 1.5 K. For the magnetic field applied along the *c* axis we observe strong changes in the Hall effect at the previously established field induced phase boundaries AFM I ↔ III and III ↔ V (see Ref. [1]). From a detailed analysis of the Hall effect, we find evidence for topological changes of the Fermi surface due to at least one Lifshitz transition. Furthermore, in the magnetoresistivity and magnetostriction data we find a distinct history dependent anomaly within phase III, indicative of a first order phase transition. We relate our findings to band structure calculations carried out under consideration of the concept of a dual nature of the uranium 5f electrons with different degrees of localization.

[1] D. Schulze Grachtrup et al., Phys. Rev. B **85** (2012) 054410

**9:12AM R22.00007 Raman scattering study on the hidden order and antiferromagnetic phases in URu<sub>2-x</sub>Fe<sub>x</sub>Si<sub>2</sub><sup>1</sup>**, HSIANG-HSI KUNG, Rutgers University, SHENG RAN, NORAVEE KANCHANAVATEE, University of California San Diego, ALEXANDER LEE, VIKTOR KRAPIVIN, KRISTJAN HAULE, Rutgers University, M. BRIAN MAPLE, University of California San Diego, GIRSH BLUMBERG, Rutgers University — The heavy fermion compound URu<sub>2</sub>Si<sub>2</sub> possesses an unusual ground state known as the “hidden order” (HO) phase below *T* = 17.5 K, which evolves into an large moment antiferromagnetic (LMAFM) phase under pressure. A recent Raman scattering study shows that an *A*<sub>2g</sub> symmetry (*D*<sub>4h</sub>) in-gap mode emerges in the HO phase, characterizing the excitation from a chirality density wave<sup>2</sup>. Here, we report Raman scattering results for single crystal URu<sub>2-x</sub>Fe<sub>x</sub>Si<sub>2</sub> with *x* ≤ 0.2, where the Fe substitution acts as chemical pressure, shifting the system’s ground state from HO to LMAFM. We found that the *A*<sub>2g</sub> mode softens with doping, vanishes at the HO and LMAFM phase boundary, then re-emerges and hardens with doping in the LMAFM phase. The relations between the *A*<sub>2g</sub> mode energy and the strength of the HO/LMAFM order parameters will be discussed in this talk.

<sup>1</sup>GB and HHK acknowledge support from DOE BES Award DE-SC0005463. AL and VK acknowledge NSF Award DMR-1104884. KH acknowledges NSF Award DMR-1405303. MBM, SR and NK acknowledge DOE BES Award DE-FG02-04ER46105 and NSF Award DMR 1206553.

<sup>2</sup>H. Kung, R.E. Baumbach, E.D. Bauer, V.K. Thorsmolle, W. Zhang, K. Haule, J.A. Mydosh and G. Blumberg *Science* **347**, 1339 (2015)

**9:24AM R22.00008 Hidden order to antiferromagnetic transition in URu<sub>2</sub>Si<sub>2</sub>**, JESSE HALL, MAHSA RAHIMI MOVASSAGH, MURRAY WILSON, GRAEME LUKE<sup>1</sup>, McMaster University, NORAVEE KANCHANAVATEE, KEVIN HUANG<sup>2</sup>, MARC JANOSCHEK<sup>3</sup>, M. BRIAN MAPLE, University of California San Diego, TOM TIMUSK<sup>4</sup>, McMaster University — The second-order phase transition in the heavy fermion compound URu<sub>2</sub>Si<sub>2</sub> continues to confound efforts to reveal its true nature, and bears the moniker “hidden order” with good reason. While the order parameter remains mysterious, antiferromagnetism is easily induced with modest chemical substitution. The proximity of these two phases offers tantalizing clues about the nature of the hidden order phase. We present data on the antiferromagnetic phase, revealing the similarities and the differences between the two phases, including evidence for effects above the transition temperature. The implications of these findings for the hidden order parameter will be discussed.

<sup>1</sup>Alternate affiliation: Canadian Institute for Advanced Research

<sup>2</sup>Present address: State Key Laboratory of Surface Physics, Department of Physics, Fudan University, Shanghai 200433, China

<sup>3</sup>Present address: MPA-CMMS, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

<sup>4</sup>Alternate affiliation: Canadian Institute for Advanced Research

**9:36AM R22.00009 Electronic tuning of URu<sub>2</sub>Si<sub>2</sub> through ligand site substitution (Si → Ga and P)**, R. E. BAUMBACH, A. GALLAGHER, K. W. CHEN, NHMFL-FSU, S. CARY, FSU - Dept Chem. And Biochem., F. KAMETANI, ASC-NHMFL-FSU, D. GRAF, NHMFL-FSU, T. ALBRECHT-SCHMITT, FSU - Dept Chem. And Biochem., S. C. RIGGS, A. SHEKHTER, NHMFL-FSU — Materials that straddle the boundary between itinerant and local electronic behavior are exemplary hosts for novel phenomena, including unconventional superconductivity, anomalous magnetism, non-Fermi liquid behavior, and exotic electronic phases. The 5f-electron intermetallic URu<sub>2</sub>Si<sub>2</sub> is a well-known example, exhibiting an exotic ordered state (“hidden order”) and unconventional superconductivity. In spite of intense experimental and theoretical interest, understanding of the origin of these phenomena remains elusive. We report a study of URu<sub>2</sub>Si<sub>2</sub> using the new tuning parameter, ligand site substitution Si → L (L = Ga and P). While phosphorous substitution quickly suppresses both hidden order and superconductivity, gallium substitution has a mild effect, illustrating the marked difference between electron- and hole-doping on the ligand site for the physics of this compound. In an effort to disentangle these phenomena, we performed electrical transport and thermodynamic measurements. Electrical transport measurements in high magnetic fields are particularly illuminating, and provide insight into the evolution of the anomalous magnetoresistance, Fermi surface topology, electronic effective masses, and *g*-factor anisotropy. We discuss trends in these quantities for electron- and hole-doping and their implications for unraveling the behavior of URu<sub>2</sub>Si<sub>2</sub>.

**9:48AM R22.00010 Thermal expansion measurements on Fe substituted URu<sub>2</sub>Si<sub>2</sub><sup>1</sup>**, SHENG RAN, CHRISTIAN WOLOWIEC, INHO JEON, NAVEEN POUSE, NORAVEE KANCHANAVATEE, KEVIN HUANG, M. BRIAN MAPLE, Department of Physics and Center for Advanced Nanoscience, University of California, San Diego, USA, TYLER DAPRON, MARK WILLIAMSEN, DAVID SNOW, DINESH MARTIEN, STEFANO SPAGNA, Quantum Design, Inc., San Diego, USA — The search for the order parameter of the hidden order (HO) phase in URu<sub>2</sub>Si<sub>2</sub> has attracted an enormous amount of attention for the past three decades. The small antiferromagnetic moment of only ~0.03  $\mu_B$ /U found in the HO phase is too small to account for the entropy of ~0.2Rln(2) derived from the second order mean field BCS-like specific heat anomaly associated with the HO transition that occurs below T<sub>0</sub> = 17.5 K. A first order transition from the HO phase to a large moment antiferromagnetic (LMAFM) phase occurs under pressure. We have recently demonstrated that tuning URu<sub>2</sub>Si<sub>2</sub> by substitution of Fe for Ru reproduces the temperature vs applied pressure phase diagram and offers an opportunity to study the HO and LMAFM phases at atmospheric pressure. Motivated by this observation, we performed thermal expansion measurements on URu<sub>2-x</sub>Fe<sub>x</sub>Si<sub>2</sub> single crystals for various values of x in both the HO and LMAFM regions of the phase diagram. Interesting preliminary results have emerged from these studies that shed light on the LMAFM phase and its relationship with the elusive HO phase.

<sup>1</sup>Research in UCSD is supported by US DOE BES under Grant No.DE-FG02-04-ER46105(materials synthesis and characterization) and US NSF under Grant No.DMR-1206553(low temperature measurements).

**10:00AM R22.00011 Magnetic excitations in URu<sub>2</sub>Si<sub>2</sub> paramagnetic and Hidden Order phases**, NICHOLAS BUTCH, NIST - Natl Inst of Stds & Tech, MICHAEL MANLEY, Oak Ridge National Laboratory, JASON JEFFRIES, Lawrence Livermore National Laboratory, MARC JANOSCHEK, Los Alamos National Laboratory, KEVIN HUANG, M. BRIAN MAPLE, UC San Diego, AYMAN SAID, BOGDAN LEU, Argonne National Laboratory, JEFFREY LYNN, NIST - Natl Inst of Stds & Tech — We have mapped the lattice and magnetic excitations in heavy fermion URu<sub>2</sub>Si<sub>2</sub> via inelastic neutron and x-ray scattering measurements in the Hidden Order and paramagnetic phases. The magnetic excitations and phonons always respect the zone edges of the paramagnetic phase, showing no signs of reduced spatial symmetry. Features of the magnetic and lattice excitation spectra are associated with effects due to electronic interactions. Our results are inconsistent with simple local order parameters and density waves, and place constraints on models invoking Brillouin zone folding of the magnetic excitations. Phys. Rev. B 91, 035128 (2015)

**10:12AM R22.00012 Spin fluctuations and hidden-order phases in Ce-based Kondo systems<sup>1</sup>**, D. S. INOSOV, P. Y. PORTNICHENKO, A. S. CAMERON, TU Dresden, Germany, S. PASCHEN, A. PROKOFIEV, Vienna Univ. of Technology, Austria, G. FRIEMEL, H. JANG, B. KEIMER, MPI for Solid State Research, Germany, V. B. FILIPOV, N. Y. SHITSEVALOVA, Institute for Problems of Materials Science, Ukraine, A. SCHNEIDEWIND, Juelich Center for Neutron Science, Germany, A. IVANOV, J. OLLIVIER, Institut Laue-Langevin, France, P. P. DEEN, European Spallation Source, Sweden, A. M. STRYDOM, University of Johannesburg, South Africa — Among heavy-fermion metals, both CeB<sub>6</sub> and Ce<sub>3</sub>Pd<sub>20</sub>Si<sub>6</sub> compounds exhibit a magnetically hidden ordered phase in their low-temperature phase diagram, which is attributed to the ordering of magnetic quadrupolar moments, known as the antiferroquadrupolar (AFQ) ordering. Using inelastic neutron scattering, we have investigated the spectrum of spin excitations in both systems. In the structurally simplest CeB<sub>6</sub>, it consists of several contributions including conventional spin waves that coexist with both ferro- and antiferromagnetic excitonic resonance-like modes. However, the structurally more complex Ce<sub>3</sub>Pd<sub>20</sub>Si<sub>6</sub> possesses a much simpler magnetic excitation spectrum with only a single contribution peaked around the AFQ wave vector. It remains quasielastic in the absence of an external magnetic field, but then develops into dispersive magnon modes whose band width scales linearly with the applied field. Furthermore, neutron diffraction measurements on the same sample at sub-Kelvin temperatures revealed diffuse magnetic scattering that can be associated with the hidden order parameter.

<sup>1</sup>Supported by DFG Grant No. IN 209/3-1

**10:24AM R22.00013 Evidence for ferroquadrupole order in YbRu<sub>2</sub>Ge<sub>2</sub> from x-ray diffraction and elastoresistivity measurements**, ELLIOTT ROSENBERG, JIUN-HAW CHU, IAN FISHER, Stanford University, JACOB RUFF, CHESS — YbRu<sub>2</sub>Ge<sub>2</sub> undergoes a non-magnetic phase transition at 10K, several Kelvin above a phase transition to a magnetically ordered state that is characterized by a unidirectional incommensurate spin density wave. Here, we show via high-resolution x-ray diffraction that the non-magnetic phase transition corresponds to a continuous tetragonal-to-orthorhombic structural phase transition. Elastoresistance measurements in the tetragonal state indicate a divergence of the quadrupolar strain susceptibility in the B<sub>1g</sub> symmetry channel, implying that the structural phase transition is driven by quadrupolar order.

**10:36AM R22.00014 Evolution of superconductivity and magnetism in La<sub>1-x</sub>Yb<sub>x</sub>Ru<sub>2</sub>P<sub>2</sub>**, CONNOR RONCAIOLI, HALYNA HODOVANETS, SHANTA SAHA, JOHNPIERRE PAGLIONE, University of Maryland — LaRu<sub>2</sub>P<sub>2</sub>, with a 4.1 K transition, is the first known pnictide-based superconductor. Sharing structural and electronic elements similar to those of the unconventional Fe-pnictide superconductors, it is of interest to investigate the parameter space in which a superconducting ground state survives. We present preliminary indications of more interesting magnetic behavior and structural tuning behavior when paramagnetic Yb is substituted for La in La<sub>1-x</sub>Yb<sub>x</sub>Ru<sub>2</sub>P<sub>2</sub>, and investigate potential heavy fermion behavior in the Yb end-member of this series.

**Thursday, March 17, 2016 8:00AM - 11:00AM –**  
**Session R23 DMP GERA DCMP: Thermoelectrics-Nanostructures** 322 - Matthew Grayson, Northwestern University

**8:00AM R23.00001 Thermoelectric properties of  $\text{Mg}_2(\text{Ge}, \text{Sn})$  solid solutions<sup>1</sup>**, JIFENG SUN, DAVID J. SINGH, University of Missouri — Intermetallic compounds  $\text{Mg}_2\text{X}$  ( $\text{X} = \text{Si}, \text{Ge}, \text{Sn}$ ) and their solid solutions have attracted much attention as they are composed of environmental friendly and naturally abundant constituent elements and can be promising thermoelectric materials at intermediate temperature range (500 K - 1000 K). The figure of merit (ZT) of n-type  $\text{Mg}_2\text{X}$  solid solutions can reach up to 1.5. However, the p-type materials have much lower ZT values up to 0.38. In this talk, we will present the evolution of the thermoelectric properties of  $\text{Mg}_2(\text{Ge}, \text{Sn})$  solid solutions with a typical composition of  $\text{Mg}_2\text{Ge}_{0.5}\text{Sn}_{0.5}$  using first principles calculations combining with the experimental data. The ZT was optimized with respect to both doping concentrations and operating temperatures. Importantly, at 500 K - 1000 K temperature range we find ZT values up to 2 are possible for optimized n-type material within  $10^{19} \text{ cm}^{-3}$  to  $10^{20} \text{ cm}^{-3}$  carrier concentrations. But the p-type counterparts show inferior performance with ZT values ranging from 0.2 to 0.7.

<sup>1</sup>Supported by DOE through the S3TEC Energy Frontier Research Center

**8:12AM R23.00002 Ab initio calculations of the vibrational and dielectric properties of  $\text{PbSnTe}$  alloys**, LUISA SCOLFARO, Texas State University, USA, A.R. REZENDE NETO, H.W. LEITE ALVES, Universidade Federal de Sao Joao del Rei, Brazil, J.E. PETERSEN, T.H. MYERS, Texas State University, USA, P.D. BORGES, Universidade Federal de Viosa, Brazil — Thermoelectric devices have promise in dealing with the challenges of the growing demand for alternative clean energy and Te-based materials well-known candidates for them. Recently [1], we have shown that the high values for the dielectric constant, together with anharmonic LA-TO coupling, reduces the lattice thermal conductivity and enhances the electronic conductivity in  $\text{PbTe}$ . Also, it was shown that by alloying this material with Se, the electronic conductivity of the alloys is also enhanced [2]. But, it is not clear if the same occurs when alloying with Sn. We show, in this work, our ab initio results for the vibrational and dielectric properties of  $\text{Pb}_{1-x}\text{Sn}_x\text{Te}$  alloys. The calculations were carried out by using the Density Functional Theory, and the alloys were described by both the Virtual Crystal Approximation and Cluster Expansion Method. Our results show that the anharmonic LA-TO coupling enhances and reach its maximum for Sn concentration values of 0.75, corresponding to the maximum value for the dielectric constant, which is higher than that obtained for  $\text{PbTe}$ . [1] H. W. Leite Alves, et al., Phys. Rev. B87, 115204 (2013). [2] Y. Pei, et al., Nature 473, 66 (2011).

**8:24AM R23.00003 Band Degeneracy, Low Thermal Conductivity, and High Thermoelectric Figure of Merit in  $\text{SnTe-CaTe}$  Alloys**, R. AL RAHAL AL ORABI, Department of Environmental Science and Engineering, Ewha Womans University, N. MECHOLSKY, Department of Physics and Vitreous State Laboratory, The Catholic University of America, J. P. HWANG, W. KIM, School of Mechanical Engineering, Yonsei University, J. S. RHYEE, Department of Applied Physics, College of Applied Science, Kyung Hee University, D. WEE, Department of Environmental Science and Engineering, Ewha Womans University, M. FORNARI, 5Department of Physics, Central Michigan University and Science of Advanced Materials Program — Pure lead-free  $\text{SnTe}$  has limited thermoelectric potentials because of the low Seebeck coefficients and the relatively large thermal conductivity. In this study, we provide experimental evidence and theoretical understanding that alloying  $\text{SnTe}$  with  $\text{Ca}$  greatly improves the transport properties leading to ZT of 1.35 at 873 K, the highest ZT value so far reported for singly doped  $\text{SnTe}$  materials. The introduction of  $\text{Ca}$  (0-9%) in  $\text{SnTe}$  induces multiple effects: (1)  $\text{Ca}$  replaces  $\text{Sn}$  and reduces the hole concentration due to  $\text{Sn}$  vacancies, (2) the energy gap increases limiting the bipolar transport, (3) several bands with larger effective masses become active in transport, and (4) the lattice thermal conductivity is reduced of about 70% due to the contribution of concomitant scattering terms associated with the alloy disorder and the presence of nanoscale precipitates. An efficiency of 10% (for  $\Delta T = 400 \text{ K}$ ) was predicted for high temperature thermoelectric power generation using  $\text{SnTe}$ -based n- and p-type materials.

**8:36AM R23.00004 Mode resolved modeling of phonon-structure interactions in semiconductor nanocomposites**, JOSEPH FESER, University of Delaware — Introducing nanoscale inhomogeneities into semiconductor alloys is a known route to enhance the scattering of long wavelength phonons and to subsequently reduce thermal conductivity. For key applications such as thermoelectric energy conversion materials, this must be done efficiently to avoid harming electronic functionality. Thus, key questions arise such as what type (i.e. contrast mechanisms), shape, size, and number density of particles should be used. This talk presents two new theoretical developments in this area from our group: (1) The use of continuum mechanics to analytically calculate exact phonon scattering cross sections of cylindrical and spherical shaped elastic discontinuities across the Mie regime, and their subsequent use in Boltzmann transport models of thermal transport and (2) the development of a new frequency-domain atomistic approach to simulate the scattering cross section of nanoparticles of arbitrary complexity for wavevectors spanning the entire Brillouin zone, and which can accommodate very large atomistic systems. Its advantages compared to Atomistic Green's functions and molecular dynamics will be discussed.

**9:12AM R23.00005 Thermal Conductivity of Nanocrystalline Silicon Prepared by Plasma-Enhanced Chemical-Vapor Deposition<sup>1</sup>**, BATTOGTOKH JUGDERSUREN, Sotera Defense Solutions, XIAO LIU, Naval Research Laboratory, BRIAN KEARNEY, DANIEL QUEEN, Natl Research Council, THOMAS METCALF, JAMES CULBERTSON, CHRISTOPHER CHERVIN, Naval Research Laboratory, MICHAEL KATZ, Natl Research Council, RHONDA STROUD, Naval Research Laboratory — Nanocrystallization by ball milling has been used successfully to reduce the thermal conductivity of silicon-germanium alloys ( $\text{SiGe}$ ) and turn them into useful thermoelectric materials at a temperature of a few hundred degrees C. Currently the smallest grain sizes in nanocrystalline  $\text{SiGe}$  are in the 10 nm range. Germanium is added to scatter short wavelength phonons by impurity scattering. In this work, we report a record low thermal conductivity in nanocrystalline silicon prepared by plasma-enhanced chemical-vapor deposition. By varying hydrogen to silane ratio, we can vary the average grain sizes from greater than 10 nm down to 3 nm, as determined by both the high resolution transmission electron microscopy and X-ray diffraction. The values of thermal conductivity, as measured by the  $3\omega$  technique, can be correspondingly modulated from that of ball-milled nanocrystalline  $\text{SiGe}$  to a record low level of 0.3 W/mK at room temperature. This low thermal conductivity is only about 1/3 of the minimum thermal conductivity limit of silicon. Possible causes of such a large reduction are discussed.

<sup>1</sup>Work supported by the Office of Naval Research

**9:24AM R23.00006 Thermal Investigations of Periodically Nanoporous Si Films — The Impact of Structure Sizes and Pore-Edge Amorphization**, DONGCHAO XU, HONGBO ZHAO, QING HAO, Department of Aerospace and Mechanical Engineering, University of Arizona — In recent years, nanoporous Si films have been intensively studied as promising thermoelectric materials, which mainly benefits from their dramatically reduced lattice thermal conductivity  $k_L$  and bulk-like electrical properties.<sup>1,2</sup> Despite many encouraging results, challenges still exist in the theoretical explanation of the observed low  $k_L$ .<sup>3</sup> Existing studies mainly attribute the low  $k_L$  to 1) phonon bandstructure modification by coherent phonon processes in a periodic structure (phononic effects), and/or 2) pore-edge defects. In this work, temperature-dependent  $k_L$  is measured for nanoporous Si films with different pore sizes and spacing to compare with model predictions. For systematic studies, two fabrication techniques are used to drill the nanopores: 1) reactive ion etching, and 2) a focus ion beam to introduce more pore-edge defects. The results from this work will provide guidance for phonon engineering in general materials with periodic interfaces or boundaries. References: 1. Tang et al., *Nano Letters* **10**, 4279-4283 (2010). 2. Yu et al., *Nature Nanotechnology* **5**, 718-721 (2010). 3. Cahill et al., *Applied Physics Reviews* **1**, 011305/1-45 (2014) Nanoscale thermal transport. II. 2003–2012.

**9:36AM R23.00007 Thermoelectric Power of Nanocrystalline Silicon Prepared by Hot-Wire Chemical-Vapor Deposition<sup>1</sup>**, BRIAN KEARNEY, Natl Research Council, XIAO LIU, Naval Research Laboratory, BATTOGTOKH JUGDER-SUREN, Sotera Defense Solutions Inc., DANIEL QUEEN, Natl Research Council, THOMAS METCALF, JAMES CULBERTSON, CHRISTOPHER CHERVIN, RHONDA STROUD, Naval Research Laboratory, WILLIAM NEMETH, QI WANG, National Renewable Energy Laboratory — Although doped bulk silicon possesses a favorable Seebeck coefficient and electrical conductivity, its thermal conductivity is too large for practical thermoelectric applications. Thin film nanocrystalline silicon prepared by hot-wire chemical-vapor deposition (HWCVD) is an established material used in multijunction amorphous silicon solar cells. Its potential in low cost and scalable thermoelectric applications depends on achieving a low thermal conductivity without sacrificing thermoelectric power and electrical conductivity. We examine the thermoelectric power of boron-doped HWCVD nanocrystalline silicon and find that it is comparable to doped nanostructured silicon alloys prepared by other methods. Given the low thermal conductivity and high electrical conductivity of these materials, they can achieve a high thermoelectric figure of merit, ZT.

<sup>1</sup>Work supported by the Office of Naval Research

**9:48AM R23.00008 Anharmonicity Rise the Thermal Conductivity in Amorphous Silicon<sup>1</sup>**, WEI LV, ASEGUN HENRY, Georgia Institute of Technology — We recently proposed a new method called Direct Green-Kubo Modal Analysis (GKMA) method, which has been shown to calculate the thermal conductivity (TC) of several amorphous materials accurately. A-F method has been widely used for amorphous materials. However, researchers have found out that it failed on several different materials. The missing component of A-F method is the harmonic approximation and considering only the interactions of modes with similar frequencies, which neglect interactions of modes with large frequency difference. On the contrary, GKMA method, which is based on molecular dynamics, intrinsically includes all types of phonon interactions. In GKMA method, each mode's TC comes from both mode self-correlations (autocorrelations) and mode-mode correlations (crosscorrelations). We have demonstrated that the GKMA predicted TC of a-Si from Tersoff potential is in excellent agreement with one of experimental results. In this work, we will present the GKMA applications on a-Si using multiple potentials and gives us more insight of the effect of anharmonicity on the TC of amorphous silicon.

<sup>1</sup>This research was supported Intel grant AGMT DTD 1-15-13 and computational resources by NSF supported XSEDE resources under allocations DMR130105 and TG- PHY130049

**10:00AM R23.00009 Designing SiGe superlattices and alloys for minimum thermal conductivity**, JIHUI NIE, PAWEL KEBLINSKI, Rensselaer Polytech Inst — We use equilibrium molecular dynamics simulations to study the thermal conductivity of SiGe alloys to design the structures for minimum thermal conductivity, which is desired, e.g., for better thermoelectric properties or thermal barriers coatings. We explore how a combination of layered/superlattice structures with a degree of random alloying is capable of effective scattering of both low frequency (long wavelength) and high frequency (short wavelength) phonons thus greatly reducing thermal conductivity. We will discuss strategies towards guided search for arrangements of alloy constituents that minimizes thermal conductivity.

**10:12AM R23.00010 Thermal Conductivity of Quantum Wires with Surface Roughness**, SELMAN HERSHFELD, KHANDKER MUTTALIB, Dept. of Physics, University of Florida — Quantum wires have been shown to have greatly reduced thermal conductivity compared to bulk systems because of the increased role of surface scattering. The lattice thermal conductance and conductivity is calculated in the harmonic approximation for a long quantum wire placed between two heat baths using the Landauer formula for phonons and a recursive Green function technique to compute the transmission probabilities. The width of the wires is varied in the transverse direction so as to have a root mean square value  $\sigma$  and correlation length  $L$ . As observed experimentally, we find that the thermal conductance is decreased with increasing  $\sigma$  and increased as  $L$  increases. The full scaling of the thermal conductance as a function of  $\sigma$ ,  $L$ , the width and the length of the sample is discussed. The simulations are also compared to approximate techniques such as modeling the surfaces as having diffusive scattering.

**10:24AM R23.00011 Probing the low thermal conductivity of single-crystalline porous Si nanowires**, YUNSHAN ZHAO, Natl Univ of Singapore, LINA YANG COLLABORATION, LINGYU KONG COLLABORATION, BAOWEN LI COLLABORATION, JOHN T L THONG COLLABORATION, KEDAR HIPPALGAONKAR COLLABORATION — Pore-like structures provide a novel way to reduce the thermal conductivity of silicon nanowires, compared to both smooth-surface VLS nanowires and rough EE nanowires. Because of enhanced phonon scattering with interface and decrease in phonon transport path, the porous nanostructures show reduction in thermal conductance by few orders of magnitude. It proves to be extremely challenging to evaluate porosity accurately in an experimental manner and further understand its effect on thermal transport. In this study, we use the newly developed electron-beam based micro-electrothermal device technique to study the porosity dependent thermal conductivity of mesoporous silicon nanowires that have single-crystalline scaffolding. Based on the Casino simulation, the power absorbed by the nanowire, coming from the loss of travelling electron energy, has a linear relationship with its cross section. The relationship has been verified experimentally as well. Monte Carlo simulation is carried out to theoretically predict the thermal conductivity of silicon nanowires with a specific value of porosity. These single-crystalline porous silicon nanowires show extremely low thermal conductivity, even below the amorphous limit. These structures together with our experimental techniques provide a particularly intriguing platform to understand the phonon transport in nanoscale and aid the performance improvement in future nanowires-based devices.

**10:36AM R23.00012 Effects of Ordered Stacking Faults on Electrical Transport Properties in Silicon Nanowires**, MARC COLLETTE, Concordia University, Montreal, OUSSAMA MOUTANABBIR, Ecole Polytechnique, Montreal, ALEXANDRE CHAMPAGNE, Concordia University, Montreal — Lattice defects in silicon nanowires (SiNWs) allow the exploration of the fundamental physics governing transport mechanisms. We study charge transport in SiNW transistors with stacking faults in the 3C sequence, producing local hexagonal ordering. This structure leads to polytype SiNWs with distinct properties for novel applications in thermoelectronics. Since charge carrier and phonon behavior depend on crystal structure, these planar defects affect the transport properties of the nanowire. We grow our SiNWs using a VLS method, with stacking faults induced during growth. Structural characterization of each SiNW is done with Raman spectroscopy to quantify hexagonality. Individual nanowires are located and contacted using different metals to understand the Schottky barrier of the contacts at the SiNWs. We suspend 2  $\mu\text{m}$ -long SiNW devices using a wet oxide etch to uncouple the SiNW from the substrate. We study the electrical properties by  $I$ - $V$  measurements across the FET device while modulating the applied back gate voltage. Our initial data show that the presence of stacking faults causes an increase in resistivity by two orders of magnitude, thus greatly hindering charge transport through the SiNW.

**10:48AM R23.00013 Electronic structures and related thermoelectric properties of  $\text{Pb}_7\text{Bi}_4\text{Se}_{13}$  using first principle calculations and Boltzmann transport theory**, MOHAMMED BENALI KANOUN, Al Faisal University, college of science — The electronic structure, optical and thermoelectric properties of  $\text{Pb}_7\text{Bi}_4\text{Se}_{13}$  have been investigated using a combination of Density functional theory and Boltzmann transport theory. We applied the generalized gradient approximation as exchange-correlation energy functional added to the Coulomb energy (U Hubbard term). The existence of Bi and Pb has required the spin-orbit coupling. The intensity data for  $\text{Pb}_7\text{Bi}_4\text{Se}_{13}$  were measured at 100 K and 300 K leading to consider  $\text{Pb}_7\text{Bi}_4\text{Se}_{13}$  in two phases. The valence band maximum emerges predominantly from Se- $p$  state with admixture of Bi- $p$  and Pb- $p$  states, while the conduction band minimum comes from Se- $d$  states. The optical absorption shows the possibility of smaller multiple direct and indirect inter-band transitions in the visible region. We computed Seebeck coefficient, electrical and thermal conductivities, figure of merit and power factor, as function of temperature using the Boltzmann transport theory.  $\text{Pb}_7\text{Bi}_4\text{Se}_{13}$  is a potential shielding material that can be used at visible and UV region for thermoelectric devices. The present results were validated by comparison with the available experimental measurements.

# Thursday, March 17, 2016 8:00AM - 11:00AM –

## Session R24 DCMF: Superfluid Helium 323 - Wei Guo, Maglab, Florida State University

### 8:00AM R24.00001 Textural domain walls in superfluid $^3\text{He-B}$ , TAKESHI MIZUSHIMA, Osaka University —

Owing to the richness of symmetry, the superfluid  $^3\text{He}$  serves as a rich repository of topological quantum phenomena. This includes the emergence of surface Majorana fermions and their quantum mass acquisition at the topological critical point.<sup>1</sup> Furthermore, the marriage of the prototype topological superfluid with nanofabrication techniques brings about a rich variety of spontaneous symmetry breaking, such as the formation of the stripe order and nontrivial domain walls. In this work, we examine the possible formation of textural domain walls in the superfluid  $^3\text{He-B}$  confined to a thin slab with a sub-micron thickness. When an applied magnetic field is much higher than the dipolar field, two nearly degenerate ground states appear, which are characterized by the Ising order associated with the spontaneous breaking of a magnetic order-two symmetry,  $\hat{\ell}_z = +1$  and  $-1$ . We here discuss the structure of the textural domain wall formed by the spatial modulation of the Ising order, such as low-lying quasiparticle excitations and spontaneous spin current. We also report bosonic modes bound to the textural domain wall.

<sup>1</sup>T. Mizushima *et al.* arXiv:1508.00787.

### 8:12AM R24.00002 Chiral pair density wave phase of confined $^3\text{He-A}$ film, HAO WU, Dept. Physics, Northwestern University, JAMES A SAULS, Dept. Physics & Astronomy, Northwestern University —

The edge states of a  $^3\text{He-A}$  film are Weyl Fermions propagating in a direction determined by the chirality of the bulk phase, which leads to a non-vanishing spontaneous mass current on the edge. We report calculations of the reduction in the edge mass currents due to hybridization as a function of lateral confinement,  $D$ . Strong lateral confinement leads to a sequence of quantum phase transitions. The A phase undergoes a transition to a pair density wave (PDW) phase with broken translational symmetry at  $D_{c2} \sim 13\xi_0$ , and a transition to a polar state at  $D_{c1} \sim 9\xi_0$ . The order parameter for  $D_{c1} < D$  is calculated self-consistently. The resulting phase is a periodic array of chiral domains with opposite chirality separated by domain walls. The mass currents on the domain walls contradict the direction of current on the edges, which leads to separation into multiple regions of circulating current in each domain. The periodicity of PDW phase increases as confinement length  $D$  increases and eventually only one domain is left in the lateral confined film when  $D$  approaches  $D_{c2}$ . We calculated and compared the free energy of the confined single domain wall and the homogeneous A phase, and determined the phase boundary  $D_{c2} - T$ .

### 8:24AM R24.00003 Equilibrium helical order in radially confined superfluid $^3\text{He}^1$ , JOSHUA WIMAN, J A SAULS, Northwestern University —

An exciting prediction of confined superfluid  $^3\text{He}$  is the presence of spontaneously broken translational symmetry, resulting in a superfluid phase that has a different translational symmetry than that of the confining geometry. Such phases have been described theoretically in films, cylinders, and ribbons. We predict an inhomogeneous superfluid phase with helical order that is energetically stable within cylindrical channels of radius comparable to the Cooper pair coherence length. By incorporating extensions to standard Ginzburg-Landau (GL) strong-coupling theory that accurately reproduce the bulk phase diagram at high pressures and allow tuneable boundary conditions<sup>2</sup>, we find this new phase to be stable at both high and low pressures and favored by boundary conditions with strong pairbreaking. We present superfluid phase diagrams as functions of pressure, temperature, and channel radius showing the regions of stability for this “spiral” phase relative to those phases previously predicted for the channel. Transverse NMR frequency shifts are a possible experimental signature of this phase, and we present calculations of these shifts as functions of rf pulse tipping angle, field orientation, and temperature.

<sup>1</sup>Supported by NSF Grant DMR-1508730.

<sup>2</sup>J. J. Wiman & J. A. Sauls, Phys. Rev. B 92, 144515 (2015)

### 8:36AM R24.00004 Order parameter texture transition in superfluid $^3\text{He-B}$ in strained aerogel<sup>1</sup>, A.M. ZIMMERMAN, Northwestern University, J.I.A. LI, Columbia University, W.P. HALPERIN, Northwestern University —

The introduction of anisotropic impurity scattering into superfluid  $^3\text{He}$  using high porosity silica aerogel has proven to be a fruitful method of engineering both the phase and the order parameter texture of the superfluid<sup>2,3</sup>. We have observed an abrupt transition between two orthogonal order parameter textures at a temperature  $T_x \approx 1.9$  mK, in  $^3\text{He-B}$  confined in aerogel samples with anisotropy induced by mechanical compression along an axis  $\vec{\epsilon}$ . At this transition the order parameter, characterized by the quantization axis of the orbital angular momentum  $\hat{l}$ , changes from a configuration with  $\hat{l} \parallel \vec{\epsilon}$  below  $T_x$  to  $\hat{l} \perp \vec{\epsilon}$  above  $T_x$ . This transition is independent of the orientation of  $\vec{\epsilon}$  relative to the external magnetic field, as well as the magnitude of the applied field. This indicates that the textural transition is due to strain alone, with the anisotropic scattering from the aerogel favoring different orientations of  $\hat{l}$  above and below  $T_x$ .

<sup>1</sup>Research was supported by the NSF DMR-1103625.

<sup>2</sup>J.I.A. Li *et al.*, Phys. Rev. Lett., **114**, 105302, (2015).

<sup>3</sup>J. Pollanen *et al.*, Phys. Rev. Lett., **107**, 235504, (2011).

### 8:48AM R24.00005 Phase diagram of a thin film of $^3\text{He}$ confined within a $1.08 \mu\text{m}$ deep cavity<sup>1</sup>, NIKOLAY ZHELEV, ABHILASH SEBASTIAN, ERIC SMITH, JEEVAK PARPIA, Cornell University —

We describe measurements of superfluid  $^3\text{He}$  confined to a high-aspect ratio cavity within the head of a high quality factor torsion pendulum. Superfluid phase diagram for the confined thin film of fluid is predicted to be radically different compared to that of the bulk. In particular, at low pressures at the onset of the A-B transition, a “stripe phase” of alternating degenerate domains of B phase is predicted to occur [1]. By tracking the torsion pendulum frequency and quality factor, we identify a well-defined superfluid transition for the fluid within the pendulum head. At lower temperatures, sharp transitions from the A phase to the B phase on cooling and a gradual transition from the B phase to the A phase on warming are observed. The values for the ratio of the cavity depth and the coherence length ( $D/\xi(T, P)$ ) at the transitions match well the values of the transitions seen in the NMR measurements of  $^3\text{He}$  confined to a 700 nm deep cavity [2]. At present, we do not see any evidence in our measurements that the “stripe phase” is realized at the A-B phase boundary.

[1] A.B. Vorontsov and J.A. Sauls, Phys. Rev. Lett. 98, 045301 (2007).

[2] L.V. Levitin, *et. al.*, Science 340, 841 (2013).

<sup>1</sup>We acknowledge support from NSF grant: DMR 1202991

## 9:00AM R24.00006 Dislocation motion in solid hcp $^3\text{He}$ <sup>1</sup>, JOHN BEAMISH, ZHI GANG CHENG, University of Alberta

— At temperatures above about 100 mK, dislocations reduce the shear modulus of hcp  $^4\text{He}$  by as much as 90%. This occurs when dislocations thermally unbind from the  $^3\text{He}$  impurities that pin them, becoming extraordinarily mobile. The elastic softening is accompanied by a thermally activated dissipation peak due to the  $^3\text{He}$  impurities. At higher temperatures the dissipation has an  $\omega T^4$  dependence caused by scattering of thermal phonons from moving dislocations. Previous measurements on the fermi solid, hcp  $^3\text{He}$ , showed a similar dislocation softening, but the corresponding dissipation was not measured. We have extended these measurements by measuring the temperature, amplitude and frequency dependence of both the shear modulus and the dissipation in hcp  $^3\text{He}$ . The dissipation behavior is very different from that of hcp  $^4\text{He}$ . Neither the impurity unbinding peak associated with the elastic softening, nor the high temperature phonon scattering dissipation, were observed. Instead, there is a large and non-thermally activated dissipation which is largest at low frequencies. We believe that this unexpected dissipation is associated with a new dislocation damping mechanism in  $^3\text{He}$ , perhaps associated with spin rearrangements caused by moving dislocations.

<sup>1</sup>This work was supported by a grant from NSERC Canada

## 9:12AM R24.00007 Symmetry breaking field in $\text{UPt}_3$ and connection to superfluid $^3\text{He}$ <sup>1</sup>, WILLIAM HALPERIN, northwestern university

— The multiple superconducting phases of  $\text{UPt}_3$  in its temperature-field phase diagram are a strong indication of its unconventional order parameter. It is generally accepted that such a complex phase diagram with 3 different vortex phases are nearly degenerate, and would be so, except for the presence of a symmetry breaking field attributed to antiferromagnetism which appears at a temperature an order of magnitude higher than the superconducting transition.[1] I propose an alternative mechanism where the symmetry breaking field can be, in large part, ascribed to anisotropic electronic scattering from stacking faults. The success of the theory[2] in accounting for stabilization of anisotropic phases of superfluid  $^3\text{He}$  in globally anisotropic aerogel[3] suggests a similar consequence from anisotropic quasiparticle scattering in  $\text{UPt}_3$ . Specific heat measurements indicate that the temperature window of the more anisotropic A-phase, a direct measure of the strength of the symmetry breaking field, decreases systematically with fewer stacking faults. [1] D.W. Hess *et al.*, J. Phys.: Condens. Matter 1, 8135 (1989). [2] E.V. Thuneberg *et al.*, Phys. Rev. Lett. 80, 2161 (1998). [3] J. Pollanen *et al.*, Nat. Phys. 8, 317 (2012).

<sup>1</sup>NSF DMR-1103625

## 9:24AM R24.00008 The Momentum Distribution of Liquid $^3\text{He}$ , Revisited<sup>1</sup>, PAUL SOKOL, MATTHEW BRYAN, Indiana Univ - Bloomington, TIMOTHY PRISK, Oak Ridge National Lab

— Liquid  $^3\text{He}$  is a system of fundamental importance to condensed matter physics because it is a prototypical example of a strongly interacting fermion system whose interactions are well known. Quantum Monte Carlo calculations predict that the atomic momentum distribution of liquid  $^3\text{He}$  contains a Fermi surface discontinuity and an average atomic kinetic energy in the range 12-13 K at saturated vapor pressure. A number of high-resolution neutron Compton scattering studies of liquid  $^3\text{He}$  have been described in the literature, with experimenters observing no Fermi surface discontinuity and obtaining kinetic energies in the range of 8-10 K. In this presentation, we reconsider measurements of the momentum distribution of liquid  $^3\text{He}$  taken at 500 mK under 0, 10, 15 bar of pressure [R.M. Dimeo *et al* Physica B 241-243, 952 (1998)]. We demonstrate that there is complete agreement between the experimental data and quantum Monte Carlo calculations when instrumental resolution and final state effect corrections are taken into account. We also consider the prospects for a direct observation of the Fermi surface discontinuity in liquid  $^3\text{He}$  using neutron Compton scattering.

<sup>1</sup>This research was supported by NSF award DGE-1069091.

## 9:36AM R24.00009 X-ray coherent diffractive imaging of quantum vortices in single helium droplets

, RICO MAYRO TANYAG, CHARLES BERNANDO, CURTIS JONES, LUIS GOMEZ, ANDREY VILESOV, University of Southern California, CAMILA BACELLAR, JAMES CRYAN, KATRIN SIEFERMANN, FELIX STURM, OLIVER GESSNER, Chemical Sciences Division, Lawrence Berkeley National Laboratory, KEN FERGUSON, SEBASTIAN CARRON, SEBASTIAN SCHORB, SLAC National Accelerator Laboratory, CHRISTOPH BOSTEDT, Argonne National Laboratory, LARS ENGLERT, Carl von Ossietzky University of Oldenburg, DENIS ANIELSKI, LUTZ FOUCAR, Max Planck Advanced Study Group at CFEL, JOACHIM ULLRICH, Physikalisch-Technische Bundesanstalt, DANIEL ROLLES, ARTEM RUDENKO, Kansas State University — Free, single, rotating superfluid  $^4\text{He}$  nanodroplets (diameter  $D = 200 - 2000$  nm, temperature  $T = 0.4$  K) containing a number of quantum vortices have been studied via ultrafast X-ray coherent diffraction imaging using a free electron laser. The droplets were doped with Xe atoms, which collect on the vortex cores and serve as a contrast agent. In order to obtain the instantaneous positions and shapes of the vortices from the diffraction images, a phase retrieval technique has been developed, which utilizes the droplet boundary as a physical support. The algorithm also uses the droplet's scattering phase as an input for the iterative phase reconstruction. The obtained reconstructions reveal a plethora of transient vortex configurations within the droplet. The details of the algorithm and the possible origin of the observed vortex configuration will be discussed.

## 9:48AM R24.00010 Investigation of Grid Turbulence in Superfluid $^4\text{He}$ with Improved Measurement Technique<sup>1</sup>, JIHEE YANG, GARY G. IHAS, University of Florida - Gainesville

— Quantum turbulence (QT), a tangle of quantized vorticity in a macroscopically correlated quantum fluid, can have many analogous aspects to classical turbulence. Understanding QT can give us insights into classical turbulence as well as fluids in general. We generate QT by pulling a grid through a  $4.6 \text{ cm} \times 4.6 \text{ cm}$  cross-section channel in superfluid  $^4\text{He}$ . Second sound, a temperature/entropy wave, is used to monitor vorticity,  $\omega$ . A resonant technique with high (3000) Q increases greatly the sensitivity of the measurement, but it requires a phase and amplitude locked tracking system which adheres to the resonant peak independent of frequency shifts. According to theories, the vorticity decays as  $\omega \sim t^{-11/10}$  or  $\omega \sim t^{-17/14}$  when the energy containing eddies are growing. When they saturate at the channel size, the vorticity begins decaying as  $\omega \sim t^{3/2}$ . These different decaying regions are examined in this large channel and compared to previous experiments that have been performed in  $1 \text{ cm}^2$  square channels<sup>2</sup>.

<sup>1</sup>US NSF DMR#1007937

<sup>2</sup>M. R. Smith, R. J. Donnelly, N. Goldenfeld, and W. F. Vinen, Phys. Rev. Lett. 71, 2583 (1993).; S. R. Stalp, Ph.D. dissertation, University of Oregon 1998.; L. Munday, Ph.D. dissertation, Lancaster University 2014.

**10:00AM R24.00011 Anomalous Elasticity of  $^4\text{He}$  Films at the Quantum Phase Transition**, KEIYA SHIRAHAMA, Keio University, DAISUKE TAKAHASHI, Ashikaga Institute of Technology, TAKAYUKI KOGURE, HITOMI YOSHIMURA, RAMA HIGASHINO, Keio University —  $^4\text{He}$  films on solid substrates exhibit a quantum phase transition between localized (nonsuperfluid) and superfluid states by changing coverage  $n$ . We have made torsional oscillator (TO) studies for  $^4\text{He}$  films adsorbed on nanoporous glasses. A TO with localized films showed an apparent "supersolid" behavior, an increase in TO frequency  $f$  with broad peak in  $Q^{-1}$ . Combining with FEM analyses for TO's with different designs, we conclude that the behavior results from the softening of adsorbed  $^4\text{He}$  films at high temperatures. The features in  $f$  and  $Q^{-1}$  are fitted well to a Debye-like activation with a distributed energy gap  $\Delta$ , so the elasticity is accounted by thermal excitation of localized atoms to an "extended" state. As the critical coverage  $n_c$  approaches the gap decreases to zero with a powerlaw  $\Delta \propto (n - n_c)^{1.2}$ . Assuming that the  $^4\text{He}$  chemical potential  $\mu(n)$  is located in the middle of the gap, we can estimate the elastic constant  $\kappa^{-1} = n^2 \partial \mu / \partial n$ . The elasticity agrees with shear moduli of  $^4\text{He}$  films obtained from the FEM analysis within factor of three. The energetics proposed from the elastic behavior naturally explains other properties of He films adsorbed on disordered substrates.

**10:12AM R24.00012 Superfluidity, Bose-Einstein condensation and dimensions of liquid  $^4\text{He}$  in nanopores**<sup>1</sup>, LEANDRA VRANJEŠ MARKIĆ, Faculty of Science, University of Split, HR-21000 Split, Croatia, EU, HENRY GLYDE, Department of Physics and Astronomy, University of Delaware, Newark, Delaware 19716-2593, USA — Path integral Monte Carlo (PIMC) calculations of the superfluid fraction,  $\rho_S/\rho$ , and the one-body density matrix (OBDM) (Bose-Einstein condensation (BEC)) of liquid  $^4\text{He}$  confined in nanopores are presented. The goal is to determine the effective dimensions of the liquid in the nanopore. We simulate a cylinder of liquid of diameter  $d_L$  surrounded by 5 Å of inert solid  $^4\text{He}$  in a nanopore of diameter  $d$ ;  $d = d_L + 10$  Å [1]. The PIMC  $\rho_S(T)/\rho$  and OBDM scales as a 1D Luttinger Liquid at extremely small liquid pore diameters only,  $d_L = 6$  Å where the liquid atoms form a 1D line at the center of the pore. In the range  $8 \leq d_L \leq 22$  Å the PIMC  $\rho_S(T)/\rho$  scales as a 2D liquid. In this  $d_L$  range the liquid fills the pores in cylindrical layers. There is a cross over from 2D to 3D scaling at larger  $d_L \simeq 22$  Å. In the range  $8 \leq d_L \leq 22$  Å, the  $T_C$  predicted using the Kosterlitz-Thouless 2D scaling criterion of the OBDM agrees well with the  $T_C$  obtained from  $\rho_S(T)/\rho$ . Superflow observed in pores of diameter (18 <  $d$  < 32 Å) is apparently standard static superflow with the low  $T_C$  arising from its 2D character.

1. L. Vranješ Markić and H. R. Glyde, Phys. Rev. B92, 064510 (2015)

<sup>1</sup>Supported by Office of Basic Energy Sciences, USDOE, ER46680

**10:24AM R24.00013 Dissipation in Nanoscale Superfluids**, ADRIAN DEL MAESTRO, University of Vermont, BERND ROSENOW, University of Leipzig — Pressure driven flow of a superfluid inside a narrow channel can be maintained by the nucleation of vortices and their resulting motion across the flow lines. The maximum velocity of the superfluid is set by a nucleation rate which crucially depends on the microscopic details of the vortices and flow profile. Within the kinetic vortex theory, we have determined the critical superfluid velocity inside a nanoscale constriction and obtain agreement with experimental results for superfluid helium-4 in nanopores. In the small pore limit, when the ratio of pore radius to correlation length is of order unity, we find a drastic suppression of the superfluid velocity that can be understood within the Langer-Ambegaokar-McCumber-Halperin theory of resistive fluctuations in thin superconducting wires.

**10:36AM R24.00014 High-Resolution Measurements of the Roton Lifetime in Nano-Confinement**<sup>1</sup>, MATTHEW BRYAN, Indiana University - Bloomington, TIMOTHY PRISK, SOULEYMANE DIALLO, EUGENE MAMONTOV, Oak Ridge National Lab, PAUL SOKOL, Indiana University - Bloomington — At very low temperatures, the phonon-roton spectrum of bulk superfluid helium is sharp and well-defined in energy. As the temperature is increased, the roton energy gap becomes smaller and the roton peak acquires a finite linewidth. The conventional understanding of this effect is that roton-roton scattering drives the softening and broadening of the roton mode where the mean free path is governed by the thermal population of rotons. It is an open question whether the roton mode follows the same behavior when the liquid is confined within sufficiently small mesopores. It is possible that the restricted geometry introduces a new length scale which controls the roton mean free path at low temperatures. We report high-resolution (4  $\mu\text{eV}$ ) measurements of the roton energy and linewidth within tubular, silica nanopores 2.8 nm in diameter. The new results provide a critical test of the idea that tight, nanoscale confinement modifies the energy and linewidth of the roton excitation.

<sup>1</sup>This research was supported by NSF award DGE-1069091 and the experiment at ORNLs Spallation Neutron Source was sponsored by the U.S. Department of Energy.

**10:48AM R24.00015 Pressure driven flow studies of superfluid helium-4 through single, high aspect ratio nanopipes**, JEFFREY BOTIMER, PETER TABOREK, Univ of California - Irvine — We have measured flow rates of helium-4 through high aspect ratio (>10,000) single glass nanopipes and etched nanopores under the influence of a pressure drop. The initial diameter of the glass pipes is 200nm while the initial diameter of the nanopores is approximately 80nm; the diameter of both types of nanopipe were reduced using atomic layer deposition(ALD) of Al<sub>2</sub>O<sub>3</sub>. Flow rates were measured for a wide range of temperatures (0.8K to 3.0K), pressures (up to 40 atm), and pipe lengths (0.8 mm to 30 mm). We observed flow velocities in the range of 1-6 m/s which has a power law dependence on pressure. Flow appears to be governed by turbulence at low temperatures. We have found evidence for a critical pressure above which turbulent flow is eliminated. This critical pressure appears to depend on temperature.

**Thursday, March 17, 2016 8:00AM - 10:48AM —**

**Session R25 DCMP: Superconductivity: Less Common Materials I** 324 - Harald Jeschke, Goethe-Universitt Frankfurt

**8:00AM R25.00001 Spin triplet superconductivity in a weak-coupling Hubbard model for the quasi-one-dimensional compound Li<sub>0.9</sub>Mo<sub>6</sub>O<sub>17</sub>**, CHRISTIAN PLATT, WEEJEE CHO, Department of Physics, Stanford University, ROSS H. MCKENZIE, School of Mathematics and Physics, University of Queensland, SRI RAGHU, Department of Physics, Stanford University — The purple bronze Li<sub>0.9</sub>Mo<sub>6</sub>O<sub>17</sub> is of interest due to its quasi-one-dimensional electronic structure and the possible Luttinger liquid behavior resulting from it. For sufficiently low temperatures, it is a superconductor with a pairing symmetry that is still to be determined. To shed light on this issue, we analyze a minimal Hubbard model for this material involving four Molybdenum orbitals per unit cell near quarter filling, using asymptotically exact perturbative renormalization group methods. We find that spin triplet odd-parity superconductivity is the dominant instability. Approximate nesting properties of the two quasi-one-dimensional Fermi surfaces enhance certain second-order processes, which play crucial roles in determining the structure of the pairing gap. Notably, we find that the gap has accidental nodes, i.e. it has more sign changes than required by the point-group symmetry.

**8:12AM R25.00002 Geometrical structures and electronic properties of Sm, K-doped chrysene**, XIAOHUI WANG, Beijing CSRC, SIMULATIONS OF PHYSICAL SYSTEM DIVISION TEAM — The discovery of superconductivity in potassium-doped picene (KxC<sub>22</sub>H<sub>14</sub>) has revitalized the research interest in polycyclic aromatic hydrocarbons (PAHs), and a large variety of PAHs superconductors have been reported afterwards, such as phenanthrene, coronene and 1,2,8, 9-dibenzopentacene. Recently a new PAHs superconductor, Sm-doped chrysene, with T<sub>c</sub> = 5 K was reported experimentally whose precise nature is still unknown. In this work, crystal structure search and electronic structure of A-doped chrysene, Ax-C<sub>18</sub>H<sub>12</sub> (A=Sm, K), have been studied by the first-principles density-functional theory using the projector augmented wave method based on the generalized gradient approximation implemented in the VASP package. We also include with van der Waals (vdW) corrections in the calculations, thus clarifying the dopant atoms positions and optimized crystal structures of doped superconducting chrysene. Our findings represent a significant step toward the understanding of superconductivity of PAHs.

**8:24AM R25.00003 Coulomb-induced pairing in a quarter-filled band model for  $\kappa$ -(BEDT-TTF)<sub>2</sub>X<sup>1</sup>**, W. WASANTHI DE SILVA, Mississippi State Univ, NILADRI GOMES, SUMIT MAZUMDAR, Univ of Arizona, R. TORSTEN CLAY, Mississippi State Univ —  $\kappa$ -(BEDT-TTF)<sub>2</sub>X is a two dimensional organic charge transfer solid superconductor with a hole density of one half per (BEDT-TTF) molecule. With one hole per dimer of molecules, the material is frequently described using an effective 1/2-filled band Hubbard model on an anisotropic triangular lattice. Within this effective model a metal to antiferromagnetic (AFM) semiconductor phase transition is found. Calculations beyond the mean field level, however, have shown absence of superconductivity within the model. We present the results of correlated-electron calculations on the  $\kappa$ -lattice for up to 64 BEDT-TTF molecules using the Constrained Path Monte Carlo (CPMC) and Path Integral Renormalization Group (PIRG) methods over a wide range of carrier density. We show that superconducting pair-pair correlations in this model are enhanced by electron-electron (e-e) interactions for d-wave pairing symmetry uniquely for hole density close to quarter-filling. Our results indicate that this enhancement of superconductivity is not related to the presence of AFM order, but to the strong tendency to spin-singlet formation in the quarter-filled band.

<sup>1</sup>Supported by DOE Grant DE-FG02-06ER46315 and NSF-CHE-151475

**8:36AM R25.00004 Quarter-filled systems with frustration: Candidate for correlated electron superconductivity<sup>1</sup>**, NILADRI GOMES, Univ of Arizona, W. WASANTHI DE SILVA, Mississippi State Univ, TIRTHANKAR DUTTA, Univ of Arizona, R. TORSTEN CLAY, Mississippi State Univ, SUMIT MAZUMDAR, Univ of Arizona — A necessary condition for superconductivity (SC) driven by electron correlation is that electron electron (e-e) interactions enhance superconducting pair-pair correlations, relative to the non-interacting limit. We present the results of high-precision calculations of superconducting pair-pair correlations on four different frustrated lattices over the complete range of carrier density  $0 < \rho < 1$  in each case. We find that pair correlations are enhanced relative to the noninteracting limit only for density  $\rho$  equal to or close to 0.5 (1/4 filling). At all other  $\rho$  pair correlations are suppressed by interactions. This enhancement is due to the proximity to a spin-gapped paired-electron crystal (PEC) state that occurs at  $\rho = 0.5$ . Our theory explains the pseudogap observed at high temperatures in many organic superconductors. The remarkable bandfilling specificity is an essential ingredient to understanding the mechanism of superconductivity in the two-dimensional organic charge-transfer solids as well as the many different families of other unconventional superconductors that share this bandfilling.

<sup>1</sup>Supported by DOE Grant DE-FG02-06ER46315 and NSF-CHE-151475

**8:48AM R25.00005 Quantum critical origin of the superconducting dome and the isotope effect in SrTiO<sub>3</sub><sup>1</sup>**, YARON KEDEM, JONATHAN EDGE, NORDITA, ULRICH ASCHAUER, NICOLA SPALDIN, ETH Zurich, ALEXANDER BALATSKY, NORDITA, Los Alamos National Laboratory — We expand the notion that quantum criticality can induce superconductivity, by proposing a concrete mechanism for superconductivity due to quantum ferroelectric fluctuations. To this end, we investigate the origin of superconductivity in doped SrTiO<sub>3</sub> (STO) using a combination of density functional and strong coupling theories within the framework of quantum criticality. Our density functional calculations of the ferroelectric soft mode frequency as a function of doping reveal a crossover related to quantum paraelectricity at a doping level coincident with the experimentally observed top of the superconducting dome. Thus, we suggest a model in which the soft mode fluctuations provide the pairing interaction for superconductivity carriers. Within our model, the low doping limit of the superconducting dome is explained by the emergence of the Fermi surface, and the high doping limit by departure from the quantum critical regime. This results in a prediction that the highest critical temperature will increase and shift to lower carrier doping with increasing <sup>18</sup>O isotope substitution, a scenario that is experimentally verifiable. In addition we show a connection between the isotope exponent of superconductivity and the critical exponent pertaining to quantum phase transition.

<sup>1</sup>This work was supported by US DOE BES E304, by the ETH Zürich (NAS and UA) and by the ERC Advanced Grant Program, No. 291151 (NAS and UA), No321031, KAW and LDRD (YK).

**9:00AM R25.00006 Structure and magnetism of oxygen-deficient SrTiO<sub>3</sub> surface**, SOHAM GHOSH, EFSTRATIOS MANOUSAKIS, Florida State Univ — Using density functional theory within a fully relaxed spin generalized gradient approximation we have investigated the structural, electronic and magnetic properties of the oxygen-deficient STO surface. We also study the role of the Rashba interaction to explain the observed momentum-spin correlations by spin and angle resolved photoemission spectroscopy.

**9:12AM R25.00007 Screening of the electron-phonon interaction in STO**, ALEXANDER EDELMAN, PETER LITTLEWOOD, Univ of Chicago — Strontium titanate is a bulk insulator that becomes superconducting at remarkably low carrier densities. Even more enigmatic properties become apparent at the strontium titanate/lanthanum aluminate (STO/LAO) interface and it is important to disentangle the effects of reduced dimensionality from the poorly-understood pairing mechanism. Recent experiments<sup>1</sup> measuring the electronic structure of the analogous strontium titanate surface have found a cross-over as a function of carrier density from a series well-resolved phonon replica bands to a single quasiparticle dispersion, with the crossover occurring at densities that correspond to the disappearance of superconductivity in the STO/LAO system. We interpret these results in a simple analytical model that extends an Engelsberg-Schrieffer theory of electrons coupled to a single longitudinal optic phonon mode to include the effects of electronic screening. As the carrier density increases, the effective dielectric function cuts off the long-range phonon interaction beyond the Thomas-Fermi screening length, eventually leaving only a uniform short-range coupling to the phonon bath. We additionally incorporate the effects of carrier density on the static dielectric properties of the interface.

<sup>1</sup>Z. Wang et al, arXiv:1506.01191

**9:24AM R25.00008 A DFT study of electron-phonon mediated superconductivity in doped Mott-Hubbard proxy cubic-tetragonal copper monoxide**, PAUL GRANT, W2AGZ Technologies — We report our preliminary study of electron-phonon mediated Cooper pairing as a component underlying high temperature superconductivity, in the presence of a Hubbard U driven antiferromagnetic ground state, subject to itinerant carrier doping, in the copper oxide perovskites. Our model is based on a proxy CuO fcc cubic-tetragonal structure that contains the basic physics of the electronic structure of copper oxide perovskites readily amenable to numerical analysis. We explore its phase diagram as a function of carrier concentration and coulomb repulsion ranging from the pure Mott-Hubbard AF insulating state to that of a metallic Fermi liquid, focusing on those conditions which might manifest high temperature superconducting behavior. In the Fermi liquid state, we find clear evidence that superconductivity arises from Jahn-Teller instabilities in the CuO bond which guided Bednorz and Mueller on the path to their 1986 discovery.

**9:36AM R25.00009 The effect of pressure and doping on SrPt<sub>3</sub>P superconductor: First-principles calculations.**, ARMINDO S. CUAMBA, HONG-YAN LU, CHIN S. TING, Univ of Houston, ARMINDO S. CUAMBA, HONG-YAN LU, C.S. TING TEAM — Recently, experiments of resistivity and magnetization on SrPt<sub>3</sub>P under pressure and doping have been conducted by B. Jawdat et al., (Phys.RevB.91,094514(2015)), it was found that with the increase of pressure, the superconducting transition temperature T<sub>c</sub> first increases with the maximal at 0.99 Gpa and then decreases, while the Si doping suppress T<sub>c</sub>. In this work, we investigate the electronic and phonon properties of SrPt<sub>3</sub>P under pressure and partial replacement of P by Si, using first-principles method. When pressure increases from 0 to 0.7 Gpa the electron phonon coupling and T<sub>c</sub> increases, the calculated T<sub>c</sub> agrees with the experiments. For the doped case, SrPt<sub>3</sub>P<sub>0.5</sub>Si<sub>0.5</sub>, an additional hole pocket around M point in Brillouin zone is formed, almost all the phonon modes shifts into lower energy, and the density of states at the Fermi level decreases, which may explains the drop in T<sub>c</sub> observed experimentally.

**9:48AM R25.00010 Real-time study of light-enhanced superconductivity**, MICHAEL SENTEF, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, ALEXANDER KEMPER, North Carolina State University, ANTOINE GEORGES, Ecole Polytechnique and College de France, Paris, CORINNA KOLLATH, HISKP, University of Bonn — Resonant pumping of IR-active phonons with lasers enables the ultrafast control of the crystal lattice in solids [1]. It has been shown that transient states with significantly modified electronic properties can be created on picosecond time scales, such as a light-induced state at elevated temperatures with optical properties in close resemblance to those of a superconductor [2]. In our work, we investigate theoretically a situation in which a change of the electronic hopping leads to a modified density of states in real time [3]. This modification, together with electron-phonon coupling, enhances superconductivity if the system is at thermal equilibrium. Our study monitors the out-of-equilibrium time evolution of the electronic momentum distribution and the superconducting order parameter. We show that the condensate dynamics dominates the initial enhancement of superconducting order, and that energy dissipation through electron-phonon scattering helps this enhancement. [1] M. Frst et al., Nature Phys. 7, 854 (2011) [2] M. Mitrano et al., arXiv:1505.04529 [3] M. A. Sentef et al., arXiv:1505.07575

**10:00AM R25.00011 Ising Superconductivity and Majorana Fermions in Transition Metal Dichalcogenides**, TONG ZHOU, HONG-LIANG JIANG, NOAH, FANQI YUAN, KAM TUEN LAW, Physics Department, the Hong Kong University of Science and Technology — In monolayer transition metal dichalcogenides (TMDs), electrons in opposite K valleys are subject to opposite effective Zeeman fields, which are referred to as Ising spin-orbit coupling (SOC) fields. The Ising SOC, originated from in-plane mirror symmetry breaking, pins the electron spins in out-of-plane directions, and results in the newly discovered Ising superconducting states with strongly enhanced upper critical fields. In this work, we show that the Ising SOC generates equal-spin triplet Cooper pairs with spin polarization in the in-plane directions. Importantly, the spin-triplet Cooper pairs can induce superconducting pairings in a half-metal wire placed on top of the TMD and result in a topological superconductor with Majorana end states. Direct ways to detect equal-spin triplet Cooper pairs and the differences between Ising superconductors and Rashba superconductors are discussed.

**10:12AM R25.00012 A DMRG Study of MoS<sub>2</sub>**, JORDAN VENDERLEY, Cornell University — In a recent work, Hsu, Vaezi, and Kim predicted spatially modulated, topological superconductivity in a class of materials known as transition metal dichalcogenides (TMDs) by studying RG flow.<sup>1</sup> Since electrons can readily develop topological superconductivity at low temperatures when spin-degeneracy is lifted, their insight was to exploit the spin-splitting of the TMD valance band in k-space in order to induce p-wave pairing. With experimental efforts currently underway to realize this phenomenon, particularly in monolayer, hole-doped MoS<sub>2</sub>, it is important to have a non-perturbative check on this result. To this end, we employ a density matrix renormalization group (DMRG) approach to study MoS<sub>2</sub>. We probe the superconducting susceptibility of the system and explore the properties of its order parameter in order to confirm the predicted FF (Fulde-Ferrell) p<sub>x</sub>+ip<sub>y</sub> phase. A quantitative understanding of the Hamiltonian parameters will provide guidance in experimental efforts to realize this topological superconductor and help ensure that the proposed material will indeed exhibit the expected order. 1.) Y.-T. Hsu, A. Vaezi, E.-A. Kim. Topological modulated superconductivity in monolayer transition metal dichalcogenides, in preparation (2015).

**10:24AM R25.00013 Superconductivity in quasi-2d organic doped Mott insulators: a superconducting dome without an antiferromagnetic quantum critical point<sup>1</sup>**, A. -M. S. TREMBLAY, CHARLES-DAVID HÉBERT, Université de Sherbrooke, PATRICK SÉMON, Université de Sherbrooke and Rutgers University — Layered organic superconductors of the BEDT family are model systems for understanding the interplay of the Mott transition with superconductivity, magnetic order and frustration. Recent experimental studies on a hole-doped compound reveal an enhancement of superconductivity and a rapid crossover between two different conducting phases above the superconducting dome. Using plaquette cellular dynamical mean field theory with state of the art continuous-time quantum Monte Carlo calculations, we study this problem with the two-dimensional Hubbard model on the anisotropic triangular lattice. Phase diagrams are in broad agreement with experiment. As in the case of the cuprates, we find, at finite doping in the unstable normal state, a first-order transition between a pseudogap and a correlated metal. We make several experimental predictions. This work also clearly shows that the superconducting dome in organic superconductors is tied to the Mott transition and its continuation as a transition separating pseudogap phase from correlated metal in doped compounds, as in the cuprates. Contrary to heavy fermions for example, the maximum T<sub>c</sub> is definitely not attached to an antiferromagnetic quantum critical point. That can also be verified experimentally.

<sup>1</sup>Supported by NSERC, CIFAR and the Tier I Canada Research Chair Program

**10:36AM R25.00014 On the equilibrium of a extremely extended and diluted magneto-matter state subject to its weight.**, DANIEL BERDICHEVSKY, Independent Scholar — Solutions to the force relationship between the magnetic stresses and the self-gravitational force are discussed for a simple homogeneous distribution of matter coalescent to a magnetic field in a cylindrical geometry. Consideration are given to the needed permeability of the medium to make it capable of supporting many times the mass of the Sun, on an extension of several parsecs to kiloparsec. This state of self organization of matter and magnetic field (magneto-matter state) has proven useful interpretation for the explanation of anomalous thermodynamic of the gas of electrons contained in flux-tubes with a twist, low-beta, often observed at 1 AU in the interplanetary medium, Berdichevsky and Shefers, 2015. This state of matter, which most basic property, the freezing in the magnetic field, see e.g., Chew et al, 1956, has proved to exist in the regions where robotic observations in the near and far space perform detailed observations of magnetic fields, and extreme dilute plasma (commonly about 1000 to 0.1 or less ionized particles per cubic cm). This work is in many ways an extension of Alfven work on magnetized space plasmas, Alven, 1942. Berdichevsky, D.B., and K., Schefers, ApJ, 803, 70, 2015, doi: 10.1088/0004-637X/805/1/70 Chew, G.F., M.L., Goldberger, and F.E. Low, 1956, the Royal Soc. London, section Math & Phys Sc., 236, pp. 112. Alfven, H (1942). "Existence of electromagnetic-hydrodynamic waves." *Nature* 150: 405.. doi:10.1038/150405d0

**Thursday, March 17, 2016 8:00AM - 10:12AM –**  
**Session R26 DMP DCOMP: Complex Structured Materials - Computational** 325 - Arunima Singh,  
NIST

**8:00AM R26.00001 Topological Phonon-Plasmon Modes in Two-Dimensional Ferromagnetic Wigner Crystal of Electrons**, WENCHENG JI, JUNREN SHI, Peking Univ — We show that a two-dimensional ferromagnetic Wigner crystal of electrons confined in a semiconductor quantum well/heterostructure with spin-orbit coupling and an appropriate sign of  $g$ -factor could be transformed to a topological phonon-plasmon system by applying a weak perpendicular magnetic field. The competition between the magnetic field and the spin-orbit coupling will drive a topological phase transition, resulting in a topologically trivial phonon-plasmon system in the high magnetic field. We demonstrate the existence of chiral edge phonon-plasmon modes in finite size samples for both phases, and the robustness of the chiral edge modes in the topological phase. We estimate parameters for a few commonly used semiconductors, such as GaAs, GaAl, InAs and InSb. Moreover, we rule out the possibility of Wigner crystal of holes as a topological phonon-plasmon system, due to the unfavorable form of spin-orbit coupling in hole bands dictated by symmetry.

**8:12AM R26.00002 Electron transport calculations with Wannier functions in van der Waals heterostructures**, WUSHI DONG, ALEJANDRO LOPEZ-BEZANILLA, PETER LITTLEWOOD, University of Chicago, Argonne National Laboratory, ANDREAS ROELOFS' GROUP AT ARGONNE NATIONAL LAB COLLABORATION — The vertical stacking of 2D materials forming van der Waals heterostructures (vdWHs) exhibits a wide range of interesting properties. A combined approach based on the Green's function formalism and a mean-field description of the electronic structure is used to calculate vertical electron transport in vdWHs. Tight-binding parameters obtained from Maximally Localized Wannier Functions enable us to model quantum electron transport at low computational costs. Our analysis of electron transport efficiencies provides the foundation and motivation for experimental works.

**8:24AM R26.00003 Interlayer coupling in few-layers transition metal dichalcogenides**, BOXIAO CAO, TIANSHU LI, George Washington Univ — The vertically heterostructured transition metal dichalcogenides (TMD) few-layers may display a wide range of lattice registry. By density functional theory and numerical structural analysis, we examined both the atomic and electronic structures of arbitrarily stacked TMD few-layers. It is shown [1] that the variation of indirect band gap in MoS<sub>2</sub> bilayers is mainly attributed to the interlayer sulfur-sulfur (S-S) interaction. We developed a structural model that allows understanding such interaction under an arbitrary stacking sequence. It is shown the arbitrarily stacked MoS<sub>2</sub> bilayers should exhibit a weak twist angle dependence on the magnitude of its indirect band gap, except for those special twist angles that recover high symmetry stacking sequences. Our analysis provides a thorough theoretical explanation to the recently measured photoluminescence spectroscopy and can form the basis for understanding the coupling in other vertically heterostructured TMD few-layers. For example, through a close experimental collaboration, we have recently identified the electronic origin for the metallization of WS<sub>2</sub> under high hydrostatic pressure (up to 35 GPa) [2].

1. B. Cao and T. Li, J. Phys. Chem. C 119, 1247 (2015)
2. A. Nayak, *et. al.*, ACS Nano 9, 9117 (2015)

**8:36AM R26.00004 First-principles study of electric and magnetic properties of an F4TCNQ ribbon on graphene**, HYUNGJU OH, SINISA COH, Univ of California - Berkeley, YOUNG-WOO SON, Korea Institute for Advanced Study, MARVIN COHEN, Univ of California - Berkeley — We present density functional calculations on the electrical and magnetic properties of a ribbon of tetrafluoro-tetracyanoquinodimethan (F4TCNQ) molecules deposited on a graphene sheet. We find that doping the system with electrons results in a spatial variation of the Dirac point energy along the direction perpendicular to the ribbon, which makes a p-n junction configuration in the graphene sheet. In addition, ferromagnetism appears in the ribbon and the ferromagnetic moments can be controlled by the electron doping. This work was supported by NSF Grant No. DMR10-1006184 and the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. Computational resources have been provided by the DOE at Lawrence Berkeley National Laboratory's NERSC facility.

**8:48AM R26.00005 RKKY interaction in triangular MoS<sub>2</sub> nanoflakes<sup>1</sup>**, DIEGO MASTROGIUSEPPE, Instituto de Fisica Rosario, OSCAR AVALOS-OVANDO, SERGIO ULLOA, Ohio University — Transition-metal dichalcogenides (TMDs), such as MoS<sub>2</sub>, possess unique electronic and optical properties, making them promising for optospintronics. Exfoliation and CVD growth processes produce nanoflakes of different shapes, often triangular with zigzag edges [1]. Magnetic impurities in this material interact indirectly through the TMD conduction electrons/holes. Using an effective 3-orbital tight-binding model [2], we study the Ruderman-Kittel-Kasuya-Yosida interaction between magnetic impurities in p-doped triangular flakes with zigzag termination. We analyze the interaction as function of impurity separation along high symmetry directions in the nanoflake, considering hybridization to different Mo orbitals, and different fillings. The interaction is anisotropic for impurities in the interior of the flake. However, when impurities lie on the edges of the crystallite, the effective exchange is Ising-like, reflecting the presence of z<sup>2</sup>-orbitals associated with edge states. Other interactions are possible by selecting impurity positions and orbital character of the states in their neighborhood. Our results can be tested with local probes, such as spin-polarized STM. [1] A. M. van der Zande *et al.*, Nat. Mat. 12, 554 (2013). [2] G. B. Liu *et al.*, PRB 88, 085433 (2013).

<sup>1</sup>Supported by NSF DMR-1508325

**9:00AM R26.00006 Symmetry origins of the 'caldera' valence band distortion in 2D semiconductors**, PENGKE LI, IAN APPELBAUM, Univ of Maryland-College Park, PHYSICS DEPARTMENT TEAM — The electronic structures of many two-dimensional van der Waals semiconductors exhibit various fascinating properties distinct from their three-dimensional bulk counterparts. Through an examination of their lattice symmetries, we identify several universal factors dictating their band dispersion in the monolayer limit, where in-plane mirror symmetry and quantum confinement play critical roles. Taking group-III metal monochalcogenides (such as GaSe) as an example, we reveal the origin of the unusual 'caldera' shape of the valence band edge (otherwise inelegantly dubbed an 'upside down Mexican hat'), which we show is surprisingly common among other 2D semiconductors (such as in phosphorene for  $\text{S}_k\text{S}_k$  along its zigzag direction). Reference: arXiv:1508.06963

**9:12AM R26.00007 First-principles simulations of Graphene/Transition-metal-Dichalcogenides/Graphene Field-Effect Transistor<sup>1</sup>**, XIANGGUO LI, YUN-PENG WANG, X. -G ZHANG, HAI-PING CHENG, Univ of Florida - Gainesville — A prototype field-effect transistor (FET) with fascinating properties can be made by assembling graphene and two-dimensional insulating crystals into three-dimensional stacks with atomic layer precision. Transition metal dichalcogenides (TMDCs) such as WS<sub>2</sub>, MoS<sub>2</sub> are good candidates for the atomically thin barrier between two layers of graphene in the vertical FET due to their sizable bandgaps. We investigate the electronic properties of the Graphene/TMDCs/Graphene sandwich structure using first-principles method. We find that the effective tunnel barrier height of the TMDC layers in contact with the graphene electrodes has a layer dependence and can be modulated by a gate voltage. Consequently a very high ON/OFF ratio can be achieved with appropriate number of TMDC layers and a suitable range of the gate voltage. The spin-orbit coupling in TMDC layers is also layer dependent but unaffected by the gate voltage. These properties can be important in future nanoelectronic device designs.

<sup>1</sup>DOE/BES-DE-FG02-02ER45995; NERSC

**9:24AM R26.00008 ABSTRACT MOVED TO P5.012 —**

**9:36AM R26.00009 Optical Properties of the  $\alpha$ -T<sub>3</sub> Model**, EMILIA ILLES, University of Guelph, JULES CARBOTTE, McMaster University, ELISABETH NICOL, University of Guelph — The  $\alpha$ -T<sub>3</sub> model, recently introduced by Raoux et. al [1], provides a continuous evolution between the honeycomb lattice of graphene and the T<sub>3</sub> or dice lattice. It is characterized by a variable Berry phase that changes continuously from  $\pi$  to 0. We present our calculations of optical properties of the  $\alpha$ -T<sub>3</sub> model, including the Hall quantization and optical conductivity, with an emphasis on the effect of the variable Berrys phase of the model. In particular, we describe the continuous evolution of the Hall quantization from a relativistic to a non-relativistic regime. [1] A. Raoux, M. Morigi, J.-N. Fuchs, F. Piechon, and G. Montambaux, Phys. Rev. Lett. 112, 026402 (2014)

**9:48AM R26.00010 Microscopic modeling of nitride intersubband absorbance<sup>1</sup>**, INES MONTANO, A.A. ALLERMAN, Sandia Natl Labs, J.J. WIERER, Lehigh University, M. MOSELEY, E.J. SKOGEN, A. TAUKE-PEDRETTI, G.A. VAWTER, Sandia Natl Labs — III-nitride intersubband structures have recently attracted much interest because of their potential for a wide variety of applications ranging from electro-optical modulators to terahertz quantum cascade lasers. To overcome present simulation limitations we have developed a microscopic absorbance simulator for nitride intersubband devices. Our simulator calculates the band structure of nitride intersubband systems using a fully coupled 8x8 k.p Hamiltonian and determines the material response of a single period in a density-matrix-formalism by solving the Heisenberg equation including many-body and dephasing contributions. After calculating the polarization due to intersubband transitions in a single period, the resulting absorbance of a superlattice structure including radiative coupling between the different periods is determined using a non-local Green's-function formalism. As a result our simulator allows us to predict intersubband absorbance of superlattice structures with microscopically determined lineshapes and linewidths accounting for both many-body and correlation contributions.

<sup>1</sup>This work is funded by Sandia National Laboratories Laboratory Directed Research and Development program. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin

**10:00AM R26.00011 Enhancement of bulk photovoltaic effect in band inversion topological phase transitions**, LIANG TAN, ANDREW RAPPE, Univ of Pennsylvania — The bulk photovoltaic effect (BPVE) is the generation of photocurrents in the bulk of a single-phase material. The dominant mechanism for the BPVE is the shift current, a non-linear optical effect which involves the excitation of carriers into current-carrying coherent superpositions. This mechanism has a number of advantages over traditional photovoltaics, such as above-band gap photovoltages, and current generation in the bulk. In this work, we show that the shift current BPVE can be enhanced in materials with band inversion topological phase transitions. Using first-principles calculations, we show that the magnitude of the shift current is sharply increased in the vicinity of the band inversion transition, and that the direction of the shift current changes abruptly at the band inversion transition. Taking as examples layered BiTeI and perovskite CsPbI<sub>3</sub>, we demonstrate that this effect is robust across different materials systems. To understand these results, we analyze our results using a low-energy effective Hamiltonian and derive the functional form of the shift current lineshape near the band gap energy.

**Thursday, March 17, 2016 8:00AM - 11:00AM —**  
**Session R27 DCMP: Non-Fermi-liquids** 326 - Arkady Shekhter, Maglab, Florida State University

**8:00AM R27.00001 New phases from interacting Majorana fermions in one dimension**, MARCEL FRANZ, ARMIN RAHMANI, XIAOYU ZHU, IAN AFFLECK, University of British Columbia — Vortices in the Fu-Kane model (describing a superconducting surface of a 3D topological insulator) are known to host Majorana zero modes. By adjusting a single system parameter – the global chemical potential – the zero modes can be tuned to the regime of strong interactions. The simplest interacting system that can be built from these ingredients is a 1D Majorana chain with nearest neighbor hopping and the most local 4-fermion interaction. The system exhibits a complex phase diagram with interesting phases and phase transitions between them. For repulsive interactions we find an interesting gapless phase with coexisting Luttinger liquid and Ising degrees of freedom. The latter is separated from a 4-fold degenerate gapped phase at strong coupling by a novel generalization of the commensurate-incommensurate transition.

**8:12AM R27.00002 Supersymmetry from Strongly Interacting Majoranas<sup>1</sup>**, ARMIN RAHMANI, XIAOYU ZHU, MARCEL FRANZ, IAN AFFLECK, UBC — We show that a strongly interacting chain of Majorana zero modes exhibits a supersymmetric quantum critical point corresponding to the tricritical Ising model, separating the Ising critical phase from a doubly degenerate gapped phase. The supersymmetry extends into a gapped phase. We identify the signatures of our predictions in tunneling experiments.

<sup>1</sup>NSERC, Max Planck-UBC Centre for Quantum Materials

**8:24AM R27.00003 Quantum phase transition in a strongly interacting 2D model of Majorana fermions**, BO-HAI LI, SHAO-KAI JIAN, HONG YAO, Institute for Advanced Study, Tsinghua Univ — Abstract: We study a 2D strongly-interacting time-reversal-invariant system consisting of Majorana fermions on the square lattice. This model may be realized as an Abrikosov vortex lattice in the superconducting surface state of a strong topological insulator. From the mean-field calculations, we show that for strong interactions a time-reversal-symmetry breaking phase occurs with chiral edge states. We further investigate the quantum critical behavior at the phase transition point by renormalization group analysis.

**8:36AM R27.00004 Landau levels of Majorana fermions in a spin liquid**, STEPHAN RACHEL, TU Dresden, LARS FRITZ, Utrecht University, MATTHIAS VOJTA, TU Dresden — Majorana fermions, originally proposed as elementary particles acting as their own antiparticles, can be realized in condensed-matter systems as emergent quasiparticles, a situation often accompanied by topological order. Here we propose a physical system which realizes Landau levels highly degenerate single-particle states usually resulting from an orbital magnetic field acting on charged particles for Majorana fermions. This is achieved in a variant of a quantum spin system due to Kitaev which is distorted by triaxial strain. This strained Kitaev model displays a spin-liquid phase with charge-neutral Majorana-fermion excitations whose spectrum corresponds to that of Landau levels, here arising from a tailored pseudo-magnetic field. We show that measuring the dynamic spin susceptibility reveals the Landau-level structure by a remarkable mechanism of probe-induced bound-state formation.

**8:48AM R27.00005 MOVED TO M1.377 —**

**9:00AM R27.00006 Johnson noise thermometry reveals the Dirac fluid in graphene**, JESSE CROSSNO, JING SHI, KE WANG, XIAOMENG LIU, ACHIM HARZHEIM, ANDREW LUCAS, SUBIR SACHDEV, PHILIP KIM, Harvard University, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Material Science, Japan, THOMAS OHKI, KIN CHUNG FONG, Raytheon BBN Technologies — Near the charge neutrality point in graphene, the Fermi surface vanishes leading to the formation of a strongly-interacting quasi-relativistic electron-hole plasma, known as a Dirac fluid. These non-Fermi liquids share many features with quantum critical systems including a fast electron-electron scattering rate which makes them well suited to hydrodynamic descriptions. A number of exotic properties have been predicted including a diverging thermal conductivity resulting in the breakdown of the Wiedemann-Franz (WF) law. I will discuss the experimental technique—based on Johnson noise thermometry—used to measure the electronic thermal conductivity of graphene and probe the unique transport dynamics of the Dirac fluid.

**9:12AM R27.00007 Transport in inhomogeneous quantum critical fluids and in the Dirac fluid in graphene**, ANDREW LUCAS, JESSE CROSSNO, PHILIP KIM, SUBIR SACHDEV, Harvard University, KIN CHUNG FONG, Raytheon BBN — We present a hydrodynamic theory of transport in quantum critical fluids, disordered on long wavelengths due to fluctuations in the chemical potential. We argue that this approach is also well-suited to the Dirac fluid in graphene near the charge-neutrality point. Numerical simulations of this theory are compared to recent experiments on thermal and electric transport in clean samples of charge-neutral graphene. We obtain substantially improved quantitative agreement with data over existing hydrodynamic models. This provides evidence that the Dirac fluid behaves as a strongly interacting electronic fluid with transport governed by essentially classical collective phenomena. This work makes quantitative contact between AdS/CMT-inspired models of transport and an experimentally realized condensed matter system for the first time.

**9:24AM R27.00008 Dimensional Crossover from 2D Fermi liquids to 1D Luttinger liquids<sup>1</sup>**, JIA-HUA GU, KAI SUN, Univ of Michigan - Ann Arbor — We demonstrate an analytic theory for the crossover between Fermi liquids and Luttinger liquids. By deforming the Fermi surface of a 2D Fermi liquid towards perfect nesting, we show that signatures of Luttinger liquids arise. In the crossover regime, bosonic particles emerge from the fermionic theory, whose the spectral weight characterize the crossover towards 1D Luttinger liquids. At perfect nesting, these bosonic modes recover the bosonization formalism for Luttinger liquids. Spin-charge separation and instabilities due to attractive interactions are also studied.

<sup>1</sup>This work was supported by the National Science Foundation under grant PHY-1402971.

**9:36AM R27.00009 Numerical study on a random 4-fermion interaction model of a strange metal**, WENBO FU, SUBIR SACHDEV, Department of Physics, Harvard University — We use exact diagonalization (ED) method to study the infinite range random 4 fermion model [1] of a strange metal. We examine the Greens function and show that ED result is in agreement with the large N result in the scaling limit [2]. We also examine the thermal entropy; this has an increasing trend as we increase the system size in the low temperature regime, and is consistent with large N high temperature expansion in the high temperature regime. [1] S. Sachdev, arXiv:1506.05111 [2] S. Sachdev and J. Ye, Phys. Rev. Lett. 70, 3339 (1993)

**9:48AM R27.00010 Electronic transport and Luttinger behavior in polymer thin films in the quasi-atomic limit<sup>1</sup>**, AARON SZASZ, RONI ILAN, Univ of California - Berkeley, JOEL MOORE, Univ of California - Berkeley, Lawrence Berkeley National Laboratory — Recent experiments have shown two-dimensional polymer films to be promising materials for thermoelectric devices, but some of the observed properties are not well understood. To better understand these materials, we introduce a new model in which each polymer is a Luttinger liquid and the polymers are weakly coupled to each other. This approximation of strong interactions within each polymer and weak coupling between them is the “quasi-atomic limit.” We find integral expressions for transport coefficients, including the electrical and thermal conductivities and the thermopower, and we extract their power law dependencies on temperature. Luttinger liquid physics is manifested in a violation of the Wiedemann-Franz law.

<sup>1</sup>This research was supported by the AFOSR MURI program.

**10:00AM R27.00011 Fractionalization beyond Luttinger Liquid in the spectroscopy of Lithium Purple Bronze<sup>1</sup>**, LERA NATALIA, CIC nanoGUNE San Sebastian Spain, ALVAREZ JOSE, Universidad Autonoma de Madrid — We offer an interpretation for the departures of ARPES and STS spectroscopies experiments in quasi-one-dimensional Lithium Purple Bronze (LiPB) from single-band Luttinger Liquid (LL) theory. We base our calculation on a phenomenological description of the published data proposed in the original experiments and consider two bands crossing the Fermi level. We discuss the breakdown of the LL scaling relation  $\eta = \alpha - 1$ , the separation of the spinon edge and the holon peak, the phenomenological TL fit to the Energy Distribution Curves (EDC) and the survival of power-like density of states down to 4K. We consider non-critical fluctuations in one of the separated modes in which the electron fractionalize, and discuss under which conditions could be related with the upturn in the resistivity at 20-30K. We discuss the possibility of a gap in such separated mode and its role on the robust one-dimensional behavior. The connection with the proposed triplet superconductivity is at  $T = 1.4K$  is also studied.

<sup>1</sup>We acknowledge financial support from MINECO FIS2012-37549-C05-03.

**10:12AM R27.00012 Universal Symmetry-Protected Resonances in a Spinful Luttinger Liquid**, YICHEN HU, CHARLES KANE, Univ of Pennsylvania — We study the problem of resonant tunneling through a quantum dot in a spinful Luttinger liquid. It provides the simplest example of a  $(0+1)$ d system with symmetry-protected topological phases. Transitions between different symmetry-protected topological phases separated by fixed points are achieved by tuning the system through resonance. For a particular interaction strength (Luttinger parameter  $g_\rho = \frac{1}{3}$ ,  $g_\sigma = 1$ ), we show that the problem is equivalent to a two channel  $SU(3)$  Kondo problem. Both problems can be mapped to a quantum Brownian motion model on a Kagome lattice, which in turn is related to quantum Brownian motion on a honeycomb lattice and the three channel  $SU(2)$  Kondo problem. Utilizing boundary conformal field theory, we find the universal peak conductance  $g^* \frac{e^2}{h}$  as well as dimensions of the leading relevant operators of the problem. This allows us to compute the scaling behavior of the resonance line-shape as a function of temperature. We also established the fact that the fixed point quantum Brownian motion on both generalized honeycomb lattice( $SU(2)_k$  Kondo) and generalized Kagome lattice( $SU(k)_2$  Kondo) flow into are the same (with  $k = 3$  our original resonant tunneling problem).

**10:24AM R27.00013 Structure of Inert Gases Adsorbed in MCM-41<sup>1</sup>**, DYLAN EVANS, PAUL SOKOL, Indiana Univ - Bloomington — One-dimensional quantum liquids of  $^3\text{He}$  or  $^4\text{He}$  have generated recent interest for investigation in the Luttinger liquid model. Unfortunately, current studies lack a clear demonstration of definitively one-dimensional behavior. We propose using the templated, porous material, MCM-41, as a host for an atomic Luttinger liquid. In general, the pores of MCM-41 are too wide to provide a strictly one-dimensional environment, so we investigate preplating these pores with inert gases to effectively reduce their diameter. We present the results of studies of the structure of inert gases in MCM-41. Nitrogen sorption isotherms were used to characterize the sample. Then, using inert gases as adsorbates, we determined the minimum effective pore diameter that can be achieved in our sample before capillary condensation takes over. X-ray powder diffraction (XRD) was performed on the ideally preplated sample to investigate the structure of the adsorbates in the nanopores. The XRD measurements are compared to simulations of core-shell cylinder model scattering, and the validity of the model is assessed. The prospects for creating a definitively one-dimensional channel for the application of studying the structure and dynamics of helium confined in one dimension are discussed.

<sup>1</sup>This work was supported by the National Science Foundation under Grant DGE-1069091.

**10:36AM R27.00014 Fractionally Charged Solitons in the t-J model on a diagonal two-leg ladder**, YIFAN JIANG, Institute for Advanced Study, Tsinghua University, HONGCHEN JIANG, Department of Physics, Stanford University, HONG YAO, Institute for Advanced Study, Tsinghua University, STEVEN KIVELSON, Department of Physics, Stanford University — We define a new class of "diagonal" t-J ladders rotated by  $\pi/4$  relatively to the canonical lattice directions of the square lattice, and study it using density matrix renormalization group (DMRG). We focus on the two-leg ladder with a doped hole concentration near  $x = 1/4$ . At exactly  $x = 1/4$ , the system forms a period 4 CDW and exhibits spin-charge separation. Slightly away from  $1/4$  doping, we observe several topologically distinct types of solitons with well defined fractionalized quantum numbers. Remarkably, given the absence of any small parameters, the effective masses of the various emergent solitons differ by over four orders of magnitude.

**10:48AM R27.00015 Non Fermi Liquid Crossovers in a Quasi-One-Dimensional Conductor in an Inclined Magnetic Field<sup>1</sup>**, ANDREI LEBED<sup>2</sup>, Department of Physics, University of Arizona — We consider a theoretical problem of electron-electron scattering time in a quasi-one-dimensional (Q1D) conductor in a magnetic field, perpendicular to its conducting axis. We show that inverse electron-electron scattering time becomes of the order of characteristic electron energy,  $1/\tau \sim \epsilon \sim T$ , in a high magnetic field, directed far from the main crystallographic axes, which indicates breakdown of the Fermi liquid theory. In a magnetic field, directed close to one of the main crystallographic axis, inverse electron-electron scattering time becomes much smaller than characteristic electron energy and, thus, applicability of Fermi liquid theory restores. We suggest that there exist crossovers between Fermi liquid and some non Fermi liquid states in a strong enough inclined magnetic field. Application of our results to the Q1D conductor  $(\text{Per})_2\text{Au}(\text{mnt})_2$  shows that it has to be possible to observe the above mentioned phenomenon in feasibly high magnetic fields of the order of  $H \geq H^* \simeq 25 T$ .

<sup>1</sup>It was partially supported by NFS grant DMR-1104512

<sup>2</sup>Please, schedule my talk in the section "Non Fermi liquids".

**Thursday, March 17, 2016 8:00AM - 11:00AM –**  
**Session R28 DCMP: Semiconductor Films, Defects, and Topological Materials** 327 - Kenjiro Gomes, University of Notre Dame

**8:00AM R28.00001 Nanoscopic oxidation of p-type and un-doped Si (100) surfaces using un-externally biased atomic force microscope tips (AFM) in the presence of selected organic solvents**, JEFFREY MCCAUSLAND, SAJEEVI WITHANAGE, ROBERT MALLIK, SERGEI LYUKSYUTOV, University of Akron — A conductive un-biased AFM tip oscillating above p-type or un-doped Si (100) treated with toluene, butan-2-ol, and propan-2-ol creates nanostructures ranging in height from 1-100 nm. The tip was oscillated in ambient conditions (30-70% Rel. Humidity) at frequencies in the  $10^2$  kHz range. It was repeatable with various concentrations of solvent in aqueous solution. It is suggested that mechanical oscillations of the AFM tip polarizes the solvent molecules deposited on the surface resulting in electron transfer from the tip to the surface followed by feature formation. This process effectively creates an electrochemical cell at the microscopic level and the miscibility of the solvents is the key to enabling the process. Species which ionize during the process may be consumed in irreversible reactions whereas the alcohols act as catalysts and are not consumed. The influence of boron defects in the Si substrates is also discussed. It appears that the observed oxidation is different from all other similar reported phenomena including local anodic oxidation, and chemo-mechanical lithographic techniques utilizing AFM.

**8:12AM R28.00002 Interface investigation of solution processed high- $\kappa$   $\text{ZrO}_2/\text{Si}$  MOS structure by DLTS**, ARVIND KUMAR, SANDIP MONDAL, KSR KOTESWARA RAO, Dept of Physics, IISc, India — The interfacial region is dominating due to the continuous downscaling and integration of high- $\kappa$  oxides in CMOS applications. The accurate characterization of high- $\kappa$  oxides/semiconductor interface has the significant importance towards its usage in memory and thin film devices. The interface traps at the high- $\kappa$ /semiconductor interface can be quantified by deep level transient spectroscopy (DLTS) with better accuracy in contrast to capacitance-voltage (CV) and conductance technique. We report the fabrication of high- $\kappa$   $\text{ZrO}_2$  films on p-Si substrate by a simple and inexpensive sol-gel spin-coating technique. Further, the  $\text{ZrO}_2/\text{Si}$  interface is characterized through DLTS. The flat-band voltage ( $V_{\text{FB}}$ ) and the density of slow interface states (oxide trapped charges) extracted from CV characteristics are 0.37 V and  $2 \times 10^{-11} \text{ C/cm}^2$ , respectively. The activation energy, interface state density and capture cross-section quantified by DLTS are  $E_{\text{V}} + 0.42 \text{ eV}$ ,  $3.4 \times 10^{11} \text{ eV}^{-1} \text{ cm}^{-2}$  and  $5.8 \times 10^{-18} \text{ cm}^2$ , respectively. The high quality  $\text{ZrO}_2$  films own high dielectric constant 15 with low leakage current density might be an appropriate insulating layer in future electronic application. The low value of interface state density and capture cross-section are the indication of high quality interface and the defect present at the interface may not affect the device performance to a great extent. The DLTS study provides a broad understanding about the traps present at the interface of spin-coated  $\text{ZrO}_2/\text{Si}$ .

**8:24AM R28.00003 A New Approach for Surface Energy Calculations Applicable to High-throughput Design of New Interfaces<sup>1</sup>**, CHRISTIAN RATSCH, JAKUB KAMINSKI, UCLA — In this talk we will present a new approach for the calculation of surface energies of periodic crystal. For non-polar materials slabs (which are terminated by two identical surfaces) the task of calculating the surface energy is trivial. But it is more problematic for polar systems where both terminating surfaces are different, as there is no single established method allowing for equal treatment of a wide range of surface morphologies and orientations. Our proposed new approach addresses this problem. It relies on carefully chosen capping atoms and the assumptions that their bond energy contributions can be used to approximate the total energy of the surface. The choice of the capping atoms is governed by a set of simple guidelines that are applicable for surfaces with different terminations. We present the results for different semiconductor materials and show that our approach leads to surface energies with errors as low as 2%. We show that hydrogen is not always the best choice for a capping atom if accurate surface energies are the target of the calculations. Our approach is suitable for high-throughput screening of new material interfaces, as accurate calculations of surface energies can be performed in an unsupervised algorithm.

<sup>1</sup>A New Approach for Surface Energy Calculations Applicable to High-throughput Design of New Interfaces

**8:36AM R28.00004 Schottky Barrier Mapping to Nanoscale Dimensions Utilizing Ballistic Electron Emission Microscopy**, VINCENT LABELLA, SUNY Polytechnic Institute, ROBERT BALSANO, CHRIS DURCAN, WES NOLTING, University at Albany - SUNY — The Schottky barrier is the electrostatic barrier between a metal and a semiconductor that results in rectification and is found in many types of devices such as source drain contacts to sub 20-nm-node transistors. Nanoscale fluctuations in the Schottky barrier height can occur due to variations in bonding, compositional fluctuations in the materials, and the presence of defects. Measuring and mapping these electrostatic fluctuations to nanoscale dimensions can be achieved with ballistic electron emission microscopy (BEEM) an STM based technique. This presentation will demonstrate how the Schottky barrier height can be mapped to nanoscale dimensions using BEEM at 77K and under ultra-high vacuum. The STM tip is positioned on a regularly spaced grid and BEEM spectra are acquired from which the barrier height can be extracted. Maps and histograms can be generated by measuring and fitting thousands of these spectra. These maps provide detailed insight into the electrostatic fluctuations occurring at the buried interface with nanoscale resolution that cannot be accomplished with other bulk measurements.

**8:48AM R28.00005 Hot Electron Scattering in Thin Metal Films Utilizing Ballistic Electron Emission Microscopy**, CHRISTOPHER DURCAN, WESTLY NOLTING, ROBERT BALSANO, State Univ of NY - Albany, VINCENT LABELLA, SUNY Polytechnic Institute — Electron scattering in nm-thick metal films has fundamental and technological importance. Ballistic Electron Emission Microscopy (BEEM) an STM based technique can be utilized to measure the scattering rate and understand the scattering mechanisms. By injecting electrons from the STM tip in the energy range of 0.2 eV- 1.5 eV into the metal base of a metal semiconductor diode and measuring the amount of current collected in the semiconductor a Schottky barrier height can be measured. In addition, by measuring the decay in the collector or BEEM current vs. metal film thickness, an electron attenuation length can be measured. One question has always been; what are these BEEM attenuation lengths sensitive to? Intrinsic properties of the metal, or extrinsic effects such as the structure of the film? By measuring the attenuation length of W and Cr and comparing to prior measurements of Cu, Ag, Au a comparison between the BEEM attenuation length and resistivity can be achieved over an order of magnitude in resistivity. The results show an inverse relationship that one expects for mean free path and resistivity, indicating that BEEM measurements are sensitive to the intrinsic properties of the metal and not solely the structure of the films.

**9:00AM R28.00006 Surface phase stability and surfactant behavior of InAsSb alloy surfaces.<sup>1</sup>**, EVAN M ANDERSON, ADAM M LUNDQUIST, Materials Science and Engineering, University of Michigan, CHRIS PEARSON, Computer Science, Engineering, and Physics, University of Michigan-Flint, JOANNA M MILLUNCHICK, Materials Science and Engineering, University of Michigan — InAsSb has the narrowest bandgap of any of the conventional III-V semiconductors: low enough for long wavelength infrared applications. Such devices are sensitive to point defects, which can be detrimental to performance. To control these defects, all aspects of synthesis must be considered, especially the atomic bonding at the surface. We use an *ab initio* statistical mechanics approach that combines density functional theory with a cluster expansion formalism to determine the stable surface reconstructions of Sb (As) on InAs (InSb) substrates. The surface phase diagram of Sb on InAs is dominated by Sb-dimer termination  $\alpha 2(2 \times 4)$  and  $\beta 2(2 \times 4)$  and  $c(4 \times 4)$ . Smaller regions of mixed Sb-As dimers appear for high Sb chemical potentials and intermediate As chemical potential. We propose that InAsSb films could be grown on  $(2 \times 4)$ , which maintain bulk-like stoichiometry, to eliminate the formation of typically observed n-type defects. Scanning tunneling microscopy and reflection high energy electron diffraction confirm the calculated phase diagram. Based on these calculations, we propose a new mechanism for the surfactant behavior of Sb in these materials.

<sup>1</sup>We gratefully acknowledge Chakrapani Varanasi and the support of the Department of Defense, Army Research Office via the grant number W911NF-12-1-0338.

**9:12AM R28.00007 Formation, properties, and function of vacancies in Si/Ge Clathrates: The importance of broken symmetries**, AMRITA BHATTACHARYA, CHRISTIAN CARBOGNO, MATTHIAS SCHEFFLER, Fritz Haber Institute of the Max Planck Society — Inclusion compounds, such as clathrates, are cage-like crystal structures that can encapsulate guest atoms. Since this allows to tune their electronic and vibrational properties, they are regarded as interesting materials for thermoelectric applications. Progress in this field is, however, hindered by the fact that filling of group-IV clathrates often results in complex and unexpected structural changes, e.g., the spontaneous formation of vacancies in certain hosts: In Ge<sub>46</sub> clathrates filled with K or Ba, the most favourable phases K<sub>8</sub>Ge<sub>44</sub>/Ba<sub>8</sub>Ge<sub>43</sub> feature two/three vacancies. Conversely, the framework of the isoelectronic Si<sub>46</sub> clathrate remains intact (K<sub>8</sub>Si<sub>46</sub>/Ba<sub>8</sub>Si<sub>46</sub>) upon filling with the exact same guests. Our first-principles calculations of the formation energies and of the thermodynamic phase stabilities confirm this experimental scenario and shed light on the underlying mechanisms. Due to the spatially more delocalized 4sp<sup>3</sup> orbitals in Ge compared to the more localized 3sp<sup>3</sup> orbitals in Si, fundamentally different symmetry breaking distortions become possible to stabilize the vacancies. Eventually, we discuss the implications of these findings for the thermoelectric properties of clathrates.

**9:24AM R28.00008 Symmetry of Highly Strained ZnSnN<sub>2</sub> Thin Films<sup>1</sup>**, NANCY SENABULYA, Univ of Michigan - Ann Arbor, YONGSOO YANG, Univ of California, Los Angeles, CHRISTIAN SCHLEPUTZ, Swiss Light Source, Paul Scherrer Institut, NATHANIEL FELDBERG, Univ of Buffalo, ROBERT MAKIN, Western Michigan Univ, CHRISTINA JONES, Univ of Michigan - Ann Arbor, STEVEN DURBIN, Western Michigan Univ, ROY CLARKE, Univ of Michigan - Ann Arbor — Zinc Tin Nitride (ZnSnN<sub>2</sub>) is a member of the ternary class of II-IV-V<sub>2</sub> semiconducting materials that have gained significant research interest in the recent past as a cheaper, earth abundant and environmentally friendly alternative to Indium-based materials used in photovoltaic and solid state lighting applications. Surface x-ray diffraction measurements performed at Argonne National Laboratory on single crystal thin films of ZnSnN<sub>2</sub> grown on (111)yttria stabilized zirconia(YSZ) substrates show a structural change from the wurtzite to the orthorhombic phase in films grown under low values of nitrogen flux and high substrate temperatures. This orthorhombic phase is characterized by in plane contraction and out of plane elongation of the unit cell lattice parameters, a phenomenon that theoretically results from the doubling of the wurtzite unit cell in the basal plane and ordering on the cation sub lattice [APL 103,042109(2013)]. We are currently studying the crystal structure of ZnSnN<sub>2</sub> thin films using 3-dimensional reciprocal space maps and pole figure measurements in order to characterize the high symmetry orthorhombic phase achieved using epitaxy.

<sup>1</sup>Work is supported by Schlumberger Faculty for the Future Grant

**9:36AM R28.00009 Surface charge transport in Silicon (111) nanomembranes<sup>1</sup>**, WEIWEI HU, SHELLEY SCOTT, RB JACOBSON, DONALD SAVAGE, MAX LAGALLY, University of Wisconsin-Madison, THE LAGALLY GROUP TEAM — Using thin sheets (nanomembranes) of atomically flat crystalline semiconductors [1], we are able to investigate surface electronic properties, using back-gated van der Pauw measurement in UHV. The thinness of the sheet diminishes the bulk contribution, and the back gate tunes the conductivity until the surface dominates, enabling experimental determination of surface conductance [2]. We have previously shown that Si(001) surface states interact with the body of the membrane altering the conductivity of the system. Here, we extended our prior measurements to Si(111) in order to probe the electronic transport properties of the Si(111)  $7\times 7$  reconstruction. Sharp ( $7\times 7$ ) LEED images attest to the cleanliness of the Si(111) surface. Preliminary results reveal a highly conductive Si(111)  $7\times 7$  surface with a sheet conductance  $R_s$  of order of  $\mu S/\square$ , for 110nm thick membrane, and  $R_s$  is a very slowly varying function of the back gate voltage. This is in strong contrast to Si(001) nanomembranes which have a minimum conductance several orders of magnitude lower, and hints to the metallic nature of the Si(111) surface. 1. Zhang, P. P. *et al.*, Nature 439, 703-706 (2006); 2. W. Peng, *et al.*, Nature Commun. 4, 1339 (2013).

<sup>1</sup>Research supported by DOE

**9:48AM R28.00010 Detection of a History Dependent Topological Hall Effect Due to Skyrmion Formation in FeGe Thin Films**, JAMES GALLAGHER, MICHAEL PAGE, VIDYA BHALLAMUDI, JACK BRANGHAM, KENG YUAN MENG, BRYAN ESSER, HAILONG WANG, DAVE MCCOMB, CHRIS HAMMEL, FENGYUAN YANG, Ohio State Univ - Columbus — B20 phase crystal structures, such as FeGe and MnSi, have been of interest because they enable magnetic skyrmion phases, which can potentially lead to low energy cost spintronic device applications. We report the synthesis of pure phase FeGe epitaxial thin films grown on Si (111) substrates by ultra-high vacuum off-axis magnetron sputtering. The FeGe films were characterized by x-ray diffraction, scanning transmission electron microscopy (STEM) and Hall effect measurements. The topological Hall effect (THE) signals were extracted by subtracting out the anomalous Hall effect and ordinary Hall effect, demonstrating the existence of the skyrmion phase in FeGe films between 5 and 275 K. Topological hall effect was observed at zero field at all temperatures below the Curie temperature, showing the possibility of metastable skyrmion particles at zero field and high temperatures. We will also discuss the study of dynamics of the ferromagnetic phases using ferromagnetic resonance.

**10:00AM R28.00011 Topological Imbert-Fedorov Shift in Weyl Semimetals<sup>1</sup>**, QING-DONG JIANG, Peking Univ, HUA JIANG, Soochow Univ, HAIWEN LIU, QING-FENG SUN, XIN-CHENG XIE, Peking Univ — The Goos-Hnchen (GH) shift and the Imbert-Fedorov (IF) shift are optical phenomena which describe the longitudinal and transverse lateral shifts at the reflection interface, respectively. Here, we predict the GHIF shifts in Weyl semimetals (WSMs) a promising material harboring low energy Weyl fermions, afemionic cousin of photons. Our results show that the GH shift in WSMs is valley independent, is analogous to that discovered in a 2D relativistic material graphene. However, the IF shift has been explored in nonoptical systems, and here we show that it is valley dependent. Furthermore, we show that the IF shift actually originates from the topological effect of the system. Experimentally, the IF shift can be utilized to characterize the Weyl semimetals, design valleytronic devices of high, and measure the Berry curvature. Moreover, we investigate the transport properties of topological semimetal using the wave-packet dynamics, which give some interesting results.

<sup>1</sup>NBRP of China, NSF-China

**10:12AM R28.00012 Hybridization-induced interface states in a topological insulator - ferromagnetic metal bilayer<sup>1</sup>**, YI-TING HSU, PRIYAMVADA JADAUN, CRAIG FENNIE, EUN-AH KIM, Cornell University — Recent experiments demonstrating large spin-torque in topological insulator (TI)/ferromagnetic metal (FM) bilayer, revealing their potential for spintronic applications raised much excitement. However, there is little understanding on the impact of the bilayer formation on the TI surface state and whether it is possible to represent such bilayer using a simple model. Moreover, due to the large charge-transfer from the FM layer, these Dirac surface states are unlikely to be anywhere near the Fermi level to contribute to the observed spin-torque. In order to establish a theoretical starting point, we calculated the band structure of a TI-FM bilayer using density functional theory (DFT) and built a simple effective model that captures the essence of the DFT results. Through this double-pronged approach, we find new surface states we dubbed reflection states to form close to chemical potential due to level-repulsion between the original Dirac surface states and the energetically close-by FM states with the same momentum. Depending on the coupling strength, the reflection states can carry a large weight of the original surface states and thus inherit not only the spatial localization but also the spin-winding of the original Dirac surface state.

<sup>1</sup>This work was supported by the Cornell Center for Materials Research with funding from the NSF MRSEC program (DMR-1120296).

**10:24AM R28.00013 Local electronic structures and 2D topological phase transition of ultra-thin Sb films<sup>1</sup>**, SUNGHWAN KIM, Center for Artificial Low Dimensional Electronic Systems, Institute for Basic Science, Korea, KYUNG-HWAN JIN, JOONBUM PARK, JUN SUNG KIM, SEUNG-HOON JHI, Department of Physics, Pohang University of Science and Technology, Korea, HAN WOONG YEOM, Center for Artificial Low Dimensional Electronic Systems, Institute for Basic Science, Korea — We investigate local electronic structures of ultrathin Sb islands and their edges grown on Bi<sub>2</sub>Te<sub>2</sub>Se by scanning tunneling microscopy/spectroscopy (STM/STS) and density functional theory (DFT) calculations. The Sb islands of various thickness are grown with atomically well ordered edge structure over the 3 bilayers (BL). On the surfaces and edges of these islands, we clearly resolve edge-localized electronic states by STS measurements, which depend on the thickness. The DFT calculations identify that the strongly localized edge states of 4 and 5 BL films correspond to a quantum spin Hall (QSH) states while the edge states of 3 BL are trivial. Our experimental and theoretical results confirm the 2D topological phase transition of the ultrathin Sb films from trivial to QSH phase.

<sup>1</sup>Center for Artificial Low Dimensional Electronic Systems, Institute for Basic Science and Department of Physics, Pohang University of Science and Technology, Korea

**10:36AM R28.00014 The novel properties of epitaxial bismuth ultra-thin films on superconducting substrate NbSe<sub>2</sub>**, DANDAN GUAN, HAOHUA SUN, MEIXIAO WANG, GUANYONG WANG, DAN XU, Shanghai Jiao Tong Univ, XIAOJUN YANG, ZHU-AN XU, Zhejiang University, YAOYI LI, CANHUA LIU, DONG QIAN, JIN-FENG JIA, Shanghai Jiao Tong Univ, SHANGHAI JIAO TONG UNIVERSITY TEAM, ZHEJIANG UNIVERSITY COLLABORATION, COLLABORATIVE INNOVATION CENTER OF ADVANCED MICROSTRUCTURE COLLABORATION — Bismuth is theoretically predicted to be a quantum spin Hall (QSH) system. Such a QSH system, interesting itself with the genuine spin degenerated backscattering forbidden transport property, is also a potential platform to study the 2D topological superconductor with superconductivity induced by proximity effect. The epitaxial growth of ultra-thin Bi(111) film on superconductor NbSe<sub>2</sub> was investigated by scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS). The orientation transition from Bi(110) phase to Bi(111) phase has been observed. One-dimensional topological edge states on the zig-zag edge of Bi(111) bilayers and proximity effect-induced superconductivity were also revealed by STS analysis.

**10:48AM R28.00015 Vertical electrical field induced island growth in layered TiSe<sub>2</sub>.**<sup>1</sup>, HUSONG ZHENG, Virginia Tech, SALVADOR VALTIERRA, NANA OPOKU, McGill University, CHUANHUI CHEN, Virginia Tech, LIYING JIAO, Tsinghua University, KIRK BEVAN, McGill University, CHENGGANG TAO, Virginia Tech — For practical applications of atomically thin transition metal dichalcogenides, it is essential to characterize the structural stability under external stimuli such as electrical fields. Using vacancy monolayer islands on TiSe<sub>2</sub> surfaces as a model system, we experimentally and theoretically investigated the shape evolution and growth rate by using scanning tunneling microscopy. The growth rate that depends on the tunneling current is experimentally determined. Our simulations of monolayer island evolution using a phase-field model are consistent with the experimental observations. The results could be potentially important for electronic device applications of ultrathin transition metal dichalcogenides and other 2D materials.

<sup>1</sup>This work is supported by ARO grant W911NF-15-1-0414.

**Thursday, March 17, 2016 8:00AM - 11:00AM –**  
**Session R29 DCMP: Disordered and Floquet Topological Phases** 328 - Andrew Potter, University of California, Berkeley

**8:00AM R29.00001 Spin susceptibility function of helical metal and RKKY interaction**<sup>1</sup>, CHUNXIAO LIU, BITAN ROY, JAY SAU, university of maryland, CMTc AND JQI TEAM — Topological insulator is a peculiar material, which is insulating in the bulk, while conducting on the surface due to the topology in momentum space. Here, we study the surface of 3D topological insulator, which is also called helical metal. The Hamiltonian of the surface electrons is  $H = k \times \sigma$ , which has spin-momentum locking and Dirac dispersion. The property that we are interested in is the spin susceptibility function of the helical metal. It describes how the system responds to the external magnetic field in the linear response regime. However, because the dispersion of helical metal is linear in momentum  $k$ , the spin susceptibility is easily divergent in terms of UV momentum cutoff. The talk we will present is focusing on how we renormalize the spin susceptibility function in the particular renormalization scheme we choose. In the second part of the talk, we will make use of the renormalized spin susceptibility to show how external magnetic impurities on the surface would interact with each other, with the interaction mediated by electrons of helical metal. This interaction is also called RKKY interaction. Treating impurities as classical spins, we show the pattern of ground state with numerical simulations.

<sup>1</sup>grants by NSF

**8:12AM R29.00002 NonSymmorphic Symmetry Protected Topological Order in Many-body Localized Systems**, KHALID ASHRAF, UC Berkeley — Many-body localized systems have many interesting physical properties such as localization protected quantum order, symmetry protected topological order, area law in entanglement spectrum etc. [1]. Specifically, it has been shown that closed quantum system in 1D i.e. p-wave superconducting wires host localization protected topological order [2]. In this work, we explore the interplay between non-symmorphic symmetry which protects topological order and localization due to disorder. Using a Bogoliubov-de Gennes (BdG) description of p-wave superconductors, we study the topological edge states on a 2D non-symmorphic crystal. We show that a localization protected topological order can exist at high energy in a 2D non-symmorphic crystal. The system goes between topologically trivial and non-trivial phases based on the degree of disorder and shift between the adjacent atoms in the bipartite lattice. We further explore the nature of this phase transition by calculating the entanglement spectrum of the two phases. Finally, the effect of dimensionality on the realization of these phases are discussed. Nandkishore et al. Annual Rev. Cond. Matt. Phys., vol 6 (2015). 2. Huse et al., Phys. Rev. B 88, 014206 (2013).

**8:24AM R29.00003 Effect of disorder on the decreasing the critical value of magnetic field in proximity induced topological superconductors**<sup>1</sup>, YAHYA ALAVIRAD, CHING-KAI CHIU, JAY SAU, Univ of Maryland-College Park — Here we investigate how adding disorder changes the critical value of magnetic field  $B_c$  required to observe the topological phase transition in proximity induced topological superconductors. We consider disordered topological superconductors in  $D = 1, 2$  spatial dimensions and use numerical analysis to directly calculate the topological invariant. Qualitatively different behavior are found depending on the dimensionality of the system. In contrast to  $D = 2$  for  $D = 1$  we show that adding disorder gradually decreases  $B_c$  from the clean case limit of  $B_c = \sqrt{\mu^2 + \Delta^2}$  to  $B_c = \Delta$ . A discussion of why these results are expected is provided. These findings, specially in  $D = 1$  dimension are of experimental interest since they show that the topological phase transition might be observable at values of magnetic field  $B_c$  much smaller than previously expected.

<sup>1</sup>This work was supported by LPS-CMTC, JQI-NSF-PFC and University of Maryland startup grants

**8:36AM R29.00004 Anderson Chern Insulators**, JAMES JUN HE, TONG ZHOU, Hong Kong Univ of Sci & Tech, Z. C. GU, Perimeter Institute, K. T. LAW, Hong Kong Univ of Sci & Tech — When a magnetic field is applied to a quantum spin Hall insulator (QSHI) without inversion symmetry, the edge states become gapful due to the breaking of time reversal symmetry (TRS) and the QSHI becomes a trivial spin Hall insulator (SHI) whose Chern number is  $N = 0$ . In this work we show that disorder can drive such a SHI to a Chern insulator (CI) with  $N = 1$  which supports a gapless chiral edge state. This CI exists in a finite range of disorder strength. Interestingly, the edge state is protected by the bulk mobility gap instead of an energy gap. For this reason, the new phase is called an Anderson Chern insulator (ACI).

**8:48AM R29.00005 Disorder-driven breakdown of topological protection in Bi<sub>2</sub>Se<sub>3</sub> films.**, JISOO MOON, Rutgers University, MATTHEW BRAHLEK, Pennsylvania State University, NIKESH KOIRALA, MARYAM SALEHI, Rutgers University, LIANG WU, N. PETER ARMITAGE, The Johns Hopkins University, SEONGSHIK OH, Rutgers University — In topological insulators (TI), there are unusual metallic states on their surfaces, so-called topological surface states (TSS). They are protected by time reversal symmetry through strong spin-orbit coupling, making them immune to disorder-related localization effects. However, in highly-disordered TIs the crystal momentum becomes ill-defined because translational invariance is broken. In those materials, it is doubtful that topological protection is still valid. In this presentation, we show that high level of disorder drives breakdown of topological protection in Bi<sub>2</sub>Se<sub>3</sub> films. TSS in the films are not protected above a critical level of disorder, and the films become trivial insulators. The films are grown by Molecular Beam Epitaxy (MBE), and the level of disorder in the films is controlled by annealing after the films are grown at room temperature.

**9:00AM R29.00006 Disordered topological crystalline phases**, IAN MONDRAGON-SHEM, TAYLOR L. HUGHES, University of Illinois at Urbana-Champaign — We study topological crystalline phases in the presence of disorder potentials that are invariant under the point group symmetries that protect the corresponding nontrivial phase. Topological states protected by spatial symmetries have so far only been clearly defined for translationally invariant systems. It has been proposed that the stability of such phases against disorder can be inferred from the existence of robust delocalized states at the boundary. However, a bulk characterization is still lacking that can provide a more complete and fundamental understanding of how these phases remain topological in the presence of disorder. We study this problem by focusing on models for which the disorder potential preserves exactly mirror and rotational symmetries. We generalize the expressions of the corresponding topological invariants to the case of broken translational invariance, and analyze their spatial distribution in the bulk of the system. We further study critical behavior in the bulk and at the boundary to determine how these states of matter undergo disorder-induced topological phase transitions. Finally, we discuss how our results could offer a bulk understanding of topological crystalline phases protected by average spatial symmetries.

**9:12AM R29.00007 Disorder-induced WAL-WL transition and anomalous Hall effect in undoped thin  $\text{Sb}_2\text{Te}_3$  films**<sup>1</sup>, INNA KORZHOVSKA, CUNY-Graduate Ctr, The City College of New York, YURY DESHKO, LUKAS ZHAO, ZHIYI CHEN, LIA KRUSIN-EBAUM, The City College of New York, SIMONE RAOUX, Helmholtz-Zentrum, Berlin, Germany — We examine the effects of disorder on charge transport in thin (20-50 nm) films of topological insulator (TI)  $\text{Sb}_2\text{Te}_3$ , where, uniquely, structural disorder can be controllably tuned over a huge range - from amorphous to crystalline - by a suitable annealing schedule. We report on the observation of disorder-induced transition from weak localization-like state (WL-like) to weak anti-localization (WAL), at which conductance changes its character from 3D in the WL-like state to 2D in the WAL (crystalline) state. Near the transition, the conductance is  $G \approx e^2/h$ , suggestive of the transport through a surface channel that is decoupled from the bulk by disorder. Quite remarkably, the onset of the WL state (where bulk transport is of variable range hopping type) is found to be concurrent with the appearance of anomalous Hall signal (AHE) which grows with increased disorder, with Hall resistivity  $\rho_{xy}$  scaling as the longitudinal resistivity squared,  $\rho_{xy} \propto \rho_{xx}^2$ . The nature of spin correlations (probed directly by the arrays of micro Hall sensors) responsible for AHE in disordered TI films in the absence of magnetic dopants will be discussed.

<sup>1</sup>Supported by NSF-DMR-1420634, NSF-DMR-1312483-MWN, and DOD-W911NF-13-1-0159

**9:24AM R29.00008 Anderson localization at the edge of a 2D topological insulator**, ESLAM KHALAF, PAVEL OSTROVSKY, Max Planck Institute for Solid State Research, Stuttgart — We study transport via edge modes in a disordered 2D topological insulator allowing for the presence of non-protected diffusive channels in addition to the topologically protected edge channels. This scenario can be realized at the interface between two quantum Hall system, in a Weyl semimetal in a magnetic field or at the edge of a quantum spin Hall system. The edge transport is described by a one-dimensional field theory in the form of a supersymmetric non-linear sigma model with a topological term. The transfer-matrix formalism is employed to map the problem to the problem of finding the eigenfunctions of a certain operator on a symmetric superspace. The latter problem is solved exactly for all symmetry classes, enabling us to obtain the full counting statistics and mesoscopic conductance fluctuations in the system. Our main finding is that disorder is much more effective in localizing the diffusive (non-protected) channels in the presence of topologically protected ones. This manifests itself as a suppression of the shot noise and conductance fluctuations at scales much shorter than the localization length.

**9:36AM R29.00009 Superconductivity and disorder in the potential topological superconductor  $(\text{Sn,In})\text{Te}^1$** , MATTHEW SMYLIE, Univ of Notre Dame, BING SHEN, HELMUT CLAUS, ALEXEY SNEZHKO, ULRICH WELP, WAI-KWONG KWOK, Argonne National Lab, MORTEN ESKILDSEN, ELIZABETH DE WAARD, Univ of Notre Dame, MICHAEL SUSNER, ATHENA SEFAT, Oak Ridge National Lab — In-doped SnTe has been proposed as a candidate topological superconductor. It has been suggested that the superconducting critical temperature ( $T_c$ ) is strongly enhanced with impurity scattering in this material, with the pairing mechanism perhaps changing with doping. To access information on the pairing symmetry of the superconducting order parameter, ultra-sensitive magnetic field penetration measurements have been conducted by means of a Tunnel-Diode-Oscillator (TDO) technique. Particle irradiation with low MeV protons was used as a controllable source of disorder, but no enhancement of  $T_c$  was observed in cubic-phase material as scattering increased. Detailed characterization measurements and analysis were performed before and after irradiation of the samples.

<sup>1</sup>Tunnel diode oscillator and magnetization measurements were supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

**9:48AM R29.00010 Characterization & Transport Signatures of Periodically Driven Topological Phases**, MICHEL FRUCHART, PIERRE DELPLACE, KRZYSZTOF GAWEDZKI, DAVID CARPENTIER, Laboratoire de Physique, ENS de Lyon — The discovery of the Quantum Hall Effect in the 80's opened the field of topological phases of matter, which has been renewed by the discovery of a new kind of topological insulator in 2005, this time in a time-reversal invariant system. In order to obtain a material with tunable topological properties, research were carried out on out-of-equilibrium systems subject to a periodic drive. Such periodically driven topological phases turn out to be richer than their equilibrium counterparts. We consider a 2D crystal subject to a drive periodic in time, constrained so that it is time-reversal invariant and show that such a system is characterized by  $\mathbb{Z}_2$  indices attached to a gap (and not to a band), which we explicitly construct. To probe these out-of-equilibrium phases in a phase coherent regime, we use standard transport measurements. With the help of numerical simulations, we show that the running time-averaged differential conductances are quantized in a topological gap, and that multi-terminal setups enable to probe the chirality of the out-of-equilibrium topological states.

**10:00AM R29.00011 Floquet topological phases coupled to environments**, SZABOLCS VAJNA, Department of Physics, Boston University and Budapest University of Technology and Economics, BARUCH HOROVITZ, Department of Physics, Ben-Gurion University of the Negev — We consider the fate of a helical edge state of a spin Hall insulator and its topological transition in presence of a circularly polarized light when coupled to various forms of environments. A Lindblad type equation is developed to determine the fermion occupation of the Floquet bands. We find that non-secular terms, corresponding to 2-photon transitions lead to a mixing of the band occupations, hence the light induced photocurrent is in general not perfectly quantized, although deviations are small in the adiabatic limit. Sharp crossovers are identified at frequencies  $\Omega$  and  $1/2 \Omega$  ( $\Omega$  is the strength of light-matter coupling) with the former corresponding to a phase transition on the level of the 2nd order theory.

**10:12AM R29.00012 Time periodic perturbations and transport signatures in Floquet topological insulators**, AARON FARRELL, T. PEREG-BARNEA, McGill Univ — A Floquet topological insulator represents an out-of-equilibrium topological state. The topology of these systems emerges only when a time periodic perturbation is carefully applied. In time-periodic systems one can define quasi-energy states, which replace equilibrium stationary states (i.e. energy eigenstates). For appropriate time periodic potential strengths, a Floquet topological insulator exhibits edge localized quasi-energy states which lie in a gap of its quasi-energy spectrum. These edge states are a non-equilibrium analogue of the topologically protected edge-states in equilibrium topological insulators. In an equilibrium system such edge states lead to robust signature transport properties, e.g. a two-terminal conductivity of  $2e^2/h$ . This talk will explore how these transport signatures translate to Floquet topological insulators. We will do this by developing and generalizing intuition borrowed from the field of photon-assisted tunneling. We show that ultimately the signature transport properties of an equilibrium topological insulator do not directly hold in the out-of-equilibrium setting. This fact notwithstanding, we will provide an indirect way of retaining these transport signatures by using a so-called Floquet sum rule.

**10:24AM R29.00013 Selective scattering between Floquet-Bloch and Volkov states in a topological insulator**, FAHAD MAHMOOD, CHING-KIT CHAN, ZHANYBEK ALPICHSEV, DILLON GARDNER, YOUNG LEE, PATRICK LEE, NUH GEDIK, Massachusetts Inst of Tech-MIT — The coherent optical manipulation of solids is emerging as a promising way to engineer novel quantum states of matter. The strong time periodic potential of intense laser light can be used to generate hybrid photon-electron states. Interaction of light with Bloch states leads to Floquet-Bloch states which are essential in realizing new photo-induced quantum phases. Similarly, dressing of free electron states near the surface of a solid generates Volkov states which are used to study non-linear optics in atoms and semiconductors. The interaction of these two dynamic states with each other remains an open experimental problem. Here we use Time and Angle Resolved Photoemission Spectroscopy (TR-ARPES) to selectively study the transition between these two states on the surface of the topological insulator  $\text{Bi}_2\text{Se}_3$ . We find that the coupling between the two strongly depends on the electron momentum, providing a route to enhance or inhibit it. Moreover, by controlling the light polarization we can negate Volkov states in order to generate pure Floquet-Bloch states. This work establishes a systematic path for the coherent manipulation of solids via light-matter interaction.

**10:36AM R29.00014 Anisotropic ultrafast dynamics in  $\text{BiSbTe}_2\text{S}$  topological insulator investigated by time-resolved photoemission spectroscopy**, F. BOSCHINI, M. ZONNO, E. DA SILVA NETO, S. ZHDANOVICH, M. SCHNEIDER, B. ZWARTSENBURG, G. LEVY, A. MILLS, D. JONES, A. DAMASCELLI, University of British Columbia, S. KUSHWAHA, R. J. CAVA, Department of Chemistry, Princeton University — Topological insulating phases in 3-dimensional bulk materials are characterized by the presence of a Dirac-like dispersive surface state – with a specific momentum-locked spin structure – localized within the bulk insulating band gap [1,2] Here we will present time-resolved photoemission (TR-ARPES) experimental results from a new topological insulator,  $\text{BiSbTe}_2\text{S}$ .  $\text{BiSbTe}_2\text{S}$  exhibits superior chemical stability, as evidenced by the lack of any measurable energy shift of the Dirac point over time. The TR-ARPES signal (1.55-eV pump and 6.2-eV probe) reveals a direct optical population/depopulation of the Dirac states followed by slow recombination processes on a ps-timescale with a marked dependence of the relaxation time on crystallographic orientation. In addition, we also observe an ultrafast pump-induced modification of the equilibrium Dirac state energy dispersion. These effects can be ascribed to an anisotropic pump-induced modification of the phonon population, which in turn leads to an anisotropic electron-phonon assisted scattering of the hot electrons populating the unoccupied Dirac states. [1] Y. Xia et al. Nat. Phys. **5**, 398 (2009) [2] Z.-H. Zhu et al. Phys. Rev. Lett. **112**, 076802 (2014)

**10:48AM R29.00015 Using Non-Equilibrium Dynamics to Probe Competing Orders in a Mott-Peierls System**, YAO WANG, Stanford University, BRIAN MORITZ, SIMES SLAC National Accelerator Laboratory, CHENG-CHIEN CHEN, Argonne National Laboratory, CHUNJING JIA, SIMES SLAC National Accelerator Laboratory, MICHEL VAN VEENENDAAL, Argonne National Laboratory/Northern Illinois University, THOMAS DEVEREAUX, SIMES SLAC National Accelerator Laboratory — The competition between ordered phases and the associated quantum criticality are significant in the study of strongly correlated systems. Here we examine one aspect, the non-equilibrium dynamics of a photoexcited Mott-Peierls system, using an effective Hubbard-bond-phonon model and exact diagonalization. Near the quantum phase transition where spin and charge become intertwined, we observe anti-phase dynamics and coupling-strength-dependent suppression or enhancement in the static structure factors. The renormalized bosonic excitations coupled to a photoemitted electron can be extracted from the spin and charge dynamics, providing an approach for characterizing the underlying bosonic modes. The results from this analysis for different electron momenta show uneven softening of bosonic modes due to a stronger coupling near  $k_F$ . This behavior reflects the strong link between the fermionic momenta, the coupling vertices, and ultimately the bosonic susceptibilities near a quantum phase transition.

**Thursday, March 17, 2016 8:00AM - 10:48AM —**

**Session R30 DMP DCMP: Properties of Multiferroic Materials** 329 - Sergey Artyukhin, Rutgers University

**8:00AM R30.00001 Large-amplitude spin dynamics driven by a THz pulse in resonance with an electromagnon**, STEVEN JOHNSON, ETH Zurich — With femtosecond time resolution, x-ray diffraction offers unique capabilities to observe directly the dynamics of long range order. When the x-ray energy is tuned near a core-level transition it is possible in many systems to selectively study the dynamics of long-range order of valence properties such as orbital ordering or magnetic spin. Here I discuss how resonantly enhanced magnetic scattering can be used to quantitatively measure the character and magnitude of spin motion in a coherent electromagnon in  $\text{TbMnO}_3$  driven by a THz frequency electromagnetic field. We observe a  $4^\circ$  rotation of the antiferromagnetically ordered spin spiral plane, a result consistent with a previously published model that suggests this may be a viable route for ultrafast domain switching in multiferroics.

**8:36AM R30.00002 Terahertz excitations of spin-orbital ground state in multiferroic  $\text{Sr}_2\text{FeSi}_2\text{O}_7$** , THUC MAI, C. SVOBODA, E.V. JASPER, M.T. WARREN, J. BRANGHAM, Department of Physics, The Ohio State University, Columbus OH 43210, S-W. CHEONG, Rutgers Center for Emergent Materials, Rutgers University, T-H. HWAN, POSTECH, South Korea, R. VALDÉS AGUILAR, Department of Physics, The Ohio State University, Columbus OH 43210 — We studied the elementary excitations in  $\text{Sr}_2\text{FeSi}_2\text{O}_7$ , a novel multiferroic material, using time domain terahertz spectroscopy. We found 3 absorption modes above the Néel temperature. These modes can be described as optical transitions between the  $\text{Fe}^{2+} 3d^6$  energy levels, that are split by the compressive tetrahedral crystal field and spin orbit coupling. The excitations from the singlet spin-orbital ground state to the upper doublets are both magnetic and electric dipole active. We explored the behavior of these transitions at temperatures below  $T_{N\acute{e}el}$ , and as a function of external magnetic field, applied along different crystalline axes.

**8:48AM R30.00003 Non-reciprocal directional dichroism in the AFM phase of  $\text{BiFeO}_3$  at THz frequencies<sup>1</sup>**, URMAS NAGEL, T. RÖÖM, Natl Inst of Chem Phys & Biophys, Tallinn, D. FARKAS, D. SZALLER, S. BORDÁCS, I. KÉZSMÁRKI, Budapest University of Technology and Economics, Hungary, H. ENGELKAMP, HFML, Radboud University Nijmegen, The Netherlands, Y. OZAKI, Y. TOMIAKI, T. ITO, Electronics and Photonics Research Institute, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan, RANDY S. FISHMAN, Oak Ridge National Laboratory, Tennessee, USA — We did THz absorption spectroscopy of  $\text{BiFeO}_3$  single crystals in the AFM phase, where the spin cycloid is destroyed in magnetic fields between 18 T and 32 T in Voigt geometry at 1.6 K. If  $\mathbf{B}_0 \parallel [1\bar{1}0]$ , we see strong directional dichroism (DD) of absorption of the magnon mode with light propagating along the direction of the ferroelectric polarization  $\mathbf{k} \parallel \mathbf{P} \parallel [111]$  and  $\mathbf{e}^\omega \parallel [1\bar{1}0]$ ,  $\mathbf{b}^\omega \parallel [\bar{1}12]$ . The sign of DD can be reversed (i) by reversing the direction of  $\mathbf{B}_0$  or (ii) by flipping the sample, thus reversing the propagation direction of light. The observed effect is caused by the strong magneto-electric coupling in the collinear AFM phase.

<sup>1</sup>Research sponsored by the Estonian Ministry of Education and Research (IUT23-3).

**9:00AM R30.00004 Ultrafast Anisotropic Optical Response and Coherent Acoustic Phonon Generation in Polycrystalline BaTiO<sub>3</sub>-BiFeO<sub>3</sub><sup>1</sup>**, B. A. MAGILL, G. A. KHODAPARAST, M. GYU KANG, Y. ZHOU, H-C SONG, S. PRIYA, Virginia Tech — Ultrafast optical spectroscopy can provide insight into fundamental microscopic interactions, dynamics and the coupling of several degrees of freedom. Pump/ probe studies can reveal the answer to questions like What are the achievable switching speeds in multiferroics?, What is the influence of the crystallographic orientation and domain states on the available switching states?, and What is the effect of the hetrostructure on promoting the coupling between the varying field excitations?. In this presentation, we report on two color (400/800nm) ultrafast pump-probe differential reflectance spectroscopy of *BiFeO<sub>3</sub> – BaTiO<sub>3</sub>* structures. The (001) – *BiFeO<sub>3</sub> – BaTiO<sub>3</sub>* thin films were prepared using pulsed laser deposition on vicinal *SrTiO<sub>3</sub>* substrates using LSMO bottom electrodes. Crystal orientation and topography were analyzed by x-ray diffraction and atomic force microscopy. The films were found to exhibit perovskite phase and in our study, we introduce the first observation of photoexcited strain waves, with the frequencies in the GHz range.

<sup>1</sup>Supported by the AFOSR through grant FA9550-14-1-0376.

**9:12AM R30.00005 Optical diode effect at THz frequencies of spin-wave excitations in the room-temperature multiferroic BiFeO<sub>3</sub><sup>1</sup>**, TOOMAS RÕÖM, U. NAGEL, National Institute of Chemical Physics and Biophysics, Tallinn, Estonia, S. BORDÁCS, I. KÉZSMÁRKI, Budapest University of Technology and Economics, Budapest, Hungary, H.T. YI, S.-W. CHEONG, Rutgers Univ., New Jersey, J. H. LEE, R.S. FISHMAN, Oak Ridge National Laboratory, Tennessee — We studied the unidirectional transmission of THz radiation in BiFeO<sub>3</sub> crystals, the unique multiferroic compound offering a real potential for room-temperature applications. We found that the optical magnetoelectric effect generated by spin waves in BiFeO<sub>3</sub> is robust enough to cause considerable nonreciprocal directional dichroism in the GHz-THz range even at room temperature. The optical magnetoelectric effect in BiFeO<sub>3</sub> is dominated by two types of spin-current induced polarizations, while the exchange-striction and single-ion polarization terms do not significantly contribute to it. Our work demonstrates that the nonreciprocal directional dichroism spectra and their theoretical analysis provide microscopic model of the magnetoelectric couplings in multiferroic materials.

<sup>1</sup>We acknowledge the Estonian Grant IUT23-3; the Hungarian OTKA K 108918, OTKA PD 111756, Bolyai 00565/14/11; the DOE, Office of Sciences, Basic Energy Sciences, Mat. Sciences and Eng. Div., and the DOE Grant DE-FG02-07ER46382

**9:24AM R30.00006 Magnetoelectric coupling in hexagonal LuFeO<sub>3</sub> thin films**, HAO LIU, Fudan University — The magnetic and polar properties of single-crystalline hexagonal LuFeO<sub>3</sub> films have been studied. Both theoretical and experimental approaches indicated the coexisting of multiple ferroic orders. The spontaneous electric polarization is associated with a structural change, which also influences the magnetic properties, predicting a strong magnetoelectric coupling in these films. To investigate the magnetoelectric coupling, the micro capacitance structures were fabricated by photolithography combined with Ar ion beam etching method. The capacitance vs voltage curves show significant magnetic field effect, indicating strong magnetoelectric coupling in this system.

**9:36AM R30.00007 Temperature Dependent Atomic and Electronic Structure of LuFe<sub>2</sub>O<sub>4</sub>**, SIZHAN LIU, HAN ZHANG, New Jersey Institute of Technology, SANJIT GHOSE, Brookhaven National Laboratory, THOMAS EMGE, Rutgers University, DANIEL KAPLAN, U.S Army RDECOM-ARDEC, CHERNO JAYE, DANIEL FISHER, NIST, SANG-WOOK CHEONG, Rutgers University, TREVOR TYSON, New Jersey Institute of Technology — Structural measurements on multiple length scales have been conducted over a broad range of temperatures. These measurements have been complemented by optical and thermal measurements. The nature of the observed local atomic and electronic structural changes will be discussed and compared with previous work. This work is supported by DOE Grant DE-FG02-07ER46402.

**9:48AM R30.00008 Structure of Multiferroic RAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> and RFe<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> in the Region of High Electric Polarization**, HAN ZHANG, TIAN YU, New Jersey Institute of Technology, ZHIQIANG CHEN, Center for High Pressure Science and Technology Advanced Research, China, CHRISTIE NELSON, Brookhaven National Laboratory, LEONARD BEZMATERNYKH, L.V. Kirensky Institute of Physics, YU-SHENG CHEN, Advanced Photon Source, Argonne National Laboratory, MILINDA ABEYKOON, Brookhaven National Laboratory, TREVOR TYSON, New Jersey Institute of Technology — The multiferroic system RAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub> is known to exhibit a strong coupling of magnetic field to the electrical polarization at low temperature (below ~100 K). A giant magnetoelectric effect was found in this system. Recent work by us (PRB B 92 104108) reveals evidence for changes in the local structure at low temperature. In this work we explore the structural changes using single crystal diffraction and other structural probes. Comparisons between the Fe and Al based systems will be made. This work is supported by DOE Grant DE-FG02-07ER46402.

**10:00AM R30.00009 Optical and Electro-Optical Properties of RFe<sub>2</sub>O<sub>4</sub> (R = Y and Yb) Thin Films<sup>1</sup>**, RAM RAI, MICHELLE PASCOLINI, JOSHUA HINZ, SUNY Buffalo State — We present optical, and electro-optical properties of RFe<sub>2</sub>O<sub>4</sub> (R = Y and Yb) thin films deposited on sapphire and YSZ substrates by reactive electron-beam deposition. In order to investigate the electronic transitions and optical properties, we measured transmittance and reflectance of the RFe<sub>2</sub>O<sub>4</sub> thin films in the 1 – 6 eV photon energy range and at temperatures from 10 to 400 K. The optical spectra of RFe<sub>2</sub>O<sub>4</sub> show several electronic peaks arising from Fe 2p<sup>+</sup> to d<sub>on</sub>-site and O 2p to Fe 3d, Y 4d and Y 5s (Yb 5d and 6s) charge-transfer transitions. Interestingly, the electronic excitations display strong temperature dependence with an anomaly between 170 K and 190 K, indicating a structural distortion. Moreover, the electro-optical effects up to 10 % have been observed in the RFe<sub>2</sub>O<sub>4</sub> thin films at 10 K for applied electric fields below 1 kV/cm. These electro-optical effects mostly occur between the photon energy of 1 and 3 eV, vary almost linearly with applied fields, and the effects disappear above 150 K. We will discuss the driving mechanism for the observed electro-optical effects of these compounds.

<sup>1</sup>National Science Foundation (DMR-1406766)

**10:12AM R30.00010 Magnetically induced ferroelectricity in single crystalline ferrimagnet, Mn<sub>2</sub>Mo<sub>3</sub>O<sub>8</sub><sup>1</sup>**, SHALINEE CHIKARA, JOHN SINGLETON, National High Magnetic Field Lab, Los Alamos National Laboratory, Los Alamos, NM 87544, USA, BIN GAO, YAZHONG WANG, SANG-WOOK CHEONG, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA, VIVIEN ZAPF, National High Magnetic Field Lab, Los Alamos National Laboratory, Los Alamos, NM 87544, USA — We present magnetization and electric polarization results on multiferroic ferrimagnet molybdate system, Mn<sub>2</sub>Mo<sub>3</sub>O<sub>8</sub> in pulsed magnetic fields. Mn<sub>2</sub>Mo<sub>3</sub>O<sub>8</sub>, also known as the mineral isiemite crystallizes in a hexagonal P6<sub>3</sub>mc space group. The magnetism is attributed to the Mn ions whereas the Mo is diamagnetic. The Mo and Mn atoms are stacked alternately along c-axis. The Mn ions form a hexagonal lattice and occur in octahedral and tetragonal coordination. The spins on two different Mn sites give rise to ferrimagnetism. The system orders at about 42 K accompanied by a lambda like anomaly in heat capacity. Mn<sub>2</sub>Mo<sub>3</sub>O<sub>8</sub> shows anisotropic magnetization with a change in slope at 40 K signaling possibly an AFM to ferrimagnet ordering. We observe magnetic field induced electric polarization in our preliminary results and an anomaly at 40 K corresponding to T<sub>N</sub>.

<sup>1</sup> A portion of this work was performed at the NHMFL, which is supported by National Science Foundation Cooperative Agreement No. DMR-1157490, the State of Florida, and the U.S. Department of Energy.

**10:24AM R30.00011 Temperature Dependent Structure of BiFeO<sub>3</sub>: Probing For Spin Lattice Correlations**, TREVOR TYSON, TIAN YU, HAN ZHANG, NJIT, MILINDA ABEYKOON, Photon Sciences, Brookhaven National Laboratory — The local structure of BiFeO<sub>3</sub> has been measured over a broad range of temperatures and in magnetic fields. This detailed study explores the nature of the coupling of magnetism and with the lattice on crossing magnetic transitions. Estimates on the structural changes are given. This work is supported by DOE Grant DE-FG02-07ER46402.

**10:36AM R30.00012 Lattice and magnetic excitations in NdFe<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub>**, RICARDO LOBO, ESPCI PSL, CNRS, UPMC — We measured the temperature dependent polarized infrared spectra of multiferroic NdFe<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub>. The spectra is mostly temperature independent except for the lowest energy phonon in the hexagonal plane. This phonon splits into two at around 60 K, a temperature sensibly larger than the system Néel temperature of 31 K. X-ray scattering indicates that the lattice parameters have an anomaly at the same temperature that the phonon splits. Using inelastic neutron scattering we looked for magnetic excitations that could explain be coupled to phonons. Momentum and energy dispersion curves around the magnetic Bragg peaks show magnetic excitations at energies comparable to the split phonon. We will discuss these results in terms of magnetic fluctuations and activation of Brillouin zone boundary modes.

**Thursday, March 17, 2016 8:00AM - 11:00AM —**  
**Session R32 DCP: Plasmonics and Beyond II: Ultrafast Dynamics** 332 - Teri Odom, Northwestern University

**8:00AM R32.00001 Quantum theory for plasmon-assisted local field enhancement**, ILYA GRIG-ORENKO, New York City College of Technology — We applied quantum theory for nonlocal response and plasmon-assisted field enhancement near a small metallic nanoscale antenna in the limit of weak incoming fields. A simple asymmetric bio-inspired design of the nanoantenna for polarization-resolved measurement is proposed. The spatial field intensity distribution was calculated for different field frequencies and polarizations. We have shown that the proposed design the antenna allows us to resolve the polarization of incoming photons.

**8:12AM R32.00002 Propagating and localized surface plasmons in Ag nanostructures**, MACIEJ DABROWSKI, YANAN DAI, HRVOJE PETEK, Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA 15260 — Plasmonic excitations strongly depend on the size, geometry and dielectric environment of nanoscale metals. Here, we study an epitaxially grown Ag nanostructures on Si(001) and Si(111) surfaces by Low Energy Electron Microscopy/Photoemission Electron Microscopy (LEEM/PEEM). Using the combination of LEEM and broadly tunable femtosecond laser excited multiphoton PEEM we image how single crystalline metallic nanostructures form and how plasmon excitations depend on the particle structure and laser excitation parameters. For Ag pyramids with the dimensions of few hundreds nanometers, dipolar and quadrupolar localized surface plasmons are observed. For Ag wires with several micrometer lengths, both localized and propagating surface plasmons can be excited, depending on the polarization, particle orientation and energy of the excitation. Finally, in larger Ag islands, several micrometers in size, the interference patterns are created by plasmon waves excited at the island edges. In addition to plasmonic response, light diffraction patterns around the Ag nanostructures are discussed.

**8:24AM R32.00003 Plasmon-exciton coupling at Ag nanocluster decorated TiO<sub>2</sub>(110) surface studied by time-resolved two-photon photoemission spectroscopy**, SHIJING TAN, ADAM ARGONDISO, HRVOJE PETEK, Department of Physics and Astronomy, University of Pittsburgh — We study the spectroscopy and electron dynamics at Ag nanocluster decorated TiO<sub>2</sub>(110) surface upon photoexcitation of plasmonic modes by two-photon photoemission spectroscopy (2PP). Depositing Ag onto a reduced rutile TiO<sub>2</sub>(110) surface at room temperature forms pancake-like Ag particles with an average diameter of 4 nm and height of 1.5 nm. Measurements of the 2PP yield from Ag/TiO<sub>2</sub> surface with tunable femtosecond laser excitation show enhancement at plasmonic resonances. Exciting with s-polarization ( $\vec{S}$ ) the plasmonic resonance enhancement has a single peak at 3.1 eV, whereas with p-polarization ( $\vec{P}$ ) there is an additional more intense resonance at 3.8 eV. We attribute the 3.1 and 3.8 eV peaks to the in-plane and the surface-normal plasmon modes respectively. Crystal azimuth orientation dependent excitation with ( $\vec{S}$ ) shows an anisotropy in the 2PP spectra for the 3.1 eV in-plane plasmon mode when the laser electric field is aligned in the [001] vs. [110] directions. The existence of two plasmon modes and the in-plane plasmon anisotropy imply that the plasmon modes are perturbed by coherent coupling with excitons in the rutile TiO<sub>2</sub> substrate. We speculate that plasmon-exciton resonant energy transfer could play an important role in the plasmonically enhanced photocatalysis at the Ag/TiO<sub>2</sub> surface.

**8:36AM R32.00004 Plasmonics at the Space-Time Limit**, MARTIN AESCHLIMANN, Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Germany — The optical response of metallic nanostructures exhibits fascinating properties: local field interference effects that lead to strong variations of the near field distribution on a subwavelength scale, local field enhancement, and long lasting electronic coherences. Coherent control in general exploits the phase properties of light fields to manipulate coherent processes. Originally developed for molecular systems these concepts have recently been adapted also to nano-optical phenomena. Consequently, the combination of ultrafast laser spectroscopy, i.e. illumination with broadband coherent light sources, and near-field optics, opens a new realm for nonlinear optics on the nanoscale. To circumvent the experimental limitation of optical diffraction we use a photoemission electron microscope (PEEM) that has been proved to be a versatile tool for the investigation of near field properties of nanostructures with a spatial resolution of only a few nanometers and that allows for new spectroscopy techniques with ultrafast time resolution [1,2]. We introduce a new spectroscopic method that determines nonlinear quantum-mechanical response functions beyond the optical diffraction limit. While in established coherent two-dimensional (2D) spectroscopy a four-wave-mixing response is measured using three ingoing and one outgoing wave, in 2D nanoscopy we employ four ingoing and no outgoing waves. This allows studying a broad range of phenomena not accessible otherwise such as space-time resolved coupling, transport, and Anderson localized photon modes [3, 4]. [1] M. Aeschlimann et al, Nature **446**, 301 (2007) [2] M. Aeschlimann et al, PNAS **107** (12), 5329 (2010) [3] M. Aeschlimann et al, Science **333**, 1723-1726 (2011) [4] M. Aeschlimann et al, Nature Photonics **9**, 663, (2015)

**9:12AM R32.00005 Imaging of Surface Plasmons by Ultrafast Multi-Photon Photoemission Electron Microscopy**, YANAN DAI, MACIEJ DABROWSKI, HRVOJE PETEK, Department of Physics and Astronomy, University of Pittsburgh, Pittsburgh, PA 15260 — Silver nanostructures on silicon substrates are characterized by Low Energy Electron Microscopy (LEEM) and their plasmonic modes are imaged by ultrafast femtosecond laser pulse with Multi-Photon Photoemission Electron Microscopy (mP-PEEM). Simulations of Surface Plasmon Polariton (SPP) and Localized Surface Plasmon (LSP) mP-PEEM images are performed by 3D finite difference time domain (FDTD) method in order to characterize the plasmonic excitations. We imaged and simulated the interference patterns of multiple SPPs launched at the edges of microns scale single-crystal Ag islands with excitation wavelengths covering whole visible range. In addition, we studied the plasmonically enhanced excitation and plasmonic field distributions on single-crystal Ag wires of a few microns in length. Finally, we studied plasmon dynamics by recording plasmon field evolution on Ag structures from FDTD simulation.

**9:24AM R32.00006 EELS study of plasmon excitations in LPNE aluminum nanowires**, RODOLFO LOPEZ JR, JAY SHARPING, ERIK MENKE, Univ of California - Merced — We present our current experimental investigations of plasmonic resonances of aluminum nanowire arrays. Ordered nanowires with well-defined shape and size distributions are fabricated on silicon wafers and TEM apertures using lithographically patterned nanowire electrodeposition (LPNE). The structures, which have sizes down to 40 nm in the z direction, and planar sizes varying up to 200nm, exhibit prominent and tunable plasmon resonances which are visible in EELS spectra. The electron energy loss spectra is correlated to the native oxide layer thickness as well as growth parameters of the nanowire array.

**9:36AM R32.00007 Excited carrier dynamics and transport in plasmonic nanostructures<sup>1</sup>**, RAVIS-HANKAR SUNDARARAMAN, PRINEHA NARANG, ADAM JERMYN, HARRY ATWATER, WILLIAM GODDARD III, Joint Center for Artificial Photosynthesis, California Institute of Technology — Surface plasmon resonances provide a pathway to efficiently capture electromagnetic radiation in sub-wavelength structures for energy conversion and photodetection at the nano scale. The complete mechanism involves several microscopic steps spanning length scales from atomic dimensions to tens or hundreds of nanometers, posing challenges for experimental characterization and for first-principles predictions. To provide the basis for predicting and optimizing the complex interplay of materials and geometric effects in plasmon decay-induced excited carrier phenomena, we combined *ab initio* electronic structure calculations, electromagnetic simulations and Boltzmann transport models. In Au, Ag, Cu and Al nanostructures, we find that initial carrier distributions as well as their subsequent transport, relaxation and thermalization are sensitive to electronic structure, exhibiting strong asymmetries between electrons and holes. We predict energy-dependent spatially-resolved carrier distributions collected in plasmonic nanostructures with strong field inhomogeneities, and explore the possibility of tailoring materials and geometry to collect the carrier distributions needed for such applications as photochemically driven CO<sub>2</sub> reduction and water splitting.

<sup>1</sup>This material is based upon work performed by JCAP, a DOE Energy Innovation Hub, supported through the Office of Science of the U.S. Department of Energy under Award Number DE-SC0004993.

**9:48AM R32.00008 Solar upconversion with plasmonic hot carriers**, JENNIFER A. DIONNE, Stanford University — Upconversion of sub-bandgap photons is a promising approach to exceed the Shockley-Queisser limit in solar technologies. Placed behind a solar cell, upconverting materials convert lower-energy photons transmitted through the cell to higher-energy above-bandgap photons that can then be absorbed by the cell and contribute to photocurrent. Because the upconverter is electrically isolated from the active cell, it need not be current-matched to the cell, nor will it add mid-gap recombination pathways. Calculations have indicated that single-junction cell efficiencies can exceed 44% upon addition of an upconverter – a significant improvement over the maximum cell efficiency of 30% without an upconverter. However, due to the low quantum efficiencies and narrow absorption bandwidths of existing upconverters, such significant cell improvements have yet to be observed experimentally. In this presentation, we will describe an entirely new solar upconverting scheme based on hot-carrier injection from a plasmonic absorber to an adjacent semiconductor. The plasmonic system both induces upconversion based on injection of hot-electrons and hot-holes and also enhances light-matter interactions. Low-energy photons incident on a plasmonic particle generate hot electrons and hot holes, which are injected into a semiconducting quantum well and subsequently radiatively recombine. Importantly, the bandgap of the quantum well can be higher than the energy of the incident photon, enabling emission of a higher-energy photon than that absorbed. First, we present analytic calculations showing that efficiencies as high as 25% are possible, significantly higher than existing solid-state upconverters, which are only 2-5% efficient. We also describe how further improvements in the efficiency are possible by employing materials and geometries that allow for more efficient carrier injection. Then, we describe experiments on InGaN/GaN quantum wells decorated with Au disks. On their own, the InGaN/GaN quantum wells do not upconvert. With the addition of the gold disks, strong upconversion is observed. We show how this new upconversion scheme offers spectral tunability across visible and near-infrared frequencies, does not require coherent illumination, is a linear process, and can be broadband. Contributing authors include Guru Naik and Alex Welch, Stanford University

**10:24AM R32.00009 Detecting antibody-antigen reaction using nano ripple gold LSPR based biosensor**, IRAM SALEEM, DHARSHANA WIJESUNDERA, BUDDHI TILAKARATNE, Department of Physics, University of Houston and Texas center for superconductivity TcSUH, WILLIAM WIDGER, Department of Biology and Biochemistry, University of Houston and Texas center for superconductivity TcSUH, WEI-KAN CHU, Department of Physics, University of Houston and Texas center for superconductivity TcSUH — We introduce a simple and cost-effective scheme for bio-sensing using nano-ripple structures. One-dimension metallic nano-ripple structures formed by gas cluster ion beam irradiation have shown polarization of light as well as the localized surface plasmon resonance. These localized surface plasmon resonance (LSPR) based bio sensors not only are capable of label free real time analytical detection but also show high sensitivity. The nano surface morphology determines the changes in the plasmonic properties of nanostructures hence the plasmonic response is tunable. By immobilizing a stable and sterically accessible monolayer of antibody on the surface of these substrates and loading different concentrations of the specific antigen we identified the shift in the LSPR peaks triggered by the change of dielectric function in the neighborhood of the structures. These plasmonic nano-metallic structures can be utilized to observe the shift in the LSPR resonance frequency due to the cycle of adsorption, re-adsorption and reactions taking place on the surface that can potentially be mapped in to reaction mechanics. The bio-sensor has monolayer molecule-coating sensitivity and specific selectivity.

**10:36AM R32.00010 Unique signature of bivalent analyte surface plasmon resonance model: A model governed by non-linear differential equations<sup>1</sup>**, PURUSHOTTAM TIWARI, Georgetown University, XUEWEN WANG, YESIM DARICI, JIN HE, Florida International University, AYKUT UREN, Georgetown University — Surface plasmon resonance (SPR) is a biophysical technique for the quantitative analysis of bimolecular interactions. Correct identification of the binding model is crucial for the interpretation of SPR data. Bivalent SPR model is governed by non-linear differential equations, which, in general, have no analytical solutions. Therefore, an analytical based approach cannot be employed in order to identify this particular model. There exists a unique signature in the bivalent analyte model, existence of an 'optimal analyte concentration', which can distinguish this model from other biphasic models. The unambiguous identification and related analysis of the bivalent analyte model is demonstrated by using theoretical simulations and experimentally measured SPR sensorgrams.

<sup>1</sup>Experimental SPR sensorgrams were measured by using Biacore T200 instrument available in Biacore Molecular Interaction Shared Resource facility, supported by NIH Grant P30CA51008, at Georgetown University

**10:48AM R32.00011 Selective plasmon enhancement of fluorescence towards point of care disease diagnostics**, BISHWAMBHAR SENGUPTA, JINGYI ZHU, Clemson University, RAMAKRISHNA PODILA, APPARAO RAO, Clemson University — Surface plasmon coupled emission (SPCE) is a novel analytical technique in which the isotropic emission of a fluorophore is combined with the surface plasmon resonance of a metal thin film to yield highly directional emission from the so-called plasmaphore and thus greatly increased sensitivity. The optimal SPCE enhancement is achieved by introducing a spacer layer to mitigate fluorescence-quenching arising from metal-fluorophore interactions. Here we report a >10-fold amplification of rhodamine B (RhB) fluorophore when carbon nanomaterials are used as the spacer layer. By combining experimental and density functional theory studies, we found that the rehybridization between CNMs and RhB results in emission redshift. We present SPCE-based biosensors for smart-phone based sensing of different analytes including biomarkers for diseases such as tuberculosis.

**Thursday, March 17, 2016 8:00AM - 11:00AM –**

**Session R33 DPOLY: Organic Electronics and Photonics - Organic Photovoltaics** 336 - Daniel Sinkovits, University of Wisconsin, Stout

**8:00AM R33.00001 ABSTRACT MOVED TO V4.002 –**

**8:36AM R33.00002 Multiple Charge Transfer States at Ordered and Disordered Donor/Acceptor Interfaces**, MICHAEL FUSELLA, BRETT VERRETT, YUNHUI LIN, Princeton University, ALYSSA BRIGEMAN, The Pennsylvania State University, GEOFFREY PURDUM, YUEH-LIN LOO, Princeton University, NOEL GIEBINK, The Pennsylvania State University, BARRY RAND, Princeton University — The presence of charge transfer (CT) states in organic solar cells is accepted, but their role in photocurrent generation is not well understood. Here we investigate solar cells based on rubrene and C<sub>60</sub> to show that CT state properties are influenced by molecular ordering at the donor/acceptor (D/A) interface. Crystalline rubrene films are produced with domains of 100s of microns adopting the orthorhombic phase, as confirmed by grazing incidence XRD, with the (h00) planes parallel to the substrate. C<sub>60</sub> grown atop these films adopts a highly oriented face-centered cubic phase with the (111) plane parallel to the substrate. For this highly ordered system we have discovered the presence of four CT states. Polarized external quantum efficiency (EQE) measurements assign three of these to crystalline origins with the remaining one well aligned with the disordered CT state. Varying the thickness of a disordered blend of rubrene:C<sub>60</sub> atop the rubrene template modulates the degree of crystallinity at the D/A interface. Strikingly, this process alters the prominence of the four CT states measured via EQE, and results in a transition from single to multiple electroluminescence peaks. These results underscore the impact of molecular structure at the heterojunction on charge photogeneration.

**8:48AM R33.00003 Charge Photogeneration in Organic Photovoltaics: Role of Hot versus Cold Charge Transfer Excitons**, KENAN GUNDOĞDU, BHOJ GAUTAM, ROBERT YOUNTS, NC State University, LIANG YAN, UNC, ROBERT YOUNTS, HARALD ADE, NC State University, WEI YOU, UNC, NC STATE UNIVERSITY TEAM, UNIVERSITY OF NORTH CAROLINA TEAM — The role of excess excitation energy on long-range charge separation in organic donor/acceptor bulk heterojunctions continues to be unclear. While ultrafast spectroscopy results argue for efficient charge separation through high energy CT states within the first picosecond (ps) of excitation, charge collection measurements suggest excess photon energy does not increase the current density in bulk heterojunction (BHJ) devices. Here we studied the population dynamics of charge separated polarons upon excitation of high energy polymer states and low energy interfacial CT states in two polymer/fullerene blends from ps to nanosecond (ns) time scales. We observed that the charge separation dynamics do not show significant dependence on excitation energy. These results confirm that excess exciton energy is not necessary for the effective generation of charges.

**9:00AM R33.00004 Fully conjugated donor-acceptor block copolymers as model systems for studies of charge transfer<sup>1</sup>**, MELISSA APLAN, YOUNGMIN LEE, CHRISTOPHER GRAY, THOMAS MALLOUK, ENRIQUE GOMEZ, Pennsylvania State University — Fully conjugated block copolymers, consisting of an electron donor and an electron acceptor block, can serve as the active layer in organic photovoltaic devices. Incorporating the donor-acceptor interface within the chemical structure enables model studies of charge transfer. We synthesized a series of block copolymers consisting of a P3HT electron donor and a push-pull polymer electron acceptor, yielding: poly(3-hexylthiophene)-block-poly-((9-(9-heptadecanyl)-9H-carbazole)-1,4-diyl-alt-[4,7-bis(3-hexylthiophen-5-yl)-2,1,3-benzothiadiazole]-2',2''-diyl) (P3HT-b-PCT6BT), poly(3-hexylthiophene)-block-poly-((9,9-dioctylfluorene)-2,7-diyl-alt-[4,7-bis(3-hexylthiophen-5-yl)-2,1,3-benzothiadiazole]-2',2''-diyl) (P3HT-b-PFT6BT), and poly(3-hexylthiophene)-block-poly-((2,5-dihexylphenylene)-1,4-diyl-alt-[4,7-bis(3-hexylthiophen-5-yl)-2,1,3-benzothiadiazole]-2',2''-diyl) (P3HT-b-PPT6BT). By altering the electron rich unit of the acceptor, we adjust the energy difference between donor and acceptor HOMOs. Using photoluminescence, we observe no evidence of exciton dissociation to a charge transfer state in P3HT-b-PCT6BT. In P3HT-b-PFT6BT and P3HT-b-PPT6BT we observe varying degrees of intrachain charge transfer. These results measure the critical driving force needed for charge transfer.

<sup>1</sup>Fully conjugated donor-acceptor block copolymers as model systems for studies of charge transfer

**9:12AM R33.00005 Morphology-insensitive Performance Facilitates Transition from Spin-Coating to Roll-to-Roll Coating For High-Performance, Solution-Processed Solar Cells**, DEAN DELONGCHAMP, National Institute of Standards and Technology — Solution processing via roll-to-roll (R2R) coating promises a low cost, low thermal-budget, sustainable revolution for the production of solar cells. Yet virtually all high efficiency solution processed research cells have been demonstrated by spin-coating, a low-volume deposition process. We present detailed device and morphology studies of an organic photovoltaic (OPV) system deposited by a high volume manufacturing technique, blade-coating, that achieves greater than 9.5 % power conversion efficiency (PCE). The average crystal domain orientation and characteristic phase separation length distribution are markedly different when deposited by blade-coating rather than spin-coating. This result allows us to determine which aspects of morphology are not relevant to the PCE of this system. Whether the crystallites are “face on” or “edge on” does not appear to impact the PCE of system, nor does the length scale or “hierarchical” nature of the phase length scale. Persistent morphological qualities that may be associated with high PCE in this system are relatively pure phases and relatively strong diffraction. We posit that OPV systems in which the PCE is less sensitive to morphology may also be less sensitive to film thickness, enabling some to maintain high PCE in active layers thicker than greater than ~200 nm. We confirm that blade-coating is a suitable prototyping technique for R2R coating by demonstrating nominally identical morphologies for both piece blade-coating and continuous-web, slot-die coating.

**9:48AM R33.00006 Contorted hexabenzocoronene derivatives enable fullerene-free, semi-transparent solar cells with record-breaking single-junction photovoltage**, NICHOLAS DAVY, MELDA SEZEN, YUEH-LIN LOO, Department of Chemical and Biological Engineering, Princeton University — Recent work on tuning the chemical structure of contorted hexabenzocoronene (cHBC) in our group has yielded derivatives with a spectrum of energy levels and absorption profiles, greatly improving the utility of these materials as donor and/or acceptor constituents in organic solar cells. Here, we report planar-heterojunction solar cells comprising an extended heterocyclic cHBC donor and a halogenated cHBC acceptor. By harvesting primarily near-UV light, these devices exhibit a record open-circuit voltage of 1.5 V; this value is higher than any previously reported value for a single-junction organic solar cell. Our active layers are molecularly smooth and pinhole-free; these devices should be scalable to large areas without incurring substantial loss to performance. With a transmittance of 79% across the visible, our devices can be vertically integrated to directly drive the switching of electrochromic windows, where existing prototypes depend on tandem solar cells having near-infrared absorbers.

**10:00AM R33.00007 Layer-by-layer fabrication of supramolecular dyes on TiO<sub>2</sub> surfaces for optoelectronic applications**, XIAOQING KONG, SHAWN MAGUIRE, Stevens Institute of Technology, DIANE LYE, MARCUS WECK, New York University, STEPHANIE LEE, Stevens Institute of Technology — We present a modular layer-by-layer approach based on metal coordination chemistry to assemble supramolecular dyes exhibiting increased absorption in the visible range on electrode surfaces. Specifically, palladiated bis-pincer complexes (Pd-BPCs) were employed as linkers between pyridyl-terminated organic molecules via dative bonding. By alternately immersing mesoporous TiO<sub>2</sub>-coated glass substrates in solutions containing dissolved zinc porphyrin (ZnP) and Pd-BPCs, supramolecular dyes were assembled layer-by-layer on the TiO<sub>2</sub> surfaces. UV-visible absorption spectra of these assembled structures revealed a linear increase in the Soret and Q bands of ZnP after each immersion of the substrate in the ZnP solution. Coordination of the ZnP layers with Pd-BPC resulted in a slight red shift (<10 nm) of the absorption bands. The modular nature of the assembly process afforded the incorporation of other pyridyl-terminated organic molecules in specific layers of the supramolecular assemblies. By assembling unique organic dyes that absorb different wavelengths of light, we expect to expand light absorption across the visible region of the solar spectrum for solar cell applications.

**10:12AM R33.00008 Surprising increase in photostability of organic amorphous materials by efficient molecular packing**, YUE QIU, Univ of Wisconsin, Madison, LUCAS ANTONY, JUAN DE PABLO, University of Chicago, MARK EDIGER, Univ of Wisconsin, Madison — Photochemically robust materials are desired for organic electronics. Previous work has demonstrated that crystal packing can strongly influence photochemical reactivity. In amorphous materials, however, similar efforts to tune photostability have not been successful. In this work, we show that organic glasses prepared by physical vapor deposition can be highly stable against photo-isomerization. Disperse orange 37 (DO37), an azobenzene derivative, is studied as a model molecule. The thickness and molecular orientation of DO37 thin films can be altered by the photo-isomerization reaction. We use spectroscopic ellipsometry to measure sample thickness and molecular orientation during light irradiation. By changing the substrate temperature during the deposition, photostability can increase 2 to 3 orders of magnitude relative to the liquid-cooled glass. We find that photostability correlates with density of packing, with density increases of up to 1.3%. Simulations also show that glasses with higher density can be significantly more photo-stable. These results show for the first time that photostability of glasses can be significantly modulated by molecular packing. And they may provide insight in designing organic photovoltaics and light emission devices with longer lifetimes.

**10:24AM R33.00009 Fixed Junction Photovoltaic Devices Based On Polymerizable Ionic Liquids<sup>1</sup>**, AUSTIN LIMANEK, DR. JANELLE LEGER, Western Washington University — Recently, polymer-based photovoltaic devices (PPVs) have received significant attention as a possible affordable, large area and flexible solar energy technology. In particular, research on chemically fixed p-i-n junctions in polymer photovoltaic devices has shown promising results. These devices are composed of ionic monomers in a polymer matrix sandwiched between two electrodes. When a potential is applied, the ionic monomers migrate towards their corresponding electrodes, enabling electrochemical doping of the polymer. This leads to the formation of bonds between the polymer and ionic monomers, resulting in the formation of a chemically fixed p-i-n junction. However, early devices suffered from long charging times and low overall response. This has been attributed to the low phase compatibility between the ionic monomers and the polymer. It has been shown for light-emitting electrochemical cells, replacing the ionic monomers with polymerizable ionic liquids (PILs) mitigates these challenges. We will present the use of PILs as the dopant in fixed junction PPV devices. Preliminary devices demonstrate significantly improved performance, decreased charging times, and high open circuit voltages.

<sup>1</sup>This research supported by the National Science Foundation DMR-1057209

**10:36AM R33.00010 Physical and electrical models for interpreting AC and DC transport measurements in polymer solar cells**, MAX MCINTYRE, MARIAN TZOLOV, RAQUEL COSSEL, SETH PEELER, Lock Haven Univ — We have fabricated and studied bulk heterojunction solar cells using a mixture of the low bandgap material PCPDTBT and PCBM-C60. Our transport studies show that the devices in dark have good rectification and they respond to AC voltage as a simple RC circuit. The illumination causes an additional contribution to the impedance, which varies with the level of illumination. One proposed model is that photo-generated charges can become trapped in potential wells. These charges then follow a Debye relaxation process, which contributes to a varying dielectric constant. Another proposed model is based on a RC circuit model with two capacitors which can describe the varying capacitance behavior. The physical mechanism for this model is that photo-generated charges become accumulated at the interface between PCPDTBT and PCBM-C60 and form an additional layer of charge. We will show that our circuit models and their analogous physical models can predict the AC and DC responses of polymer solar cells.

**10:48AM R33.00011 Dye-Sensitized Carbon Nano-Yarn Based Photovoltaic Cells with Enhanced Electron-Hole Separation and Barrier Characteristics<sup>1</sup>**, H. JUSTIN MOORE, MIGUEL LEAL, GLENN GRIS-SOM, TAREK TRAD, NAZMUL ISLAM, AHMED TOUHAMI, M. JASIM UDDIN, University Texas Rio Grande Valley — Over the last 30 years dye-sensitized solar cells have received considerable interest as an alternative energy source due to their low-cost, environmental sustainability, flexibility, and an abundant number of other practical applications. Flexible carbon nanotube-yarn based photo voltaic cells have shown considerable advantages over metal wire based solar cells or non-flexible substrates like indium-doped tin oxide glass. Carbon nanotubes are superior for photo voltaic cells due to their lower electrical resistance, excellent electrocatalytic activity, and high mechanical integrity. Here, we introduce the use of poly(3-hexylthiophene-2,5-diyl), [6.6] diphenyl C<sub>62</sub> bis(butyric acid methyl ester), cadmium sulfide-cadmium selenide quantum dots, and ruthenium-based dye N719 to locally increase electron generation, decrease electron-hole pair recombination, as well as enhancing barrier characteristics. Our prototype 3-dimensional carbon nano-yarn based photovoltaic cells show an enhancement in photon to energy conversion efficiency (>6.5%). This along with prolonged environmental stability makes for a very promising solar cell.

<sup>1</sup>NIH, NSF, Welch Foundation

**Thursday, March 17, 2016 8:00AM - 11:00AM –**  
**Session R34 DPOLY: Polymer Glasses** 337 - Rob Hoy, University of South Florida

**8:00AM R34.00001 Elastic yielding after  $\gamma$ -irradiation of cold-drawn polymer glasses<sup>1</sup>**, PANPAN LIN, Univ of Akron, QUAN XU, China University of Petroleum, ABRAHAM JOY, SHI-QING WANG, Univ of Akron — Elastic yielding shows up when a considerable retractive stress rises from a piece of cold-drawn polymer glass during annealing at temperatures above storage temperature .....[1,2]. This phenomenon indicates significant chain tension built up during cold drawing. To explore the role of chain networking, we applied  $\gamma$ -irradiation to produce chain scission and cause partial breakdown of the chain network in the pre-necked polymer glasses. To demonstrate universality, four different glasses, i.e., polycarbonate (PC), polystyrene (PS), poly(methyl methacrylate) (PMMA), and poly(2,6-dimethyl-1,4-phenylene oxide) (PPE) were first subjected to uniaxial extension at room temperature before the irradiation. Our data shows that the retractive stress significantly decreases in magnitude with increasing dosage of the  $\gamma$ -irradiation. The diminishing elastic yielding effect may be due to the loss of chain tension by chain scission brought about by the irradiation. [1] S. Cheng and S.-Q. Wang, Phys. Rev. Lett. **110**, 065506 (2013). [2] S. Cheng and S.-Q. Wang, Macromolecules **47**, 3661 (2014).

<sup>1</sup>This work is support, in part, by ACS-PRF (54047-ND7).

**8:12AM R34.00002 To explore the nature of mechanical stress of polymeric glass by stress relaxation tests<sup>1</sup>**, XIAOXIAO LI, JIANNING LIU, PANPAN LIN, SHI-QING WANG, University of Akron — In a glassy polymer intermolecular interactions glue all segments into one single macroscopic piece thanks to attractive van der Waals bonding. The cohesive strength of such a primary structure is rather weak. If the molecular weight is sufficiently high, the covalent bonding can "magically" take part in the cohesion of the polymer glass through formation of a chain network. This picture of hybrid structure enables us to delineate the nature of mechanical stress [1]. Under either extension or compression, we performed stress relaxation experiments in both pre-yield and post-yield regimes to illustrate how inter-segmental and intra-segmental components of stress emerge in the different regimes. [1] S.-Q. Wang, S. Cheng, P. Lin, and X. Li, J. Chem. Phys. 141, 094905 (2014).

<sup>1</sup>This work is supported, in part, by a NSF grant (DMR-EAGER-1444859).

**8:24AM R34.00003 Role of dynamical heterogeneities on the viscoelastic spectrum of polymers: a stochastic continuum mechanics model**, ROBIN MASUREL, CNRS UPMC ESPCI ParisTech PSL Res Univ, Lab SIMM, SABINE CANTOURNET, MINES ParisTech, PSL-Research University, MAT Centre des matériaux, ALAIN DEQUIDT, Univ Clermont Ferrand, Inst Chim Clermont Ferrand, DIDIER LONG, Laboratoire Polymères et Matériaux Avancés, HELNE MONTES, FRANOIS LEQUEUX, CNRS UPMC ESPCI ParisTech PSL Res Univ, Lab SIMM — Amorphous polymers in their glass transition regime can be described as a tiling of nanometric domains. Each domain exhibits its own relaxation time which is distributed over at least 4 decades. These domains are known as dynamical heterogeneities. This article will describe the mechanics of amorphous polymers using a stochastic continuum mechanics model that includes their heterogeneous dynamics. Solving this model both by finite elements and using a self-consistent method, we find a viscoelastic relaxation spectrum quantitatively similar to that of an experimentally measured one in a polymer. We show evidence that elastic couplings between domains control the stress relaxation after a step strain and result in a narrowing of the long-time region of the viscoelastic spectrum (as compared to that of dynamical heterogeneities).

**8:36AM R34.00004 Recovery from nonlinear creep provides a window into physics of polymer glasses**, JAMES CARUTHERS, GRIGORI MEDVEDEV, Purdue University — Creep under constant applied stress is one of the most basic mechanical experiments, where it exhibits extremely rich relaxation behavior for polymer glasses. As many as five distinct stages of nonlinear creep are observed, [1] where the rate of creep dramatically slows down, accelerates and then slows down again. Modeling efforts to-date has primarily focused on predicting the intricacies of the nonlinear creep curve. We argue that as much attention should be paid to the creep recovery response, when the stress is removed. The experimental creep recovery curve is smooth, where the rate of recovery is initially quite rapid and then progressively decreases. In contrast, the majority of the traditional constitutive models predict recovery curves that are much too abrupt. A recently developed stochastic constitutive model that takes into account the dynamic heterogeneity of glasses produces a smooth creep recovery response that is consistent with experiment. 1. G. A. Medvedev and J. M. Caruthers, Polymer 74, 235 (2015)

**8:48AM R34.00005 Multi-step deformations – a stringent test for constitutive models for polymer glasses**, GRIGORI MEDVEDEV, JAMES CARUTHERS, Purdue University — A number of constitutive models have been proposed to describe mechanical behavior of polymer glasses, where the focus has been on the stress-strain curve observed in a constant strain rate deformation. The stress-strain curve possesses several prominent features, including yield, post-yield softening, flow, and hardening, which have proven challenging to predict. As a result, both viscoplastic and nonlinear viscoelastic constitutive models have become quite intricate, where a new mechanism is invoked for each bend of the stress-strain curve. We demonstrate on several examples that when the models are used to describe the multi-step deformations vs. the more common single strain rate deformation, they produce responses that are qualitatively incorrect, revealing the existing models to be parameterizations of a single-step curve. A recently developed stochastic constitutive model has fewer problems than the traditional viscoelastic/viscoplastic models, but it also has difficulties. The implications for the mechanics and physics of glassy polymers will be discussed.

**9:00AM R34.00006 Brittle-ductile transition under compression of glassy polymers<sup>1</sup>**, JIANNING LIU, XIAOXIAO LI, PANPAN LIN, Univ of Akron, SHIWANG CHENG, Oak Ridge National Laboratory, WEIYU WANG, Univ of Tennessee, JIMMY MAYS, Oak Ridge National Laboratory, SHI-QING WANG, Univ of Akron — Polymeric glasses of high molecular weight are always ductile in compression. Even the most brittle (in tensile extension) polystyrene is ordinarily ductile in uniaxial compression. Thus, it seems that theoretical studies only need to develop a description of yielding and post-yield plastic deformation for polymer glasses. But can yielding take place in compression if the molecular weight is sufficiently reduced? In other words, can alpha processes be greatly accelerated during external deformation in absence of chain networking? Must a new paradigm account for the role of chain networking that only takes place in polymers of high molecular weight? To address these questions, we systematically explored the response over a range of temperature to uniaxial compression at different rates of polystyrene with various molecular weights and molecular weight distributions. Our preliminary results [1] show that PS of low molecular weight is brittle in compression and chain networking is necessary (but not sufficient) to ensure a ductile response. [1] Liu, J.; Lin, P.; Cheng, S.; Wang, W.; Mays, J. W.; Wang, S.-Q. Polystyrene glasses under compression: Ductile and brittle responses. *ACS Macro Letters* 2015, 1072-1076.

<sup>1</sup>This work is supported, in part, by a NSF grant (DMR-EAGER-1444859).

**9:12AM R34.00007 Incorporating the effect of orientation hardening in an effective temperature nonequilibrium theory for glassy polymers**, JINGKAI GUO, Johns Hopkins Univ, RUI XIAO, Hohai Univ, THAO NGUYEN, Johns Hopkins Univ — Amorphous polymers exhibit a wide range of time and temperature dependent behavior. Recently, Xiao and Nguyen developed an effective temperature theory that can capture a wide variety of nonequilibrium behaviors at moderate strains. At large strains, the stress response of glassy polymers is dominated by strain hardening as a result of chain alignment. The goal of this study was to extend the effective temperature theory to large deformation and make it capable of modeling strain hardening from deformation-induced molecular alignment. We compared two approaches. In the spirit of internal state variable thermodynamics theory, we introduced a series of stretch-like internal state variables to characterize the molecular resistance to plastic flow associated with each inelastic mechanism. The dependence of free energy on the internal state variables naturally gives rise to a deformation dependent back stress. The flow rule and the evolution of effective temperatures were derived in a thermodynamically consistent manner. In the second approach, we introduced a steady-state limit in the evolution of the effective temperature characterizing the nonequilibrium structure of the material. Both approaches can well capture the experimentally measured phenomena of orientation hardening, including the development of deformation-induced anisotropy in the yield strength and hardening modulus, the Bauschinger effect, and differences in the hardening moduli in tension and compression of pre-oriented specimens.

**9:24AM R34.00008 An effective temperature theory coupling structural evolution and viscoplastic deformation of glassy polymers**, THAO NGUYEN, Department of Mechanical Engineering, Johns Hopkins University, RUI XIAO, Department of Engineering Mechanics, Hohai University — Glassy polymers are amorphous polymers that have been driven out of equilibrium below the glass transition temperature. In the nonequilibrium state, the polymer chains continue to slowly rearrange towards a lower entropy state, which causes physical properties to change with time in a process referred to as physical aging. Physical aging can be reversed by plastic deformation, which moves the material further away from equilibrium. Though structural evolution and viscoplasticity are interdependent, they have been treated as separate processes and described by different theoretical approaches. Here, we introduce a new theory that strongly couples viscoplasticity and structural evolution through an effective temperature thermodynamic framework and a constitutive model for the dependence of the relaxation time on the configurational structure. The theory can describe a wide range of nonequilibrium behaviors, including viscoplasticity, physical aging, mechanical rejuvenation, and the glass transition, using a common set of parameters. We will show comparisons of theoretical predictions and experimental measurements of the effect of cold work and aging on the viscoplastic stress response and energy storage as measured by dynamic scanning calorimetry.

**9:36AM R34.00009 Entropy Theory of Polymer Glass-Formation in Variable Spatial Dimension.**, WEN-SHENG XU, Univ of Chicago, JACK DOUGLAS, National Institute of Standards and Technology, KARL FREED, Univ of Chicago — The importance of packing frustration is broadly appreciated to be an important aspect of glass-formation. Recently, great interest has focused on using spatial dimensionality ( $d$ ) as a theoretical tool for exploring this and other aspects of glass-forming liquids. We explore glass-formation in variable based on the generalized entropy theory, a synthesis of the Adam-Gibbs model with direct computation of the configurational entropy of polymer fluids using an established analytical statistical thermodynamic model. We find that structural relaxation in the fluid state asymptotically becomes Arrhenius in the limit and that the fluid transforms upon sufficient cooling above a critical dimension near into a dense amorphous state with a finite positive residual configurational entropy. The GET also predicts the variation with measures of fragility and of the characteristic temperatures of glass-formation demarking the onset, middle, and end, of the broad glass transition. Direct computations of the isothermal compressibility and thermal expansion coefficient, which are physical measures of packing frustration, demonstrate that these fluid properties strongly correlate with the fragility of glass-formation. Back to three dimensions, we deduce apparently universal relationships between  $d$ , a measure of the breadth of the glass-formation and both the isothermal compressibility and thermal expansion coefficient of polymer melts at  $T_g$ .

**9:48AM R34.00010 Free Volume, Energy, and Entropy at the Polymer Glass Transition: New Results and Connections with Widely Used Treatments**<sup>1</sup>, RONALD WHITE, JANE LIPSON, Dartmouth College — Free volume has a storied history in polymer physics. To introduce our own results, we consider how free volume has been defined in the past, e.g. in the works of Fox and Flory, Doolittle, and the equation of Williams, Landel, and Ferry. We contrast these perspectives with our own analysis using our Locally Correlated Lattice (LCL) model where we have found a striking connection between polymer free volume (analyzed using *PVT* data) and the polymer's corresponding glass transition temperature,  $T_g$ . The pattern, covering over 50 different polymers, is robust enough to be reasonably predictive based on melt properties alone; when a melt hits this  $T$ -dependent boundary of critical minimum free volume it becomes glassy. We will present a broad selection of results from our thermodynamic analysis, and make connections with historical treatments. We will discuss patterns that have emerged across the polymers in the energy and entropy when quantified as "per LCL theoretical segment". Finally we will relate the latter trend to the point of view popularized in the theory of Adam and Gibbs.

<sup>1</sup>The authors gratefully acknowledge support from NSF DMR-1403757

**10:00AM R34.00011 The Effects of Pressure, Local Packing, and Chain Stiffness on the Polymer Glass Transition.**<sup>1</sup>, JANE LIPSON, RONALD WHITE, Dartmouth Chemistry Department — We have recently shown that thermodynamic properties like free volume, energy, and entropy in the polymer melt state can be connected to the polymer's glass transition temperature,  $T_g$ . One of the strongest correlations we have observed is that relating  $T_g$  to polymer free volume. However, isochoric results on glassifying systems, which can be accessed by taking pressure-dependent measurements, reveal that free volume cannot be the only parameter to control the approach to the glass transition. We therefore turn to the effects of pressure, local packing, and chain stiffness. Up to this point we have focused on ambient pressure; we now apply our LCL model analysis to changes in dynamical behavior with  $T$ , or  $P$ . In addition we will correlate our LCL results with various measures of chain stiffness in the context of glassy behavior.

<sup>1</sup>JEGL gratefully acknowledges support from NSF DMR-1403757

**10:12AM R34.00012 Design rules for rational control of polymer glass formation behavior and mechanical properties with small molecular additives**<sup>1</sup>, JAYACHANDRA HARI MANGALARA, DAVID SIMMONS, The University of Akron — Small molecule additives have long been employed to tune polymers' glass formation, mechanical and transport properties. For example, plasticizers are commonly employed to suppress polymer  $T_g$  and soften the glassy state, while antiplasticizers, which stiffen the glassy state of a polymer while suppressing its  $T_g$ , are employed to enhance protein and tissue preservation in sugar glasses. Recent literature indicates that additives can have a wide range of possible effects, but all of these have not been clearly understood and well appreciated. Here we employ molecular dynamics simulations to establish design rules for the selection of small molecule additives with size, molecular stiffness, and interaction energy chosen to achieve targeted effects on polymer properties. We furthermore find that a given additive's effect on a polymer's  $T_g$  can be predicted from its Debye-Waller factor  $\langle u^2 \rangle$  via a function previously found to describe nanoconfinement effects on the glass transition. These results emphasize the potential for a new generation of targeted molecular additives to contribute to more targeted rational design of polymers.

<sup>1</sup>We acknowledge the Keck Foundation and the Ohio Supercomputing Center for financial and computational support of this effort, respectively.

**10:24AM R34.00013 Molecular dynamics simulation of a model polystyrene glass**<sup>1</sup>, ZHUONAN LIU, SHIQING WANG, MESFIN TSIGE, Univ of Akron — We have performed all-atom molecular dynamics (MD) simulations of a model polystyrene glass to examine such concepts as load-bearing strands (LBSs) and activation zones (AZs) surrounding the LBSs that were proposed in a recent molecular model for yielding and failure of polymer glasses.<sup>1</sup> In our simulations, two long chains form a pair of hairpins in a matrix of short polystyrene chains. By deforming the system in different ways including pulling on the two long chains in opposite directions, we examine whether AZs emerge around the two long chains that can be taken as LBSs and how such AZs develop during deformation. 1. S. Wang, S. Cheng, P. Lin, and X. Li, J. Chem. Phys., 2014, 141, 094905.

<sup>1</sup>This work is, in part, supported by NSF grant DMR 144859

**10:36AM R34.00014 Molecular dynamics as observed with probes of different dimensions in thin polymer films<sup>1</sup>**, JIANG ZHAO, HAO ZHANG, JINGFA YANG, FUYI WANG, Institute of Chemistry, Chinese Academy of Sciences, DILIU, Department of Chemistry, Dalian University of Technology, China — Rotational motion of individual fluorescence molecules doped in thin films of polyvinylacetate (PVAc) was monitored by single molecule fluorescence de-focus microscopy. Perylendiimide and its derivatives of different dimension were chosen as probes for local dynamics. The results demonstrate that the local vibration mode detected by different molecules probe depends on dimension of the probes the larger probes the lower frequency. The population of rotating probes is found to increase with temperature elevation, depending on the molecular dimension as well. The comparison of the results with thermo-dynamic measurements helps to shed new light on the physical picture of glass transition.

<sup>1</sup>Supported by MoST of China

**10:48AM R34.00015 Preparation of a series of model poly(*n*-alkyl styrene)s and their viscoelasticity and glass transition temperatures**, SATORU MATSUSHIMA, ATSUSHI TAKANO, Department of applied chemistry, Graduate School of Engineering, Nagoya University, YOSHIKI TAKAHASHI, Institute for Materials Chemistry and Engineering, Kyushu University, YUSHU MATSUSHITA, Department of applied chemistry, Graduate School of Engineering, Nagoya University — Viscoelasticity and glass transition temperatures for linear polymers of many species have been investigated so far, and it is well-known that the melt viscosity for the linear polymers varies with molecular weight in essentially the same manner such as packing length theory. It is important to understand the relationship between the viscosity and the molecular structure of various kinds of linear polymers. To investigate the relationship deeply, viscoelastic measurements using linear polymer analogues which the molecular structure is systematically varied should be useful. For example, poly(*n*-alkyl-substituted polymers) such as poly(*n*-alkyl methacrylate)s are one of the good candidate. In this study, a series of poly(*n*-alkyl styrene)s with the different number of carbon atoms(*n*) in the side alkyl groups (*n*=1, 2, 3, 4, 6, 8, 10 and 12) were carefully synthesized by an anionic polymerization technique, and the viscoelasticity and the glass transition temperatures of the poly(*n*-alkyl styrene)s with high molecular weight ( $M_w \geq 4Me$ ) and narrow molecular weight distribution ( $M_w/M_n \leq 1.1$ ) were discussed.

**Thursday, March 17, 2016 8:00AM - 10:48AM –**

**Session R35 DBIO GSOF GSNP: Active Matter: Collective Phenomena in Living Systems III**

338 - Carl Franck, Cornell University

**8:00AM R35.00001 Phase separation dynamics during *Myxococcus xanthus* fruiting body formation**, GUANNAN LIU, Princeton University, FATMAGUL BAHAR, ADAM PATCH, Syracuse University, SHASHI THUTUPALLI, Princeton University, DAVID YLLANES, M. CRISTINA MARCHETTI, ROY WELCH, Syracuse University, JOSHUA SHAEVITZ, Princeton University — Many living systems take advantage of collective behavior for group survival. We use the soil-dwelling bacterium *Myxococcus xanthus* as a model to study out-of-equilibrium phase separation during fruiting body formation. *M. xanthus* cells have the ability to glide on solid surfaces and reverse their direction periodically. When starved, *M. xanthus* cells aggregate together and form structures called fruiting bodies, inside of which cells sporulate to survive stressful conditions. We show that at high cell density the formation of fruiting bodies is a phase separation process. From experimental data that combines single-cell tracking, population-scale imaging, mutants, and drug applications, we construct the phase diagram of *M. xanthus* in the space of Péclet number and cell density. When wild type cells are starved, we find that they actively increase their Péclet number by modulating gliding speed and reversal frequency which induces a phase separation from a gas-like state to an aggregated fruiting body state.

**8:12AM R35.00002 Active matter model of *Myxococcus xanthus* aggregation**, ADAM PATCH, Department of Physics, Syracuse University, FATMAGUL BAHAR, Department of Biology, Syracuse University, GUANNAN LIU, Department of Physics, Princeton University, SHASHI THUTUPALLI, Department of Physics, Princeton University; Lewis-Sigler Institute for Integrative Genomics, Princeton University, ROY WELCH, Department of Biology, Syracuse University, DAVID YLLANES, Department of Physics, Syracuse University, JOSHUA SHAEVITZ, Department of Physics, Princeton University; Lewis-Sigler Institute for Integrative Genomics, Princeton University, M. CRISTINA MARCHETTI, Department of Physics, Syracuse University; Syracuse Biomaterials Institute, Syracuse University — *Myxococcus xanthus* is a soil-dwelling bacterium that exhibits several fascinating collective behaviors including streaming, swarming, and generation of fruiting bodies. A striking feature of *M. xanthus* is that it periodically reverses its motility direction. The first stage of fruiting body formation is characterized by the aggregation of cells on a surface into round mesoscopic structures. Experiments have shown that this aggregation relies heavily on regulation of the reversal rate and local mechanical interactions, suggesting motility-induced phase separation may play an important role. We have adapted self-propelled particle models to include cell reversal and motility suppression resulting from sporulation observed in aggregates. Using 2D molecular dynamics simulations, we map the phase behavior in the space of Péclet number and local density and examine the kinetics of aggregation for comparison to experiments.

**8:24AM R35.00003 Thermodynamics of the motility-induced phase separation**, ALEXANDRE SOLON, Massachusetts Institute of Technology, USA, JOACHIM STENHAMMAR, Lund University, Sweden, MICHAEL CATES, University of Cambridge, UK, JULIEN TAILLEUR, Université Paris Diderot, France — Self-propelled particles are known to accumulate in regions of space where their velocity is lowered. In addition, if their velocity diminishes when the local density increases (for example due to crowding effects), a positive feedback loop leads to the now well-established motility-induced phase separation (MIPS) between a dense immobile phase and a dilute motile phase. Understanding the phase equilibrium of MIPS is still a matter of debate. Although, depending on the models used to study the transition, a chemical potential or a pressure can be defined, these quantities do not play their usual thermodynamic role. In particular, the usual common tangent or equal-area constructions fail in these systems. Indeed, we will show that describing the phase equilibrium of MIPS necessitates generalized thermodynamics that include non-equilibrium contributions. This approach allows us to predict correctly the phase diagram of MIPS and to gain insight into the thermodynamics of active systems. It also sheds light on the (in)equivalence of statistical ensembles for these systems, paving the way for more efficient computational studies.

**8:36AM R35.00004 Epithelial gap closure governed by forces and geometry.**, BENOIT LADOUX, Mechanobiology Institute (Singapore) and Institut Jacques Monod (CNRS, France) — The closure of gaps within epithelia is crucial to maintain the integrity and the homeostasis of the tissue during wound healing or cell extrusion processes. Cells mediate gap closure through either the assembly of multicellular actin-based contractile cables (purse-string contraction) or the protrusive activity of border cells into the gap (cell crawling). I will present experimental data and numerical modeling that show how these mechanisms can mutually interact to promote efficient epithelial gap closure and how mechanical constraints can regulate these mechanisms. I will first present how geometrical constraints dictate mechanisms of epithelial gap closure. We determine the importance of tissue shape during closure and the role of curvature of cell boundaries in this process. An essential difference between the two closure mechanisms is that cell crawling always pulls the edge of the tissue forward (i.e. towards the gap) while purse string pulls the edge forward or backwards depending on the local geometry. Our study demonstrates how the interplay between these two mechanisms is crucial for closing gaps and wounds, which naturally come in arbitrary shapes. Then I will focus on epithelial closure mechanism during cell extrusion. Within confluent cell layers, cellular motions coupled between neighbors are tightly regulated by the packing density of the epithelium inducing drastic changes in the dynamics of these tissues. I will show how cell density and tissue mechanics regulate the extrusion of cells within a confluent epithelial cell sheet, simultaneously measuring collective movements and traction forces. Epithelial packing and collective cell dynamics dictate the modes of cellular extrusions from lamellipodia crawling of the neighboring cells at low densities to coordinated actin-based contractile purse-string mechanism at higher density.

**9:12AM R35.00005 Self-Driven Jamming of Growing Microbial Populations**, CARL SCHRECK, MORGAN DELARUE, PAWEŁ GNEIWEK, OSKAR HALLATSCHKE, University of California, Berkeley — When cells grow in confined spaces, they assemble into dense populations that interact both chemically and physically. Although in recent years scientists have uncovered a previously hidden layer of mechanical regulation in mammalian tissues that impacts gene expression and development, little is known about the consequences of mechanical constraints on single-celled microbes. This is largely due to a lack of appropriate culturing techniques and accurate computational models. Using physically explicit computer models that are developed alongside microfluidic experiments, we address two fundamental questions: (1) what structures self-assemble in confined geometries due to the cell growth and division process? and (2) how do those structures and associated stresses feed back on to cell physiology? We find that microbial growth in confinement can lead to jamming, heterogeneous stress fields, and intermittent flow that in turn result in spatially and temporally heterogeneous physiological responses. With computer simulations, we further explore the differences between this 'active' flow that is driven internally by cell growth and 'inactive' flow, such as shear and hopper flow, that is driven externally.

**9:24AM R35.00006 Cell Size Clues for the Allee Effect in Vegetative Amoeba Suspension Culture**, CARL FRANCK, BRENDAN RAPPAZZO, XIAONING WANG, IGOR SEGOTA, Cornell University — That cells proliferate at higher rates with increasing density helps us appreciate and understand the development of multicellular behavior through the study of dilute cell systems. However, arduous cell counting with a microscope reveals that in the model eukaryote, *Dictyostelium discoideum* this transition is difficult to ascertain and thereby further explore despite our earlier progress (Phys. Rev. E 77, 041905, (2008)). Here we report preliminary evidence that the slow proliferation phase is well characterized by reduced cell size compared to the wide distribution of cell sizes in the familiar exponential proliferation phase of moderate densities. This observation is enabled by a new system for characterizing cells in stirred suspension cultures. Our technique relies on quickly acquiring magnitude distributions of detected flashes of laser light scattered in situ by cell targets.

**9:36AM R35.00007 Manipulation of long-term dynamics in a colloidal active matter system using speckle light fields**, ERCAG PINCE, SABAREESH K.P. VELU, AGNESE CALLEGARI, PARVIZ ELAHI, Bilkent University, SYLVAIN GIGAN, Universit  Pierre et Marie Curie, GIOVANNI VOLPE, Bilkent University, GIORGIO VOLPE, University College London — Particles undergoing a stochastic motion within a disordered medium is a ubiquitous physical and biological phenomena. Examples can be given from organelles performing tasks in the cytoplasm to large animals moving in patchy environment. Here, we use speckle light fields to study the anomalous diffusion in an active matter system consisting of micron-sized silica particles (diameter 5 m) and motile bacterial cells (*E. coli*). The speckle light fields are generated by mode mixing inside a multimode optical fiber where a small amount of incident laser power is needed to obtain an effective disordered optical landscape for the purpose of optical manipulation. We experimentally show how complex potentials contribute to the long-term dynamics of the active matter system and observed an enhanced diffusion of particles interacting with the active bacterial bath in the speckle light fields. We showed that this effect can be tuned and controlled by varying the intensity and the statistical properties of the speckle pattern. Potentially, these results could be of interest for many technological applications, such as the manipulation of microparticles inside optically disordered media of biological interest.

**9:48AM R35.00008 A Density-Independent Flocking Transition in Confluent Tissues<sup>1</sup>**, MICHAEL CZAJKOWSKI, Syracuse Univ, DAPENG BI, Rockefeller Univ, M. LISA MANNING, M. CRISTINA MARCHETTI, Syracuse Univ — Some of us recently demonstrated a density-independent solid-liquid transition in confluent tissues controlled by cell motility and a cell shape parameter measuring the interplay of cortical tension and cell-cell adhesion. An important insight of this work is that the rigidity and dynamics of cell layers depends sensitively on cell shape. To explore the influence of cell shape on collective states, we have constructed continuum equations that couple a scalar field describing cell-shape anisotropy to cell polarization. The model displays a density independent transition to a polarized state of elongated cells driven by a cellular shape-index parameter. We map out the phase diagram using linear stability analysis and numerical solution of the nonlinear hydrodynamic equations. The proposed transition constitutes a density-independent flocking transition.

<sup>1</sup> We acknowledge support from The Simons Foundation and NSF-DGE-1068780

**10:00AM R35.00009 Multicellular contractility contributes to the emergence of mesothelioma nodules.<sup>1</sup>**, ANDRAS CZIROK, University of Kansas Medical Center — Malignant pleural mesothelioma (MPM) nodules arise from the mesothelial lining of the pleural cavity by a poorly understood mechanism. We demonstrate that macroscopic multicellular aggregates, reminiscent of the MPM nodules found in patients, develop when MPM cell lines are cultured at high cell densities for several weeks. Surprisingly, the nodule-like aggregates do not arise by excessive local cell proliferation, but by myosin II-driven cell contractility. Contractile nodules contain prominent actin cables that can span several cells. Several features of the in vitro MPM nodule development can be explained by a computational model that assumes uniform and steady intercellular contractile forces within a monolayer of cells, and a mechanical load-dependent lifetime of cell-cell contacts. The model behaves as a self-tensioned Maxwell fluid and exhibits an instability that leads to pattern formation. Altogether, our findings suggest that inhibition of the actomyosin system may provide a hitherto not utilized therapeutic approach to affect MPM growth.

<sup>1</sup> NIH R01-GM102801

**10:12AM R35.00010 Cilia driven flow networks in the brain**, YONG WANG, MPI Dynamics and Self-Organization, REGINA FAUBEL, MPI biophysical Chemistry, CHRISITIAN WESTENDORF, MPI Dynamics and Self-Organization, GREGOR EICHELE, MPI biophysical Chemistry, EBERHARD BODENSCHATZ, MPI Dynamics and Self-Organization — Neurons exchange soluble substances via the cerebrospinal fluid (CSF) that fills the ventricular system. The walls of the ventricular cavities are covered with motile cilia that constantly beat and thereby induce a directional flow. We recently discovered that cilia in the third ventricle generate a complex flow pattern leading to partitioning of the ventricular volume and site-directed transport paths along the walls. Transient and daily recurrent alterations in the cilia beating direction lead to changes in the flow pattern. This has consequences for delivery of CSF components along the near wall flow. The contribution of this cilia-induced flow to overall CSF flow remains to be investigated. The state-of-art lattice Boltzmann method is adapted for studying the CFS flow. The 3D geometry of the third ventricle at high resolution was reconstructed. Simulation of CSF flow without cilia in this geometry confirmed that the previous idea about unidirectional flow does not explain how different components of CSF can be delivered to their various target sites. We study the contribution of the cilia-induced flow pattern to overall CSF flow and identify target areas for site-specific delivery of CSF-constituents with respect to the temporal changes.

**10:24AM R35.00011 Collective motion of motile cilia: from human airways to model systems**, PIETRO CICUTA, LUIGI FERIANI, MAURIZIO CHIOCCOLI, JURIJ KOTAR, University of Cambridge — Mammalian airways are a fantastic playground of nonlinear phenomena, from the function of individual active filaments, to the emerging collective behaviour, to the rheology of the mucus solution surrounding cilia. We have been investigating the fundamental physics of this system through a variety of model system approaches, both experimental and computational. In the last year we have started measurements on living human cells, observing cilia shape during beating, and measuring speed and coherence of the collective dynamics. We report on significant differences in the collective motion in ciliated cell carpets from a variety of diseases, and we attempt to reconcile the collective dynamical phenotypes to the properties of individual filaments and the mechanics of the environment.

**10:36AM R35.00012 Active matter clusters at interfaces.** , KATHERINE COPENHAGEN, Univ of California - Merced, AJAY GOPINATHAN, University of California - Merced — Collective and directed motility or swarming is an emergent phenomenon displayed by many self-organized assemblies of active biological matter such as clusters of embryonic cells during tissue development and flocks of birds. Such clusters typically encounter very heterogeneous environments. What happens when a cluster encounters an interface between two different environments has implications for its function and fate. Here we study this problem by using a mathematical model of a cluster that treats it as a single cohesive unit whose movement depends on the nature of the local environment. We find that low speed clusters which exert forces but no active torques, encountering an interface with a moderate difference in properties can lead to refraction or even total internal reflection of the cluster. For large speeds and clusters with active torques, they show more complex behaviors crossing the interface multiple times, becoming trapped at the interface and deviating from the predictable refraction and reflection of the low velocity clusters. Our results show a wide range of behaviors that occur when collectively moving active biological matter moves across interfaces and these insights can be used to control motion by patterning environments.

**Thursday, March 17, 2016 8:00AM - 11:00AM —**

**Session R36 GSNP GSOF: Continuum Descriptions of Discrete Materials II** 339 - Paul Umbanhowar, Northwestern University

**8:00AM R36.00001 Dynamic shear jamming in dense suspensions** , IVO PETERS, University of Southampton, SAYANTAN MAJUMDAR, HEINRICH JAEGER, University of Chicago — Shear a dense suspension of cornstarch and water hard enough, and the system seems to solidify as a result. Indeed, previous studies have shown that a jamming front propagates through these systems until, after interaction with boundaries, a jammed solid spans across the system. Because these fully jammed states are only observed if the deformation is fast enough, a natural question to ask is how this phenomenon is related to the discontinuous shear thickening (DST) behavior of these suspensions. We present a single experimental setup in which we on the one hand can measure the rheological flow curves, but on the other hand also determine if the suspension is in a jammed state. This we do by using a large-gap cylindrical Couette cell, where we control the applied shear stress using a rheometer. Because our setup only applies shear, the jammed states we observe are shear-jammed, and cannot be a result of an overall increase in packing fraction. We probe for jammed states by dropping small steel spheres on the surface of the suspension, and identify elastic responses. Our experiments reveal a clear distinction between the onset of DST and Shear-Jammed states, which have qualitatively different trends with packing fraction close to the isotropic jamming point.

**8:12AM R36.00002 Rheological behavior of partially-wet granular matter** , RAMIN GHELICHI, Postdoctoral Associate, KEN KAMRIN, Assistant Professor, KAMRIN GROUP TEAM — The topic of wet granular material modeling is an open area of study. In this talk we present a comprehensive continuum model for wet granular matter, which is informed by a novel Discrete Element Method (DEM), which tracks the fluid content coating each grain as well as a variable fluid-bridge volume. We have developed a DEM simulation method with a history-dependent potential based on the Hertz-Mindlin contact in compression and evolving capillary forces in tension. The capillary bridge in the simulations forms based on the volume of the fluid on each particle. First, we determine the cohesive force between grains, which is a function of grain separation, bridge volume, grain geometry, and fluid properties. The volume of the bridges also evolves in time, which affects the cut-off distance in bridges and the force-separation function. The other important factor which has been considered in the model is the particle roughness, which has a significant effect on the capillary force function. The effect of fluid viscosity is also considered. The second step in this work is to utilize the DEM results to identify a constitutive model that can explain the plastic behavior (flow rule) of a dense granular assembly under varying degrees of wetness.

**8:24AM R36.00003 Effect of friction on shear jamming<sup>1</sup>** , DONG WANG, JONATHAN BARES, Duke University, JOSHUA DIJKSMAN, Wageningen University, JIE REN, Merck & Co, HU ZHENG, Hohai University, ROBERT BEHRINGER, Duke University — Shear jamming of granular materials was first found for systems of frictional disks, with a static friction coefficient  $\mu \approx 0.6$  (Bi et al. Nature (2011)). Jamming by shear is obtained by starting from a zero-stress state with a packing fraction  $\phi$  between  $\phi_J$  (isotropic jamming) and a lowest  $\phi_S$  for shear jamming. This phenomenon is associated with strong anisotropy in stress and the contact network in the form of force chains, which are stabilized and/or enhanced by the presence of friction. Whether shear jamming occurs for frictionless particles is under debate. The issue we address experimentally is how changing friction affects shear jamming. By applying a homogeneous simple shear, we study the effect of friction by using photoelastic disks either wrapped with Teflon to reduce friction or with fine teeth on the edge to increase friction. Shear jamming is still observed; however, the difference  $\phi_J - \phi_S$  is smaller with lower friction. We also observe larger fluctuations due to initial configurations both at the lowest and the highest friction systems studied. Ongoing work is to use particles made of gelatin to reduce the friction coefficient to the order of 0.01.

<sup>1</sup>We acknowledge support from NSF Grant DMR1206351, NASA Grant NNX15AD38G and the William M. Keck Foundation

**8:36AM R36.00004 Frictionless Shear Jamming, a finite-size phenomenon** , MARCO BAITY-JESI, Universidad Complutense de Madrid, CARL GOODRICH, Harvard University, JAMES SETHNA, Cornell University, ANDREA LIU, University of Pennsylvania — Athermal frictionless spheres jam as their density is increased. A few years ago, it was shown that at sufficiently high density, an initially unjammed system of frictional particles can jam under shear. Here we study shear jamming in packings of frictionless particles, and show that it is a finite-size effect with scalings that can be understood within a generalized scaling theory.

**8:48AM R36.00005 Slow Relaxations in Fluid-Driven Granular Flows** , CARLOS ORTIZ, DOUGLAS DURIAN, DOUGLAS JEROLMACK, Univ of Pennsylvania — Particles in a pack may appear frozen, but exhibit very slow dynamics (creep). To probe long-time dynamics, we construct an annular chamber that mimics an infinitely-long river channel. We drive the packs with a laminar flow and record dynamics by laser scanned particle tracking. The dynamics of “bed load” grains near the surface exhibit relatively fast shear and their velocity profile as a function of depth can be well-described by a local  $\mu(I)$ -rheology. However, grains deep in the pack, which appear frozen by eye, exhibit slow creep dynamics that are not captured by the local model. This transition between bed load and creep occurs at a critical value of the local relaxation time. We find that the timescale for heterogeneous dynamics increases monotonically as a function of depth, but the length scale characterized by the domain size of the heterogeneities achieves a maximum at the transition to creeping. We explore the relation between the important length and time scales of the flow in the creep phase using nonlocal rheology.

**9:00AM R36.00006 Flow of interacting colloidal suspensions through a narrow channel** , RAUL CRUZ HIDALGO, SARA ARIETALEANIZ, University of Navarra, IGNACIO PAGONABARRAGA, University of Barcelona — In this work we numerically study the constitutive behavior of interacting colloidal suspensions at intermediate and high concentrations. The influence of the interaction potential strength on the system's response is examined, in suspensions flowing through narrow channels at low Reynold's numbers. Using Lattice Boltzmann methods, we analyze the rheological response of a colloidal suspension once the steady state is established. In dilute suspensions we always recover a newtonian behavior. At higher volume fractions, the range and strength of the interaction potential has a stronger impact in the behavior of the suspension. While for short range potentials, the non-newtonian response mostly depends on colloid concentration and confinement distance, for a Lennard-Jones potential we identify two rheological responses depending on the potential strength,  $\xi_{LJ}$ , at a given concentration. For weak  $\xi_{LJ}$  the effective viscosity,  $\eta_{eff}$ , decreases until a minimum is reached. On the contrary, at large values of  $\xi_{LJ}$  the effective viscosity  $\eta_{eff}$  increases when increasing the strength of interaction. This behavior has been correlated with the local structure of this complex fluid.

**9:12AM R36.00007 Impact Fragmentation and Crushing of Concrete and Other Solids Due to Kinetic Energy of High Shear Strain Rate**, ZDENEK BAZANT, KEDAR KIRANE, Northwestern University — While numerous studies have dealt with dynamic crack propagation, they have not led to a macroscopic continuum model usable in FE analysis. Recent work on such a model is reviewed. The key idea is that comminution under high-rate shear is driven by the release local kinetic (rather than strain) energy of the shear strain rate field in forming finite-size fragments. At strain rates  $>10^3/s$ , this energy exceeds the maximum possible elastic strain energy by orders of magnitude. It is found that the particle size scales as the  $-2/3$  power of the shear strain rate and as the  $2/3$  power of interface fracture energy, and the released and dissipated kinetic energy as the  $2/3$  power of the shear strain rate. These results explain the long debated phenomenon of “dynamic overstress”. In FE simulations, this kinetic energy of strain rate field can be dissipated either by equivalent viscosity or by the work of increased strength limits. In simulating the impact of missiles into concrete walls, both approaches give nearly equivalent results. A dimensionless indicator of the comminution intensity is also formulated. The theory was inspired by noting that the local kinetic energy of shear strain rate plays a role analogous to the local kinetic energy of eddies in turbulent flow.

**9:24AM R36.00008 Explanation of nonlocal granular fluidity in terms of microscopic fluctuations**, QIONG ZHANG, KEN KAMRIN, Massachusetts Inst of Tech-MIT — A recently proposed granular constitutive law has shown capability to predict nonlocal granular rheology using a variable denoted granular fluidity. This work is aimed at finding the microscopic physical meaning of fluidity in terms of fluctuations such as fluctuation of normalized shear stress and fluctuation of velocity. We try to predict the fluidity as a function of the fluctuation of normalized shear stress, and also test Eyring equation and kinetic theory based on the theoretical prediction proposed in other work. We find a consistent definition for the fluidity to be proportional to the product of the velocity fluctuations and some function of packing fraction divided by the average diameter of the grains. This definition shows predictive ability in multiple geometries for which flow behavior is nonlocal. It is notable that the fluidity is well-defined as a function of kinematic state variables, as one would hope for a quantity of this nature.

**9:36AM R36.00009 Mesoscale poroelasticity of heterogeneous media**, SIAVASH MONFARED, HADRIEN LAUBIE, Massachusetts Inst of Tech-MIT, FARHANG RADJAI<sup>1</sup>, Universite de Montpellier, ROLAND PELLENG, FRANZ-JOSEF ULM, Massachusetts Inst of Tech-MIT — Poroelastic behavior of heterogeneous media is revisited. Lattice Element Method (LEM) is used to model interaction between solid constituents due to a pressurized pore space. Exploring beyond mean-field based theories in continuum microporomechanics, local textural variations and its contribution to the global anisotropic poroelastic behavior of real multiphase porous media are captured. To this end, statistical distributions of mesoscale poroelastic coefficients from numerical simulations on X-ray microscopy scans of two different organic-rich shales with different microtextures are presented. The results are compared with predictions using mean-field based tools of continuum micromechanics. The textural dependency of strain localization and stress chain formation captured in this framework promises a powerful tool for modeling poroelastic response of complex porous composites and a path to incorporate local textural and elastic variations into a continuum description.

<sup>1</sup>Visiting Scientist, CNRS-MIT, MIT

**9:48AM R36.00010 Low-frequency oscillations in vibrated granular columns.**, NICOLAS RIVAS, Helmholtz Institute Erlangen-Nuremberg, ANTHONY THORNTON, KIT WINDOWS-YULE, University of Twente, DAVE PARKER, University of Birmingham, STEFAN LUDING, University of Twente — We present simulations, experiments and theoretical treatments of vertically vibrated granular media. The systems considered are quasi-one-dimensional. This column geometry makes it possible to study collective oscillations of the grains with a characteristic frequency that is much lower than the frequency of energy injection (LFOs). Using event-driven molecular dynamics simulations we see that LFOs become slower and more pronounced as the shaking of the container increases. Experimental observations, using the positron emission particle tracking technique, agree well with the simulated data. The conditions necessary for the existence of LFOs are derived from a granular continuum model, which is able to relate the column density profile with the measured characteristic frequencies

**10:00AM R36.00011 Continuum model and simulation of segregating rods**, RICHARD M. LUEPTOW, Northwestern University, YONGZHI ZHAO, Zhejiang University, PAUL B. UMBANHOWAR, Northwestern University — Most studies of segregation of flowing granular materials focus on spherical particles, even though particles are often non-spherical in practical granular systems. Here we focus on the segregation of rod-like (cylindrical) particles of the same diameter but different lengths using continuum theory and DEM simulations based on super-ellipsoids. In the flowing layer of a bounded heap flow, a bidisperse mixture of long and short rods segregates such that the shorter rods percolate toward the lower portion of the flowing layer while longer rods rise toward the upper portion of the flowing layer, much like smaller spherical particles segregate from larger spherical particles. The rods tend to deposit on the underlying bed of particles in the heap such that they are aligned with the flow with the smaller rods deposited upstream of the larger rods due to segregation. The percolation velocities related to segregation for long and short rods depend on the local shear rate and the concentration of the other particle species, just as is the case for small and large spherical particles. Using this percolation velocity and an appropriate value for collisional diffusion, the advection-diffusion-segregation continuum model successfully predicts the segregation of rod-like particles.

**10:12AM R36.00012 Flow and packing properties of frictional shapes from spheres to cubes**, LEONARDO E. SILBERT, Southern Illinois University, K. MICHAEL SALERNO, DAN S. BOLINTINEANU, JEREMY B. LECHMAN, GARY GREEST, Sandia National Laboratories — Though grains in many applications are aspherical and rough, many computational studies of granular flow and packing focus on ideal spherical particles, often without friction. Following Latham [1], we optimally represent arbitrary shapes using overlapping spheres of different sizes. We use discrete element simulations to study the packing and flow of frictional granular superquadric (superball) shapes ranging from spheres to cuboids. When packing particles, friction becomes more important as particle shape becomes more angular. This leads to a larger density change between frictional and frictionless packings. Friction and shape are also important to granular flow. For a planar-shear flow different shapes have similar flow behavior in the zero-friction limit. However, with increasing friction particle shape couples to the tangential frictional forces and becomes more important. Flow results are compared with continuum theories of granular materials. Results from simulations of anisotropic particles and mixtures of shapes will also be discussed.

[1] X. Garcia, J. Xiang, J.-P. Latham, and J. P. Harrison, *Géotechnique* 59, 779 (2009).

**10:24AM R36.00013 Scaling Relations for Wheeled Locomotion in Granular Media**, JAMES SLONAKER, KEN KAMRIN, MIT — Vehicular wheel design for use on granular material has not currently been perfected. Resistive Force Theory (RFT) is a reduced-order empirical model for granular drag, which shows promise to help simulate and understand locomotion processes to design more efficient wheels. Here we explore the fundamental scaling relations derived from RFT and their experimental validation. Similar to the non-dimensional scaling relations in fluid mechanics, the relative simplicity of RFT asserts that only one material parameter, the “grain-structure coefficient”, is required, which reduces the complexity of the non-dimensional groups implied by the system. Therefore, wheels with differing input design parameters like size, mass, shape and even gravity, can be tested and their performance related to each other in predictable ways. We experimentally confirmed these relations by testing with 3D printed wheel geometries in a controlled sand bed.

replacing MAR16-2015-006074 and

### 10:36AM R36.00014 Scaling of heat transfer in granular materi

YOHANNES, Rutgers University, HEATHER EMADY, Arizona State University, INGRID PARDES, MAHAM GLASSER, FERNANDO MUZZIO, ALBERTO CUITINO, Rutgers University — Several industrial processes and powders, in devices such as rotating drums, to bring about a desired chemical and/or physical transformation. Predicting the heat transfer process can significantly improve the quality of the end product and efficiency. However, there is a need to predict the evolution of the distribution and average of the particles' temperature, particularly for the purpose of manufacturing scale productions. We used discrete element method (DEM) based simulations to study the heat transfer in rotating drums at low temperature. Various physical, mechanical, and thermal properties of particles were considered in the effect of operating conditions such as size of drum, material fill level, and speed of rotation on the heat transfer. We identified timescales relevant to the heat transfer process and developed a relationship between these timescales and the temperature of particles. We also found that the evolution of the temperature distribution, since different particles have different predicted based on these timescales. These findings can be used to predict the required time to heat up all particles.

MAR16-2015-006601

### 10:48AM R36.00015 Structural evolution of Colloidal Gels under Flow

, ARMAN BOROMAND, JOAO MAIA, Case Western Reserve University, SAFA JAMALI, Massachusetts Institute of Technology — Colloidal suspensions are ubiquitous in different industrial applications ranging from cosmetic and food industries to soft robotics and aerospace. Owing to the fact that mechanical properties of colloidal gels are controlled by its microstructure and network topology, we trace the particles in the networks formed under different attraction potentials and try to find a universal behavior in yielding of colloidal gels. Many authors have implemented different simulation techniques such as molecular dynamics (MD) and Brownian dynamics (BD) to capture better picture during phase separation and yielding mechanism in colloidal system with short-ranged attractive force. However, BD neglects multi-body hydrodynamic interactions (HI) which are believed to be responsible for the second yielding of colloidal gels. We envision using dissipative particle dynamics (DPD) with modified depletion potential and hydrodynamic interactions, as a coarse-grain model, can provide a robust simulation package to address the gel formation process and yielding in short ranged-attractive colloidal systems. The behavior of colloidal gels with different attraction potentials under flow is examined and structural fingerprints of yielding in these systems will be discussed.

## Thursday, March 17, 2016 8:00AM - 11:00AM –

Session R37 GSOFT: Liquid Crystals: Dimers and Liquid Crystal Applications 340 - Antal Jakil,

Kent State University

### 8:00AM R37.00001 The twist-bend nematic phase of bent mesogenic dimers and its mixtures<sup>1</sup>

, MICHAEL TUCHBAND, MIN SHUAI, KERI GRABER, DONG CHEN, LEO RADZIHOVSKY, ARTHUR KLITTNICK, Department of Physics, University of Colorado Boulder, LEE FOLEY, ALYSSA SCARBROUGH, JAN PORADA, MARK MORAN, EVA KORBLOVA, DAVID WALBA, Department of Chemistry, University of Colorado Boulder, MATTHEW GLASER, JOSEPH MACLENNAN, NOEL CLARK, Department of Physics, University of Colorado Boulder, SOFT MATERIALS RESEARCH CENTER TEAM — Binary mixtures of the twist-bend nematic-forming liquid crystal CB7CB with the prototypical rod-like liquid crystal 5CB exhibit a twist-bend nematic phase with properties similar to those reported for neat CB7CB. The linear dependence of the phase transition temperature on concentration indicates that these binary mixtures are nearly ideal. We confirm the presence of nanoscale modulations of the molecular orientation in the mixtures by freeze-fracture transmission electron microscopy (FFTEM). We devise and implement a statistical approach to quantitatively measure the ground state pitch of the twist-bend phase and its mixtures using FFTEM. The addition of 5CB generally shifts the measured ground-state pitch distributions towards larger pitch. The pitch apparently increases discontinuously at higher 5CB concentrations.

<sup>1</sup>This work was supported by NSF MRSEC Grant 0820579, by Institute for Complex Adaptive Matter Postdoctoral Fellowship Award OCG5711B, and by ED GAANN Award P200A120014.

### 8:12AM R37.00002 Resonant soft X-ray scattering study of twist bend nematic phase<sup>1</sup>, CHENHUI

ZHU, Advanced Light Source, Lawrence Berkeley National Laboratory, ANTHONY YOUNG, CHENG WANG, , ALEXANDER HEXEMER, Advanced Light Source, Lawrence Berkeley National Laboratory, QUAN LI, , OLEG LAVRENTOVICH, LCI, Kent State University, DAVID WALBA, Department of Chemistry and Biochemistry, University of Colorado Boulder, MICHAEL TUCHBAND, MIN SHUAI, , NOEL CLARK, Department of Physics, University of Colorado at Boulder — Liquid crystals (LCs) form many interesting nano-scale structures, many of which can be probed with X-ray scattering techniques, typically hard X-rays due to its high penetrating power. However, in the hard X-ray regime, the scattering contrast of some LC nanostructures can be extremely low due to their weak electron density modulation. Here we show it is possible to use resonant soft x-rays to probe the helical pitch of the newly discovered twist bend nematic phase [1,2], which is purely a twist bend structure with no electron density modulation. The in-situ temperature dependent measurement will be presented and discussed. This work together with our previous study on the helical nanofilament B4 phase [3] shows the great potential of soft x-ray scattering in liquid crystals. [1] D. Chen, et al. *PNAS*, DOI 1314654110 (2015). [2] V. Borshch, et al. *Nat. Comm.*, **4**, 2635 (2015). [3] C. Zhu, et al. *Nano. Lett.* **15**, 3420 (2015).

<sup>1</sup>supported by the Director of the Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

### 8:24AM R37.00003 Dynamic Light Scattering on a Twist-Bend nematic Liquid Crystal

, ZEINAB PARSOUI, SHAIKH SHAMID, VOLODYMYR BORSHCH, PAVAN CHALLA, Kent State University, GABRIELA TAMBA, GEORG MEHL, University of Hull, JAMES GLEESON, ANTAL JKLI, OLEG LAVRENTOVICH, DAVID ALLENDER, JONATHAN SELINGER, SAMUEL SPRUNT, Kent State University — We present a dynamic light scattering study performed on the uniaxial and twist-bend nematic ( $N_{TB}$ ) phases of a liquid crystal dimer/monomer mixture. In the nematic phase, in addition to the usual two hydrodynamic director modes, the results reveal a single non-hydrodynamic process that is associated with fluctuations in orientational order in the plane perpendicular to the primary (uniaxial) ordering direction. On the other hand, data from the  $N_{TB}$  phase demonstrate a pair of non-hydrodynamic modes and a single hydrodynamic mode. The non-hydrodynamic modes are strongly temperature-dependent, slowing down as the transition is approached from the  $N_{TB}$  side. Our results may be explained by a Landau-deGennes expansion of free energy for the N to  $N_{TB}$  transition in terms of a helical polarization field, which is nonzero in the  $N_{TB}$  state and is coupled to the heliconical director that characterizes the  $N_{TB}$  state. The short pitch of the structure allows a “coarse-graining” of the free energy that accounts for the observed fluctuation mode structure and properties at optical wavevectors. In the model, the helical axis is the effective director, and the helical planes become smectic-like layers. We estimate an effective compression constant,  $B = 4000$  Pa, for the  $N_{TB}$  “layer” structure.

**8:36AM R37.00004 Layer Thinning in Freely-Suspended Thin Liquid Films of a Symmetric Liquid Crystal Dimer**, SHOKIR PARDAEV, ZEINAB PARSOUZI, JAMES GLEESON, Department of Physics, Kent State Univ - Kent, ANTAL JAKLI, Chemical Physics Interdisciplinary Program and Liquid Crystal Institute, Kent State Univ-Kent, SAMUEL SPRUNT, Department of Physics, Kent State Univ - Kent — We report optical reflectivity and dynamic light scattering (DLS) studies on freely suspended smectic films of a symmetric liquid crystal dimer, which exhibits the phase sequence isotropic—nematic—twist-bend nematic—smectic in cooling. In sufficiently thin films the reflectivity  $R$  is expected to scale as the square of the number of smectic layers ( $N^2$ ) while the frequency  $f$  of underdamped layer fluctuations scales as  $N^{-1/2}$ . On heating thin films drawn in the smectic phase, we observe a sequence of layer thinning transitions, with  $R$  and  $f$  following the expected scaling relations, provided the stepwise melting involves double rather than single layers. We will describe a model to explain the unusual layer thinning process. We thank M. G. Tamba and G. Mehl for providing the liquid crystal compound: NSF grant DMR-1307674.

**8:48AM R37.00005 ABSTRACT WITHDRAWN —**

**9:00AM R37.00006 Giant Magnetic Field-induced Phase Transitions in Dimeric Liquid Crystals.**, SEYYED MUHAMMAD SALILI, MIROSLAW SALAMONCZYK, Liquid Crystal Institute, Kent State University, Kent, OH 44242, USA, MARIA-GABRIELA TAMBA, Department of Nonlinear Phenomena, Institute for Experimental Physics, Otto von Guericke University Magdeburg, Magdeburg, Germany, SAMUEL SPRUNT, Department of Physics, Kent State University, Kent, OH 44242, USA, GEORG MEHL, Department of Chemistry, University of Hull, Hull HU6 7RX, UK, ANTAL JAKLI, Liquid Crystal Institute, Kent State University, Kent, OH 44242, USA, JAMES GLEESON, Department of Physics, Kent State University, Kent, OH 44242, USA, KENT GROUP COLLABORATION, HULL GROUP COLLABORATION — Liquid crystals are responsive to external fields such as electric, magnetic fields. The first experimental observation of dependence of isotropic to nematic phase transition on the applied magnetic field was done using a strong magnetic field on bent-core nematogens and the phase transition temperature exhibited an upshift of 0.7 C at B=30 T [1]. We report on measurements of giant magnetic field-induced isotropic-nematic transition of chainsticks (nunchuks) type dimeric liquid crystals. Upon using the B=25 T split-helix resistive solenoid magnet at NHMFL, we have observed up to 18 C upshift of the isotropic to nematic phase transition temperature at B=22T. We discuss the results within the context of differential thermodynamic potential and the two basic mean-field theories. To our knowledge, this is the first observation of such huge shifts in the phase transitions of thermotropic liquid crystals. [1] T. Ostapenko et al, Phys. Rev. Lett. 101, 247801 (2008).

**9:12AM R37.00007 Smectic Phase Formed by DNA Dimers<sup>1</sup>**, MIROSLAW SALAMONCZYK, Liquid Crystal Institute, Kent State University, JAMES GLEESON, Department of Physics, Kent State University, ANTAL JAKLI, Liquid Crystal Institute, Kent State University, SAMUEL SPRUNT, Department of Physics, Kent State University, JAN DHONT, EMMANUEL STIAKAKIS, Forschungszentrum Julich, Julich, Germany — h — *abstract* — The rapidly expanding bio market is driving the development and characterization of new multifunctional materials. In particular, nucleic acids are under intense study for gene therapy, drug delivery and other bio-safe applications [1,2,3]. DNA is well-known to form a cholesteric nematic liquid crystal in its native form; however, much recent research has focused on self-assembly and mesomorphic behavior in concentrated solutions of short DNA helices [4]. Our work focuses on DNA dimers, consisting of 48 base-pair double-stranded helices connected by a 5 to 20 base flexible single strand, and suspended in a natural buffer. Depending on temperature, concentration and length of the flexible spacer, polarizing optical microscopy and small angle x-ray scattering reveal cholesteric nematic and, remarkably, smectic liquid crystalline phases. A model for smectic phase formation in this system will be presented. [1] J.-L. Lim et al., Int. J. of. Pharm. 490 (2015) 2652] D.-H. Kim et al., Nature Biotech. 23 (2005) 2223] K. Liu et al., Chem. Eur. J. 21 (2015) 48984] M. Nakata et al., Science 318 (2007) 1276\pard-/abstract-

<sup>1</sup>NSF DMR 1307674

**9:24AM R37.00008 Lipid decorated liquid crystal pressure sensors<sup>1</sup>**, TETIANA LOPATKINA, PIOTR POPOV, LAWRENCE HONAKER, ANTAL JAKLI, Chemical Physics Interdisciplinary Program and Liquid Crystal Institute, Kent State University, Kent, OH 44242, ELIZABETH MANN, Department of Physics, Kent State University, Kent, OH 44242, MANN'S GROUP COLLABORATION, JAKLI'S GROUP COLLABORATION — Surfactants usually promote the alignment of liquid crystal (LC) director parallel to the surfactant chains, and thus on average normal to the substrate (homeotropic), whereas water promotes tangential (planar) alignment. A water-LC interface is therefore very sensitive to the presence of surfactants, such as lipids: this is the principle of LC-based chemical and biological sensing introduced by Abbott et al[1]. Using a modified configuration[2], we found that at higher than 10 micro molar lipid concentration, the uniformly dark texture seen for homeotropic alignment between left-, and right-handed circular polarizers becomes unstable and slowly brightens again. This texture shows extreme sensitivity to external air pressure variations offering its use for sensitive pressure sensors. Our analysis indicates an osmotic pressure induced bending of the suspended films explaining both the birefringence and pressure sensitivity. In the talk we will discuss the experimental details of these effects. [1] J. M. Brake, M. K. Daschner, Y.-Y. Luk, and N. L. Abbott, Science (80-. ). 302, 2094 (2003). [2] P. Popov, E. K. Mann, and A. Jakli, Phys. Rev. Appl. 1, 034003 (2014).

<sup>1</sup>This work was financially supported by NSF DMR No. DMR-0907055.

**9:36AM R37.00009 2D and 3D Histioid Disclination Networks in Liquid Crystals<sup>1</sup>**, MIAO JIANG, YUBING GUO, OLEG LAVRETOVICH, QI-HUO WEI, Kent State University — Topological defects and disclination lines are of both fundamental interest and practical importance. In this paper, we will show that periodic/non-periodic 2D/3D networks of disclination lines can be created in nematic liquid crystal cells by setting well-designed alignment patterns at the top and bottom substrate surfaces. The desired complex patterns of liquid crystal molecular alignments at the substrates are obtained using a projection photoalignment technique based on plasmonic metamasks. The designs of alignment patterns and their resulting disclination line networks will be presented. These designable topological networks represent a new kind of artificial materials which could be of useful for directing colloidal and molecular assembly.

<sup>1</sup>National Science Foundation CMMI-1436565

**9:48AM R37.00010 Photophysics of guest-host liquid crystal systems containing naphthopyran derivatives**, MARIACRISTINA RUMI, Air Force Rsch Lab - WPAFB, TAMAS KOSA, LUDMILA SUKHOMLINOVA, BAHMAN TAHERI, Alpha Micron Inc., TIMOTHY WHITE, TIMOTHY BUNNING, Air Force Rsch Lab - WPAFB — Photoinduced order-increase changes can be observed in guest-host liquid crystal systems containing certain phototropic species, such as naphthopyrans. We are investigating the dynamics of the naphthopyran photoinduced interconversion reaction and the related liquid crystal order increase process as a function of excitation conditions and temperature. The thermal relaxation from different photostationary states is also been monitored. The guest-host system behavior is compared with that of the same guest species in isotropic media and other photoresponsive materials in liquid crystalline media, to determine if the naphthopyran interconversion reaction is affected by the anisotropy of the environment surrounding the guest molecules. This will provide a better understanding of the mutual influence of the guest and host molecules on the properties of the photoresponsive mixed systems.

### **10:00AM R37.00011 Plasmonic Photopatterning of Complex Molecular Orientations in Liquid Crystals<sup>1</sup>**

, YUBING GUO, MIAO JIANG, CHENHUI PENG, Liquid Crystal Institute, Kent State Univ - Kent, KAI SUN, Department of Material Science, University of Michigan, OLEG YAROSHCHUK, Institute of Physics, National Academy of Sciences of Ukraine, OLEG LAVRENTOVICH, QI-HUO WEI, Liquid Crystal Institute, Kent State Univ - Kent — Aligning liquid crystal (LC) molecules in spatially non-uniform patterns are highly demanded for applications such as programmable origami and liquid crystal enabled nonlinear electrokinetics. We developed a high resolution projection photoalignment technique for patterning arbitrary LC alignment fields. The photoalignment is based on carefully engineered metasurfaces, or dubbed as plasmonic metamasks (PMMs). When illuminated by light, the PMMs generate patterns of both light intensity and polarization. By projecting the light transmitted through the PMMs onto liquid crystal cells coated with photosensitive materials, alignment patterns predesigned in polarization patterns of the PMMs can be imposed in liquid crystals. This technique makes the liquid crystal alignment a repeatable and scalable process similar to conventional photolithography, promising various applications.

<sup>1</sup>National Science Foundation CMMI-1436565

### **10:12AM R37.00012 Flow Meter Based on Freely Suspended Smectic Liquid Crystal Films<sup>1</sup>**

, ADAM GREEN, None, ZHIYUAN QI, CHEOL PARK, MATTHEW GLASER, JOSEPH MACLENNAN, NOEL CLARK, Soft Materials Research Center, University of Colorado, Boulder, CO 80309 — We present the realization of a idealized 2D hydrodynamic system coupled to air-flow, and show that freely suspended films (FSF) of smectic liquid crystals can be used as a novel flow-meter. Freely-suspended films of liquid crystals are one of the closest physical realizations of an idealized 2D fluid. The velocity of air-flow above a film suspended above a channel can be inferred by studying the velocity profile of the smectic film. This velocity profile can be measured using digital video microscopy to track the inclusions present in the moving film. The velocity profile is then fitted to the coupled 2D solutions of an embedded fluid in air, and the velocity of the air can then be extracted. This flow meter serves as a demonstration of a robust test-bed for further exploration of 2D hydrodynamics.

<sup>1</sup> This work was supported by NASA Grant No. NNX-13AQ81G, NSF MRSEC Grant No. DMR-0820579, and DMR-1420736.

### **10:24AM R37.00013 Optical fibers based on compositions of polymers and liquid crystals for gas detection.**

, PETR SHIBAEV, ANTHONY TANTILLO, Fordham University, Department of Physics — Optical fibers based on compositions of methacrylic and vinyl polymers mixed with low molar mass liquid crystals were prepared and studied as promising gas sensors. A range of concentrations producing anisotropic fibers that are mostly sensitive to the vapors of organic solvents was determined. The fibers were prepared by stretching gel-like compositions of polymers and liquid crystals. Mechanical properties of the compositions leading to the most stable fibers were studied. It was found that under certain conditions the fibers develop multilayered structure with anisotropic (mostly liquid crystalline) core. These fibers are very sensitive to changing gaseous atmosphere and to the presence of organic solvent vapors. The sensitivity of different types of fibers to a variety of organic solvents vapors was determined. Some fibers were crosslinked by using hydrogen bonding molecules. The behavior of these optical fibers with respect to the influence of organic vapors with and without hydrogen donor/acceptor moieties was also analyzed. It was shown that hydrogen bonding increases the mechanical strength of the fibers but does not affect substantially their sensitivity to gases. Optical calculations and model discussion accompany the presentation of experimental data.

### **10:36AM R37.00014 Reorientation and isotropisation of liquid crystals induced by gas diffusion.**

, ANTHONY TANTILLO, Fordham University Department of Physics, PETR SHIBAEV, Fordham University, Department of Physics — Reorientation and isotropisation of liquid crystals induced by organic solvent vapors was studied experimentally in relation to the use of liquid crystals as gas sensors. Reorientation and isotropisation were studied in the droplets deposited on the flat surface and on the tip of the hollow fibers. The anisotropy of gas diffusion was studied in the films and droplets of different sizes deposited on the surfaces with planar and homeotropic conditions. It was revealed that the diffusion coefficients differ approximately by a factor of two for liquid crystals in planar and homeotropic orientations. It was also shown that interference pattern created by passing light in liquid crystalline droplets deposited on the planar surface and on the tip of the hollow fiber can be used in detection of very small concentration of vapors. The model of diffusion is suggested and molecular dynamics simulations of the diffusion in liquid crystals with different molecular orientation are performed. The molecular dynamics simulations were performed on a time scale of about tens nanoseconds. In general they confirm the experimental results, but provide larger differences (by a factor 2 to 4) for diffusion coefficient in liquid crystals with planar and homeotropic orientation.

### **10:48AM R37.00015 Drying, phase separation, and deposition in droplets of sunset yellow chromonic liquid crystal<sup>1</sup>**

, ADAM GROSS, ZOEY S. DAVIDSON, University of Pennsylvania, YONGYANG HUANG, Lehigh University, TIM STILL, University of Pennsylvania, CHAO ZHOU, Lehigh University, A.G. YODH, University of Pennsylvania — We investigate the drying process and the final deposition patterns of multi-phase sessile droplets containing aqueous lyotropic chromonic liquid crystal (LC). The experiments employ a variety of optical techniques including profilometry, polarization optical microscopy and optical coherence microscopy. An unusual hierarchical LC assembly is observed during drying; in particular, LC mesogens are first formed at the start of drying and then compartments of isotropic, nematic and columnar phases arise. Nonuniform evaporation creates concentration gradients in droplets such that LC phases emerge from the outer edge of the drop and advance to the center over the course of drying. Distinct outward flows associated with the “coffee-ring effect” are seen initially, but the assembly of the mesogens creates viscosity, density, and surface tension gradients that effectively introduce new convective flows and complex LC phase boundaries within the drop. Finally, we show that the final deposit shape of chromonic materials changes with rate of evaporation.

<sup>1</sup>We gratefully acknowledge financial support through NSF DMR12-05463, MRSEC DMR11-20901, NASA NNX08AO0G, and NSF DBI-1455613.

## **Thursday, March 17, 2016 8:00AM - 11:00AM —**

**Session R38 DPOLY DBIO GSOF: Biopolymers and Biohybrid Polymers: Networks and Hydrogels** 341 - Bradley Olsen, MIT

### **8:00AM R38.00001 Self-Healing Nanocomposite Hydrogel with Well-Controlled Dynamic Mechanics**

, QIAOCHU LI, Massachusetts Inst of Tech-MIT, SUMEET MISHRA, North Carolina State University, PANGKUAN CHEN, Massachusetts Inst of Tech-MIT, JOSEPH TRACY, North Carolina State University, NIELS HOLTEN-ANDERSEN, Massachusetts Inst of Tech-MIT — Network dynamics is a crucial factor that determines the macroscopic self-healing rate and efficiency in polymeric hydrogel materials, yet its controllability is seldom studied in most reported self-healing hydrogel systems. Inspired by mussel's adhesion chemistry, we developed a novel approach to assemble inorganic nanoparticles and catechol-decorated PEG polymer into a hydrogel network. When utilized as reversible polymer-particle crosslinks, catechol-metal coordination bonds yield a unique gel network with dynamic mechanics controlled directly by interfacial crosslink structure. Taking advantage of this structure-property relationship at polymer-particle interfaces, we next designed a hierarchically structured hybrid gel with two distinct relaxation timescales. By tuning the relative contribution of the two hierarchical relaxation modes, we are able to finely control the gel's dynamic mechanical behavior from a viscoelastic fluid to a stiff solid, yet preserving its fast self-healing property without the need for external stimuli.

**8:12AM R38.00002 Polymer-induced compression of biological hydrogels**, SUJIT DATTA, ASHER PRESKA STEINBERG, RUSTEM ISMAGILOV, California Institute of Technology — Hydrogels – such as mucus, blood clots, and the extracellular matrix – provide critical functions in biological systems. However, little is known about how their structure is influenced by many of the polymeric materials they come into contact with regularly. Here, we focus on one critically important biological hydrogel: colonic mucus. While several biological processes are thought to potentially regulate the mucus hydrogel structure, the polymeric composition of the gut environment has been ignored. We use Flory-Huggins solution theory to characterize polymer-mucus interactions. We find that gut polymers, including those small enough to penetrate the mucus hydrogel, can in fact alter mucus structure, changing its equilibrium degree of swelling and forcing it to compress. The extent of compression increases with increasing polymer concentration and size. We use experiments on mice to verify these predictions with common dietary and therapeutic gut polymers. Our results provide a foundation for investigating similar, previously overlooked, polymer-induced effects in other biological hydrogels.

**8:24AM R38.00003 Thermal-induced ageing of agar solutions: impact on the structural and mechanical properties of agar gels<sup>1</sup>**, BOSI MAO, Centre de Recherche Paul Pascal, AHMED BENTALEB, FRÉDÉRIC LOUERAT, THIBAUT DIVOUX, PATRICK SNABRE, Centre de Recherche Paul Pascal - CNRS — Numerous hydrogels are prepared by cooling down to ambient temperature, aqueous polymer solutions brought to a boil. Although the incubation time of the polymer solution at such a high temperature could be used as a tuning parameter, its impact on the subsequent gelation has been poorly investigated. Here we study the effect of prolonged heating at 80°C on a 1.5% wt solution of agar, a natural polysaccharide. The incubation time is varied from a few hours up to five days. We show that the agar sol. continuously degrades as the result of both the hydrolysis and the intermolecular oxidation of the polymer chains. Furthermore, electronic microscopy and X-ray diffraction experiments reveal that gels formed from older agar sols display an increasingly coarser microstructure composed of micron-sized aggregated pieces of polysaccharides, in contrast with the fibrous-like structure of gels made from fresh sols. Along with structural changes prolonged incubation time leads to weaker gels of lower shear elastic modulus. Finally, macro-indentation experiments coupled to direct visualization show that increasing the incubation time of the agar sol. decreases the yield strain of the gel by a factor of three, while the rupture scenario turns continuously from brittle to ductile-like.

<sup>1</sup>acknowledging funding from BioMérieux & CNRS

**8:36AM R38.00004 Nonlinear elasticity of alginate gels**, SEYED MEYSAM HASHEMNEJAD, SANTANU KUNDU, Mississippi State University — Alginate is a naturally occurring anionic polysaccharide extracted from brown algae. Because of biocompatibility, low toxicity, and simple gelation process, alginate gels are used in biomedical and food applications. Here, we report the rheological behavior of ionically crosslinked alginate gels, which are obtained by in situ gelation of alginates with calcium salts, in between two parallel plates of a rheometer. Strain stiffening behavior was captured using large amplitude oscillatory shear (LAOS) experiments. In addition, negative normal stress was observed for these gels, which has not been reported earlier for any polysaccharide networks. The magnitude of negative normal stress increases with applied strain and can exceed that of the shear stress at large strain. Rheological results fitted with a constitutive model that considers both stretching and bending of chains indicate that nonlinearity is likely related to the stretching of the chains between the crosslink junctions. The results provide an improved understanding of the deformation mechanism of ionically crosslinked alginate gel and the results will be important in developing synthetic extracellular matrix (ECM) from these materials.

**8:48AM R38.00005 Cryo-imaging and modeling of the super molecular structure of cross-linked gelatin and its applications.**, CLEMENT MARMORAT, State Univ of NY- Stony Brook, ARKADI ARINSTEIN, Technion Israel Institute of Technology- Mechanical Engineering, NAAMA KOIFMAN, YESHAYAHU TALMON, Technion Israel Institute of Technology- Chemical Engineering, EYAL ZUSSMAN, Technion Israel Institute of Technology- Mechanical Engineering, MIRIAM RAFILOVICH, State Univ of NY- Stony Brook — The need for naturally derived materials to synthesize bio-compatible scaffolds is growing. In its natural state, gelatin derives its properties from a network of structured, intertwined, triple helical chains. The mechanical properties can be further controlled by additional enzymatic cross-linking. But, in contrast to simple polymer systems, the response to an imposed deformation is then determined by two competing factors, the establishment of the cross-linked mesh vs. the self-assembly of the fibrils into larger and therefore stronger hierarchical structures. Properties deduced from the response functions to measurements; such as rheology or swelling, are then a combination of these two very different factors, hence impossible to model unless more precise knowledge is available regarding the internal structure. We applied cryogenic-temperature scanning electron microscopy (cryo-SEM) to image the networks. Based on these images, a theoretical model was developed, for which we obtained excellent agreement for the mesh size of both networks, and their mechanical properties. We then used these controlled scaffolds, embedding them with fluorescent beads, to image live cells traction forces at stake during cell migration.

**9:00AM R38.00006 Encoding Mechano-Memories in Actin Networks**, LOUIS FOUCARD, UCLA, dpt of chemistry and biochemistry, SAYANTAN MAJUMDAR, James Franck institute, University of Chicago, dpt of Physics, ALEX LEVINE, UCLA, dpt of chemistry and biochemistry, MARGARET GARDEL, James Franck institute, University of Chicago, dpt of Physics — The ability of cells to sense and adapt to external mechanical stimuli is vital to many of its biological functions. A critical question is therefore to understand how mechanosensory mechanisms arise in living matter, with implications in both cell biology and smart materials design. Experimental work has demonstrated that the mechanical properties of semiflexible actin networks in Eukaryotic cells can be modulated (either transiently or irreversibly) via the application of external forces. Previous work has also shown with a combination of numerical simulations and analytic calculations shows that the broken rotational symmetry of the filament orientational distribution in semiflexible networks leads to dramatic changes in the mechanical response. Here we demonstrate with a combination of numerical and analytic calculations that the observed long-lived mechano-memory in the actin networks arise from changes in the nematic order of the constituent filaments. These stress-induced changes in network topology relax slowly under zero stress and can be observed through changes in the nonlinear mechanics. Our results provide a strategy for designing a novel class of materials and demonstrate a new putative mechanism of mechanical sensing in eukaryotic cells.

**9:12AM R38.00007 Fibril Formation and Phase Separation in Aqueous Cellulose Ethers**, AMANDA MAXWELL, University of Minnesota, Department of Chemistry, PETER SCHMIDT, University of Minnesota, Department of Chemistry and Materials Science, JOHN MCALLISTER, JOSEPH LOTT, University of Minnesota, Department of Chemistry, FRANK BATES, University of Minnesota, Department of Chemistry and Materials Science, TIMOTHY LODGE, University of Minnesota, Department of Chemistry — Aqueous solutions of many cellulose ethers are known to undergo thermoreversible gelation and phase separation upon heating to form turbid hydrogels, but the mechanism and resulting structures have not been well understood. Turbidity, light scattering and small-angle neutron scattering (SANS) are used to show that hydroxypropyl methylcellulose (HPMC) chains are dissolved in water below 50 °C and undergo phase separation at higher temperatures. At 70 °C, at sufficiently high concentrations in water, HPMC orders into fibrillar structures with a well-defined radius of  $18 \pm 2$  nm, as characterized by cryogenic transmission electron microscopy and SANS. The HPMC fibril structure is independent of concentration and heating rate. However, HPMC fibrils do not form a percolating network as readily as is seen in methylcellulose, resulting in a lower hot-gel modulus, as demonstrated by rheology.

**9:24AM R38.00008 Simulation of Polymer Physical Gel With Platelet Fillers**, DI XU, DILIP GERSSAPE, Stony Brook University — Platelet filler such as clays have superior effects on the properties of polymer gels. We used molecular dynamic simulations to study platelet filled composite gels system, in which small hexagonal disks simulate the platelets and gelation is due to short-range attraction between end-monomers and platelets. The properties of platelet filled composites are studied as a function of filler concentration. The mechanism of gelation was found similar to those of pure polymer gels; the polymers and platelets formed organic-inorganic networks, which percolate at high enough filler concentration. It was observed platelets aggregated into local intercalation structure, which significantly differs from typical spherical fillers. This unique intercalation structure is examined by radial distribution function and ordering parameters. We discussed how intercalation would affect the properties of the platelet composites by comparing them with spherical fillers.

**9:36AM R38.00009 A Coarse-Grained Model for Simulating Chitosan Hydrogels**, HONGCHENG XU, Biophysics Program, University of Maryland, College Park, SILVINA MATYSIAK, Biophysics Program, Fischell Department of Engineering, University of Maryland, College Park — Hydrogels are biologically-derived materials composed of water-filled cross-linking polymer chains. It has widely been used as biodegradable material and has many applications in medical devices. The chitosan hydrogel is stimuli-responsive for undergoing pH-sensitive self-assembly process, allowing programmable tuning of the chitosan deposition through electric pulse. To explore the self-assembly mechanism of chitosan hydrogels, we have developed an explicit-solvent coarse-grained chitosan model that has roots in the MARTINI force field, and the pH change is modeled by protonating chitosan chains using the Henderson-Hasselbalch equation. The mechanism of hydrogel network formation will be presented. The self-assembled polymer network qualitatively reproduces many experimental observables such as the pH-dependent strain-stress curve, bulk moduli, and structure factor. Our model is also capable of simulating other similar polyelectrolyte polymer systems.

**9:48AM R38.00010 Bio-Inspired Metal-Coordination Dynamics: A Unique Tool for Engineering Soft Matter Mechanics**, NIELS HOLTEN-ANDERSEN, Massachusetts Institute of Technology — Growing evidence supports a critical role of metal-coordination in soft biological material properties such as self-healing, underwater adhesion and autonomous wound plugging. Using bio-inspired metal-binding polymers, initial efforts to mimic these properties with metal-coordination crosslinked polymer materials have shown promise. In addition, with polymer network mechanics strongly coupled to coordinate crosslink dynamics material properties can be easily tuned from visco-elastic fluids to solids. Given their exploitation in desirable material applications in Nature, bio-inspired metal-coordinate complex crosslinking provides an opportunity to further advance synthetic polymer materials design. Early lessons from this pursuit are presented.

**10:24AM R38.00011 A Molecular Framework for Tunable Functional Response of Programmable Polyesters<sup>1</sup>**, KSHITIJ C. JHA, ABRAHAM JOY, MESFIN TSIGE, Department of Polymer Science, The University of Akron — All-atom molecular dynamics (MD) simulations, using the OPLS force field, were carried out on a library of multifunctional polyesters with peptide-like functional pendant groups. The polyesters are structural peptidomimetics and can be utilized for applications in sensing, and separation, and as biomedical scaffolds. The modular design of the polyesters affords a range of hydrophilic and hydrophobic behavior. We used MD to quantify the hydrogen bond dynamics, end-to-end distance, and radii of gyration with changes in side group functionality, concentration, and temperature. We discerned trends for the physical behavior of polyesters with change in nature and ratio of the side groups. We also observed functional assembly for dissimilar polyesters, and correlated the assembly to the affinity of side groups. The trends in physical behavior and dissimilar assembly can be mined for iterative design towards programmatic assembly of the modular multifunctional polyesters under study.

<sup>1</sup>This work was made possible by funding from the ACS Petroleum Research Fund (ACS PRF 54801- ND5)

**10:36AM R38.00012 Effects of Crowder Structure and Salt on DNA Mobility and Conformation in Crowded Environments<sup>1</sup>**, STEPHANIE M. GORCZYCA, RAE M. ROBERTSON-ANDERSON, University of San Diego — Biological cells are crowded environments in which DNA must move through to perform specific functions. We study how the properties of crowded cell-like environments impact DNA dynamics by tracking individual 115 kbp ring and linear DNA in different crowded environments using single-molecule fluorescence microscopy. We determine the role of crowder structure and salt on DNA diffusion and conformation by measuring the mean-squared center-of-mass displacements, as well as the conformational shape, size, and fluctuations of each molecule. Previously, we used 10 and 500 kDa dextran as crowders and showed that mobility of both ring and linear DNA decreased exponentially with increased crowding, but rings compact while linear DNA elongate. These effects were dependent solely on the reduction in available volume for DNA rather than size or number of crowders. Here we use crowders of similar molecular weight, but different structure to dextran (10 kDa PEG and 400 kDa Ficoll). We find that DNA mobility reduction is independent of crowder structure and that ring and linear DNA undergo more significant compaction. Finally, we characterize the role of salt on DNA mobility and conformation to determine the relative roles of enthalpic versus entropic effects on crowding-induced DNA dynamics.

<sup>1</sup>This research was funded by the AFOSR Young Investigator Program, Grant No. FA9550-12-1-0315 and the Arnold and Mabel Beckman Scholarship Foundation.

**10:48AM R38.00013 Altered Sputum Microstructure as a Marker of Airway Obstruction in Cystic Fibrosis Patients**, GREGG DUNCAN, JAMES JUNG, NATALIE WEST, MICHAEL BOYLE, JUNG SOO SUK, JUSTIN HANES, Johns Hopkins University — In the lungs of cystic fibrosis (CF) patients, highly viscoelastic mucus remains stagnant in the lung leading to obstructed airways prone to recurrent infections. Bulk-fluid rheological measurement is primarily used to assess the pathological features of mucus. However, this approach is limited in detecting microscopic properties on the length scale of pathogens and immune cells. We have shown in prior work based on the transport of muco-inert nanoparticles (MIP) in CF sputum that patients can carry significantly different microstructural properties. In this study, we aimed to determine the factors leading to variations between patients in sputum microstructure and their clinical implications. The microrheological properties of CF sputum were measured using multi-particle tracking experiments of MIP. MIP were made by grafting polyethylene glycol onto the surface of polystyrene nanoparticles which prior work has shown prevents adhesion to CF sputum. Biochemical analyses show that sputum microstructure was significantly altered by elevated mucin and DNA content. Reduction in sputum pore size is characteristic of patients with obstructed airways as indicated by measured pulmonary function tests. Our microstructural read-out may serve as a novel biomarker for CF.

**Thursday, March 17, 2016 8:00AM - 11:00AM —**

**Session R39 DBIO DPOLY GSNP: Physics of Genome Organization: from DNA to Chromatin**

I 342 - John Marko, Northwestern University

**8:00AM R39.00001 New insights into chromatin folding and dynamics from multi-scale modeling<sup>1</sup>** , WILMA OLSON, Rutgers, the State University of New Jersey — The dynamic organization of chromatin plays an essential role in the regulation of gene expression and in other fundamental cellular processes. The underlying physical basis of these activities lies in the sequential positioning, chemical composition, and intermolecular interactions of the nucleosomes—the familiar assemblies of roughly 150 DNA base pairs and eight histone proteins—found on chromatin fibers. We have developed a mesoscale model of short nucleosomal arrays and a computational framework that make it possible to incorporate detailed structural features of DNA and histones in simulations of short chromatin constructs with 3-25 evenly spaced nucleosomes. The correspondence between the predicted and observed effects of nucleosome composition, spacing, and numbers on long-range communication between regulatory proteins bound to the ends of designed nucleosome arrays lends credence to the model and to the molecular insights gleaned from the simulated structures. We have extracted effective nucleosome-nucleosome potentials from the mesoscale simulations and introduced the potentials in a larger scale computational treatment of regularly repeating chromatin fibers. Our results reveal a remarkable influence of nucleosome spacing on chromatin flexibility. Small changes in the length of the DNA fragments linking successive nucleosomes introduce marked changes in the local interactions of the nucleosomes and in the spatial configurations of the fiber as a whole. The changes in nucleosome positioning influence the statistical properties of longer chromatin constructs with 100-10,000 nucleosomes. We are investigating the extent to which the 'local' interactions of regularly spaced nucleosomes contribute to the corresponding interactions in chains with mixed spacings as a step toward the treatment of fibers with nucleosomes positioned at the sites mapped at base-pair resolution on genomic sequences.

<sup>1</sup>Support of the work by USPHS R01 GM 34809 is gratefully acknowledged.

**8:36AM R39.00002 Mitotic chromosome compaction via active loop extrusion.<sup>1</sup>** , ANTON GOLOBORODKO, MAXIM IMAKAEV, Massachusetts Inst of Tech-MIT, JOHN MARKO, Northwestern University, LEONID MIRNY, Massachusetts Inst of Tech-MIT, MIT-NORTHWESTERN TEAM — During cell division, two copies of each chromosome are segregated from each other and compacted more than hundred-fold into the canonical X-shaped structures. According to earlier microscopic observations and the recent Hi-C study, chromosomes are compacted into arrays of consecutive loops of ~100 kilobases. Mechanisms that lead to formation of such loop arrays are largely unknown. Here we propose that, during cell division, chromosomes can be compacted by enzymes that extrude loops on chromatin fibers. First, we use computer simulations and analytical modeling to show that a system of loop-extruding enzymes on a chromatin fiber self-organizes into an array of consecutive dynamic loops. Second, we model the process of loop extrusion in 3D and show that, coupled with the topo II strand-passing activity, it leads to robust compaction and segregation of sister chromatids. This mechanism of chromosomal condensation and segregation does not require additional proteins or specific DNA markup and is robust against variations in the number and properties of such loop extruding enzymes.

<sup>1</sup>Work at NU was supported by the NSF through Grants DMR-1206868 and MCB-1022117, and by the NIH through Grants GM105847 and CA193419. Work at MIT was supported by the NIH through Grants GM114190 R01HG003143.

**8:48AM R39.00003 Multiscale modeling of three-dimensional genome** , BIN ZHANG, PETER WOLYNES, Rice University — The genome, the blueprint of life, contains nearly all the information needed to build and maintain an entire organism. A comprehensive understanding of the genome is of paramount interest to human health and will advance progress in many areas, including life sciences, medicine, and biotechnology. The overarching goal of my research is to understand the structure-dynamics-function relationships of the human genome. In this talk, I will be presenting our efforts in moving towards that goal, with a particular emphasis on studying the three-dimensional organization, the structure of the genome with multi-scale approaches. Specifically, I will discuss the reconstruction of genome structures at both interphase and metaphase by making use of data from chromosome conformation capture experiments. Computationally modeling of chromatin fiber at atomistic level from first principles will also be presented as our effort for studying the genome structure from bottom up.

**9:00AM R39.00004 The universality of nucleosome organization: from yeast to human** , RAZVAN CHEREJI, NIH — The basic units of DNA packaging are called nucleosomes. Their locations on the chromosomes play an essential role in gene regulation. We study nucleosome positioning in yeast, fly, mouse, and human, and build biophysical models in order to explain the genome-wide nucleosome organization. We show that DNA sequence alone is not able to generate the phased arrays of nucleosomes observed in vivo near the transcription start sites. We discuss simple models which can account for the formation of nucleosome depleted regions and nucleosome phasing at the gene promoters. We show that the same principles apply to different organisms. References: [1] RV Chereji, D Tolkunov, G Locke, AV Morozov - Phys. Rev. E 83, 050903 (2011) [2] RV Chereji, AV Morozov - J. Stat. Phys. 144, 379 (2011) [3] RV Chereji, AV Morozov - Proc. Natl. Acad. Sci. U.S.A. 111, 5236 (2014) [4] RV Chereji, T-W Kan, et al. - Nucleic Acids Res. (2015) doi: 10.1093/nar/gkv978 [5] RV Chereji, AV Morozov - Brief. Funct. Genomics 14, 50 (2015) [6] HA Cole, J Ocampo, JR Iben, RV Chereji, DJ Clark - Nucleic Acids Res. 42, 12512 (2014) [7] D Ganguli, RV Chereji, J Iben, HA Cole, DJ Clark - Genome Res. 24, 1637 (2014)

**9:12AM R39.00005 Elucidate Chromatin Folding at the Mesoscale** , XIANGYUN QIU, George Washington Univ — Knowledge of the three-dimensional structure of chromatin, an active participant of all gene-directed processes, is required to decode its (epi)genetics-structure-function relationships. Albeit often simplified as “beads-on-a-string”, chromatin possesses daunting complexity in its intricate intra- and inter-nucleosome interactions, as well as the myriad types of molecules acting on it. On the other hand, the folding of chromatin from an extended chain of nucleosomes is highly constrained, e.g., by rather bulky nucleosomes and semi-rigid linker dsDNAs. Further given the well-defined nucleosome and dsDNA structures at the nanometer scale, this creates an opportunity for low-resolution structural methods such as small angle scattering to obtain mesoscale structures of chromatin, which can be further refined computationally to yield atomistic structures of chromatin. Here we present results from our recent studies of recombinant nucleosome arrays with solution small angle x-ray scattering (SAXS) and ensemble structure modeling.

**9:24AM R39.00006 Formation of chromosomal domains in interphase by loop extrusion** , GEORGE FREY FUDENBERG, MIT — While genomes are often considered as one-dimensional sequences, interphase chromosomes are organized in three dimensions with an essential role for regulating gene expression. Recent studies have shown that Topologically Associating Domains (TADs) are fundamental structural and functional building blocks of human interphase chromosomes. Despite observations that architectural proteins, including CTCF, demarcate and maintain the borders of TADs, the mechanisms underlying TAD formation remain unknown. Here we propose that loop extrusion underlies the formation TADs. In this process, cis-acting loop-extruding factors, likely cohesins, form progressively larger loops, but stall at TAD boundaries due to interactions with boundary proteins, including CTCF. This process dynamically forms loops of various sizes within but not between TADs. Using polymer simulations, we find that loop extrusion can produce TADs as determined by our analyses of the highest-resolution experimental data. Moreover, we find that loop extrusion can explain many diverse experimental observations, including: the preferential orientation of CTCF motifs and enrichments of architectural proteins at TAD boundaries; TAD boundary deletion experiments; and experiments with knockdown or depletion of CTCF, cohesin, and cohesin-loading factors. Together, the emerging picture from our work is that TADs are formed by rapidly associating, growing, and dissociating loops, presenting a clear framework for understanding interphase chromosomal organization.

**9:36AM R39.00007 TBA** , XIAOWEI ZHUANG, Harvard Univ — No abstract available.

**10:12AM R39.00008 Predictive Computational Modeling of Chromatin Folding**, MIICHELE DI PIERRO, BIN ZHANG, PETER J. WOLYNES, JOSE N. ONUCHIC, Center for Theoretical Biological Physics, Rice University — In vivo, the human genome folds into well-determined and conserved three-dimensional structures. The mechanism driving the folding process remains unknown. We report a theoretical model (MiChroM) for chromatin derived by using the maximum entropy principle. The proposed model allows Molecular Dynamics simulations of the genome using as input the classification of loci into chromatin types and the presence of binding sites of loop forming protein CTCF. The model was trained to reproduce the Hi-C map of chromosome 10 of human lymphoblastoid cells. With no additional tuning the model was able to predict accurately the Hi-C maps of chromosomes 1-22 for the same cell line. Simulations show unknotted chromosomes, phase separation of chromatin types and a preference of chromatin of type A to sit at the periphery of the chromosomes.

**10:24AM R39.00009 Robustness of nucleosome patterns in the presence of DNA sequence-specific free energy landscapes and active remodeling**, JOHANNES NUEBLER, Physik-Department, Technische Universität München, BENEDIKT OBERMAYER, WOLFRAM MBIUS, Max-Delbrück-Center for Molecular Medicine, MICHAEL WOLFF, ULRICH GERLAND, Physik-Department, Technische Universität München — Proper positioning of nucleosomes in eukaryotic cells is important for transcription regulation. When averaged over many genes, nucleosome positions in coding regions follow a simple oscillatory pattern, which is described to a surprising degree of accuracy by a simple one-dimensional gas model for particles interacting via a soft-core repulsion. The quantitative agreement is surprising given that nucleosome positions are known to be determined by a complex interplay of mechanisms including DNA sequence-specific nucleosome stability and active repositioning of nucleosomes by remodeling enzymes. We rationalize the observed robustness of the simple oscillatory pattern by showing that the main effect of several known nucleosome positioning mechanisms is a renormalization of the particle interaction. For example, disorder from sequence-specific affinities leads to an apparent softening, while active remodeling can result in apparent softening for directional sliding or apparent stiffening for clamping mechanisms. We suggest that such parameter renormalization can explain the apparent difference of nucleosome properties in two yeast species, *S. cerevisiae* and *S. pombe*.

**10:36AM R39.00010 The role of Nucleosome Positions on Chromatin Structure: A multi-scale approach**, JOSHUA LEQUIEU, ANDRES CORDOBA, JUAN J. DE PABLO, University of Chicago — Nucleosomes compose the basic unit of chromatin, and their locations are central to the regulation and compaction of eukaryotic genomes. In this work, we examine the coupling between different length scales within chromatin by examining the influence of nucleosome positions on three-dimensional chromatin structure. First, using a detailed molecular model of DNA and proteins, we predict the one-dimensional positioning of nucleosomes and the repositioning mechanisms of nucleosomal DNA. We demonstrate that this mechanism is strongly dependent on DNA sequence and that DNA slides around the histone proteins by either a screw-like or loop-like rearrangement. Next, we couple this detailed model to a coarsened model of chromatin and examine the impact of DNA sequence on chromatin's three-dimensional structure. We show that both the locations of nucleosomes and the mechanisms by which they move have a significant impact on higher-order chromatin structure and that variations in DNA sequence lead to "open" or "closed" regions of chromatin. This approach represents an efficient tool towards understanding the higher order structure of chromatin and how various aspects of chromatin structure are coupled together.

**10:48AM R39.00011 Chromatin extrusion explains key features of loop and domain formation in wild-type and engineered genomes**, ADRIAN SANBORN, SUHAS RAO, Stanford, SU-CHEN HUANG, NEVA DURAND, MIRIAM HUNTLEY, ANDREW JEWETT, IVAN BOCHKOV, DHARMARAJ CHINNAPPAN, ASHOK CUTKOSKY, JIAN LI, KRISTOPHER GEETING, DOUG MCKENNA, ELENA STAMENOVA, Baylor College of Medicine, ANDREAS GNIRKE, ALEXANDRE MELNIKOV, ERIC LANDER, Broad Institute, EREZ AIDEN, Baylor College of Medicine — Our recent kilobase-resolution genome-wide maps of DNA self-contacts demonstrated that mammalian genomes are organized into domains and loops demarcated by the DNA-binding protein CTCF. Here, we combine these maps with new Hi-C, microscopy, and genome-editing experiments to study the physical structure of chromatin fibers, domains, and loops. We find that domains are inconsistent with equilibrium and fractal models. Instead, we use physical simulations to study two models of genome folding. In one, intermonomer attraction during condensation leads to formation of an anisotropic "tension globule." In the other, CTCF and cohesin act together to extrude unknotted loops. Both models are consistent with the observed domains and loops. However, the extrusion model explains a far wider array of observations, such as why the CTCF-binding motifs at pairs of loop anchors lie in the convergent orientation. Finally, we perform 13 genome-editing experiments examining the effect of altering CTCF-binding sites on chromatin folding. The extrusion model predicts *in silico* the experimental maps using only CTCF-binding sites. Thus, we show that it is possible to disrupt, restore, and move loops and domains using targeted mutations as small as a single base pair.

**Thursday, March 17, 2016 8:00AM - 11:00AM —**

**Session R40 GSNP: Systems with Large Fluctuations and Strong Correlations I** 343 - Michel Pleimling, Virginia Tech

**8:00AM R40.00001 Kinetic roughening: how directionality changes the game**, NUNO ARAUJO, Universidade de Lisboa — The nonequilibrium evolution of growing interfaces has attracted many experimental and theoretical studies over decades. One of the most popular theoretical approaches considers kinetic discrete models to describe particle aggregation on substrates. Albeit simple, these models are expected to contain the relevant physics. Inspired by recent advances in the production of functionalized colloidal particles, with attractive patches on their surface, we have proposed a stochastic model to study the effect of directionality and selective pairwise interactions on the kinetics of aggregation. We find a nontrivial dependence of the bulk and surface properties on the strength and flexibility of the patch-patch interactions, and on the spatial-patch distribution. For three-patch particles, sustained growth is only observed for a finite-range of the distance between patches, yielding two absorbing phase transitions and a tricritical flexibility. For four-patch particles with two distinct patches, i.e. strong and weak bonds, and sufficiently different bonding probabilities, the scaling properties of the interface crossover from the universality class of Kardar-Parisi-Zhang to the critical class of Kardar-Parisi-Zhang with quenched disorder. The latter is observed for an extended range of the parameters revealing the presence of a self-organized critical mechanism. Implications of our findings beyond functionalized particles are also discussed.

**8:36AM R40.00002 Exactly solvable models of growing interfaces: the Arcetri models**, XAVIER DURANG, Korean Institute for Advanced Study, MALTE HENKEL, Université de Lorraine, France — Motivated by an analogy with the spherical model of a ferromagnet, the Arcetri models present new universality classes for the growth of interfaces, distinct from the common Edwards-Wilkinson and Kardar-Parisi-Zhang universality classes. Those models are obtained by treating and replacing the non-linear term in the noisy Burgers equation or the KPZ equation by a mean spherical condition. We studied the consequences of such constraints on the Edwards-Wilkinson (EW) interface.

**8:48AM R40.00003 Infinite-noise criticality: Nonequilibrium phase transitions in fluctuating environments**<sup>1</sup>, THOMAS VOJTA, Missouri Univ of Science and Technology, JOSE HOYOS, Instituto de Física de São Carlos — We study the effects of time-varying environmental noise on nonequilibrium phase transitions in spreading and growth processes. Using the examples of the logistic evolution equation as well as the contact process, we show that such temporal disorder gives rise to a distinct type of critical points at which the effective noise amplitude diverges on long time scales. This leads to enormous density fluctuations characterized by an infinitely broad probability distribution at criticality. We develop a real-time renormalization-group theory that provides a general framework for the effects of temporal disorder on nonequilibrium processes. We also discuss how general this exotic critical behavior is, we illustrate the results by computer simulations, and we touch upon experimental applications of our theory.

<sup>1</sup>Supported by the NSF under Grant No. DMR-1205803, by Simons Foundation, by FAPESP under Grant No. 2013/09850-7, and by CNPq under Grant Nos. 590093/2011-8 and 305261/2012-6.

**9:00AM R40.00004 Random field disorder at an absorbing state transition in one and two dimensions**<sup>1</sup>, HATEM BARGHATHI, THOMAS VOJTA, Missouri S&T — We investigate the behavior of nonequilibrium phase transitions under the influence of disorder that locally breaks the symmetry between two symmetrical macroscopic absorbing states. In equilibrium systems such “random-field” disorder destroys the phase transition in low dimensions by preventing spontaneous symmetry breaking. In contrast, we show here that random-field disorder fails to destroy the nonequilibrium phase transition of the one- and two-dimensional generalized contact process. Instead, it hampers the dynamics in the symmetry-broken phase. Specifically, the dynamics in the one-dimensional case is described by a Sinai walk of the domain walls between two different absorbing states. In the two-dimensional case, we map the dynamics onto that of the well studied low-temperature random-field Ising model. We also study the critical behavior of the nonequilibrium phase transition and characterize its universality class in one dimension. We support our results by large-scale Monte-Carlo simulations and discuss the applicability of our theory to other systems.

<sup>1</sup>This work was supported by the NSF under Grants No. DMR-1205803

Department of Computer Science, Boulder, CO  
80309, USA.  
Mechanical Engineering & Mechanics,  
Drexel University,  
Philadelphia, PA 19104 USA

**9:12AM R40.00005 Leveraging large fluctuations for stochastic control in uncertain environments**<sup>1</sup>, IRA SCHWARTZ<sup>2</sup>, Naval Research Lab, CHRISTOFFER HECKMAN, University of Colorado, M. ANI HSIEH, Drexel University — We present the development of a stochastic control strategy that leverages the environmental dynamics and uncertainty to navigate in a stochastic fluidic environment. We assume that the domain is composed of the union of a collection of disjoint regions, each bounded by Lagrangian coherent structures (LCSs). We analyze a passive particle’s noise-induced transition between adjacent LCS-bounded regions and show how most probable escape trajectories with respect to the transition probability between adjacent LCS-bounded regions can be determined. Additionally, we show how the likelihood of transition can be controlled through minimal actuation. The result is an energy efficient navigation strategy that leverages the inherent uncertainty of the surrounding flow field for controlling sensors in a noisy fluidic environment. We experimentally validate the proposed control strategy and show that the single vehicle control parameter exhibits a predictable exponential scaling with respect to the escape times and is effective even in situations where the structure of the flow is not fully known and control effort is costly.

<sup>1</sup>IBS supported by ONR nos. F1ATA01098G001, N0001412WX-20083. MAH by ONR award numbers N000141211019 and N0001413-10731.

<sup>2</sup>Nonlinear Systems Dynamics Section, Code 6792, Washington, DC 20375 USA

**9:24AM R40.00006 Flux line non-equilibrium relaxation kinetics following current quenches in disordered type-II superconductors**<sup>1</sup>, HARSHWARDHAN CHATURVEDI, HIBA ASSI, Department of Physics, Virginia Tech, ULRICH DOBRAMYSL, The Gurdon Institute, University of Cambridge, U.K., MICHEL PLEIMLING, UWE TÄUBER, Department of Physics, Virginia Tech — We investigate the relaxation dynamics of magnetic vortex lines in disordered type-II superconductors following rapid changes in the external driving current by means of Langevin molecular dynamics simulations for an elastic line model. A system of driven interacting flux lines in a sample with randomly distributed point pinning centers is initially relaxed to a moving non-equilibrium steady state. The current is then instantaneously decreased, such that the final stationary state resides either still in the moving regime, or in the pinned Bragg glass phase. The ensuing non-equilibrium relaxation kinetics of the vortices is studied in detail by measuring the mean flux line gyration radius and the two-time transverse height autocorrelation function. The latter allows us to investigate the physical aging properties for quenches from the moving into the glassy phase, and to compare with non-equilibrium relaxation features obtained with different initial configurations.

<sup>1</sup>Research supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02-09ER46613.

**9:36AM R40.00007 Local temperatures and voltages in quantum systems far from equilibrium**<sup>1</sup>, ABHAY SHASTRY, CHARLES STAFFORD, University of Arizona, DEPARTMENT OF PHYSICS COLLABORATION — We show that the local measurement of temperature and voltage for a quantum system in steady state, arbitrarily far from equilibrium, with arbitrary interactions within the system, is unique when it exists. This is interpreted as a consequence of the second law of thermodynamics. We further derive a necessary and sufficient condition for the existence of a solution. In this regard, we find that a solution occurs whenever there is no net population inversion. However, when there is a net population inversion, we may characterize the system with a (unique) negative temperature. These results provide a firm mathematical foundation for our measurement protocol, and sound meaning to such measurements in the thermodynamic sense.

<sup>1</sup>Research supported by the US Department of Energy, grant DE-SC 0006699

**9:48AM R40.00008 Quasiparticle explanation of "weak thermalization" regime under quench in a non-integrable quantum spin chain** , CHENG-JU LIN, OLEXEI MOTRUNICH, Caltech — Eigenstate Thermalization Hypothesis provides one picture of thermalization in a quantum system by looking at individual eigenstates. However, it is also important to consider how local observables reach equilibrium values dynamically. Quench protocol is one of the settings to study such questions. A recent numerical study [Banuls, Cirac, and Hastings, Phys. Rev. Lett. **106**, 050405 (2011)] of a nonintegrable quantum Ising model with longitudinal field under such quench setting found different behaviors under different initial quantum states. One particular case termed weak thermalization regime showed apparently persistent oscillations of some observables. Here we provide an explanation of such oscillations. We use perturbation theory near the ground state of the model, and identify the oscillation frequency as the quasiparticle mass. With this quasiparticle picture, we can then address the long-time behavior of the oscillations.

**10:00AM R40.00009 How can an autonomous quantum Maxwell demon harness correlated information?**<sup>1</sup> , ADRIAN CHAPMAN, AKIMASA MIYAKE, Univ of New Mexico, CQUIC THERMODYNAMICS TEAM — We study an autonomous quantum system, which exhibits refrigeration under an information-work tradeoff like a Maxwell demon. The system becomes correlated as a single demon qubit interacts sequentially with memory qubits while in contact with two heat reservoirs of different temperatures. Using strong subadditivity of the von Neumann entropy, we derive a global Clausius inequality to show thermodynamical advantages from access to correlated information. It is demonstrated, in a matrix product density operator formalism, that our demon can simultaneously realize refrigeration against a thermal gradient and erasure of information from its memory, which is impossible without correlations. The phenomenon can be even enhanced by the presence of quantum coherence.

<sup>1</sup>The work was supported in part by National Science Foundation grants PHY-1212445 and PHY-1521016.

**10:12AM R40.00010 Fano-Andreev effect in Quantum Dots in Kondo regime**<sup>1</sup> , PEDRO ORELLANA, ANA MARIA CALLE, MONICA PACHECO, Universidad Tecnica Federico Santa Maria, VICTOR APEL, Universidad Catlica del Norte — In the present work, we investigate the transport through a T-shaped double quantum dot system coupled to two normal leads and to a superconducting lead. We study the role of the superconducting lead in the quantum interferometric features of the double quantum dot and by means of a slave boson mean field approximation at low temperature regime. We inquire into the influence of intradot interactions in the electronic properties of the system as well. Our results show that Fano resonances due to Andreev bound states are exhibited in the transmission from normal to normal lead as a consequence of quantum interference and proximity effect. This Fano effect produced by Andreev bound states in a side quantum dot was called Fano-Andreev effect, which remains valid even if the electron-electron interaction are taken into account, that is, the Fano-Andreev effect is robust against e-e interactions even in Kondo regime.

<sup>1</sup>We acknowledge the financial support from FONDECYT program Grants No. 3140053 and 11400571

**10:24AM R40.00011 Quantum critical temperature of a modulated oscillator** , VITTORIO PEANO, University of Erlangen-Nrnberg, LINGZHEN GUO, MICHAEL MARTHALER, Karlsruhe Institute of Technology, MARK DYKMAN, Michigan State University — We show that the rate of switching between the vibrational states of a modulated nonlinear oscillator is characterized by a quantum critical temperature  $T_c \propto \hbar^2$ . Above  $T_c$  there emerges a quantum crossover region where the switching rate displays a steep and characteristic temperature dependence, followed by a qualitatively different temperature dependence for higher  $T$ . In contrast to the crossover between tunneling and thermal activation in equilibrium systems, here the crossover occurs between different regimes of switching activated by quantum fluctuations. The results go beyond the standard real-time instanton technique of the large-deviation theory.

**10:36AM R40.00012 The interplay between universal scaling laws and vortex clustering in two-dimensional quantum turbulence** , AUDUN SKAUGEN, LUIZA ANGHELUTA, Univ of Oslo — The relationship between vortex dynamics and the turbulent energy spectrum is an active research topic in quantum turbulence of superfluids and Bose-Einstein condensates. The energy spectra in quantum turbulence exhibit a Kolmogorov -5/3 scaling law, analogous to classical turbulence. Recent developments show that in two-dimensional quantum flows, this energy spectrum corresponds to an inverse energy cascade, which is realized by clustering of like-signed quantized vortices. We investigate numerically the statistics of quantized vortices in two-dimensional quantum turbulence using the Gross-Pitaevskii equation. We find that a universal -5/3 scaling law in the turbulent energy spectrum is intimately connected with the vortex statistics, such as number fluctuations and velocity, which also show a similar scaling behavior. The -5/3 scaling law appearing in the power spectrum of the vortex number is consistent with a scenario of isolated vortices passively advected by a turbulent superfluid velocity, which is again generated by like-signed vortex clusters. The velocity probability distribution of clustered vortices is also sensitive to spatial correlations, and exhibits a power-law tail with a -5/3 exponent that we can predict analytically from the point vortex model.

**10:48AM R40.00013 Fluctuation loops in a noise-driven linear circuit model** , STEPHEN TEITSWORTH, AKHIL GHANTA, JOHN NEU, Duke University — Understanding the spatio-temporal structure of most probable fluctuation pathways to rarely occurring states is a central problem in the study of noise-driven, non-equilibrium dynamical systems. When the underlying system does not possess detailed balance, the optimal fluctuation pathway to a particular state and relaxation pathway from that state may combine to form a loop-like structure in the system phase space which we call a *fluctuation loop*. Here, we study fluctuation loops in a linear circuit model consisting of coupled RC elements, where each element is driven by its own noise source and, generally, the effective noise strengths of different elements are not equal. Using a stochastic Hamiltonian approach, we determine the optimal fluctuation pathways, and construct corresponding fluctuation loops. Analytical results agree closely with suitably averaged simulation results based on the associated Langevin equation. To better characterize fluctuation loops, we study the time-dependent area tensor that is swept out by individual stochastic trajectories in the system phase space. At long times, the area tensor scales linearly with time, with a coefficient that precisely vanishes when the system satisfies detailed balance.

**Thursday, March 17, 2016 8:00AM - 11:00AM —**

**Session R41 DBIO: Neural Control of Behavior** 344 - Gordon Berman, Emory University

**8:00AM R41.00001 Taking Action: How Small Brains Make Big Choices** , GWYNETH CARD, HHMI Janelia Research Campus — No abstract available.

**8:36AM R41.00002 Tracking *C. elegans* and its neuromuscular activity using NemaFlex** , FRANK VAN BUSSEL, Department of Mechanical Engineering, Texas Tech University, MIZANUR RAHMAN, JENNIFER HEWITT, Department of Chemical Engineering, Texas Tech University, JERZY BLAWDZIEWICZ, Department of Mechanical Engineering, Texas Tech University, MONICA DRISCOLL, Department of Molecular Biology and Biochemistry, Rutgers University, NATHANIEL SZEWCZYK, MRC/Arthritis Research UK Centre for Musculoskeletal Ageing Research, University of Nottingham, UK, SIVA VANAPALLI, Department of Chemical Engineering, Texas Tech University — Recently, a novel platform has been developed for studying the behavior and physical characteristics of the nematode *C. elegans*. This is NemaFlex, developed by the Vanapalli group at Texas Tech University to analyze movement and muscular strength of crawling *C. elegans*. NemaFlex is a microfluidic device consisting of an array of deformable PDMS pillars, with which the *C. elegans* interacts in the course of moving through the system. Deflection measurements then allow us to calculate the force exerted by the worm via EulerBernoulli beam theory. For the procedure to be fully automated a fairly sophisticated software analysis has to be developed in tandem with the physical device. In particular, the usefulness of the force calculations is highly dependent on the accuracy and volume of the deflection measurements, which would be prohibitively time-consuming if carried out by hand/eye. In order to correlate the force results with muscle activations the *C. elegans* itself has to be tracked simultaneously, and pillar deflections precisely associated with mechanical-contact on the worm's body. Here we will outline the data processing and analysis routines that have been implemented in order to automate the calculation of these forces and muscular activations.

**8:48AM R41.00003 High Throughput Interrogation of Behavioral Transitions in *C. elegans*** , MOCHI LIU, JOSHUA SHAEVITZ, ANDREW LEIFER, Princeton University — We present a high-throughput method to probe transformations from neural activity to behavior in *Caenorhabditis elegans* to better understand how organisms change behavioral states. We optogenetically deliver white-noise stimuli to target sensory or inter neurons while simultaneously recording the movement of a population of worms. Using all the postural movement data collected, we computationally classify stereotyped behaviors in *C. elegans* by clustering based on the spectral properties of the instantaneous posture. (Berman et al., 2014) Transitions between these behavioral clusters indicate discrete behavioral changes. To study the neural correlates dictating these transitions, we perform model-driven experiments and employ Linear-Nonlinear-Poisson cascades that take the white-noise stimulus as the input. The parameters of these models are fitted by reverse-correlation from our measurements. The parameterized models of behavioral transitions predict the worm's response to novel stimuli and reveal the internal computations the animal makes before carrying out behavioral decisions. Preliminary results are shown that describe the neural-behavioral transformation between neural activity in mechanosensory neurons and reversal behavior.

**9:00AM R41.00004 Influence of the Enteric Nervous System on Gut Motility Patterns in Zebrafish<sup>1</sup>** , RYAN BAKER, Dept of Physics, Univ of Oregon, JULIA GANZ, ELLIE MELANCON, JUDITH EISEN, Institute of Neuroscience, University of Oregon, RAGHUVeer PARTHASARATHY, Department of Physics, University of Oregon — The enteric nervous system (ENS), composed of diverse neuronal subtypes and glia, regulates essential gut functions including motility, secretion, and homeostasis. In humans and animals, decreased numbers of enteric neurons lead to a variety of types of gut dysfunction. However, surprisingly little is known about how the number, position, or subtype of enteric neurons affect the regulation of gut peristalsis, due to the lack of good model systems and the lack of tools for the quantitative characterization of gut motion. We have therefore developed a method of quantitative spatiotemporal mapping using differential interference contrast microscopy and particle image velocimetry, and have applied this to investigate intestinal dynamics in normal and mutant larval zebrafish. From movies of gut motility, we obtain a velocity vector field representative of gut motion, from which we can quantify parameters relating to gut peristalsis such as frequency, wave speed, deformation amplitudes, wave duration, and non-linearity of waves. We show that mutants with reduced neuron number have contractions that are more regular in time and reduced in amplitude compared to wild-type (normal) fish. We also show that feeding fish before their yolk is consumed leads to stronger motility patterns.

<sup>1</sup>We acknowledge support from NIH awards P50 GM098911 and P01 HD022486

**9:12AM R41.00005 Improved Software for Quantifying the Behavior of *Drosophila* Larvae** , NATALIE BERNAT, MARC GERSHOW, New York University — A key advantage of small crawling organisms like *C. elegans* and the *Drosophila* larva is that their behaviors may be assayed automatically using computer vision software. Current state of the art software is capable of detecting the positions and postures of crawling larvae and automatically categorize their behaviors in parallel. However, these algorithms, which are based on frame-by-frame analysis of thresholded black and white images, fail to correctly describe the postures of larvae executing sharp bends and have difficulty separating multiple larvae that are physically touching. We present new tracking software that uses intensity information in grayscale images and applies temporal smoothness constraints to positions and postures. We implemented this software as an ImageJ plugin, extending its portability and applicability.

**9:24AM R41.00006 Development of a two photon microscope for tracking *Drosophila* larvae** , DOYCHO KARAGYOZOV, MIRNA MIHOVILOVIC SKANATA, MARC GERSHOW, New York Univ NYU — Current in vivo methods for measuring neural activity in *Drosophila* larva require immobilization of the animal. Although we can record neural signals while stimulating the sensory organs, we cannot read the behavioral output because we have prevented the animal from moving. Many research questions cannot be answered without observation of neural activity in behaving (freely-moving) animals. Our project aims to develop a tracking microscope that maintains the neurons of interest in the field of view and in focus during the rapid three dimensional motion of a free larva.

**9:36AM R41.00007 Chemotaxis of *Caenorhabditis elegans* in complex media: crawling, burrowing, 2D and 3D swimming, and controlled fluctuations hypothesis<sup>1</sup>** , AMAR PATEL, ALEJANDRO BILBAO, Dept. of Mechanical Engineering, Texas Tech University, MIZANUR RAHMAN, SIVA VANAPALLI, Dept. of Chemical Engineering, Texas Tech University, JERZY BLAWDZIEWICZ, Dept. of Mechanical Engineering, Texas Tech University — *Caenorhabditis elegans* is a powerful genetic model, essential for studies in diverse areas ranging from behavior to neuroscience to aging, and locomotion and chemotaxis are the two key observables used. We combine our recently developed theory of nematode locomotion and turning maneuvers [Phys. Fluids 25, 081902 (2013)] with simple models of chemosensation to analyze nematode chemotaxis strategies in 2D and 3D environments. We show that the sharp-turn (pirouette) chemotaxis mechanism is efficient in diverse media; in particular, the nematode does not need to adjust the sensing or motion-control parameters to efficiently chemotax in 2D crawling, 3D burrowing, and 2D or 3D swimming. In contrast, the graduate-turn mechanism becomes inefficient in swimming, unless a phase-shift is introduced between the sensing signal and modulation of body wave to generate the gradual turn. We hypothesize that there exists a new "controlled fluctuations" chemotaxis mechanism, in which the nematode changes the intensity of undulation fluctuations to adjust the persistence length of the trajectory in response to a variation in chemoattractant concentration.

<sup>1</sup>Supported by NSF Grant No. CBET 1059745

**9:48AM R41.00008 Motor neurons in *Drosophila* flight control: could b1 be the one?** , SAMUEL WHITEHEAD, Department of Physics, Cornell University, TROY SHIRANGI, HHMI, Janelia Farm Campus, ITAI COHEN, Department of Physics, Cornell University — Similar to balancing a stick on ones fingertip, flapping flight is inherently unstable; maintaining stability is a delicate balancing act made possible only by near-constant, often-subtle corrective actions. For fruit flies, such corrective responses need not only be robust, but also fast: the *Drosophila* flight control reflex has a response latency time of ~5 ms, ranking it among the fastest reflexes in the animal kingdom. How is such rapid, robust control implemented physiologically? Here we present an analysis of a putatively crucial component of the *Drosophila* flight control circuit: the b1 motor neuron. Specifically, we apply mechanical perturbations to freely-flying *Drosophila* and analyze the differences in kinematics patterns between flies with manipulated and un-manipulated b1 motor neurons. Ultimately, we hope to identify the functional role of b1 in flight stabilization, with the aim of linking it to previously-proposed, reduced-order models for reflexive control.

**10:00AM R41.00009 System identification and sensorimotor determinants of flight maneuvers in an insect**, SIMON SPONBERG, Georgia Tech, ROBERT HALL, EATAI ROTH, Univ. of Washington — Locomotor maneuvers are inherently closed-loop processes. They are generally characterized by the integration of multiple sensory inputs and adaptation or learning over time. To probe sensorimotor processing we take a system identification approach treating the underlying physiological systems as dynamic processes and altering the feedback topology in experiment and analysis. As a model system, we use agile hawk moths (*Manduca sexta*), which feed from real and robotic flowers while hovering in mid air. Moths rely on vision and mechanosensation to track floral targets and can do so at exceptionally low luminance levels despite hovering being a mechanically unstable behavior that requires neural feedback to stabilize. By altering the sensory environment and placing mechanical and visual signals in conflict we show a surprisingly simple linear summation of visual and mechanosensation produces a generative prediction of behavior to novel stimuli. Tracking performance is also limited more by the mechanics of flight than the magnitude of the sensory cue. A feedback systems approach to locomotor control results in new insights into how behavior emerges from the interaction of nonlinear physiological systems.

**10:12AM R41.00010 Leveraging low-dimensional postures to resolve coiled shapes reveals new reorientation behaviors in the nematode *C. elegans*.**, GREG STEPHENS, VU Amsterdam and OIST Graduate University, ONNO BROEKMANS, VU Amsterdam and Lumicks, WILLIAM RYU, University of Toronto — Low-dimensionality is both a fundamental property of many living systems and an aid in their quantitative analysis. Here, we exploit the low-dimensionality of *C. elegans* body shape to develop a novel postural tracking algorithm which captures both simple worm shapes and also complex, self-occluding coils. We apply our algorithm to a thermally-evoked escape response with relatively simple coils and to more complex, spontaneous turns which occur during foraging. We divide the escape response into three post-stimulus phases, reversal, turn and post-turn, and find that the full distribution of reorientation angles is shaped by independent and significant contributions from all three phases, a result consistent with the release and presence of the monoamine tyramine during the entire response. In spontaneous coils we find two separable peaks of turning posture amplitudes, indicating distinct reorientation behaviors of large-amplitude ventral-side turns; large ventral bearing reorientations occur through a shape sequence similar to the escape response while large dorsal bearing reorientations are accomplished by overturning across the ventral side. We find that these large-amplitude turning events occur independently but with approximately matched rates that adapt on a similar timescale.

**10:24AM R41.00011 Slithering on sand: kinematics and controls for success on granular media.**, PERRIN E SCHIEBEL, TINGNAN ZHANG, Georgia Institute of Technology, JIN DAI, CHAOHUI GONG, MIAO YU, Carnegie Mellon University, HENRY C ASTLEY, Georgia Institute of Technology, MATTHEW TRAVERS, HOWIE CHOSSET, Carnegie Mellon University, DANIEL I GOLDMAN, Georgia Institute of Technology — Previously, we studied the *subsurface* locomotion of undulatory sand-swimming snakes and lizards; using empirical drag response of GM to subsurface intrusion of simple objects allowed us to develop a granular resistive force theory (RFT) to model the locomotion and predict optimal movement patterns. However, our knowledge of the physics of GM at the surface is limited; this makes it impossible to determine how the desert-dwelling snake *C. occipitalis* moves effectively (0.45+/-0.04 bodylengths/sec) on the surface of sand. We combine organism biomechanics studies, GM drag experiments, RFT calculations and tests of a physical model (a snake-like robot), to reveal how multiple factors acting together contribute to slithering on sandy surfaces. These include the kinematics—targeting an ideal waveform which maximizes speed while minimizing joint-level torque, the ability to modulate ground interactions by lifting body segments, and the properties of the GM. Based on the sensitive nature of the relationship between these factors, we hypothesize that having an element of force-based control, where the waveform is modulated in response to the forces acting between the body and the environment, is necessary for successful locomotion on yielding substrates.

**10:36AM R41.00012 Dynamic Control of Walking and Paw-shaking in the Cat**, JESSICA GREEN, GENNADY CYMBALYUK, Georgia State University — Multistable central pattern generators (CPGs) are capable of producing multiple rhythmic patterns with different periods. We developed a model of a half center oscillator, consisting of two reciprocally inhibitory neurons. Each neuron contains two slow inward currents, a  $\text{Na}^+$  current, and a  $\text{Ca}^{++}$  current. We found that a walking rhythm (1 Hz) and a paw-shaking rhythm (10 Hz) do coexist in this model. The kinetics of the inactivations of  $\text{I}_{\text{NaS}}$  and  $\text{I}_{\text{CaS}}$  produce this multistability. A paw-shaking response can be demonstrated as a result of a switch in the multistable model or as a transient response of a nearby monostable model. The duration of this transient paw-shaking response depends on pulse duration and the phase of walking at which the pulse is initiated. We also developed a model of two populations with 20 neurons each, in which there are random inhibitory synapses across the two populations and random excitatory synapses within each population. This population model generates similar behavior as the two neuron model.

**10:48AM R41.00013 Recovery methods of the dragonfly from irregular initial conditions.**, JAMES MELFI, Cornell University, ANTHONY LEONARDO, HHMI Janelia Farms, JANE WANG, Cornell University — We release dragonflies from a magnetic tether in a wide range of initial orientations, which results in them utilizing multiple methods to regain their typical flight orientation. Special focus is placed on dropping them while upside down, as the recovery method used is a purely rolling motion. Filming this stereotypical motion with a trio of high speed cameras at 4000 fps, we capture detailed body and wing kinematics data to determine how the dragonfly generates this motion. By replaying the flights within a computer simulation, we can isolate the significant changes to wing kinematics, and find that it is an asymmetry in the wing pitch which generates the roll. Further investigation demonstrates that this choice is highly dependent upon the state of the dragonfly, and as such our results indicate the dragonfly both tracks its current state, and changes its mid-flight control mechanisms accordingly.

**Thursday, March 17, 2016 8:00AM - 10:48AM –**

**Session R42 DPOLY: Small Molecule Transport in Polymers and Polymer Nanocomposites II**

345 - William Phillip, University of Notre Dame

**8:00AM R42.00001 Statistical Mechanical Theory of Penetrant Diffusion in Polymer Melts and Glasses**, RUI ZHANG, KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — We generalize our force-level, self-consistent nonlinear Langevin equation theory of activated diffusion of a dilute spherical penetrant in hard sphere fluids [1] to predict the long-time diffusivity of molecular penetrants in supercooled polymer liquids and non-aging glasses. Chemical complexity is treated using an a priori mapping to a temperature-dependent hard sphere mixture model where polymers are disconnected into effective spheres based on the Kuhn length as the relevant coarse graining scale. A key parameter for mobility is the penetrant to polymer segment diameter ratio,  $R$ . Our calculations agree well with experimental measurements for a wide range of temperatures, penetrant sizes (from gas molecules with  $R \sim 0.3$  to aromatic molecules with  $R \sim 1$ ) and diverse amorphous polymers, over 10 decades variation of penetrant diffusivity. Structural parameter transferability is good. We have also formulated a theory at finite penetrant loading for the coupled penetrant-polymer dynamics in chemically (nearly) matched mixtures (e.g., toluene-polystyrene) which captures well the increase of penetrant diffusivity and decrease of polymer matrix vitrification temperature with increasing loading. [1] R. Zhang and K. S. Schweizer, J. Chem. Phys., 143, 144906 (2015).

**8:12AM R42.00002 Molecular Dynamics Simulations of Penetrants in Microphase Separated Tapered Diblock Copolymers<sup>1</sup>**, YOUNGMI SEO, JONATHAN R. BROWN, LISA M. HALL, Ohio State Univ - Columbus — Tapered AB diblock copolymers contain pure A and B monomer blocks on the ends with a tapered midblock of intermediate composition, providing taper length as an additional tuning parameter to control microphase separation and interfacial behavior. We model the midblock as a statistical linear gradient from pure A to pure B. Recent experiments with salt dissolved in one of microphases show that a certain length of taper increases ion conductivity while the same length of inverse taper lowers conductivity. We perform coarse-grained molecular dynamics simulations of tapered copolymers with monomer sized penetrants, which have preferential interactions with one microphase, to better understand this observation and the general effects of tapering on dynamics. We calculate penetrant diffusion, polymer relaxation times, and other quantities over the range from 0% (diblock) to 100% (full gradient) taper length, with the taper direction either normal or inverse (with the A side of the taper connected to the pure B block). Normal taper results typically lie between those of diblocks and full gradients, while inverse tapers show strong nonmonotonic behavior as a function of taper length. For intermediate length inverse tapers, penetrant and monomer dynamics are significantly slower than those of diblocks or normal tapers, and this relates to the folding of the inverse chains back and forth across the interface. To provide further insight, we also compare to the dynamics of random copolymers of various compositions.

<sup>1</sup>Based upon work supported by NSF Grant 1454343

**8:24AM R42.00003 Mechanism of Concentration Dependence of Water Diffusivity in Polyacrylate Gels.**, SRIRAMVIGNESH MANI, FARDIN KHABAZ, RAJESH KHARE, Texas Tech University — Membrane based separation processes offer an energy efficient alternative to traditional distillation based separation processes. In this work, we focus on the molecular mechanisms underlying the process of separation of dilute ethanol-water mixture using polyacrylate gels as pervaporation membranes. The diffusivities of the components in swollen gels exhibit concentration dependence. We have used molecular dynamics (MD) simulations to study the correlation between the dynamics of solvent (water and ethanol) molecules, polymer dynamics and solvent structure in the swollen gel systems as a function of solvent concentration. Three different polyacrylate gels were studied: (1) poly n-butyl acrylate (PBA), (2) copolymer of butyl acrylate and 2-hydroxyethyl acrylate P(BA50-HEA50), and (3) poly 2-hydroxyethyl acrylate (PHEA). Simulation results show that solvent concentration has a significant effect on local structure of the solvent molecules and chain dynamics; these factors (local structure and chain dynamics), in turn, affect the diffusivity of these molecules. At low concentration, solvent molecules are well dispersed in the gel matrix and form hydrogen bonds with the polymer. Solvent mobility is correlated with polymer mobility in this configuration and consequently water and ethanol molecules exhibit slower dynamics, this effect is especially significant in PHEA gel. At high solvent concentration, water molecules form large clusters in the system accompanied by enhancement in mobility of both the gel network and the solvent molecules.

**8:36AM R42.00004 Structure/property relationships in polymer membranes for water purification and energy applications**, GEOFFREY GEISE, University of Virginia — Providing sustainable supplies of purified water and energy is a critical global challenge for the future, and polymer membranes will play a key role in addressing these clear and pressing global needs for water and energy. Polymer membrane-based processes dominate the desalination market, and polymer membranes are crucial components in several rapidly developing power generation and storage applications that rely on membranes to control rates of water and/or ion transport. Much remains unknown about the influence of polymer structure on intrinsic water and ion transport properties, and these relationships must be developed to design next generation polymer membrane materials. For desalination applications, polymers with simultaneously high water permeability and low salt permeability are desirable in order to prepare selective membranes that can efficiently desalinate water, and a tradeoff relationship between water/salt selectivity and water permeability suggests that attempts to prepare such materials should rely on approaches that do more than simply vary polymer free volume. One strategy is to functionalize hydrocarbon polymers with fixed charge groups that can ionize upon exposure to water, and the presence of charged groups in the polymer influences transport properties. Additionally, in many emerging energy applications, charged polymers are exposed to ions that are very different from sodium and chloride. Specific ion effects have been observed in charged polymers, and these effects must be understood to prepare charged polymers that will enable emerging energy technologies. This presentation discusses research aimed at further understanding fundamental structure/property relationships that govern water and ion transport in charged polymer films considered for desalination and electric potential field-driven applications that can help address global needs for clean water and energy.

**9:12AM R42.00005 Ion transferring in polyelectrolyte networks in electric fields.**, HONGHAO LI, AYKUT ERBAS, Northwestern Univ, JOS ZWANIKKEN, University of Massachusetts Lowell, MONICA OLVERA DE LA CRUZ, Northwestern Univ — Ion-conducting polyelectrolyte gels have drawn the attention of many researchers in the last few decades as they have wide applications not only in lithium batteries but also as stretchable, transparent ionic conductor or ionic cables devices. However, ion dynamics in polyelectrolyte gels has been much less studied analytically or computationally due to the complicated interplay of long-range electrostatic and short-range interactions. Here we propose a coarse-grained non-equilibrium molecular dynamics simulation to study the ion dynamics in polyelectrolyte gels under external electric fields. We found a nonlinear response region where the molar conductivity of polyelectrolyte gels increases with external fields. We propose counterion redistribution under electric fields as the driving mechanism. We also found the ionic conductivity to be modulated by changing polyelectrolyte network topology such as the chain length. Our discovery reveals the essential difference of ion dynamics between electrolytes and polyelectrolyte gels. These results will expand our understanding in charged polymeric systems and help in designing ion-conducting devices with higher conductivity.

**9:24AM R42.00006 Thermodynamics of Ionic Transport through Functionalized Membranes**, VIKRAMJIT RATHEE, SIYI QU, THEODORE DILENSCHNEIDER, WILLIAM A. PHILLIP, JONATHAN K. WHITMER, Chemical and Biomolecular Engineering, University of Notre Dame — Through microphase separation of block copolymers, highly porous solid membranes may be assembled. Further functionalization with amine and sulfonic acid groups has demonstrated promise in exquisitely controlling the flux of charged species, and in particular multivalent ions. Using coarse-grained molecular simulations, we explore the essential thermodynamics underlying salt rejection in charge-functionalized membranes, and develop a model capable of linking the performance of these membranes to their molecular character through free energy calculations.

**9:36AM R42.00007 Theoretical model of Case-II diffusion based on molecular-dynamics study of methanol in PMMA<sup>1</sup>**, JIAYUAN MIAO, Case Western Reserve University, MESFIN TSIGE, University of Akron, PHILIP TAYLOR, Case Western Reserve University — In Case-II diffusion, a sharp diffusion front moves at a nearly constant speed. An obstacle to the theoretical prediction of the form of this front lies in the large mismatch between the time scale of atomic motion, which is measured in femtoseconds, and the time scale of diffusion in a macroscopic sample, which is measured in millions of seconds. We attempt to overcome this limitation by using the short-time results of atomistic molecular-dynamics simulations to construct a stochastic model valid over all time scales. The ability of this model to yield Case-II diffusion behavior was confirmed, and it was then developed into a continuum mathematical model in which the diffusivity  $D$  has a strong dependence on the concentration of the penetrant. We anticipate that solution of the appropriate non-linear diffusion equation will yield an accurate portrayal of the characteristics of the diffusion process.

<sup>1</sup>Work supported by the Petroleum Research Fund of the American Chemical Society

**9:48AM R42.00008 Multicomponent Diffusion of Penetrant Mixtures in Rubbery Polymers: A Molecular Dynamics Study**, STEFAN BRINGUIER, MARK VARADY, OptiMetrics, Inc. a DCS Company, CRAIG KNOX, Leidos, Inc., JERRY CABALO, R&T Directorate, Edgewood Chemical Biological Center, THOMAS PEARL, OptiMetrics, Inc. a DCS Company, BRENT MANTOOTH, R&T Directorate, Edgewood Chemical Biological Center — The importance of understanding transport of chemical species across liquid-solid boundaries is of particular interest in the decontamination of harmful chemicals absorbed within polymeric materials. To characterize processes associated with liquid-phase extraction of absorbed species from polymers, it is necessary to determine an appropriate physical description of species transport in multicomponent systems. The Maxwell-Stefan (M-S) formulation is a rigorous description of mass transport in multicomponent solutions, in which, mutual diffusivities determine the degree of relative motion between interacting molecules in response to a chemical potential gradient. The work presented focuses on the determination of M-S diffusivities from molecular dynamics (MD) simulations of nerve agent O-ethyl S-[2(diisopropylamino)ethyl] methylphosphonothioate (VX), water, and methanol mixtures within a poly(dimethylsiloxane) matrix. We investigate the composition dependence of M-S diffusivities and compare the results to values predicted using empirical relations for binary and ternary mixtures. Finally, we highlight the pertinent differences in molecular mechanisms associated with species transport and employ non-equilibrium MD to probe transport across the mixture-polymer interface.

**10:00AM R42.00009 Cooperative Reformable Channel System with Unique Recognition of Small Gas Molecules in a two-dimensional ZIF-membrane**, BENYAMIN MOTEVALLI, NEDA TAHERIFAR, ZHE LIU, Department of Mechanical and Aerospace Engineering, Monash University, Clayton, Victoria 3800, Australia — We report a cooperative reformable channel system in a coordination porous polymer, named as ZIF-L. Three types of local flexible ligands coexist in the crystal structure of this polymer, resulting in ultra-flexibility. The reformable channel is able to regulate permeation of a nonspherical guest molecule, such as N<sub>2</sub> or CO<sub>2</sub>, based on its longer molecular dimension, which is in a striking contrast to conventional molecular sieves that regulate the shorter cross-sectional dimension of the guest molecules. Our density functional theory (DFT) calculations reveal that the guest molecule induces dynamic motion of the flexible ligands, leading to the channel reformation, and then the guest molecule reorients itself to fit in the reformed channel. Such a unique “induced fit-in” mechanism causes the gas molecule to pass through 6 membered-ring windows in the c- crystal direction of ZIF-L with its longer axis parallel to the window plane. Our experimental permeance of N<sub>2</sub> through the ZIF-L membranes is about three times greater than that of CO<sub>2</sub>, supporting the DFT simulation predictions.

**10:12AM R42.00010 Predicting the solubility of gases in Nitrile Butadiene Rubber in extreme conditions using molecular simulation**, MUSAB KHAWAJA, NICOLA MOLINARI, ADRIAN SUTTON, Imperial College London, Department of Physics and the Thomas Young Centre for Theory and Simulation of Materials, UK, ARASH MOSTOFI, Imperial College London, Departments of Materials and Physics and the Thomas Young Centre for Theory and Simulation of Materials, UK — In the oil and gas industry, elastomer seals play an important role in protecting sensitive monitoring equipment from contamination by gases - a problem that is exacerbated by the high pressures and temperatures found down-hole. The ability to predict and prevent such permeative failure has proved elusive to-date. Nitrile butadiene rubber (NBR) is a common choice of elastomer for seals due to its resistance to heat and fuels. In the conditions found in the well it readily absorbs small molecular weight gases. How this behaviour changes quantitatively for different gases as a function of temperature and pressure is not well-understood. In this work a series of fully atomistic simulations are performed to understand the effect of extreme conditions on gas solubility in NBR. Widom particle insertion is used to compute solubilities. The importance of sampling and allowing structural relaxation upon compression are highlighted, and qualitatively reasonable trends reproduced. Finally, while at STP it has previously been shown that the solubility of CO<sub>2</sub> is higher than that of He in NBR, we observe that under the right circumstances it is possible to reverse this trend.

**10:24AM R42.00011 Analysis of surface segregation in polymer mixtures: A combination of mean field and statistical associated fluid theories**, JAROSLAW KRAWCZYK<sup>1</sup>, SALVATORE CROCE, BUDDHAPRIYA CHAKRABARTI, Department of Mathematical Sciences, Durham University, South Road, Durham DH1 3LE, United Kingdom., JOS TASCHE, Department of Chemistry, Durham University, South Road, Durham DH1 3LE, United Kingdom. — The surface segregation in polymer mixtures remains a challenging problem for both academic exploration as well as industrial applications. Despite its ubiquity and several theoretical attempts a good agreement between computed and experimentally observed profiles has not yet been achieved. A simple theoretical model proposed in this context by Schmidt and Binder combines Flory-Huggins free energy of mixing with the square gradient theory of wetting of a wall by fluid. While the theory gives us a qualitative understanding of the surface induced segregation and the surface enrichment it lacks the quantitative comparison with the experiment. The statistical associating fluid theory (SAFT) allows us to calculate accurate free energy for a real polymeric materials. In an earlier work we had shown that increasing the bulk modulus of a polymer matrix through which small molecules migrate to the free surface causes reduction in the surface migrant fraction using Schmidt-Binder and self-consistent field theories. In this work we validate this idea by combining mean field theories and SAFT to identify parameter ranges where such an effect should be observable.

<sup>1</sup>Department of Molecular Physics, Łódź University of Technology, Żeromskiego 116, 90-924 Łódź, Poland

**10:36AM R42.00012 Continuum Model for Decontamination of Chemical Warfare Agent from a Rubbery Polymer using the Maxwell-Stefan Formulation**, MARK VARADY, STEFAN BRINGUIER, THOMAS PEARL, OptiMetrics, Inc., a DCS Company, SHAWN STEVENSON, BRENT MANTOOTH, RT Directorate, Edgewood Chemical Biological Center — Decontamination of polymers exposed to chemical warfare agents (CWA) often proceeds by application of a liquid solution. Absorption of some decontaminant components proceed concurrently with extraction of the CWA, resulting in multicomponent diffusion in the polymer. In this work, the Maxwell-Stefan equations were used with the Flory-Huggins model of species activity to mathematically describe the transport of two species within a polymer. This model was used to predict the extraction of the nerve agent O-ethyl S-[2(diisopropylamino)ethyl] methylphosphonothioate (VX) from a silicone elastomer into both water and methanol. Comparisons with experimental results show good agreement with minimal fitting of model parameters from pure component uptake data. Reaction of the extracted VX with sodium hydroxide in the liquid-phase was also modeled and used to predict the overall rate of destruction of VX. Although the reaction proceeds more slowly in the methanol-based solution compared to the aqueous solution, the extraction rate is faster due to increasing VX mobility as methanol absorbs into the silicone, resulting in an overall faster rate of VX destruction.

**Thursday, March 17, 2016 8:00AM - 10:48AM –**

**Session R43 GSNP: Nonlinear Dynamics in Networks | 346 - Adilson Motter, Northwestern University**

**8:00AM R43.00001 Collective Dynamics of Oscillator Networks: Why do we suffer from heavy jet lag?** , HIROSHI KORI, Ochanomizu University — The circadian rhythm of the entire body in mammals is orchestrated by a small tissue in the brain called the suprachiasmatic nucleus (SCN). The SCN consists of a population of neurons, each of which exhibit circadian (i.e., approximately 24 h) gene expression. Neurons form a complex network and interact with each other using various types of neurotransmitters. The rhythmic gene expressions of individual cells in the SCN synchronize through such interaction. Jet-lag symptoms arise from temporal mismatch between the internal circadian clock orchestrated by the SCN and external solar time. It may take about one week or even longer to recover from jet lag after a long-distance trip. We recently found that recovery from jet lag is considerably accelerated in the knocked-out (KO) mice lacking the receptors of a certain neurotransmitter in the SCN [1]. Importantly, all other properties of mice including sleep-awake rhythms and breeding seem to be intact. Only the response to the jet lag changes. It was also found that after a few days of jet lag, cells in the SCN desynchronize in the wild type (WT) mice, whereas they do not in KO mice. This desynchrony might be a main reason for heavy jet lag symptoms. To understand the mechanism underlying jet lag, we propose a simple model of the SCN, which is a network of phase oscillators [1]. Despite its simplicity, this model can reproduce important dynamical properties of the SCN. For example, this model reproduces the desynchrony of oscillators after jet lag. Moreover, when intercellular interaction is weaker, this desynchrony is suppressed and the recover from jet lag is considerably accelerated. Our mathematical study provides a deeper understanding of jet lag and an idea how to circumvent heavy jet lag symptoms. [1] Y. Yamaguchi, T. Suzuki, Y. Mizoro, H. Kori, K. Okada, Y. Chen, J.M. Fustin, F. Yamazaki, N. Mizuguchi, J. Zhang, X. Dong, G. Tsujimoto, Y. Okuno, M. Doi, H. Okamura: Mice Genetically Deficient in Vasopressin V1a and V1b Receptors Are Resistant to Jet Lag, *Science* 342, pp. 85-90 (2013).

**8:36AM R43.00002 Synchronization in neuronal oscillator networks with input heterogeneity and arbitrary network structure** , ELIZABETH DAVISON, BISWADIP DEY, NAOMI LEONARD, Princeton University — Mathematical studies of synchronization in networks of neuronal oscillators offer insight into neuronal ensemble behavior in the brain. Systematic means to understand how network structure and external input affect synchronization in network models have the potential to improve methods for treating synchronization-related neurological disorders such as epilepsy and Parkinson's disease. To elucidate the complex relationships between network structure, external input, and synchronization, we investigate synchronous firing patterns in arbitrary networks of neuronal oscillators coupled through gap junctions with heterogeneous external inputs. We first apply a passivity-based Lyapunov analysis to undirected networks of homogeneous FitzHugh-Nagumo (FN) oscillators with homogeneous inputs and derive a sufficient condition on coupling strength that guarantees complete synchronization. In biologically relevant regimes, we employ Gronwall's inequality to obtain a bound tighter than those previously reported. We extend both analyses to a homogeneous FN network with heterogeneous inputs and show how cluster synchronization emerges under conditions on the symmetry of the coupling matrix and external inputs. Our results can be generalized to any network of semi-passive oscillators.

**8:48AM R43.00003 Independent Noise Can Synchronize Interacting Networks of Pulse-Coupled Oscillators<sup>1</sup>** , HERMANN RIECKE, JOHN MENG, Northwestern University — Structured networks comprised of subnetwork modules are ubiquitous. Motivated by the observation of rhythms and their interaction in different brain areas, we study a network consisting of two subnetworks of pulse-coupled integrate-fire neurons. Through mutual inhibition the neurons in the individual subnetworks can become synchronized and each subnetwork can exhibit coherent oscillatory dynamics, e.g. an ING-rhythm. In the absence of coupling between the networks the rhythms will in general have different frequencies. We investigate the interaction between these different rhythms. Strikingly, we find that increasing the noise level in the input to the individual neurons can synchronize the rhythms of the two networks, even though the inputs to different neurons are uncorrelated, sharing no common component. A heuristic phase model for the coupled networks shows that this synchronization hinges on the fact that only a fraction of the neurons may spike in a given cycle. Thus, the synchronization of the network rhythms differs qualitatively from that of individual oscillators.

<sup>1</sup>supported by NSF-CMMI 1435358

**9:00AM R43.00004 A simple experimental realization of the Sakaguchi-Kuramoto model** , DAVID MERTENS, ZHUWEI ZENG, LARS ENGLISH, Dickinson College — We explore the collective phase dynamics of Wien-bridge oscillators coupled resistively. The dynamics of these oscillators were recently shown to follow Sakaguchi's modification to the Kuramoto model. In this talk we outline the steps of that analysis. We then examine results for a variety of experimentally obtained coupling arrangements, including all-to-all and some-to-all. In particular, we provide evidence for the emergence of synchronized clusters, a finite-size effect that is not accounted for in the traditional theories for the Sakaguchi-Kuramoto model.

**9:12AM R43.00005 Experimental studies of a chain of Sakaguchi-Kuramoto oscillators** , HANYU MA, DAVID MERTENS, LARS ENGLISH, Dickinson College, HANYU MA TEAM, LARS ENGLISH COLLABORATION, DAVID MERTENS COLLABORATION — The collective phase dynamics of Wien-bridge oscillators, coupled resistively, were recently shown to follow the Sakaguchi-Kuramoto model. In this talk we present experimental findings for the dynamics of rings of oscillators. For identical speeds and uni-directional nearest-neighbor coupling, we find that the system quickly approaches a steady state of identical nearest-neighbor phase offsets. We then present the effects of adding disorder to the natural speeds. We also discuss the case of bi-directional coupling, in which case chimera behavior is expected.

**9:24AM R43.00006 Title: Chimeras in small, globally coupled networks: Experiments and stability analysis** , JOSEPH D. HART, University of Maryland, College Park, KANIKA BANSAL, None, THOMAS E. MURPHY, RAJARSHI ROY, University of Maryland, College Park — Since the initial observation of chimera states, there has been much discussion of the conditions under which these states emerge. The emphasis thus far has mainly been to analyze large networks of coupled oscillators; however, recent studies have begun to focus on the opposite limit: what is the smallest system of coupled oscillators in which chimeras can exist? We experimentally observe chimeras and other partially synchronous patterns in a network of four globally-coupled chaotic opto-electronic oscillators. By examining the equations of motion, we demonstrate that symmetries in the network topology allow a variety of synchronous states to exist, including cluster synchronous states and a chimera state. Using the group theoretical approach recently developed for analyzing cluster synchronization, we show how to derive the variational equations for these synchronous patterns and calculate their linear stability. The stability analysis gives good agreement with our experimental results. Both experiments and simulations suggest that these chimera states often appear in regions of multistability between global, cluster, and desynchronized states.

**9:36AM R43.00007 ABSTRACT WITHDRAWN** —

**9:48AM R43.00008 Emerging hierarchies in dynamically adapting webs** , ELENI KATIFORI, University of Pennsylvania, JOHANNES GRAEWER, Max-Planck Institute for Dynamics and Self-Organization, MARCELO MAGNASCO, CARL MODES, Rockefeller University — Transport networks play a key role across four realms of eukaryotic life: slime molds, fungi, plants, and animals. In addition to the developmental algorithms that build them, many also employ adaptive strategies to respond to stimuli, damage, and other environmental changes. We model these adapting network architectures using a generic dynamical system on weighted graphs and find in simulation that these networks ultimately develop a hierarchical organization of the final weighted architecture accompanied by the formation of a system-spanning backbone. We quantify the hierarchical organization of the networks by developing an algorithm that decomposes the architecture to multiple scales and analyzes how the organization in each scale relates to that of the scale above and below it. The methodologies developed in this work are applicable to a wide range of systems including the slime mold *Physarum polycephalum*, human microvasculature, and force chains in granular media.

**10:00AM R43.00009 Hybrid percolation transition in complex networks** , BYUNGNAM KAHNG, Seoul National University — Percolation has been one of the most applied statistical models. Percolation transition is one of the most robust continuous transitions known thus far. However, recent extensive researches reveal that it exhibits diverse types of phase transitions such as discontinuous and hybrid phase transitions. Here hybrid phase transition means the phase transition exhibiting natures of both continuous and discontinuous phase transitions simultaneously. Examples include k-core percolation, cascading failures in interdependent networks, synchronization, etc. Thus far, it is not manifest if the critical behavior of hybrid percolation transitions conforms to the conventional scaling laws of second-order phase transition. Here, we investigate the critical behaviors of hybrid percolation transitions in the cascading failure model in inter-dependent networks and the restricted Erdos-Renyi model. We find that the critical behaviors of the hybrid percolation transitions contain some features that cannot be described by the conventional theory of second-order percolation transitions.

**10:12AM R43.00010 Phase Transitions in Networks of Memristive Elements** , FORREST SHELDON, MASSIMILIANO DI VENTRA, Univ of California - San Diego — The memory features of memristive elements (resistors with memory), analogous to those found in biological synapses, have spurred the development of neuromorphic systems based on them (see, e.g., [1]). In turn, this requires a fundamental understanding of the collective dynamics of networks of memristive systems. Here, we study an experimentally-inspired model of disordered memristive networks in the limit of a slowly ramped voltage and show through simulations that these networks undergo a first-order phase transition in the conductivity for sufficiently high values of memory, as quantified by the memristive ON/OFF ratio. We provide also a mean-field theory that reproduces many features of the transition and particularly examine the role of boundary conditions and current- vs. voltage-controlled networks. The dynamics of the mean-field theory suggest a distribution of conductance jumps which may be accessible experimentally. We finally discuss the ability of these networks to support massively-parallel computation. Work supported in part by the Center for Memory and Recording Research at UCSD. [1] Y.V. Pershin and M. Di Ventra, Proc. IEEE, 100, 2071 (2012).

**10:24AM R43.00011 ABSTRACT WITHDRAWN —**

**10:36AM R43.00012 A network model of human aging: Limits, errors, and information** , SPENCER FARRELL, ARNOLD MITNITSKI, KENNETH ROCKWOOD, ANDREW RUTENBERG, Dalhousie University — The Frailty Index (FI) quantifies human aging using the fraction of accumulated age-related deficits. The FI correlates strongly with mortality and accumulates non-linearly and stochastically with age. Clinical data shows a nearly universal limit of  $FI \leq 0.7$ . We computationally model an aging population using a network model of interacting deficits. Deficits damage and repair at rates that depend upon the average damage of connected nodes. The model is parametrized to fit clinical data. We find that attribution errors, especially false negative, allow the model to recover the frailty limit. Mutual information allows us to assess how well the FI can predict mortality. Mutual information provides a non-parametric measure of how the FI predicts mortality. We find that attribution errors have a small effect on the mutual information when many deficits are included in the model. The mutual information of our model and of the clinical data are comparable.

**Thursday, March 17, 2016 8:00AM - 11:00AM —**

**Session R44 GQI: Quantum Information and Thermodynamics** 347 - Mohammad Ansari, Delft University of Technology

**8:00AM R44.00001 Quantum thermodynamics for arbitrarily small devices** , STEPHANIE WEHNER, Delft Univ of Tech — Quantum thermodynamics for arbitrarily small devices.

**8:36AM R44.00002 Exceeding the Carnot efficiency** , NELLY HUEI YING NG, Delft Univ of Tech, MISCHA WOODS, University College of London, Department of Physics and Astronomy, London WC1E 6BT, United Kingdom, STEPHANIE WEHNER, Delft Univ of Tech — A suitable way of quantifying work for microscopic quantum systems has been constantly debated in the field of quantum thermodynamics. One natural approach is to measure the average increase in energy of an ancillary system, called the battery, after a work extraction protocol. The quality of work extracted is usually argued to be good by quantifying higher moments of the energy distribution, or by restricting the amount of entropy to be low. This limits the amount of heat contribution to the energy extracted, but does not completely prevent it. We show that if one allows for a definition of work that tolerates a non-negligible entropy increase in the battery, then a small scale heat engine (with a similar set up to that of arXiv:1506.02322) can possibly exceed the Carnot efficiency. This can be done without using any additional resources such as coherence or correlations, and furthermore can be achieved by using finite-size quantum heat baths as well.

**8:48AM R44.00003 The maximum efficiency of nano heat engines depends on more than temperature<sup>1</sup>** , MISCHA WOODS, Uni Coll London, & TU Delft, Netherlands & National Uni Singapore, NELLY NG, TU Delft, Netherlands & National Uni Singapore, STEPHANIE WEHNER, TU Delft, Netherlands — Sadi Carnots theorem regarding the maximum efficiency of heat engines is considered to be of fundamental importance in the theory of heat engines and thermodynamics. Here, we show that at the nano and quantum scale, this law needs to be revised in the sense that more information about the bath other than its temperature is required to decide whether maximum efficiency can be achieved. In particular, we derive new fundamental limitations of the efficiency of heat engines at the nano and quantum scale that show that the Carnot efficiency can only be achieved under special circumstances, and we derive a new maximum efficiency for others. A preprint can be found here arXiv:1506.02322 [quant-ph]

<sup>1</sup> Singapore MOE Tier 3A Grant & STW, Netherlands

**9:00AM R44.00004 Autonomous quantum thermal machines and quantum to classical energy flow** , MAX FRENZEL, DAVID JENNINGS, TERRY RUDOLPH, Imperial College London — We address the issue of autonomous quantum thermal machines that are tailored to achieve some specific thermodynamic primitive, such as work extraction in the presence of a thermal environment, while having minimal or no control from the macroscopic regime. Beyond experimental implementations, this provides an arena in which to address certain foundational aspects such as the role of coherence in thermodynamics, the use of clock degrees of freedom and the simulation of local time-dependent Hamiltonians in a particular quantum subsystem. For small-scale systems additional issues arise. Firstly, it is not clear to what degree genuine ordered thermodynamic work has been extracted, and secondly non-trivial back-actions on the thermal machine must be accounted for. We find that both these aspects can be resolved through a judicious choice of quantum measurements that magnify thermodynamic properties up the ladder of length-scales, while simultaneously stabilizing the quantum thermal machine. Within this framework we show that thermodynamic reversibility is obtained in a particular Zeno limit, and finally illustrate these concepts with a concrete example involving spin-systems.

### 9:12AM R44.00005 Stochastic Independence as a Resource for Small-Scale Thermodynamics

, MATTEO LOSTAGLIO, Imperial College London, MARKUS P. MUELLER, Western Ontario University and Perimeter Institute for Theoretical Physics, MICHELE PASTENA, Heidelberg University — It is well-known in thermodynamics that the creation of correlations costs work. It seems then a truism that if a thermodynamic transformation  $A \rightarrow B$  is impossible, so will be any transformation that in sending  $A$  to  $B$  also correlates among them some auxiliary systems  $C$ . Surprisingly, we show that this is not the case for non-equilibrium thermodynamics of microscopic systems. On the contrary, the creation of correlations greatly extends the set of accessible states, to the point that we can perform on individual systems and in a single shot any transformation that would otherwise be possible only if the number of systems involved was very large. We also show that one only ever needs to create a vanishingly small amount of correlations (as measured by mutual information) among a small number of auxiliary systems (never more than three). The many, severe constraints of microscopic thermodynamics are reduced to the sole requirement that the non-equilibrium free energy decreases in the transformation. This shows that, in principle, reliable extraction of work equal to the free energy of a system can be performed by microscopic engines.

### 9:24AM R44.00006 Quantum coherence, time-translation symmetry and thermodynamics

, KAMIL KORZEKWA, MATTEO LOSTAGLIO, DAVID JENNINGS, TERRY RUDOLPH, Imperial College London — The first law of thermodynamics imposes not just a constraint on the energy content of systems in extreme quantum regimes but also symmetry constraints related to the thermodynamic processing of quantum coherence. We show that this thermodynamic symmetry decomposes any quantum state into mode operators that quantify the coherence present in the state. We then establish general upper and lower bounds for the evolution of quantum coherence under arbitrary thermal operations, valid for any temperature. We identify primitive coherence manipulations and show that the transfer of coherence between energy levels manifests irreversibility not captured by free energy. Moreover, the recently developed thermomajorization relations on block-diagonal quantum states are observed to be special cases of this symmetry analysis.

### 9:36AM R44.00007 Quantum work statistics of charged Dirac particles in time-dependent fields<sup>1</sup>

, SEBASTIAN DEFFNER, AVADH SAXENA, Los Alamos Natl Lab — The quantum Jarzynski equality is an important theorem of modern quantum thermodynamics. We show that the Jarzynski equality readily generalizes to relativistic quantum mechanics described by the Dirac equation. After establishing the conceptual framework we solve a pedagogical, yet experimentally relevant, system analytically. As a main result we obtain the exact quantum work distributions for charged particles traveling through a time-dependent vector potential evolving under Schrödinger as well as under Dirac dynamics, and for which the Jarzynski equality is verified. Special emphasis is put on the conceptual and technical subtleties arising from relativistic quantum mechanics.

<sup>1</sup>SD acknowledges financial support by the U.S. Department of Energy through a LANL Director's Funded Fellowship.

### 9:48AM R44.00008 The second law of quantum thermodynamics as an equality

, JONATHAN OPPENHEIM, University College London — The traditional second law of thermodynamics says that the average amount of work required to change one state into another while in contact with a heat reservoir, must be at least as large as the change in free energy of the system. Here, we consider a fine-grained notion of the free energy, and show that in terms of it, the second law can be written as an equality. We also obtain a generalisation of the Jarzynski fluctuation theorem which holds for arbitrary initial states, not just the case of an initial thermal state. We derive a generalisation of Gibbs-stochasticity, a condition originally found in the approach to thermodynamics inspired by quantum information theory. This generalisation directly incorporates the case of fluctuating work and serves as a parent equation which can be used to derive the second law equality and the generalisation of the Jarzynski equation. We further show that each of these three generalisations can be seen as the quasi-classical limit of three fully quantum identities. This allows for more general and fully quantum fluctuation relations from the information theoretic approach to quantum thermodynamics.

### 10:24AM R44.00009 Recoverability in quantum information theory<sup>1</sup>

, MARK WILDE, Louisiana State Univ - Baton Rouge — The fact that the quantum relative entropy is non-increasing with respect to quantum physical evolutions lies at the core of many optimality theorems in quantum information theory and has applications in other areas of physics. In this work, we establish improvements of this entropy inequality in the form of physically meaningful remainder terms. One of the main results can be summarized informally as follows: if the decrease in quantum relative entropy between two quantum states after a quantum physical evolution is relatively small, then it is possible to perform a recovery operation, such that one can perfectly recover one state while approximately recovering the other. This can be interpreted as quantifying how well one can reverse a quantum physical evolution. Our proof method is elementary, relying on the method of complex interpolation, basic linear algebra, and the recently introduced Renyi generalization of a relative entropy difference. The theorem has a number of applications in quantum information theory, which have to do with providing physically meaningful improvements to many known entropy inequalities. This is based on arXiv:1505.04661, now accepted for publication in Proceedings of the Royal Society A.

<sup>1</sup>I acknowledge support from startup funds from the Department of Physics and Astronomy at LSU, the NSF under Award No. CCF-1350397, and the DARPA Quiness Program through US Army Research Office award W31P4Q-12-1-0019.

### 10:36AM R44.00010 Quantum Decoherence at Finite Temperatures: Theory and Computations<sup>1</sup>

, M.A. NOVOTNY, Mississippi State University, FENGPING JIN, Jülich Supercomputing Centre, SEIJI MIYASHITA, University of Tokyo, SHENGJUN YUAN, Radboud Universiteit, HANS DE RAEDT, University of Groningen, KRISTEL MICHIELSEN, Jülich Supercomputing Centre — The decoherence of a finite quantum system  $S$  coupled to a finite quantum environment  $E$  is considered, where the entirety  $S+E$  is a closed quantum system. The entirety is prepared in a canonical thermal state at a finite temperature. By applying perturbation theory, we find closed form expressions for measures of decoherence and thermalization of  $S$  in terms of the free energies of  $S$  and  $E$ . Hence we have quantified how difficult it is to decohere a particular finite quantum system  $S$  at a fixed temperature, the result being a function of the free energy of  $S$ . We have also quantified how potent a particular finite Hilbert space environment  $E$  at a fixed temperature is at decohering a generic quantum system. To test these predictions, we performed both real and imaginary time calculations for the Schrödinger equation for an entirety with up to 40 quantum spins. The large-scale calculations (vectors in Hilbert space with length up to  $2^{40} \approx 10^{12}$ ) validate our predictions for all temperatures. Preprint arXiv:1502.03996.

<sup>1</sup>MAN supported in part by NSF DMR-1206233.

### 10:48AM R44.00011 Dynamical and thermodynamical control of open quantum Brownian motion<sup>1</sup>

, FRANCESCO PETRUCCIONE, University of KwaZulu-Natal, ILYA SINAYSKIY, National Institute for Theoretical Physics — Open quantum Brownian motion was introduced as a new type of quantum Brownian motion for Brownian particles with internal quantum degrees of freedom. Recently, an example of the microscopic derivation of open quantum Brownian motion has been presented [I. Sinayskiy and F. Petruccione, Phys. Scr. T165, 014017 (2015)]. The microscopic derivation allows to relate the dynamical properties of open Quantum Brownian motion and the thermodynamical properties of the environment. In the present work, we study the possibility of control of the external degrees of freedom of the "walker" (position) by manipulating the internal one, e.g. spin, polarization, occupation numbers. In the particular example of the known microscopic derivation the connection between dynamics of the "walker" and thermodynamical parameters of the system is established. For the system of open Brownian walkers coupled to the same environment controllable creation of quantum correlations is investigated.

<sup>1</sup>This work is based upon research supported by the South African Research Chair Initiative of the Department of Science and Technology and National Research Foundation.

**Thursday, March 17, 2016 8:00AM - 10:48AM –**

**Session R45 GQI DAMOP: Hybrid Quantum Systems III** 348 - Guido Burkard, University of Konstanz, Germany

**8:00AM R45.00001 Investigations of a transmon-coupled nanoresonator in a CPW cavity.**

, YU HAO, Syracuse University, FRANCISCO ROXINAL, University of Campinas, MATT LAHAYE, Syracuse University — In this work, we describe our progress developing a qubit-coupled nanomechanical resonator(nmr), which has potential both for fundamental studies in quantum measurement and quantum thermodynamics and applications in quantum information. The hybrid system is composed of a superconducting charge-type transmon qubit and a ultra-high-frequency flexural nmr; both are embedded in, and measured through, a superconducting coplanar-wave-guide(CPW) resonator. Transmission measurements of the CPW cavity allow us to probe the state of transmon as it interacts resonantly with the NMR. In the talk, we'll present the latest measurements of this device at low NMR thermal occupation factors and discuss future prospects for developing this system for more advanced quantum measurements.

**8:12AM R45.00002 Surface acoustic wave resonators in the quantum regime**, RICCARDO MANENTI,

MICHAEL PETERER, ANI NERSISYAN, EINAR MAGNUSSON, ANDREW PATTERSON, PETER LEEK, University of Oxford — Surface acoustic waves (SAWs) are mechanical modes confined to the surface of a piezoelectric crystal that can be excited and detected by electric circuits. These mechanical waves can be trapped between two reflectors producing a SAW resonator. In this talk, I will present an experimental study of SAW resonators at 10 mK [1], in which we find that internal quality factors  $Q_i$  approaching 0.5 million can be reached at 0.5 GHz and that  $Q_i > 10^4$  is achievable above 4 GHz, making SAW resonators promising devices for integration into quantum circuits. I will discuss the loss mechanisms that may be currently limiting these Q-factors, and report on our progress towards coupling these mechanical resonators to superconducting qubits. [1] R. Manenti et al., arXiv:1510.04965

**8:24AM R45.00003 Cavity magnomechanics**, XUFENG ZHANG, CHANGLING ZOU, LIANG JIANG, HONG X. TANG, Yale

University — Mechanical oscillators have been recently widely utilized to couple with optical and microwave photons in a variety of hybrid quantum systems, but they all lack the tunability. The magnetostrictive force provides an alternative mechanism to allow phonon to couple with a different type of information carrier magnon, the collective excitation of magnetization whose frequency can be tuned by a bias magnetic field. Here, we demonstrate an intriguing hybrid system that consists of a magnonic, a mechanical, and a microwave resonator. The magnon-phonon interaction results in hallmark coherent phenomena such as magnomechanically induced transparency/absorption and magnomechanical parametric amplification. The magnetic field dependence of magnon provides our system with unprecedented tunability. Moreover, the great flexibility of our system allows us to achieve triple resonance among magnon, phonon and photon, which drastically enhances the magnomechanical interaction. Our work demonstrates the fundamental principle of cavity magnetomechanics, opening up great opportunities in various applications, such as tunable microwave filter and amplifier, long-lifetime quantum memories, microwave-to-optics conversion.

**8:36AM R45.00004 Continuous dynamical decoupling of a single diamond nitrogen-vacancy center spin with a mechanical resonator<sup>1</sup>**, EVAN MACQUARRIE, TANAY GOSAVI, Cornell University, SUNIL BHAVE, Purdue

University, GREGORY FUCHS, Cornell University — We use coherent interactions between a diamond mechanical resonator and a single nitrogen-vacancy (NV) center spin qubit to engineer a decoherence-protected spin basis. For solid state spin qubits such as the NV center, a dominant source of inhomogeneous dephasing is magnetic field fluctuations due to nearby paramagnetic impurities or instabilities in a magnetic bias field. By dressing the NV center spin states with a  $581 \pm 2$  kHz mechanical Rabi field, we decrease the spin's sensitivity to magnetic fluctuations in a thermally isolated subspace, thus prolonging the Ramsey coherence time from  $T_2^* = 2.7 \pm 0.1 \mu\text{s}$  to  $15 \pm 1 \mu\text{s}$ . We develop a model that quantitatively predicts the relationship between the mechanical Rabi field and the dephasing time. Our model shows that a combination of random magnetic field fluctuations and hyperfine coupling limits the protected coherence time over the range of mechanical dressing fields accessed in our experiment. Finally, we show that amplitude noise in the dressing field will dominate over magnetic noise for larger driving fields.

<sup>1</sup>We acknowledge research support from the Office of Naval Research.

**8:48AM R45.00005 Towards a highly efficient quantum spin-photon interface for an NV centre based quantum network**, STEFAN BOGDANOVIC, CRISTIAN BONATO, SUZANNE VAN DAM, ANDREAS REISERER, ANNE-MARIJE

ZWERVER, RONALD HANSON, Kavli Institute of Nanoscience Delft, Delft University of Technology, QUANTUM TRANSPORT TEAM — Nitrogen-vacancy (NV) centers in diamond recently emerged as promising candidates for realizing quantum information algorithms due to their remarkable versatility. The spin of these optically active defects can be entangled with their emitted photons, making them an excellent optical interface from the perspective of quantum communication.

Recently, we have demonstrated the first building blocks of such networks, performing kilometer scale entanglement of two NV centers and teleportation of quantum information.(1) However, our current protocols are inefficient due to the low emission of NV centers resonant photons into the zero phonon line (ZPL). Here we present our efforts of coupling a single NV center emitter in a diamond membrane to a fiber-based Fabry-Perot microcavity with high finesse ( $F > 10^4$ ) at cryogenic temperatures. This approach allows spectral tuning of the cavity resonance to the ZPL emission of the NV center, thereby significantly enhancing the resonant photon emission via Purcell effect. Furthermore, the bulk environment of the NV centers protects their spin properties against surface proximity effects, which is of crucial importance for quantum information processing applications.

(1) B.Hensen et al, *Nature* **526**, 682 (2015)

**9:00AM R45.00006 Investigating the positively charged nitrogen-vacancy center in diamond as a long lived quantum memory**, MATTHIAS PFENDER, NABEEL ASLAM, SINA BURK, HELMUT FEDDER, PHILIPP NEUMANN, 3rd

Institute of Physics, University of Stuttgart, PATRICK SIMON, JOS A. GARRIDO, Walter Schottky Institut, Technische Universität München, JRG WRACHTRUP, 3rd Institute of Physics, University of Stuttgart, 3RD INSTITUTE OF PHYSICS, UNIVERSITY OF STUTTGART TEAM, WALTER SCHOTTKY INSTITUT, TECHNISCHE UNIVERSITÄT MÜNCHEN TEAM — The nitrogen-vacancy (NV) defect in diamond is one of the major candidates for a solid-state quantum processor. Its electron spin is readout and initialized optically. Proximal nuclear spins (e.g.  $^{14}\text{N}$ ,  $^{15}\text{N}$ ,  $^{13}\text{C}$ ) serve as inherently robust qubits, their readout is facilitated via the electron spin in a QND measurement and they exhibit  $T_1$  lifetimes of several minutes. However, for strongly coupled nuclear spins, the coherence time is limited by the electron spin's  $T_1$  lifetime (5 ms @ roomtemperature). In Si:P, this obstacle is overcome by ionizing the P donor into a spinless charge-state. In this work, we employ in-plane gate structures on the diamond surface for deterministic charge state switching of near-surface NVs from  $\text{NV}^-$  over  $\text{NV}^0$  to  $\text{NV}^+$ , while investigating the electron spin properties using the nitrogen nuclear spin as a probe. The positive charge state happens to have no unpaired electrons, therefore the nuclear spin coherence time is prolonged beyond the 5ms-limit imposed by the  $\text{NV}^-$  electron spin. Proper charge state control removes an important roadblock for achieving minute-long coherence times at room-temperature and deterministic quantum system initialization.

**9:12AM R45.00007 Coupling a single InAs quantum dot to mechanical motion of a photonic crystal membrane**, SAMUEL CARTER, ALLAN BRACKER, Naval Research Laboratory, MIJIN KIM, Sotera Defense Solutions, Inc, CHUL SOO KIM, MAXIM ZALALUTDINOV, BRENNAN PURSLEY, Naval Research Laboratory, SOPHIA ECONOMOU, Department of Physics, Virginia Tech, CYPRIAN CZARNOCKI, CAMERON JENNINGS, MICHAEL SCHEIBNER, School of Natural Sciences, University of California, Merced, DANIEL GAMMON, Naval Research Laboratory — Coupling quantum mechanical systems to mechanical motion is attractive for fundamental science, quantum information applications, and sensing. Semiconductor quantum dots (QDs) embedded in suspended photonic crystal structures provide a versatile system for advances in this area. Flexural modes of the suspended membrane as well as localized mechanical modes surrounding optical cavities couple to QDs through strain, with the photonic crystal used to maximize collection of photons from QDs. We have performed high resolution spectroscopy of InAs QDs embedded in photonic crystal structures while optically driving mechanical motion. Using time-correlated photon counting, the strain-induced shift of the QD optical transitions is measured as a function of time. For QDs at the center of the membrane (along the growth direction), the strain is minimum, and the optical transitions shift by only a few  $\mu\text{eV}$ . For QDs shifted 30 nm from the center, the strain induces larger shifts of  $50\mu\text{eV}$ . Measurements in a magnetic field are being performed on charged QDs to determine the coupling of mechanical motion to electron and hole spin transitions.

**9:24AM R45.00008 Inductive cooling in quantum magnetomechanics.**<sup>1</sup>, ERICK ROMERO-SANCHEZ, University of Queensland, JASON TWAMLEY, Macquarie University, WARWICK P. BOWEN, University of Queensland, MICHAEL R. VANNER, University of Oxford — Coupling to light or microwave fields allows quantum control of the motion of a mechanical oscillator, and offers prospects for precision sensing, quantum information systems, and tests of fundamental physics. In cavity electromechanics ground state cooling has been achieved using resolved sideband cooling. Here we present an alternative approach based on a magnetomechanical system that inductively couples an  $LC$  resonator to a mechanical oscillator. The experimental setup consists of a micro cantilever with a pyramidal magnetic tip attached at the end of the beam. The sharp end of the magnetic tip is positioned close to the planar microfabricated inductor of the  $LC$  resonator. The displacement in the position of the end of the cantilever generates a change in flux through the coil inducing an electromotive force in the circuit. The current in the  $LC$  resonator generates a magnetic field, and then a force between the tip and the coil. When they are strongly coupled and the mechanical resonance frequency  $\omega_m$  exceeds the electrical decay rate of the resonator  $\gamma_e$ , resolved sideband cooling can be used to cool the mechanics. We present estimations for the coupling rates and the experimental parameters required for these experiments.

<sup>1</sup>E. Romero acknowledges to CONACyT

**9:36AM R45.00009 Strain coupling of a mechanical resonator to a single quantum emitter in diamond**<sup>1</sup>, KENNETH LEE, DONGHUN LEE, PREETI OVARTCHAIYAPONG, ANIA JAYICH, University of California Santa Barbara — Hybrid quantum devices are central to the advancement of several emerging quantum technologies, including quantum information science and quantum-assisted sensing. Here, we present a hybrid quantum device in which strain fields associated with resonant vibrations of a diamond cantilever dynamically modulate the energy and polarization dependence of the optical transitions of a single nitrogen-vacancy defect center in diamond. With mechanical driving, we observe optomechanical couplings exceeding 10 GHz. Through resonant excitation spectroscopy, we quantitatively characterize the intrinsic strain environment of a single defect, and use this optomechanical coupling to tune the zero-phonon line of the defect. Through stroboscopic measurements, we show that we are able to match the frequency and polarization dependence of the optical zero-phonon lines of two separate NV centers. The experiments demonstrated here mark an important step toward realizing a monolithic hybrid quantum device capable of realizing and probing the dynamics of non-classical states of mechanical resonators, spin-systems, and photons.

<sup>1</sup>This work was supported with grants from the AFOSR, NSF and DARPA

**9:48AM R45.00010 Microwave-frequency electromechanical resonators incorporating phononic crystals**, K. J. SATZINGER, G. PEAIRS, A. VAINSENER, University of California, Santa Barbara, A. N. CLELAND, University of Chicago — Piezoelectric micromechanical resonators at gigahertz frequencies have been operated in the quantum limit, with quantum control and measurement achieved using superconducting qubits. However, experiments to date have been limited by mechanical dissipation, due to a combination of internal and radiative losses. In this talk, we explore the incorporation of phononic crystals into resonator designs. In phononic crystals, periodic patterning manipulates the acoustic band structure of the material. Through appropriately chosen geometries, these periodic patterns lead to full acoustic bandgaps which can be used to greatly reduce radiation losses from resonant structures. Alternatively, the crystal geometry can be manipulated to allow isolated modes within the bandgap, giving fine control over the spatial structure of the resonator modes. In this talk, we will describe the design, fabrication, and measurement of resonators with phononic crystals.

**10:00AM R45.00011 Superconducting-circuit quantum heat engine with frequency resolved thermal baths**, PATRICK P. HOFER, JEAN-RENÉ SOUQUET, AASHISH A. CLERK, McGill University — The study of quantum heat engines promises to unravel deep, fundamental concepts in quantum thermodynamics. With this in mind, we propose a novel, realistic device that efficiently converts heat into work while maintaining reasonably large output powers. The key concept in our proposal is a highly peaked spectral density in both the thermal baths as well as the working fluid. This allows for a complete separation of the heat current from the working fluid. In our setup, Cooper pairs tunnelling across a Josephson junction serve as the the working fluid, while two resonant cavities coupled to the junction act as frequency-resolved thermal baths. The device is operated such that a heat flux carried entirely by the photons induces an electrical current against a voltage bias, providing work.

**10:12AM R45.00012 Strong nonlinearity of mesoscopic vibrational modes induced by electron-phonon coupling**, KIRILL MOSKOVTSOV, M. I. DYKMAN, Michigan State University — We show that the electron-phonon coupling can lead to a strong nonlinearity of vibrational modes in semiconductor nano- and micro-resonators. For typical mode frequencies, the electron distribution adiabatically follows lattice strain. Therefore strain leads to redistribution of the electron density over the valleys of the conduction band. It also leads to the onset of a spatial charge. The parameter that controls the distribution is the ratio of the deformation potential to the electron chemical potential or temperature. It is  $\sim 10^2$  for many semiconductors of interest even when they are heavily doped. Therefore the change of the electron distribution is strongly nonlinear in the strain. As a consequence, the stress induced by the electron-phonon coupling is also strongly nonlinear. We have found the vibration nonlinearity parameters for  $n$ -doped Si and calculated the amplitude dependence of the frequencies of several low-lying Si resonator modes with account taken of their spatial structure. The results are compared with the recent experimental data that shows strong effect of doping on the vibration nonlinearity.

**10:24AM R45.00013 Novel High Cooperativity Photon-Magnon Cavity QED**, MICHAEL TOBAR, JEREMY BOURHILL, NIKITA KOSTYLEV, MAXIM G. DANIEL CREEDON, School of Physics, University of Western Australia, ARC Centre of Excellence for Engineered Quantum Systems — Novel microwave cavities are presented, which couple photons and magnons in YIG spheres in a super- and ultra-strong way at around 20 mK in temperature. Few/Single photon couplings (or normal mode splitting, 2g) of more than 6 GHz at microwave frequencies are obtained. Types of cavities include multiple post reentrant cavities, which co-couple photons at different frequencies with a coupling greater than the free spectral range, as well as spherical loaded dielectric cavity resonators. In such cavities we show that the bare dielectric properties can be obtained by polarizing all magnon modes to high energy using a 7 Tesla magnet. We also show that at zero-field, collective effects of the spins significantly perturb the photon modes. Other effects like time-reversal symmetry breaking are observed.

**10:36AM R45.00014 Cavity QED with ferromagnetic magnons in a small YIG sphere**, DENGKE ZHANG, Beijing Computational Science Research Center, XIN-MING WANG, Research Center of Laser Fusion, CAEP, TIE-FU LI, Institute of Microelectronics, Tsinghua University, XIAO-QING LUO, Beijing Computational Science Research Center, WEIDONG WU, Research Center of Laser Fusion, CAEP, FRANCO NORI, Center for Emergent Matter Science, RIKEN, J. Q. YOU, Beijing Computational Science Research Center — Hybridizing collective spin excitations in ferromagnetic crystals and a cavity with high cooperativity provides a new research subject in the field of cavity quantum electrodynamics and can also have potential applications to quantum information. In contrast to spin ensembles based on dilute paramagnetic impurities, these spins are strongly exchange-coupled and have a much higher density. Here we report a direct observation of the strong coupling between magnons and microwave photons at both cryogenic and room temperatures by using the same small yttrium-iron-garnet (YIG) ferromagnetic sphere in a 3D copper cavity. We observed strong couplings of the same cavity mode to both ferromagnetic-resonance (FMR, uniform precession) mode and a magnetostatic (MS, non-uniform precession) mode in the quantum limit at 22 mK. Then, at room temperature, we observed a strong coupling of the cavity mode to the FMR mode with slightly increased damping rate. This reveals the robustness of the FMR mode against temperature. However, the coupling to MS mode disappears at room temperature and numerically simulations show that this is due to a drastic increase of the damping rate of the MS mode. Our work unveils quantum-coherence properties of the magnons.

**Thursday, March 17, 2016 8:00AM - 11:00AM –**

**Session R46 GIMS: Optical Spectroscopic Measurements of 2D Materials** 311 - Erin Wood, NIST

**8:00AM R46.00001 Internal Photoemission Spectroscopy of 2-D Materials**, NHAN NGUYEN, National Institute of Standards and Technology, MINGDA LI, SURESH VISHWANATH, RUSEN YAN, SHUDONG XIAO, HUILI XING, Cornell University, GUANGJUN CHENG, ANGELA HIGHT WALKER, QIN ZHANG, National Institute of Standards and Technology — Recent research has shown the great benefits of using 2-D materials in the tunnel field-effect transistor (TFET), which is considered a promising candidate for the beyond-CMOS technology. The on-state current of TFET can be enhanced by engineering the band alignment of different 2D-2D or 2D-3D heterostructures. Here we present the internal photoemission spectroscopy (IPE) approach to determine the band alignments of various 2-D materials, in particular SnSe<sub>2</sub> and WSe<sub>2</sub>, which have been proposed for new TFET designs. The metal-oxide-2-D semiconductor test structures are fabricated and characterized by IPE, where the band offsets from the 2-D semiconductor to the oxide conduction band minimum are determined by the threshold of the cube root of IPE yields as a function of photon energy. In particular, we find that SnSe<sub>2</sub> has a larger electron affinity than most semiconductors and can be combined with other semiconductors to form near broken-gap heterojunctions with low barrier heights which can produce a higher on-state current. The details of data analysis of IPE and the results from Raman spectroscopy and spectroscopic ellipsometry measurements will also be presented and discussed.

**8:12AM R46.00002 Optical Parameter Extraction of Nano-Layered Materials Using Terahertz Time-Domain Spectroscopy<sup>1</sup>**, FARAH VANDREVALA, ERIK EINARSSON, University at Buffalo — We report a data analysis technique for reflection-mode terahertz time-domain spectroscopy (THz-TDS) to extract the complex refractive index of nano-layered materials deposited on optically thick substrates. We measure the Fabry-Perot resonances occurring inside the substrate to determine the Fresnel coefficients at the interface of the material and the substrate. Based on these values, we extract the frequency-dependent optical parameters, including surface conductivity, of the nano-layered materials for frequencies up to 3 THz.

<sup>1</sup>Air Force Research Laboratory award FA8750-15-1-0050

**8:24AM R46.00003 Broadband THz Spectroscopy of 2D Nanoscale Materials<sup>1</sup>**, LU CHEN, SHIVENDRA TRIPATHI, MENGCHEN HUANG, JEN-FENG HSU, BRIAN D'URSO, University of Pittsburgh, HYUNGWOO LEE, CHANG-BEOM EOM, University of Wisconsin-Madison, PATRICK IRVIN, JEREMY LEVY, University of Pittsburgh — Two-dimensional (2D) materials such as graphene and transition-metal dichalcogenides (TMDC) have attracted intense research interest in the past decade. Their unique electronic and optical properties offer the promise of novel optoelectronic applications in the terahertz regime. Recently, generation and detection of broadband terahertz (10 THz bandwidth) emission from 10-nm-scale LaAlO<sub>3</sub>/SrTiO<sub>3</sub> nanostructures created by conductive atomic force microscope (c-AFM) lithography has been demonstrated<sup>2</sup>. This unprecedented control of THz emission at 10 nm length scales creates a pathway toward hybrid THz functionality in 2D-material/LaAlO<sub>3</sub>/SrTiO<sub>3</sub> heterostructures. Here we report initial efforts in THz spectroscopy of 2D nanoscale materials with resolution comparable to the dimensions of the nanowire (10 nm). Systems under investigation include graphene, single-layer molybdenum disulfide (MoS<sub>2</sub>), and tungsten diselenide (WSe<sub>2</sub>) nanoflakes.

<sup>1</sup>We gratefully acknowledge financial support from the following agencies and grants: AFOSR (FA9550-12-1-0268 (JL, PRI), FA9550-12-1-0342 (CBE)), ONR (N00014-13-1-0806 (JL, CBE), N00014-15-1-2847 (JL)), NSF DMR-1124131 (JL, CBE) and DMR-1234096 (CBE)

<sup>2</sup>Y. Ma, *et al.*, Nano Lett. **13**, 2884 (2013)

**8:36AM R46.00004 A novel grating-imaging method to measure carrier diffusion coefficient in graphene**, KE CHEN, YAGUO WANG, Department of Mechanical Engineering, Texas Materials Institute, University of Texas at Austin, DEJI AKINWANDE, SETH BANK, Department of Electrical and Computer Engineering, Microelectronics Research Center, University of Texas at Austin, JUNG-FU LIN, Department of Geological Sciences, Jackson School of Geosciences, University of Texas at Austin — Similar to carrier mobility, carrier diffusion coefficient in graphene determines the response rate of future graphene-based electronics. Here we present a simple, sensitive and non-destructive technique integrated with ultrafast pump-probe spectroscopy to measure carrier diffusion in CVD-grown graphene. In the method, the pump and the probe beams pass through the same area of a photomask with metal strips i.e. a transmission amplitude grating, and get diffracted. The diffracted light is collected by an objective lens and focused onto the sample to generate carrier density grating. Relaxation of this carrier density grating is governed by both carrier recombination and carrier diffusion in the sample. Transient transmission change of the probe beams, which reflects this relaxation process, is recorded. The measured diffusion coefficients of multilayer and monolayer CVD-grown graphene are 2000cm<sup>2</sup>/s and 10000cm<sup>2</sup>/s, respectively, comparable with the reported values of epitaxial graphene and reduced graphene. This transmission grating technique can be used to measure carrier dynamics in versatile 2D materials.

**8:48AM R46.00005 Temperature, Magnetic Field, and Dimensionality Effects on the Raman Spectra of TaSe<sub>2</sub>**, J. R. SIMPSON, Towson University, S. CHOWDHURY, Catholic University of America, A. R. HIGHT WALKER, NIST — In bulk form, TaSe<sub>2</sub> exhibits transitions between commensurate and incommensurate charge-density wave (CDW) phases, and is attracting interest for advanced device applications. In order to explore the evolution of the groundstate CDW phase with layer number, mechanical exfoliation of bulk crystals provides few- to single-layer flakes. In the present work, we extend our opto-thermal Raman measurements<sup>1</sup> on MoS<sub>2</sub> to include other TMDs, specifically TaSe<sub>2</sub>, in both 1T and 2H crystallographic phases. A novel, magneto-Raman microscope system affords measurement of low-frequency (down to 10 cm<sup>-1</sup>) vibrational modes as a function of both temperature (100 to 400) K and magnetic field (0 to 9) T. The dependence of the observed Raman-active phonons on temperature and magnetic field will be discussed and compared with earlier results on MoS<sub>2</sub>. Specifically, we observe the appearance of low-frequency, zone-folded modes in the CDW state, which soften with temperature similar to the higher frequency, in-plane E<sub>2g</sub> mode. Additionally, we compare the measured magneto-Raman results to calculations using *ab initio*, density functional theory.

<sup>1</sup>R. Yan, J. R. Simpson, *et al.*, ACS Nano **8**, 986 (2014).

**9:00AM R46.00006 Ultralow-frequency interlayer Raman modes to probe interfacial coupling in twisted bilayer MoS<sub>2</sub>**<sup>1</sup>, SHENGXI HUANG, MIT, LIANGBO LIANG, RPI, ORNL, XI LING, MIT, ALEXANDER PURETZKY, DAVID GEOHEGAN, BOBBY SUMPTER, ORNL, JING KONG, MIT, VINCENT MEUNIER, RPI, MILDRED DRESSELHAUS, MIT — Interlayer coupling strength plays an important role in tuning the optoelectronic properties of transition metal dichalcogenides (TMDs), which can be studied in twisted bilayer TMDs due to their various stacking configurations. In this work, ultralow-frequency interlayer shear and breathing Raman modes were investigated in twisted bilayer MoS<sub>2</sub>. We found both twisted angle and translational shift can significantly influence the interlayer coupling, leading to notable frequency and intensity changes of low-frequency Raman modes, as confirmed by first-principles density functional theory calculations. Large frequency and intensity variations occur near twisted angles 0° and 60°, but not between 20° and 40°, indicating translational shift does not induce much change of the coupling strength within the latter angle range. In contrast to low-frequency interlayer modes, high-frequency intralayer Raman modes are much less sensitive to interlayer coupling. Therefore, interlayer Raman modes can be used as an effective probe to study the interlayer coupling of 2D materials with different stacking configurations.

<sup>1</sup>The work is supported by DE-SC0001299, NYSTAR C080117.

**9:12AM R46.00007 Photocurrent spectroscopy of 2D materials**, DAVID COBDEN, University of Washington, Seattle — Confocal photocurrent measurements provide a powerful means of studying many aspects of the optoelectronic and electrical properties of a 2D device or material. At a diffraction-limited point they can provide a detailed absorption spectrum, and they can probe local symmetry, ultrafast relaxation rates and processes, electron-electron interaction strengths, and transport coefficients. We illustrate this with several examples, once being the photo-Nernst effect. In gapless 2D materials, such as graphene, in a perpendicular magnetic field a photocurrent antisymmetric in the field is generated near to the free edges, with opposite sign at opposite edges. Its origin is the transverse thermoelectric current associated with the laser-induced electron temperature gradient. This effect provides an unambiguous demonstration of the Shockley-Ramo nature of long-range photocurrent generation in gapless materials. It also provides a means of investigating quasiparticle properties. For example, in the case of graphene on hBN, it can be used to probe the Lifshitz transition that occurs due to the minibands formed by the Moire superlattice. We also observe and discuss photocurrent generated in other semimetallic (WTe<sub>2</sub>) and semiconducting (WSe<sub>2</sub>) monolayers. Work supported by DoE BES and NSF EFRI grants.

**9:48AM R46.00008 Two-Dimensional Transition Metal Dichalcogenides: Controlled Synthesis and Optical Characterization**, ZHONG LIN, The Pennsylvania State University, YONGJI GONG, GONGLAN YE, GANG SHI, Rice University, MICHAEL THEE, ANA LAURA ELIAS, NESTOR PEREA-LOPEZ, SIMIN FENG, YU LEI, CHANJING ZHOU, KAZUNORI FUJISAWA, VICTOR CAROZO, The Pennsylvania State University, ROBERT VAJTAI, Rice University, HUMBERTO TERRONES, Rensselaer Polytechnic Institute, ZHENG LIU, Nanyang Technological University, PULICKEL AJAYAN, Rice University, MAURICIO TERRONES, The Pennsylvania State University — Chemical vapor deposition (CVD) is a bottom-up approach suitable for the synthesis of MoS<sub>2</sub> and WS<sub>2</sub> monolayers. In order to extend the application of CVD, we modified the precursors used during the deposition. We show that by using mixed transition metal precursors of MoS<sub>2</sub>/WO<sub>3</sub> powders, alloyed monolayers of Mo<sub>x</sub>W<sub>1-x</sub>S<sub>2</sub> islands can be synthesized exhibiting a compositional gradient and a tunable optical band gap, as confirmed by Raman and photoluminescence measurements. We further show that adding tellurium powders into the transition metal precursors can lead to a 200 °C reduction in the synthesis temperature for MoS<sub>2</sub> and WS<sub>2</sub> monolayers. The materials synthesized at a reduced temperature maintain a high degree of crystallinity and optical properties.

**10:00AM R46.00009 Accuracy of the 2D sheet model for atomically thin layers**, YILEI LI, TONY HEINZ, Stanford Univ./SLAC National Accelerator Laboratory — The 2D sheet model provides a useful and concise description of the optics of atomically thin layers. The 2D sheet model is mathematically equivalent to the conventional thin slab model in the limit where the optical thickness of the layer is negligible. In this paper, we present a detailed analysis of the accuracy of the 2D sheet model for atomically thin layers by comparing numerically the predicted optical response for representative monolayer 2D materials to that obtained from the conventional thin slab model. The agreement between the optical responses produced by the two models is found to be within 0.1%, demonstrating excellent accuracy of the sheet model. Based on the 2D sheet model, we then derive the frequently applied linearized relations between the optical contrasts and the sheet conductivity. The linearized relations provides good accuracy when the material response is weak, but is shown to produce an inaccuracy of more than 25% in certain wavelength window for even a single atomic layer of MoS<sub>2</sub>. With the expression for optical transmission from the sheet model, we will clarify a confusion that occasionally arises when determining the optical attenuation by a thin layer.

**10:12AM R46.00010 Ultrasensitive Molecular Sensor Using N-doped Graphene through Enhanced Raman Scattering**, SIMIN FENG, Penn State University, MARIA CRISTINA DOS SANTOS, Universidade de Sao Paulo, BRUNO R. CARVALHO, Penn State University, RUITAO LV, Tsinghua University, KAZUNORI FUJISAWA, ANA LAURA ELIAS, MAURICIO TERRONES, Penn State University — As a novel and efficient surface analysis technique, graphene enhanced Raman scattering (GERS) has attracted increasing research attention in recent years. In particular, chemically doped graphene demonstrates much enhanced GERS effects than pristine graphene (PG) and it can be used to efficiently detect trace amount of molecules. However, the GERS mechanism is still an open question. Here, we present a comprehensive study on the GERS effect of PG and nitrogen-doped graphene (NG). By controlling the N-doping in NG, the Fermi level of graphene shifts, and if this shift aligns with the lower unoccupied molecular orbital (LUMO) of a molecule, charge transfer is enhanced, thus significantly amplifying the molecule vibrational Raman modes. We confirmed these findings using different organic fluorescent molecules. Interestingly, Raman signals from these dye molecules can be detected even for concentrations as low as 10<sup>-11</sup> mol/L, thus providing excellent molecular sensing capabilities. In order to explain our results, these NG-molecule systems were modeled using dispersion corrected density functional theory. Furthermore, we demonstrated that when using different laser excitations, it is possible to determine the gaps between the HOMO and LUMO of different molecules.

**10:24AM R46.00011 Optical/Electronic Heterogeneity of WSe<sub>2</sub> at the Nanoscale**, KYOUNG-DUCK PARK, OMAR KHATIB, VASILY KRAVTSOV, RONALD ULBRICHT, Department of Physics, Department of Chemistry, and JILA, University of Colorado at Boulder, GENEVIEVE CLARK, XIAODONG XU, Department of Physics, Department of Materials Science and Engineering, University of Washington at Seattle, MARKUS RASCHKE, Department of Physics, Department of Chemistry, and JILA, University of Colorado at Boulder — Many classes of two-dimensional (2D) materials have emerged as a potential platform for novel electronic and optical devices. However, the physical properties are strongly influenced by nanoscale heterogeneities in the form of nucleation sites, defects, strains, and edges. Here we demonstrate nano-optical imaging of the associated influence on structure and electronic properties with sub-20 nm spatial resolution from combined tip-enhanced Raman scattering (TERS) and photoluminescence (TEPL) spectroscopy and imaging. In monolayer WSe<sub>2</sub> micro-crystals grown by physical vapor deposition (PVD), we observe significant variations in TERS and TEPL near crystal edges and atomic-scale grain boundaries (GBs), consistent with variations in strain and/or exciton diffusion. Specifically, theoretical exciton diffusion lengths (25 nm) at GBs and heterogeneous nanoscale (30-80 nm) PL emission including a spectral blue-shift at edges are experimentally probed. Further, we are able to engineer the local bandgap of WSe<sub>2</sub> crystals by dynamic AFM-control in reversible (24 meV) and irreversible (48 meV) fashions, enabling systematic in-situ studies of the coupling of mechanical degrees of freedom to the nanoscale electronic properties in layered 2D materials.

**10:36AM R46.00012 Photovoltaic Response from Multilayered Transition Metal Dichalcogenides p-n Junctions**, SHAHRIAR MEMARAN, NIHAR PRADHAN, ZHENG GUANG LU, DANIEL RHODES, JONATHAN LUDWIG, QIONG ZHOU, National High Magnetic Field Laboratory, Florida State University, OMOTOLA OGUNSOLU, Department of Chemistry & Biochemistry, FSU, PULICKEL AJAYAN, Department of Mechanical Engineering and Materials Science, Rice University, DMITRY SMIRNOV, NHMFL, ANTONIO FERNANDEZ-DOMINGUEZ, FRANCISCO GARCIA-VIDAL, IFIMAC, Universidad Autonoma de Madrid, LUIS BALICAS, NHMFL — Transition metal dichalcogenides (TMDs) are layered semiconductors with indirect band gaps comparable to Si. These compounds can be grown in large area, while their gap(s) can be tuned by changing their chemical composition or by applying a gate voltage. The experimental evidence collected so far points toward a strong interaction with light, which contrasts with the small photovoltaic efficiencies  $\eta \leq 1\%$  extracted from bulk crystals or exfoliated monolayers. Here, we evaluate the potential of these compounds by studying the photovoltaic response of electrostatically generated p-n junctions composed of approximately 10 atomic layers of MoSe<sub>2</sub> stacked onto the dielectric h-BN. In addition to ideal diode-like response, we find that these junctions can yield, under AM-1.5 illumination, photovoltaic efficiencies  $\eta$  exceeding 14%, with fill factors of  $\sim 70\%$ . Given the available strategies for increasing  $\eta$  such as gap tuning, improving the quality of the electrical contacts, or the fabrication of tandem cells, our study suggests a remarkable potential for photovoltaic applications based on TMDs.

**10:48AM R46.00013 Raman 2D response of graphene in hBN sandwich as a function of doping**<sup>1</sup>, XUANYE WANG, Department of Electrical and Computer Engineering, Boston University, JASON CHRISTOPHER, Department of Physics, Boston University, ANNA SWAN, Department of Electrical and Computer Engineering, Boston University — Graphene on SiO<sub>2</sub> is plagued by accidental strain and charge doping which cause significant deterioration in electrical, thermal and optical properties. The stacking of Van der Waals layers can not only provide better properties, e.g., electrical mobility, but can also be used for novel interactions between layers. Here we use gated and contacted hBN-graphene-hBN heterostructures to calibrate the 2D Raman response to doping, particularly the low doping region less than  $1 \times 10^{12} \text{ cm}^{-2}$ . This will enable the use of the correlation between Raman G and 2D band to determine effects from doping and strain or compression separately. The dielectric environment of hBN as compared to SiO<sub>2</sub> affects the phonon dispersion and the Fermi velocity which results in approximately  $7 \text{ cm}^{-1}$  blue shift in 2D band per side of graphene contacted with hBN. Charge dependent Raman measurements of the G band provide the means to determine the electron-phonon coupling and the Fermi velocity for graphene in an hBN sandwich.

<sup>1</sup>NSF DMR 1411008

## Thursday, March 17, 2016 8:00AM - 11:00AM – Session R47 DCMF: Kondo Insulator and Semimetal 312 -

**8:00AM R47.00001 Non-universal weak antilocalization effect in cubic topological Kondo insulators**, MAXIM DZERO, Kent State University, MAXIM VAVILOV, University of Wisconsin-Madison, KOSTYANTIN KECHEZH, QuAIL and USRA, NASA Ames Research Center, VICTOR GALITSKI, University of Maryland — In this talk we present the results of our study of the quantum correction to conductivity on the surface of cubic topological Kondo insulators with multiple Dirac bands. We considered the model of time-reversal invariant disorder which induces the scattering of the electrons within the Dirac bands as well as between the bands. When only intraband scattering is present we found three long-range diffusion modes leading to weak antilocalization correction to conductivity which remains independent of the microscopic details such as Fermi velocities and relaxation times. Interband scattering gaps out two diffusion modes leaving only one long-range mode. Depending on the value of the phase coherence time, either three or only one long-range diffusion modes contribute to weak localization correction rendering the quantum correction to conductivity non-universal.

**8:12AM R47.00002 The tunable chirality and circular dichroism of topological Kondo insulator SmB<sub>6</sub> with C<sub>2v</sub> symmetry as a function of Rashba and Dresselhaus parameters**, PARIJAT SENGUPTA, ENRICO BELLOTTI, Boston University — A manifestation of optical chirality is circular dichroism (CD) due to a differential absorption of left- and right-circularly polarized light. This effect is an enabler for the design of meta-materials used in polarization sensitive imaging devices and display technologies. Concurrently, topological insulators with helical surface states offer an active control over chiral handedness that can be observed through a varying degree of polarization-dependent absorption. We show that in a band gap open topological Kondo insulator SmB<sub>6</sub> with C<sub>2v</sub> symmetry at the X point of the surface Brillouin zone, CD can be smoothly varied without any microscopic reconfiguration of the surface. We also show that CD, measured by the degree of circular polarization, can assume both positive and negative values. These findings suggest that left- and right- circularly polarized light can be selectively absorbed in the vicinity of the Dirac point by an adjustment of the Rashba- and Dresselhaus-like parameters that describe the Hamiltonian at the X point. The CD is an experimentally measurable quantity and related to Berry curvature which is an outcome of the parameter-dependent Hamiltonian. We calculate the Berry curvature and establish a pathway to alter CD through the Hamiltonian parameters.

**8:24AM R47.00003 Nonsymmorphic crystalline Kondo semimetals**<sup>1</sup>, PO-YAO CHANG, ONUR ERTEN, PIERS COLEMAN, Center for Materials Theory, Rutgers University — Kondo semimetals, such as CeNiSn and CeRhSb are a class of "failed" heavy fermion insulator that appear to develop line-nodes in the hybridization between the localized f-states and mobile conduction electrons. The classic theory[1,2] for node formation depends on angular momentum blocking in a continuum, and provides no insight into why the node should be stable in a crystalline environment. Here we examine how the semimetallic phase emerges in orthorhombic Kondo systems with nonsymmorphic symmetries. Using a periodic Anderson model that incorporates the key crystallographic symmetries of CeNiSn, we show that hybridization nodal lines are naturally protected within mirror symmetry planes. The shape of the Fermi surface around the nodes in our model agrees with observations in Shubnikov-de Haas oscillations.

[1] H. Ikeda and K. Miyake, J. Phys. Soc. Jpn. 65, 1769 (1996).

[2] J. Moreno and P. Coleman, Phys. Rev. Lett. 84, 342 (2000).

<sup>1</sup>This work is supported by NSF DMR 1309929

**8:36AM R47.00004 Spin fluctuations in the anisotropic Kondo insulator  $\text{CeRu}_4\text{Sn}_6$ <sup>1</sup>**, WESLEY T. FUHRMAN, Institute for Quantum Matter and Johns Hopkins University, J. HAENEL, Vienna University of Technology, J. RODRIGUEZ, NIST NCNR, S. PASCHEN, Vienna University of Technology, C. L. BROHOLM, Institute for Quantum Matter, Johns Hopkins University, NIST — We report and model anisotropic quasi-elastic magnetic neutron scattering from single crystalline  $\text{CeRu}_4\text{Sn}_6$ . For  $T \approx 2\text{K}$  the magnetic neutron scattering is broad in momentum ( $\mathbf{Q}$ ) with a persistent  $1/\hbar\omega$  spectrum throughout the Brillouin zone. This indicates a lack of spatial coherence and no characteristic energy scale beyond the 0.2 meV resolution of the measurement. We find the Q-dependence of the scattering can be modeled by a Kondo-Heisenberg Hamiltonian that describes residual carriers and incompletely compensated localized electrons. These findings support the interpretation of tetragonal  $\text{CeRu}_4\text{Sn}_6$  as an anisotropic or nodal Kondo insulator, markedly different from typical cubic Kondo insulators. We further discuss potential topological implications.

<sup>1</sup>Work at IQM was supported by the U.S. Department of Energy, office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02-08ER4654. W.T.F. thanks the ARCS foundation and Lockheed Martin for additional support.

**8:48AM R47.00005 Nanoscale Conducting and Insulating Domains on  $\text{YbB}_6$ <sup>1</sup>**, JENNIFER HOFFMAN, University of British Columbia, ZHIHUI ZHU, YANG HE, Harvard University, DAE-JEONG KIM, ZACHARY FISK, University of California, Irvine — Recent photoemission studies on  $\text{YbB}_6$  reported a metallic surface but without f-states pinned at the Fermi level, in contradiction to the theoretical prediction of  $\text{YbB}_6$  as a topological Kondo insulator. Thus the topological nature of  $\text{YbB}_6$  remains unclear and requires a study that can distinguish trivial surface structure and non-trivial topological effects derived from the bulk. We use scanning tunneling microscopy and spectroscopy (STM/STS) to provide a real-space microscopic picture of the surface electronic structure in  $\text{YbB}_6$ . We observe coexisting nanoscale metallic and insulating surface terminations. The surface conductivity of each termination reflects the degree of downward or upward band bending that is determined by the surface polarity. In addition to demonstrating that surface metallic in  $\text{YbB}_6$  stems from band bending at the polar surface, our study suggests the utility of  $\text{YbB}_6$  for creating spin-polarized p-n junctions at the atomic scale.

<sup>1</sup>We acknowledge funding from the National Science Foundation, DMR-1410480.

**9:00AM R47.00006 Quasiparticle Interference Imaging on  $\text{SmB}_6$ <sup>1</sup>**, HARRIS PIRIE, University of British Columbia, Harvard University, YANG HE, Harvard University, MOHAMMAD HAMIDIAN, Harvard University, Cornell University, MICHAEL YEE, Harvard University, DAE-JEONG KIM, ZACHARY FISK, University of California, Irvine, JENNIFER HOFFMAN, University of British Columbia, Harvard University — Theoretical interest in  $\text{SmB}_6$  as a possible topological Kondo insulator with spin-textured Dirac surface states spanning the bulk hybridization gap has been well supported by recent transport, quantum oscillation, and spin-resolved ARPES experiments. However, the influence of surface reconstruction and polarization on the observed dispersion remains unclear. Scanning tunneling microscopy (STM) and spectroscopy (STS) enable simultaneous measurement of local real- and momentum-space structure through quasiparticle interference (QPI) imaging. We use QPI imaging to detect and measure the dispersion of states near the hybridization gap on a non-polar,  $2 \times 1$  reconstructed surface of  $\text{SmB}_6$ . We compare these results with recent theoretical predictions to gain insight into the low energy excitations of  $\text{SmB}_6$ .

<sup>1</sup>This work was supported by the US National Science Foundation under the grant DMR-1410480.

**9:12AM R47.00007 Topological surface states in Kondo insulator  $\text{SmB}_6$  via planar tunneling spectroscopy<sup>\*</sup>**, WAN KYU PARK, LUNAN SUN, ALEX NODDINGS, University of Illinois at Urbana-Champaign, LAURA GREENE, National High Magnetic Field Laboratory and Florida State University, DAE-JEONG KIM, ZACHARY FISK, University of California, Irvine — Samarium hexaboride ( $\text{SmB}_6$ ) belongs to a class of materials called Kondo insulators in which the hybridization between itinerant electrons and local moments leads to an emergent state of matter. With inherently large spin-orbit coupling along with strong correlation,  $\text{SmB}_6$  has been recently predicted to be topological meaning that topologically robust conducting states should exist at its surfaces. Although extensive investigations have provided growing evidence for the existence of such states, corroborative spectroscopic evidences are still lacking unlike in the weakly correlated counterparts. We adopt planar tunneling spectroscopy to unveil their detailed nature and behavior utilizing its inherently high energy resolution. Measurements of tunneling conductance on two different crystal surfaces (001) and (011) reveal the expected linear density of states for two and one Dirac cones, respectively. Moreover, it is found that these topological states cease to be protected well before they merge into the bulk states at the gap edges. Microscopic modeling of the tunneling processes accounting for the interaction with spin excitons as predicted by a recent theory [1] provide consistent explanations for all the observed features, corroborating the proposed picture on the incompletely protected surface states in  $\text{SmB}_6$ . [1] Kapilevich *et al.*, Phys. Rev. B **92**, 085133 (2015). <sup>\*</sup>The work at UIUC is supported by the NSF DMR 12-06766.

**9:24AM R47.00008 Finite temperature topological phase transitions and emergence of Dirac semi-metallic phases in a Kondo lattice<sup>1</sup>**, PO-HAO CHOU, LIANG-JUN ZHAI, Department of Physics, National Tsing Hua University, Taiwan, ROC, CHUNG-HOU CHUNG, Electrophysics Department, National Chiao-Tung University, Taiwan, ROC, TING-KUO LEE, Institute of Physics, Academia Sinica, Nankang, Taiwan, ROC, CHUNG-YU MOU, Department of Physics, National Tsing Hua University, Taiwan, ROC — The energy gap in Dirac materials controls the topology and critical behaviors of the quantum phase transition associated with the critical point when the gap vanishes. However, it is often difficult to access the critical point as it requires tunability of electronic structures. Here by exploiting the many-body screening interaction of localized spins and conduction electrons in a Kondo lattice, we demonstrate that the electronic band structures in a Kondo lattice are tunable in temperature. When spin-orbit interactions are included, we find that below the Kondo temperature, the Kondo lattice is a strong topological insulator at low temperature and undergoes a topological transition to a weak topological insulator at a higher temperature  $T_D$ . At  $T_D$ , Dirac points emerge and the Kondo lattice becomes a Dirac semimetal. Our results indicate that the topological phase transition through a Dirac semi-metallic phase at finite temperatures also manifests profound physics and results in critical-like behavior both in magnetic and transport properties near  $T_D$ .

<sup>1</sup>We acknowledge support from NCTS and Ministry of Science and Technology (MoST), Taiwan.

**9:36AM R47.00009 Pressure-induced exotic states in mixed-valence rare earth hexaborides**, LILING SUN, YAZHOU ZHOU, QI WU, YI-FENG YANG, ZHONGXIAN ZHAO, Institute of Physics, CAS, DAE-JEONG KIM, PRISCILA ROSA, ZACHARY FISK, Department of Physics and Astronomy, University of California, Irvine, RONG YU, Department of Physics, Renmin University of China, QIMAO SI, Department of Physics & Astronomy, Rice University, Houston, JOE THOMPSON, Los Alamos National Laboratory, Los Alamos — Recently, a unique type of well-known compounds, mixed-valence rare earth hexaborides  $\text{RB}_6$  ( $\text{R} = \text{Sm}$  and  $\text{Yb}$ ), receive new interests due to the discovery of the coexistence of metallic surface state and insulating bulk state in  $\text{SmB}_6$ . This encourages people to revisit the  $\text{RB}_6$  with an attempt to establish a new physics that links the correlated electron systems and topological insulators. Pressure is a way to help understanding the underlying mechanism, therefore it is specially needed in establishing this link because the valence state of  $\text{RB}_6$  is sensitive to pressure. In this talk, we will report some progress of high pressure studies on the  $\text{RB}_6$ , mainly focusing on the phenomena of pressure-induced exotic states and corresponding quantum phase transitions. The connections between the related phenomena and the valence states are revealed.

### 9:48AM R47.00010 Tunable Kondo effect and spin textures on topological insulators surfaces<sup>1</sup>

, ILYA VEKHTER, Department of Physics and Astronomy, Louisiana State University, GERARDO ORTIZ, Department of Physics and Center for Exploration of Energy and Matter, Indiana University Bloomington, LEONID ISAEV, JILA, NIST and Department of Physics, University of Colorado Boulder — We consider screening of a spin-1/2 impurity at the surface of a topological insulator, and show that the very existence of Kondo screening strongly depend on details of the bulk material and surface preparation whose details are encoded in time-reversal preserving boundary conditions for electronic wavefunctions. We investigate in detail the formation of the Kondo resonance by studying the "orbital-flip" processes that screen the impurity spin in the resulting strongly spin-orbit coupled system. This mechanism gives rise to spin textures that can be used to experimentally probe signatures of a Kondo resonance in topological insulators, and we give examples relevant to specific materials.

<sup>1</sup>L.I. was supported by the NSF (PIF-1211914 and PFC-1125844), AFOSR, AFOSR-MURI, NIST and ARO individual investigator awards, and also in part by ICAM. I.V. acknowledges support from NSF Grant DMR-1105339.

### 10:00AM R47.00011 Incomplete Protection of the Surface Weyl Cones of Kondo Insulators: Spin Exciton Scattering<sup>1</sup>

, PETER RISEBOROUGH, GARY A<sub>2</sub> KAPILEVICH, ALEX GRAY, Temple Univ, MIKLOS GULACSI, Max Planck Institute for the Physics of Complex Systems, TOMASZ DURAKIEWICZ, Los Alamos National Lab, JAMES L. SMITH, Los Alamos National lab. — The material SmB<sub>6</sub> is a Kondo Insulator, where the lowest-energy bulk electronic excitations are spin excitons. The material also has surface states which are subjected to strong spin-orbit coupling. It has been suggested that SmB<sub>6</sub> is also a topological insulator. Here we show that, despite the absence of time-reversal symmetry breaking and the presence of strong spin-orbit coupling, the chiral spin texture of the Weyl cone is not completely protected. In particular, we show that the spin-exciton mediated scattering produces features in the surface electronic spectrum at energies separated from the surface Fermi-energy by the spin-exciton energy. Despite the features being far removed from the surface Fermi-energy, the features are extremely temperature dependent. The temperature variation occurs over a characteristic scale determined by the dispersion of the spin exciton. The structures may be observed by electron spectroscopy at low temperatures.

<sup>1</sup>US Department of Energy, Office of Basic Energy Science, via the award DE-FG02-01ER45872

### 10:12AM R47.00012 Magnetotransport properties of topological surface states in the presence of ferromagnetic order

, KUNAL TIWARI, WILLIAM COISH, TAMI PEREG-BARNEA, McGill University — The surface of a 3D topological insulator hosts a two dimensional Dirac cone which is robust to weak, non-magnetic perturbation. Its presence will dominate low energy transport since the bulk is gapped. However, once magnetic impurities are introduced to the surface they may gap the Dirac dispersion, suppressing or modifying the systems surface transport properties. In particular, in the presence of uniform ferromagnetic order, the Dirac cone becomes massive and should not conduct for energies near the Dirac point. On the other hand, if the ferromagnetic order has domains with different magnetization directions, current may be carried on the domain walls where the Dirac mass vanishes. Our research aims to elucidate the transport properties of topological insulators in the presence of magnetic domain structures. Our work may be relevant to recent studies on the Kondo topological insulator SmB<sub>6</sub>.

### 10:24AM R47.00013 Universal edge information from wavefunction deformation

, WEN WEI HO<sup>1</sup>, Department of Theoretical Physics, University of Geneva, LUKASZ CINCIO, HEIDAR MORADI, GUIFRE VIDAL, Perimeter Inst for Theo Phys — It is well known that the bulk physics of a topological phase constrains its possible edge physics through the bulk-edge correspondence. Therefore, the different types of edge theories that a topological phase can host is a universal piece of data which can be used to characterize topological order. Here, we argue that beginning from only the fixed point wavefunction (FPW) of a nonchiral topological phase and by locally deforming it, all possible edge theories can be extracted from its entanglement Hamiltonian (EH). We illustrate our claim by deforming the FPW of the Wen-plaquette model, the quantum double of Z<sub>2</sub>. We show that the possible EHs of the deformed FPWs reflect the known possible types of edge theories, which are generically gapped, but gapless if translational symmetry is preserved. We stress that our results do not require an underlying Hamiltonian — thus, this lends support to the notion that a topological phase is indeed characterized by only a set of quantum states and can be studied through its FPWs.

<sup>1</sup>Also affiliated to Perimeter Inst for Theo Phys

### 10:36AM R47.00014 Landau quantization and spin-momentum locking in topological Kondo insulators<sup>1</sup>

, PEDRO SCHLOTTMANN, Florida State University — SmB<sub>6</sub> has been predicted to be a strong topological Kondo insulator and experimentally it has been confirmed that at low temperatures the electrical conductivity only takes place at the surfaces of the crystal. Quantum oscillations and ARPES measurements revealed several Dirac cones on the (001) and (101) surfaces of the crystal. We considered three types of surface Dirac cones with an additional parabolic dispersion and studied their Landau quantization and the expectation value of the spin of the electrons. The Landau quantization is quite similar in all three cases and would give rise to very similar de Haas-van Alphen oscillations [1]. The spin-momentum locking, on the other hand, differs dramatically. Without the additional parabolic dispersion the spins are locked in the plane of the surface. The parabolic dispersion, however, produces a gradual canting of the spins out of the surface plane.

[1] P. Schlottmann, Phys. Rev. B **90**, 165127 (2014).

<sup>1</sup>Work supported by the Department of Energy under grant No. DE-FG02-98ER45707.

### 10:48AM R47.00015 Strong correlations in Kondo topological insulators: Two-dimensional heavy fermions, and beyond

, PREDRAG NIKOLIC, George Mason Univ — Samarium hexaboride (SmB<sub>6</sub>) is a candidate topological insulator with strong electron correlations. Empowered by the time-reversal (TR) symmetry and topology, the low-energy surface states of hybridized samarium's d and f orbitals can exhibit a rich two-dimensional heavy-fermion phenomenology. This talk will survey several interesting possibilities for correlated surface states, which depend on microscopic surface conditions. A pronounced participation of the f orbitals is expected to create a heavy-fermion Dirac metal, possibly unstable to spin density waves, superconductivity, or exotic Mott insulators (e.g. algebraic and non-Abelian spin liquids). The opposite limit of localized magnetic moments can produce a non-Fermi liquid of d electrons that exhibits two-dimensional quantum electrodynamics. Ultrathin films made from topological Kondo insulators can host lattices of SU(2) vortices, which need not break the TR symmetry. Landau-Ginzburg theory and numerical model calculations reveal the nature and stability of such vortex lattices, while field theory arguments predict that their quantum melting could yield novel incompressible quantum liquids with non-Abelian fractional excitations.

## Thursday, March 17, 2016 8:00AM - 11:00AM —

Session R48 GQI: Decoherence in Superconducting Qubits: Junctions and Fluxonium 349 - Britton Plourde, Syracuse University

**8:00AM R48.00001 Novel Josephson circuit elements for high magnetic field parity detection**, MAJA CASSIDY, Delft University of Technology — Evidence for Majorana modes in semiconductor nanowires to date has relied on DC transport measurements that probe their zero-energy characteristics. However, in order to unambiguously demonstrate the non-Abelian nature of Majoranas, it is necessary to braid them and measure their parity. Superconducting transmon qubits have been shown to be sensitive parity detectors, however traditional designs are incompatible with the strong magnetic fields required for the creation of Majoranas in nanowires. In this talk I will discuss our development of novel superconducting circuit elements such as CPW resonators, tunnel junctions, transmon qubits and on-chip microwave sources that survive magnetic fields in excess of 1T.

**8:36AM R48.00002 Decoherence and Decay of Two-level Systems due to Non-equilibrium Quasiparticles**<sup>1</sup>, SEBASTIAN ZANKER, MICHAEL MARTHALER, GERD SCHN, Karlsruhe Institute of Technology, INSTITUT FÜR THEORETISCHE FESTKÖRPERPHYSIK TEAM — It is frequently observed that even at very low temperatures the number of quasiparticles in superconducting materials is higher than predicted by standard BCS-theory. These quasiparticles can interact with two-level systems, such as superconducting qubits or two-level systems (TLS) in the amorphous oxide layer of a Josephson junction. This interaction leads to decay and decoherence of the TLS, with specific results, such as the time dependence, depending on the distribution of quasiparticles and the form of the interaction. We study the resulting decay laws for different experimentally relevant protocols.

<sup>1</sup>This work was supported by the German-Israeli Foundation for Scientific Research and Development (GIF).

**8:48AM R48.00003 Superconducting resonators with trapped vortices under direct injection of quasiparticles**, IBRAHIM NSANZINEZA, Syracuse University, UMESH PATEL, University of Wisconsin, K. R. DODGE, Syracuse University, R. F. MCDERMOTT, University of Wisconsin, B. L. T. PLOURDE, Syracuse University — Nonequilibrium quasiparticles and trapped magnetic flux vortices can significantly impact the performance of superconducting microwave resonant circuits and qubits at millikelvin temperatures. Quasiparticles result in excess loss, reducing resonator quality factors and qubit lifetimes. Vortices trapped near regions of large microwave currents also contribute excess loss. However, vortices located in current-free areas in the resonator or in the ground plane of a device can actually trap quasiparticles and lead to a reduction in the quasiparticle loss. We will describe experiments involving the controlled trapping of vortices in superconducting resonators with direct injection of quasiparticles using Normal metal-Insulator-Superconductor (NIS)-tunnel junctions.

**9:00AM R48.00004 Robustness of superconducting quantum modes against direct quasiparticle injection**, U. PATEL, Department of Physics, University of Wisconsin, Madison, Wisconsin 53706, I. NSANZINEZA, Department of Physics, Syracuse University, Syracuse, New York 13244, M. G. VAVILOV, Department of Physics, University of Wisconsin, Madison, Wisconsin 53706, B. L. T. PLOURDE, Department of Physics, Syracuse University, Syracuse, New York 13244, R. MCDERMOTT, Department of Physics, University of Wisconsin, Madison, Wisconsin 53706 — Classical Josephson digital logic based on Single Flux Quantum (SFQ) pulses offers a path to high-fidelity coherent control of large-scale superconducting quantum machines. However, an SFQ pulse driver generates nonequilibrium quasiparticles that contribute to qubit relaxation, and steps must be taken to protect the qubit from this decoherence channel. Here we describe experiments to characterize the robustness of high-Q superconducting linear resonators and qubits against direct quasiparticle injection. We use NIS junctions and SFQ elements to controllably inject quasiparticles into the groundplane of superconducting resonator and qubit chips, and we characterize the quasiparticle contribution to dissipation. We examine the effectiveness of groundplane cuts, normal metal quasiparticle traps, and spatially-varying superconducting gaps at protecting the quantum modes against quasiparticle loss. Finally, we discuss strategies for the integration of multiqubit circuits with on-chip SFQ control elements.

**9:12AM R48.00005 Normal Metal Quasiparticle Traps in 3D-Transmon Qubits**<sup>1</sup>, LUKE D. BURKHART, YVONNE Y. GAO, CHEN WANG, KYLE SERNIK, GJS DE LANGE, YIWEN CHU, URI VOOL, LUIGI FRUNZIO, MICHEL H. DEVORET, Department of Applied Physics and Physics, Yale University, GIANLUIGI CATELANI, Peter Grunberg Institut (PGI-2), Forschungszentrum Jülich, LEONID I. GLAZMAN, ROBERT J. SCHOELKOPF, Department of Applied Physics and Physics, Yale University — Quasiparticles are a known source of decoherence in Josephson-junction based superconducting qubits. While equilibrium quasiparticles should not be present in devices operated at dilution refrigeration temperatures well below the superconducting energy gap, non-thermal quasiparticles have been observed in many different superconducting qubits, including 3D-transmons and fluxonium qubits. Vortices induced by applied magnetic fields have been shown to improve non-equilibrium quasiparticle decay rates and improve coherence times by creating regions of the superconductor with vanishing energy gap, which act as quasiparticle traps. We aim to further mitigate quasiparticle-induced limits on coherence by engineering strong trapping via the introduction of normal metal to the superconducting qubit. In this talk, we present recent results regarding normal metal quasiparticle traps in 3D-transmon qubits.

<sup>1</sup>Work supported by ARO, A\*STAR

**9:24AM R48.00006 Gap-engineered quasiparticle traps in the fluxonium artificial atom**<sup>1</sup>, K. SERNIK, G. DE LANGE, U. VOOL, M. HAYS, L.D. BURKHART, Y.Y. GAO, C. WANG, K.M. SLIWA, Department of Applied Physics, Yale University, I.M. POP, Department of Applied Physics, Yale University, and Physikalisches Institut, Karlsruhe Institute of Technology, L. FRUNZIO, L.I. GLAZMAN, R.J. SCHOELKOPF, M.H. DEVORET, Department of Applied Physics, Yale University — Recent experiments have shown that the density of quasiparticles in superconducting quantum circuits exceeds the expected thermal density. In Josephson junction based superconducting qubits, these non-equilibrium quasiparticles can tunnel through the junctions of the circuit, causing decoherence. Quasiparticle traps aim to reduce the density of quasiparticles near the junctions, and therefore the rate of energy loss and dephasing due to tunneling events. These traps must be designed to not introduce any additional losses in the qubit. In this talk we will discuss recent progress in the design and implementation of quasiparticle traps in the fluxonium artificial atom.

<sup>1</sup>Work supported by ARO, ONR, YINQE, and the European Union

**9:36AM R48.00007 Spectroscopy and decoherence of plasmons and fluxons in superconducting fluxonium qubit.**, LONG NGUYEN, YEN-HSIANG LIN, NICHOLAS GRABON, NATALYA SOLOVYIEVA, VLADIMIR MANUCHARYAN, Univ of Maryland-College Park, SUPERCONDUCTING CIRCUITS LAB TEAM — Transition spectrum of a fluxonium circuit changes drastically with respect to the  $p=EJ/EC$  parameter of the small junction, remaining charge-insensitive at all values of  $p$ . At larger values of  $p$ , the spectrum consists of exponentially decoupled fluxon and plasmon transitions. At smaller values, fluxons no longer exist, and plasmons reside mostly in the array inductance. We present spectroscopy of tunable fluxoniums and discuss our findings from the decoherence measurements of various transitions.

**9:48AM R48.00008 The fluxonium as a lambda system<sup>1</sup>**, U. VOOL, A. KOU, W.C. SMITH, K. SERNIAK, S. SHANKAR, S.M. GIRVIN, M.H. DEVORET, Department of Applied Physics, Yale University — A lambda system is a 3-level system in which two low-energy states can transition to a third higher-energy state by a coherent drive but not to each other. Lambda systems are commonly implemented in systems relying on atomic transitions. In the field of superconducting quantum circuits, the fluxonium qubit, an artificial atom consisting of a Josephson junction shunted by a superinductance, is a unique artificial atom with highly non-linear energy levels. At half-flux quantum it has two low-energy states with a long energy lifetime, but it is difficult to perform fast quantum gates in this manifold. Employing the higher 2nd excited state as an intermediate level would be much more efficient. However, selection rules in the fluxonium qubit prohibit transitions between low-energy states and higher-energy states of the same parity. In this talk, we will introduce a way to create formerly forbidden transitions between levels of the fluxonium qubit - thus creating a more interesting artificial atom and a useful tool for future superconducting quantum circuits.

<sup>1</sup>Work supported by ARO, ONR, AFOSR and YINQE

**10:00AM R48.00009 Simultaneous monitoring of fluxonium qubits in a waveguide<sup>1</sup>**, A. KOU, W.C. SMITH, U. VOOL, I.M. POP, K.M. SLIWA, M. HATRIDGE, R.J. SCHOEKOPF, M.H. DEVORET, Department of Applied Physics, Yale University — Building quantum computers and quantum simulators requires separate control and readout of multiple qubits. We present an architecture for multiplexed readout of fluxonium qubits. We measured lifetimes in excess of 100 us for such artificial atoms placed in a wide-bandwidth electromagnetic environment. We use cascaded Josephson parametric converters to measure the quantum jumps of two fluxonium qubits simultaneously. Our method can access correlations between different qubits and can easily be scaled to read out larger numbers of qubits.

<sup>1</sup>Work supported by: ARO, ONR, AFOSR, and YINQE.

**10:12AM R48.00010 A disordered kinetic superinductor<sup>1</sup>**, M. HAYS, G. DE LANGE, K. SERNIAK, Z. WANG, U. VOOL, L. FRUNZIO, M.H. DEVORET, Department of Applied Physics, Yale University — The superinductance is a superconducting circuit element whose reactance exceeds the resistance quantum at the relevant microwave operation frequencies of quantum circuits. It must also be as non-dissipative as possible. Such an element is key to the fluxonium artificial atom, a highly anharmonic, charge insensitive superconducting qubit that has been proposed as the detection circuit for Majorana Fermions. So far fluxonium qubits are made exclusively from arrays of Al-AIOx-Al Josephson junctions. However, aluminium is difficult to employ in conjunction with the strong magnetic fields required in Majorana Fermion experiments. The large kinetic inductance of highly resistive disordered superconducting alloys, such as NbTiN, is currently explored as an alternative material for superinductance in quantum electronic circuits. We report the results of measurement of quality factors and phase-slip rates of high-impedance resonators made from thin-film NbTiN.

<sup>1</sup>Work supported by: ARO, ONR, AFOSR and YINQE

**10:24AM R48.00011 Fabrication and characterization of low loss and high inductance Josephson tunnel junction chains for quantum circuits**, NICHOLAS GRABON, NATALYA SOLOVYEV, LONG NGUYEN, YEN-HSIANG LIN, VLADIMIR MANUCHARYAN, University of Maryland — Linear chains of tightly packed Josephson junctions can realize a very high kinetic inductance circuit element, superinductance, with minimal losses. Superinductance is used in a conventional fluxonium qubit, but it has also been put forward as a key element of a fault-tolerant quantum circuits toolbox [1]. We report fabrication and microwave characterization of linear Al/AIOx/Al Josephson tunnel junction chains and discuss their advantages and limitations as superinductors. [1]: 10.1103/PhysRevA.87.052306

**10:36AM R48.00012 Extending quantum coherence of superconducting flux<sup>1</sup>**, FEI YAN, ARCHANA KAMAL, TERRY ORLANDO, SIMON GUSTAVSSON, Massachusetts Inst of Tech-MIT, WILLIAM OLIVER, Massachusetts Inst of Tech-MIT, Lincoln Laboratory, ENGINEERING QUANTUM SYSTEMS, MIT TEAM — We present the design of a superconducting qubit with multiple Josephson junctions. The design starts with a capacitively shunted flux qubit, and it incorporates particular junction parameter choices for the purpose of simultaneously optimizing over transition frequency, anharmonicity, flux- and charge-noise sensitivity around flux degeneracy. By studying the scaling properties with design parameters, we identify directions to extend coherence substantially.

<sup>1</sup>This research was funded by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA) via MIT Lincoln Laboratory under Air Force Contract No. FA8721-05-C-0002.

**10:48AM R48.00013 Quantum memristor in a superconducting circuit<sup>1</sup>**, JUHA SALMILEHTO, Department of Physics, Yale University, New Haven, Connecticut 06520, USA, MIKEL SANZ, University of the Basque Country UPV/EHU, Apartado 644, E-48080 Bilbao, Spain, MASSIMILIANO DI VENTRA, Department of Physics, University of California, San Diego, La Jolla, CA 92093, USA, ENRIQUE SOLANO, University of the Basque Country UPV/EHU, Apartado 644, E-48080 Bilbao, Spain — Memristors, resistive elements that retain information of their past, have garnered interest due to their paradigm-changing potential in information processing and electronics. The emergent hysteretic behaviour allows for novel architectural applications and has recently been classically demonstrated in a simplified superconducting setup using the phase-dependent conductance in the tunnel-junction-microscopic model[1]. In this contribution, we present a truly quantum model for a memristor constructed using established elements and techniques in superconducting nanoelectronics, and explore the parameters for feasible operation as well as refine the methods for quantifying the memory retention. In particular, the memristive behaviour is shown to arise from quasiparticle-induced tunneling in the full dissipative model and can be observed in the phase-driven tunneling current. The relevant hysteretic behaviour should be observable using current state-of-the-art measurements for detecting quasiparticle excitations. Our theoretical findings constitute the first quantum memristor in a superconducting circuit and act as the starting point for designing further circuit elements that have non-Markovian characteristics. [1] S. Peotta and M. Di Ventra, Phys. Rev. Applied 2, 034011 (2014).

<sup>1</sup>The authors acknowledge support from the CCQED EU project and the Finnish Cultural Foundation.

**Thursday, March 17, 2016 8:00AM - 11:00AM –**  
**Session R50 DAMOP: Quantum Gases in Reduced Dimension, Ladders, and other Novel Geometries** Hilton Baltimore Holiday Ballroom 1 - M. Rigol, Pennsylvania State University

**8:00AM R50.00001 Exploring Quantum Many-Body Spin Dynamics with Truncated Wigner Methods** , JOHANNES SCHACHENMAYER, JILA, NIST & Department of Physics, University of Colorado, Boulder — Recent experiments in atomic, molecular, and optical physics offer controlled and clean environments to experimentally study non-equilibrium dynamics of large many-body quantum spin-models with variable range interactions. Thus, efficient computation of such dynamics is of great importance. While in one dimension, time-dependent density matrix renormalization group methods (t-DMRG) have proven effective under certain conditions, computing dynamics in higher dimensional systems remains an outstanding challenge. Recently we formulated the discrete truncated Wigner approximation (DTWA), a semiclassical method based on the truncated Wigner approximation (TWA) that has been proven to be surprisingly accurate in predicting quench dynamics in high-dimensional lattices with up to tens of thousands of quantum spins. Here, we introduce the DTWA and show how it can compute time-evolution of quantum states in experiments that engineer spin-models with polar molecules in optical lattices or with ions in two-dimensional Penning traps. We show, how the DTWA can provide results for the time-evolution of classical and quantum correlations in quench experiments in regimes where other numerical methods are generally unreliable. We report on progress of how to incorporate higher order corrections to the method, and how to adapt it to systems with both spin and bosonic degrees of freedom.

**8:36AM R50.00002 A Quantum Dipolar Spin Liquid** , NORMAN YAO, Department of Physics, UC Berkeley, MICHAEL ZALETEL, Station Q, Microsoft Research, DAN STAMPER-KURN, ASHVIN VISHWANATH, Department of Physics, UC Berkeley — Quantum spin liquids are a new class of magnetic ground state in which spins are quantum mechanically entangled over macroscopic scales. Motivated by recent advances in the control of polar molecules, we show that dipolar interactions between  $S=1/2$  moments stabilize spin liquids on the triangular and kagome lattices. In the latter case, the moments spontaneously break time-reversal, forming a chiral spin liquid with robust edge modes and emergent semions. We propose a simple route toward synthesizing a dipolar Heisenberg antiferromagnet from lattice-trapped polar molecules using only a single pair of rotational states and a constant electric field.

**8:48AM R50.00003 Intrinsic topological superfluidity – fluctuations and response** , K LEVIN, CHIEN-TE WU, BRANDON ANDERSON, RUFUS BOYACK, James Franck Institute — Recent interest in topological superconductivity is based primarily on exploiting proximity effects to obtain this important phase. However, in cold gases it is possible to contemplate “intrinsic” topological superfluidity produced with a synthetic spin-orbit coupling and Zeeman field. It is important for such future experiments to establish how low in temperature one needs to go to reach the ordered phase. Similarly, it will be helpful to have a probe of the normal (pseudogap) phase to determine if the ultimate superfluid order will be topological or trivial. In this talk, we address these issues by considering fluctuation effects in such a superfluid, and calculate the critical transition temperature and response functions. We see qualitative signatures of topological superfluidity in spin and charge response functions. We also explore the suppression of superfluidity due to fluctuations, and importantly find that the temperature scales necessary to reach topological superfluidity are reasonably accessible [1]. [1] Phys. Rev. B 92, 134523 (2015)

**9:00AM R50.00004 Phase diagrams of spinor bosons in two-leg ladders.**<sup>1</sup> , JERESON SILVA VALENCIA, ROBERTO FRANCO, Universidad Nacional de Colombia, MARCOS SERGIO FIGUEIRA, Universidade Federal Fluminense — In the last, years different experimental groups have reported the realization of atomic ladders in the presence of a homogeneous flux [Nat. Phys. 10, 588 (2014)]. These experiments have motivated theoretical calculations on 2-leg ladders with spinless bosons under magnetic fields [PRB 91, 140406(R) (2015)]. In this paper, we consider spinor boson atoms with spin  $S=1$ , such as Rb and Na. Gases of these atoms can be described by the spinor Bose-Hubbard Hamiltonian which has three terms: the kinetic energy, local density-density interaction and local spin-dependent term. Using DMRG, we study  $S=1$  bosons on 2-leg ladders, taking into account both antiferromagnetic and ferromagnetic spin interaction. When both legs are ferromagnetic or antiferromagnetic, we obtained Mott insulator and superfluid phases, similar to the one-dimensional case, but the insulator areas decrease due to the additional kinetic term. The even-odd asymmetry is still observed in the antiferromagnetic case. However, when the local spin interaction has a different sign on each leg, charge density waves for densities  $3/2$  and  $5/2$  appear. The Mott insulator phase for density 1 (2) correspond to the antiferromagnetic-leg (ferromagnetic-leg).

<sup>1</sup> COLCIENCIAS (grant No. FP44842-057-2015)

**9:12AM R50.00005 XY-sliding phases – mirage of the Renormalization Group**<sup>1</sup> , STEVEN VAYL, ANATOLY KUKLOV, VADIM OGANESYAN, CSI and the Graduate Center, CUNY — The so called sliding XY phases in layered systems are predicted to occur if the one loop renormalization group (RG) flow renders the interlayer Josephson coupling irrelevant, while each layer still features broken  $U(1)$  symmetry<sup>2</sup>. In other words, such a layered system remains essentially two-dimensional despite the presence of inter-layer Josephson coupling. We have analyzed numerically a layered system consisting of groups of asymmetric layers where the RG analysis predicts sliding phases to occur. Monte Carlo simulations of such a system have been conducted in the dual representation by Worm Algorithm<sup>3</sup> in terms of the closed loops of J-currents<sup>4</sup> for layer sizes varying from  $4 \times 4$  to  $640 \times 640$  and the number of layers – from 2 to 40. The resulting flow of the inter-layer XY-stiffness has been found to be inconsistent with the RG prediction and fully consistent with the behavior of the 3D standard XY model where the bare inter-layer Josephson coupling is much smaller than the intra-layer stiffness. This result emphasizes the importance of the compactness of the  $U(1)$  variable for 2D to 3D transformation.

<sup>1</sup> This work was supported by the NSF grant PHY1314469

<sup>2</sup> C.S.OHern, et al. PRL **83**, 2745 (1999)

<sup>3</sup> N.V.Prokof'ev, B.V.Svistunov, PRL **87**, 160601 (2001)

<sup>4</sup> M.Wallin, et.al., PRB **49**, 12115 (1994)

**9:24AM R50.00006 Spontaneous increase of magnetic flux and chiral-current reversal in bosonic ladders: Swimming against the tide** , TEIMURAZ VEKUA, SEBASTIAN GRESCHNER, Leibniz University of Hannover, MARIE PIRAUD, FABIAN HEIDRICH-MEISNER, Ludwig-Maximilians-University of Munich, IAN MCCULLOCH, The University of Queensland, ULI SCHOLLWOECK, Ludwig-Maximilians-University of Munich — The interplay between the spontaneous symmetry breaking and the wave-like nature of quantum particles in lattice produces an extraordinary behavior of the chiral current of interacting bosonic particles in the presence of a uniform magnetic flux defined on a two-leg ladder. While non-interacting as well as strongly interacting particles, stirred by the magnetic field circulate along the system's boundary in the counterclockwise direction, for certain interactions between particles and at sufficiently low temperature, the circulation direction of chiral current can be spontaneously reversed in vortex lattice states. Chiral-current reversal is counter-intuitive many-body effect produced by synthetic magnetism and it can be observed up to temperatures  $T=0.5J$ , where  $J$  is a hopping rate along ladder. Besides this effect we present first numerical evidence of vortex lattice states in interacting bosonic ladders with flux and a state with spontaneously imbalanced density between the ladder legs.

**9:36AM R50.00007 Dimensional phase transition from 1D behavior to a 3D Bose-Einstein condensate**, AXEL PELSTER, DENIS MORATH, DOMINIK STRAßEL, SEBASTIAN EGGERT, Univ Kaiserslautern, Germany — The emergence of new properties from low-dimensional building blocks is a universal theme in different areas in physics. The investigation of transitions between isolated and coupled low-dimensional systems promises to reveal new phenomena and exotic phases. Interacting 1D bosons, which are coupled in a two-dimensional array, are maybe the most fundamental example of a system which illustrates the concept of a dimensional phase transition. However, recent experiments using ultracold gases have shown a surprising discrepancy between theory and experiment [1] and it is far from obvious if the power laws from the underlying 1D theory can predict the transition temperature and order parameter correctly for all interaction strengths. Using a combination of large-scale Quantum Monte-Carlo simulations and chain mean-field calculations, we show that the behavior of the ordering temperature as a function of inter-chain coupling strength does not follow a universal powerlaw, but also depends strongly on the filling. [1] A. Vogler, R. Labouvie, G. Barontini, S. Eggert, V. Guarrera, and H. Ott, Phys. Rev. Lett. 113, 215301 (2014)

**9:48AM R50.00008 Solving a quantum many-body problem by experiment**, THOMAS SCHWEIGLER, Vienna Center for Quantum Science and Technology, Atominstitut, TU Wien, VALENTIN KASPER, Institut für Theoretische Physik, Universität Heidelberg, SEBASTIAN ERNE, BERNHARD RAUER, TIM LANGEN, Vienna Center for Quantum Science and Technology, Atominstitut, TU Wien, THOMAS GASENZER, Kirchhoff-Institut für Physik, Universität Heidelberg, JÜRGEN BERGES, Institut für Theoretische Physik, Universität Heidelberg, JÖRG SCHMIEDMAYER, Vienna Center for Quantum Science and Technology, Atominstitut, TU Wien — We experimentally study a pair of tunnel-coupled one-dimensional atomic superfluids, which realize the quantum sine-Gordon/massive Thirring models relevant for a wide variety of disciplines from particle to condensed-matter physics. From measured interference patterns we extract phase correlation functions and analyze if, and under which conditions, the higher-order correlation functions factorize into lower ones. This allows us to characterize the essential features of the model solely from our experimental measurements, detecting the relevant quasiparticles, their interactions and the topologically distinct vacua. Our method provides comprehensive insights into a non-trivial quantum field theory and establishes a general method to analyze quantum many-body systems through experiments. The method is also used to investigate the non-equilibrium dynamics following a quench in the tunnel-coupling between the superfluids.

**10:00AM R50.00009 Meissner and Laughlin Phases in bosonic Ladders**, ALEXANDRU PETRESCU, Princeton University, Department of Electrical Engineering, MARIE PIRAUD, Department of Physics and Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, IAN MCCULLOCH, ARC Centre for Engineered Quantum Systems, School of Mathematics and Physics, The University of Queensland, GUILLAUME ROUX, LPTMS, Univ. Paris-Sud and CNRS, UMR 8626, KARYN LE HUR, CPHT and CNRS, Ecole Polytechnique — We introduce a hard core boson model on a ladder lattice in uniform orbital magnetic flux. This model supports the Meissner effect in the presence of insulating behavior [1,2,3]. When the ratio of particle and flux densities  $\nu$  is close to  $1/2$ , the ground state is a low-dimensional equivalent of the Laughlin state of fractional quantum Hall effect [3]. Using exact analytical methods, the density matrix renormalization group method and exact diagonalization, we identify local observables that distinguish the Laughlin phase from the surrounding vortex and Meissner phases. At  $\nu = 1/2$  the antisymmetric current, currently accessible in ultracold atom experiments [5,6], saturates. Thus remnants of topological order in quasi one dimensional systems can be probed using local observables. Secondly, we show how ground state degeneracy and topology can be probed with Thouless pump experiments on the ladder geometry. [1] A. Petrescu and K. Le Hur, PRL 111, 150601 [2] M. Piraud, F. Heidrich-Meisner, I. P. McCulloch, S. Greschner, T. Vekua, and U. Schollwöck, PRB 91, 140406R [3] A. Petrescu and K. Le Hur, PRB 91, 054520 [4] M. Atala et al, Nat. Phys. 10, 588; B. K. Stuhl et al, Science 349, 1514; M. Mancini et al, Science 349, 1510.

**10:12AM R50.00010 Entanglement entropy of the ground state of the Lieb-Liniger model**, c. M. HERDMAN, P.-N. ROY, University of Waterloo, ROGER MELKO, University of Waterloo and Perimeter Institute for Theoretical Physics, ADRIAN DEL MAESTRO, University of Vermont — We consider the entanglement between two spatial subsystems in the Lieb-Liniger model of contact interacting bosons in continuous space in one dimension. Using a continuous-space ground state path integral quantum Monte Carlo method, we numerically compute the Rényi entropy of the reduced density matrix of the subsystem as a measure of entanglement. Our numerical algorithm is based on the replica method previously introduced by the authors, which we have extended to efficiently study large spatial subsystems using a ratio approach. We confirm a logarithmic scaling of the Rényi entropy with subsystem size that is expected from conformal field theory and compute the non-universal sub-leading constant for interaction strengths ranging over several orders of magnitude. In the strongly interacting limit, we find agreement with the known free fermion result.

**10:24AM R50.00011 Diagrammatic Monte Carlo study of Fermi-polaron systems**, PETER KROISS, LODE POLLET, Department of Physics, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-University Munich — We apply the diagrammatic Monte Carlo approach to three-dimensional Fermi-polaron systems with mass-imbalance, where an impurity interacts resonantly with a noninteracting Fermi sea whose atoms have a different mass. This method allows to go beyond frequently used variational techniques by stochastically summing all relevant impurity Feynman diagrams up to a maximum expansion order limited by the sign problem. Polaron energy and quasiparticle residue can be accurately determined over a broad range of impurity masses. The quantitative exactness of two-particle-hole wave-functions is investigated, resulting in a relative lowering of polaronic energies in the mass-imbalance phase diagram. The application of the method to two-dimensional Fermi-polaron systems is presented.

**10:36AM R50.00012 Recent developments in auxiliary-field quantum Monte Carlo methods for cold atoms<sup>1</sup>**, HAO SHI, PETER ROSENBERG, ETTORE VITALI, SIMONE CHIESA, SHIWEI ZHANG, College of William and Mary — Exact calculations are performed on the two-dimensional strongly interacting, unpolarized, uniform Fermi gas with a zero-range attractive interaction. We describe recent advances in auxiliary-field quantum Monte Carlo techniques, which eliminate an infinite variance problem in the standard algorithm, and improve both acceptance ratio and efficiency. The new methods enable calculations on large enough lattices to reliably compute ground-state properties in the thermodynamic limit. An equation of state is obtained, with a parametrization provided, which can serve as a benchmark and allow accurate comparisons with experiments. The pressure, contact parameter, condensate fraction, and pairing gap will be presented. The same methods are also applied to obtain exact results on the two-dimensional strongly interacting Fermi gas in the presence of Rashba spin-orbit (SOC), providing insights on the interplay between pairing and SOC.

<sup>1</sup>Supported by NSF, DOE, and the Simons Foundation.

**10:48AM R50.00013 Multiband effects in one-dimensional bosons in optical lattices**, WEI XU, MARCOS RIGOL, Department of Physics, The Pennsylvania State University, University Park, PA 16802, USA — We use path integral quantum Monte Carlo simulations to study quantum phase transitions of ultracold bosons in optical lattices. We restrict our study to one-dimensional systems where, in the absence of the lattice, we recover analytic results for the Lieb-Liniger model. The latter is the model that describes one-dimensional bosons with contact interactions. We first discuss how cold finite systems need to be in order for one to observe ground state physics. We then show that, in shallow lattice potentials, higher Bloch bands lead to renormalized two-body interactions. We present a study the phase diagram of these systems at intermediate interaction strengths in shallow lattice potentials, and report a detailed comparison with the phase diagram of the one-band Bose-Hubbard model.

**Thursday, March 17, 2016 8:00AM - 11:24AM –**  
**Session R52 GERA FIAP: Materials for Energy Storage Devices II** Hilton Baltimore Holiday Ballroom 3 -

**8:00AM R52.00001 Azobenzene-based Polymers for Solar Thermal Batteries** , DHANDAPANI VENKATARAMAN, University of Massachusetts Amherst — Azobenzene exists as two isomers, a higher energy cis-isomer and a lower energy trans-isomer. The isomers interconvert under light or heat. Recently, there is a renewed interest in capturing the difference in the energies of the isomers and using azobenzene-based molecules as active layers for solar thermal batteries. My research group has been exploring azobenzene-based polymers as candidates for solar thermal batteries. In this talk, I will show that the azo-benzene moieties can be converted to the cis-form using light and converted back to the trans form using mechanical force. I will provide some of our recent results that indicate that high energy densities can be achieved in these polymers.

**8:36AM R52.00002 Lithiation of  $\text{Ag}_x\text{MnO}_2$ : Insights from first principles** , MERZUK KALTAK, MARIVI FERNANDEZ-SERRA, State Univ of NY- Stony Brook, MARK HYBERTSEN, Center for Functional Nanomaterials, Brookhaven National Laboratory — Stable electrode materials being able to capture high lithium concentrations are attracting considerable interest in science as well as industry. Recently hollandite  $\alpha\text{-MnO}_2$  based structures are moving into the focus of electrochemists and are considered to be promising electrodes for increasing the capacity and efficiency of rechargeable lithium batteries. These favorable properties are mainly due to the tunnel structure consisting out of stacked  $1\times 1$  and  $2\times 2$   $\text{MnO}_2$  octahedra in the z-axis. It has been shown that large ions such as silver or potassium can stabilize and increase the cyclicity of pure hollandite  $\alpha\text{-MnO}_2$  considerably. In this work we present new insights from first principles for lithiated silver hollandite  $\text{Li}_y\text{Ag}_x\text{MnO}_2$  and demonstrate that the formation of oxygen vacancies play an important role for lithium diffusion.

**8:48AM R52.00003 First Principles Investigation of the Geometrical and Electrochemical Properties of  $\text{Na}_4\text{P}_2\text{S}_6$  and  $\text{Li}_4\text{P}_2\text{S}_6$** <sup>1</sup> , LARRY E. RUSH JR., N.A.W. HOLZWARTH, Wake Forest University — First principles simulations are used to examine the structural and physical properties of  $\text{Na}_4\text{P}_2\text{S}_6$  in comparison with its  $\text{Li}_4\text{P}_2\text{S}_6$  analog. Four model structures are considered including the  $C2/m$  structure recently reported by Kuhn and co-workers<sup>2</sup> from their analysis of single crystals of  $\text{Na}_4\text{P}_2\text{S}_6$ , and three structures related to the  $P6_3/mcm$  structure with P site disorder found in 1982 by Mercier and co-workers<sup>3</sup> from their analysis of single crystals of  $\text{Li}_4\text{P}_2\text{S}_6$ . The computational results indicate that both  $\text{Na}_4\text{P}_2\text{S}_6$  and  $\text{Li}_4\text{P}_2\text{S}_6$  have the same disordered ground state structures consistent with the  $P6_3/mcm$  space group, while the optimized  $C2/m$  structures have higher energies by 0.1 eV and 0.4 eV per formula unit for  $\text{Na}_4\text{P}_2\text{S}_6$  and  $\text{Li}_4\text{P}_2\text{S}_6$ , respectively. Simulations of ion migration suggest that  $\text{Na}_4\text{P}_2\text{S}_6$  may have more favorable ionic conductivity compared to  $\text{Li}_4\text{P}_2\text{S}_6$ .

<sup>1</sup>Supported by NSF grant DMR-1105485 and DMR-1507942.

<sup>2</sup>ZAAC **640**(5):689-692 (2014)

<sup>3</sup>JSSC **43**:151-162 (1982)

**9:00AM R52.00004 Quinone Derivatives for Lithium-Ion Batteries: First-Principles Density Functional Theory Modeling** , SEUNG SOON JANG, KI CHUL KIM, School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA 30332-0245, USA, TIANYUAN LIU, SEUNG WOO LEE, G. W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA 30332-0405, USA — The Li binding thermodynamics and redox potentials of seven different quinone derivatives are investigated as positive electrode candidates for lithium-ion batteries. First, using the density functional theory (DFT) calculations on the interactions between the quinone derivatives and Li ions, it is found that Li ions are dominantly bound with carbonyl groups of the molecules. Second, it is revealed that the redox chemistry of the quinone derivatives can be tuned by the modification of their chemical structures. Further DFT-based investigations on the redox potentials of the Li-bound quinone derivatives provide an insight on the change in their redox chemistry during the discharging processes. The redox potential and charge capacity are improved by modifying the quinone derivatives with electron-withdrawing carboxylic groups. Through this study, it is also found that the cathodic activity of a quinone derivative during the discharging processes strongly relies on the solvation free energy effect as well as the number of available carbonyl groups for further Li binding. To the best of our knowledge, the changes in the redox potential of the redox-active molecules during the discharging processes is reported for the first time.

**9:12AM R52.00005 Lithiation of  $\text{Li}_2\text{SnO}_3$  and  $\text{Li}_2\text{SnS}_3$  in context of Li-ion battery materials**<sup>1</sup> , JASON HOWARD, N. A. W. HOLZWARTH, Wake Forest University — The closed pack layered crystal material (space group 15 ( $C2/c$ ))  $\text{Li}_2\text{SnO}_3$  has been studied as a possible anode material since the late 1990s.<sup>2,3,4</sup> The material undergoes an irreversible decomposition to  $\text{Li}_2\text{O}$  and  $\text{Li}_x\text{Sn}$  alloys during the first lithiation cycle. The crystal material  $\text{Li}_2\text{SnS}_3$  of the same structure was recently proposed as an electrolyte material.<sup>5</sup> The question is posed whether  $\text{Li}_2\text{SnS}_3$  would be a good electrolyte or whether it could function as an anode material similar to  $\text{Li}_2\text{SnO}_3$ . In this research a model is proposed for the lithiation process of  $\text{Li}_2\text{SnO}_3$  and  $\text{Li}_2\text{SnS}_3$ ;  $\text{Li} - \text{Li}_2\text{SnS}_3$  interfaces are also examined. The results show  $\text{Li}_2\text{SnO}_3$  begins to decompose at approximately  $\text{Li}_{2+0.5}\text{SnO}_3$ . In  $\text{Li}_2\text{SnS}_3$  the lithiation process shows it can lithiate to  $\text{Li}_{2+1}\text{SnS}_3$  without significant lattice distortion, volume expansion, or decomposition.  $\text{Li} - \text{Li}_2\text{SnS}_3$  interfaces are shown to be unstable, showing the formation of  $\text{Li}_2\text{S}$ .

<sup>1</sup>Supported by NSF grant DMR-1105485 and DMR-1507942

<sup>2</sup>Courtney & Dahn, JES **144**, 2045(1997)

<sup>3</sup>Zhang et al., J. Alloy compd. **415**, 229(2006)

<sup>4</sup>Wang et al., Surf. Interface Anal. **45**, 1297(2013)

<sup>5</sup>Brant et al., Chem.Mater. **27**,189 (2015)

**9:24AM R52.00006 Accelerated materials design of fast oxygen ionic conductors based on first principles calculations** , XINGFENG HE, YIFEI MO, Department of Materials Science and Engineering, University of Maryland, College Park — Over the past decades, significant research efforts have been dedicated to seeking fast oxygen ion conductor materials, which have important technological applications in electrochemical devices such as solid oxide fuel cells, oxygen separation membranes, and sensors. Recently,  $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$  (NBT) was reported as a new family of fast oxygen ionic conductor. We will present our first principles computation study aims to understand the O diffusion mechanisms in the NBT material and to design this material with enhanced oxygen ionic conductivity. Using the NBT materials as an example, we demonstrate the computation capability to evaluate the phase stability, chemical stability, and ionic diffusion of the ionic conductor materials. We reveal the effects of local atomistic configurations and dopants on oxygen diffusion and identify the intrinsic limiting factors in increasing the ionic conductivity of the NBT materials. Novel doping strategies were predicted and demonstrated by the first principles calculations. In particular, the K doped NBT compound achieved good phase stability and an order of magnitude increase in oxygen ionic conductivity of up to  $0.1 \text{ S cm}^{-1}$  at 900 K compared to the experimental Mg doped compositions. Our results provide new avenues for the future design of the NBT materials and demonstrate the accelerated design of new ionic conductor materials based on first principles techniques. This computation methodology and workflow can be applied to the materials design of any (e.g.  $\text{Li}^+$ ,  $\text{Na}^+$ ) fast ion-conducting materials.

**9:36AM R52.00007 TiC<sub>2</sub>: A New Two-Dimensional Sheet beyond MXenes**, TIANSHAN ZHAO, Virginia Commonwealth Univ, SHUNHONG ZHANG, YAGUANG GUO, QIAN WANG, Peking University — MXenes are attracting attention due to their rich chemistry and intriguing properties. Here a new type of metal-carbon-based sheet composed of transition metal centers and C<sub>2</sub> dimers rather than individual C atoms is designed. Taking the Ti system as a test case, density functional theory calculations combined with a thermodynamic analysis uncover the thermal and dynamic stability of the sheet, as well as a metallic band structure, anisotropic Young's modulus and Poisson's ratio, a high heat capacity, and a large Debye stiffness. Moreover, the TiC<sub>2</sub> sheet has excellent Li storage capacity with a small migration barrier, a lower mass density compared with standard MXenes, and better chemical stability as compared to the MXene Ti<sub>2</sub>C sheet. When Ti is replaced with other transition metal centers, diverse new MC<sub>2</sub> sheets containing C=C dimers can be formed, the properties of which merit further investigation.

**9:48AM R52.00008 Diffusion of lithium in titanium oxide**, PATRICK SHEA, Dalhousie University, JIANCHAO YE, BRANDON WOOD, STANIMIR BONEV, Lawrence Livermore National Laboratory — Titanium oxide has generated interest lately as a promising anode candidate for use in lithium-ion batteries. We report first principles calculations on the mobility of lithium atoms in both crystalline and amorphous phases of titanium oxide. Density functional theory calculations of structural properties and diffusion energy barriers are combined with rate theory and a lattice gas model to study diffusion of lithium over a range of concentrations. A summary of results, including significant differences in the mobility between amorphous and crystalline phases, will be presented and discussed.

**10:00AM R52.00009 Computational modeling of the structure and the ionic conductivity of the solid electrolyte materials Li<sub>3</sub>AsS<sub>4</sub> and its Ge substitutions<sup>1</sup>**, AHMAD AL-QAWASMEH, N. A. W. HOLZWARTH, Wake Forest University — Oak Ridge National Laboratory (G. Sahu et al.)<sup>2</sup> reported that the substitution of Ge into Li<sub>3</sub>AsS<sub>4</sub> leads to the composition Li<sub>3.334</sub>Ge<sub>0.334</sub>As<sub>0.666</sub>S<sub>4</sub> with impressively high ionic conductivity. We use ab initio calculations to examine the structural relationships and the ionic conductivity mechanisms for pure Li<sub>3</sub>AsS<sub>4</sub>, Li<sub>3.334</sub>Ge<sub>0.334</sub>As<sub>0.666</sub>S<sub>4</sub>, and other compositions of these electrolytes.

<sup>1</sup>Supported by NSF grant DMR-1105485 and 1507942 and WFU's DEAC cluster.

<sup>2</sup>J. Matter. Chem. A. 2014, 2, 10396

**10:12AM R52.00010 Kinetics and Mechanism of Proton Transfer in Molten Lithium Carbonate: Insights from Static and Dynamic DFT Studies**, XUELING LEI, Benedict College, KEVIN HUANG, University of South Carolina, CHANGYONG QIN, Benedict College — Using static and dynamic DFT methods and a cluster model, the mechanism and kinetics of proton transfer in lithium molten carbonate (MC) were investigated. The migration of proton prefers an inter-carbonate pathway with an energy barrier of 8.0 kcal/mol. At TS, a linkage of O—H—O involving O 2p and H 1s orbitals is formed between two carbonate ions. It is noticeable that the solvation of proton in an ionic liquid is beyond the capacity of a simple cluster model and that the FPMD method is more suitable for such a molecular system. Corrections on the calculated energies using an extracted cluster were performed and the results displayed good consistency with the value of 7.6 kcal/mol and 7.8 kcal/mol from experiment and FPMD simulation, respectively. The calculated trajectory of H indicates that proton has a good mobility in MC, while both carbon and oxygen only move slightly to facilitate the proton migration. Small geometric variations were observed on all involved ions, not just on the local structure where the proton transfer occurs, implying a synergetic process. A better description of this synergetic step can be displayed in the Lewis diagram. Overall, the results indicate that the combination of the static and dynamic DFT methods is of great advantages in treating such ionic liquid systems and can improve the reliability of the calculated results.

**10:24AM R52.00011 A formalism for modeling solid electrolyte/electrode interfaces using first principles methods<sup>1</sup>**, NICHOLAS LEPLEY, Wake Forest Univ, NATALIE HOLZWARTH, Wake Forest University — We describe a scheme based on the interface energy for analyzing interfaces between crystalline solids, quantitatively including the effect of lattice strain. This scheme is applied to the modeling of likely interface geometries of several solid state battery materials including Li metal, Li<sub>3</sub>PO<sub>4</sub>, Li<sub>3</sub>PS<sub>4</sub>, Li<sub>2</sub>O, and Li<sub>2</sub>S. We find that all of the interfaces in this study are stable with the exception of Li<sub>3</sub>PS<sub>4</sub>/Li. For this chemically unstable interface, the partial density of states helps to identify mechanisms associated with the interface reactions. We also consider the case of charged defects at the interface, and show that accurately modeling them requires a careful treatment of the resulting electric fields. Our energetic measure of interfaces and our analysis of the band alignment between interface materials indicate multiple factors which may be predictors of interface stability, an important property of solid electrolyte systems.

<sup>1</sup>Supported by NSF Grant DMR-1105485 and DMR-1507942

**10:36AM R52.00012 Hexagonal BC<sub>3</sub> as a Robust Electrode Material for Li, Na, and K Ion Batteries<sup>1</sup>**, RAJENDRA JOSHI, Department of Physics and Science of Advanced Materials, Central Michigan University, Mount Pleasant, MI, 48859, USA, BURAK ÖZDEMİR, Science of Advanced Materials, Central Michigan University, Mount Pleasant, MI, 48859, USA, JUAN PERALTA, VERONICA BARONE, Department of Physics and Science of Advanced Materials, Central Michigan University, Mount Pleasant, MI, 48859, USA — We propose hexagonal BC<sub>3</sub> as a robust electrode material for Li, Na, and K ion batteries based on first-principles density functional theory calculations. We show that, by intercalating Li, Na, and K in BC<sub>3</sub>, it is possible to form Li<sub>1.5</sub>BC<sub>3</sub>, Na<sub>1</sub>BC<sub>3</sub>, and K<sub>1.5</sub>BC<sub>3</sub> which correspond to a high theoretical capacity of 858 mA h/g, 572 mA h/g, 858 mA h/g, respectively. In addition, this material presents small open circuit voltage variations of 0.49, 0.12, and 0.16 V when used as electrode for Li, Na, and K ion batteries, respectively.

<sup>1</sup>NSF CBET-1335944, NSF DMR-0906617, DOE DE-FG02-10ER16203

**10:48AM R52.00013 Computational Investigation of Chevrel Phase Cathodes for Ca<sup>2+</sup> Ion Batteries**, MANUEL SMEU, Binghamton University - SUNY — While batteries employing Li ions are best suited for applications where portability is important, less expensive alternatives may be employed when size and weight are less critical. Batteries utilizing Ca ions have received very little attention to date due to difficulties in identifying adequate anode materials and electrolytes, although advancements have been made on both fronts. If these challenges can be overcome, Ca can offer an abundant and affordable alternative to Li for grid storage and in other applications where portability is not a priority. For such technologies, appropriate cathodes need to be identified that will allow for reversible intercalation of Ca<sup>2+</sup> ions and that can provide a desirable voltage. To this end, we investigate the Chevrel phase (CP) compounds Mo<sub>6</sub>X<sub>8</sub> (X = S, Se, Te), which can intercalate Mg<sup>2+</sup> and Ca<sup>2+</sup>, among many other ions. We use density functional theory (DFT) to calculate the voltage profiles of various guest intercalation ions (Mg, Ca, Sr, Ba) in the CP material. The electronic properties of this material will be discussed, along with the capacity and the energetics associated with ions diffusing through the CP structure. This work also offers insights into how the cathode properties may be fine-tuned by carefully selecting its constituents.

**11:00AM R52.00014 Investigation of ionic transport in sodium scandium phosphate (NSP) and related compounds**, KAUSTUBH BHAT, STEFAN BLÜGEL, HANS LUSTFELD, Peter Grünberg Institut (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany — Sodium ionic conductors offer significant advantages for application in large scale energy storage systems. In this study, we investigate the different pathways available for sodium ion conduction in NSP and calculate energy barriers for ionic transport using Density Functional Theory (DFT) and the Nudged Elastic Band Method [2]. We identify the structural parameters that reduce the energy barrier, by calculating the influence of positive and negative external pressure on the energy barrier [3]. Lattice strain can be introduced by cation or anion substitution within the NASICON structure. We substitute the scandium atom with other trivalent atoms such as aluminium and yttrium, and calculate the resulting energy barriers. Sodium thiophosphate ( $Na_3PS_4$ ) has previously shown about two orders of magnitude higher ionic conductivity than sodium phosphate ( $Na_3PO_4$ ) [4]. We investigate the effect of substituting oxygen with sulphur in NSP. We acknowledge discussions with our experimental colleagues F. Tietz and M. Guin toward this work. [1] Hong, MRB **11**, 173-182 (1976). [2] Henkelman et al. JCP **113**, 9901-9904 (2000). [3] Hirschfeld et al. PRB **84**, 224308 (2011). [4] Hayashi et al. Nat. Comm. **3**, 856 (2012).

**11:12AM R52.00015 Effects on the optical properties of titanium dioxide by doping with sulfur**, JORGE HERNANDEZ ZELEDON, JAMES LEWIS, West Virginia University —  $TiO_2$  is an attractive material for photocatalytic and photovoltaic applications like water splitting or self cleaning surfaces, but its maximum absorption happens around 4 eV, and the sunlight irradiance peak is between 1.5eV and 3.1eV. In this work we look for the effects of doping  $TiO_2$  with sulfur, as one way to reduce the gap between the conduction and the valence states, in order to increase the efficiency of Sun light absorption. To modify the optic properties we took the  $TiO_2$  rutile structure as basis for random substitutions, in which we randomly select some oxygen atoms and we replace them with sulfur, making  $TiO_2(1-x)S_2x$  for  $x = 0.1$  and  $x = 0.25$ . Here we present our results for the computational calculations of the band gap and absorption as function of concentration. All the process and calculations are made using the FIREBALL software.

**Thursday, March 17, 2016 8:00AM - 11:00AM –**  
**Session R53 FEd FIAP: Building New Pathways in Physics Innovation and Entrepreneurship Education** Hilton Baltimore Holiday Ballroom 4 - Job Ganem, Loyola University Maryland

**8:00AM R53.00001 Tinker, Thinker, Maker and CEO: Reimagining the Physics Student as Engineer, Inventor, and Entrepreneur**, CRYSTAL BAILEY, American Physical Society — Physics degree holders are among the most employable in the world, often doing everything from managing a research lab at a multi-million dollar corporation, to developing solutions to global problems in their own small startups. Employers know that with a physics training, a potential hire has acquired a broad problem-solving skill set that translates to almost any environment, as well as an ability to be self-guided and -motivated so that they can learn whatever skills are needed to successfully achieve their goals. Therefore it's no surprise that the majority of physics graduates find employment in private sector, industrial settings. Yet at the same time, only about 25% of graduating PhDs will take a permanent faculty position—while academic careers are usually the only track to which students are exposed while earning their degrees. In this talk, I will examine the role of physicist as innovator and how this role intersects with other similar STEM disciplines (such as engineering), and provide some insight into how implementing physics innovation and entrepreneurship (PIE) education will benefit both physics departments and the students they serve, regardless of students' eventual career choices. Additionally, I will provide resources to help faculty mentors give their students better information and training for a broader scope of career possibilities, and information about how educators can get involved in the growing community of PIE educators.

**8:36AM R53.00002 Impact of the Joint Task Force on Undergraduate Physics Programs for Innovation and Entrepreneurship Education in Physics**, DOUGLAS ARION, Carthage College and Galileoscope LLC — The Joint Task Force on Undergraduate Physics Programs has worked diligently to develop recommendations for what physics programs could and should be doing to prepare graduates for 21st century careers. While the 'traditional' physics curriculum has served for many years, the demands of the new workforce, and the recognition that only a few percent of physics students actually become faculty - the vast majority entering the workforce and applying their skills to a very diverse range of problems, projects, and products - implies that a review of the education undergraduates receives is in order. The outcomes of this study point to the need to provide greater connection between the education process and the actual skills, knowledge, and abilities that the workplace demands. This presentation will summarize these considerations, and show how entrepreneurship and innovation programs and curricula are a particularly effective means of bringing these elements to physics students.

**9:12AM R53.00003 Introducing a Framework for Physics Innovation and Entrepreneurship (PIE) Education.**<sup>1</sup>, BAHRAM ROUGHANI, Loyola University Maryland — A desired outcome for Physics Innovation and Entrepreneurship (PIE) education is preparing physics majors with an innovative and entrepreneurial mindset who are capable of opportunity recognition and adept in leveraging physics knowledge to address specific needs. Physics as a discipline is well-recognized to prepare students who become problem solvers and critical thinkers, gifted in dealing with abstract ideas and ambiguities in the context of complex and real-world problems. These characteristics when enhanced through appropriate combinations of curricular, co-curricular, and extra-curricular programs can prepare physics majors for careers and future challenges that may involve translating physics knowledge into useful products and services either as part of a technical team within an organization or through startups. A viable PIE education model prepares graduates for various career paths in addition to the traditional options such as pursuing graduate studies or becoming a science teacher. Having a well-defined "third option" for physics will benefit the robustness of the physics discipline through recruitment and retention of prospective students who in principle are interested in physics as a subject, but in practice they may overlook physics as their preferred major primarily because they are uncertain about a viable career path based on an undergraduate physics education.

<sup>1</sup>The "Pathways to Innovation" at Loyola is established based on the program developed by VentureWell and Epicenter (NSF Supported).

**9:48AM R53.00004 Resources to Support Physicists as Versatile and Progressive Innovators**, RANDALL TAGG, University of Colorado Denver — Physicists are trained first with broad fundamental knowledge and then through experience with exquisitely refined and specialized models and instrumentation. This is a superb platform from which to address real-world problems when it is augmented by ready access to additional practical resources. We have explored a systematic three-part approach to providing those resources: (1) creating an organized environment that stockpiles technical artifacts, tools, and instruments; (2) developing curriculum for on-demand learning of new technical competencies; (3) providing a community of like-minded physicists who enjoy connecting physics with innovation. For physicists early in their training or careers, we hope that this is a particularly attractive basis for exploring a wider range of professional options.

**10:24AM R53.00005 Lessons Learned in Student Venture Creation** , EDWARD CANER, Case Western Reserve University — The Physics Entrepreneurship Master's Program (PEP) at Case Western Reserve University is now in its 15th year of operation. PEP is a 27 credit-hour Master of Science in Physics, Entrepreneurship Track. The curriculum can be tailored to the needs of each student. Coursework consists of graduate-level classes in science, business, intellectual property law, and innovation. A master's thesis is required that is based on a real-world project in innovation or entrepreneurship within an existing company or startup (possibly the student's). PEP faculty help students connect with mentors, advisors, partners, funding sources and job opportunities. In this talk I will chronicle several pitfalls that we have encountered with our "real world" student projects and start-up businesses, several of which met their complete demise despite showing great promise for success. I will discuss how we have learned to avoid most of these pitfalls by taking surprisingly simple actions.

**10:36AM R53.00006 Advancing Successful Physics Majors - The Physics First Year Seminar Experience.** , JASON DEIBEL<sup>1</sup>, DOUGLAS PETKIE<sup>2</sup>, Wright State University — In 2012, the Wright State University physics curriculum introduced a new year-long seminar course required for all new physics majors. The goal of this course is to improve student retention and success via building a community of physics majors and provide them with the skills, mindset, and advising necessary to successfully complete a degree and transition to the next part of their careers. This new course sequence assembles a new cohort of majors annually. To prepare each cohort, students engage in a variety of activities that span from student success skills to more specific physics content while building an entrepreneurial mindset. Students participate in activities including study skills, career night, course planning, campus services, and a department social function. More importantly, students gain exposure to programming, literature searches, data analysis, technical writing, elevator pitches, and experimental design via hands-on projects. This includes the students proposing, designing, and conducting their own experiments. Preliminary evidence indicates increased retention, student success, and an enhanced sense of community among physics undergraduate students. The overall number of majors and students eventually completing their physics degrees has nearly tripled.

<sup>1</sup>Associate Professor, Department of Physics

<sup>2</sup>Chair, Department of Physics

**10:48AM R53.00007 Towson University's Professional Science Master's Program in Applied Physics: The first 5 years<sup>1</sup>** , RAJESWARI KOLAGANI, Towson University — It is a well-established fact that the scientific knowledge and skills acquired in the process of obtaining a degree in physics meet the needs of a variety of positions in multiple science and technology sectors. However, in addition to scientific competence, challenging careers often call for skills in advanced communication, leadership and team functions. The professional science master's degree, which has been nick-named as the 'Science MBA', aims at providing science graduates an edge both in terms of employability and earning levels by imparting such skills. Our Professional Science Master's Program in Applied Physics is designed to develop these 'plus' skills through multiple avenues. In addition to advanced courses in Applied Physics, the curriculum includes graduate courses in project management, business and technical writing, together with research and internship components. I will discuss our experience and lessons learned over the 5 years since the inception of the program in 2010.

<sup>1</sup>The author acknowledges support from the Elkins Professorship of the University System of Maryland

**Thursday, March 17, 2016 8:00AM - 11:00AM —**  
**Session R55 FPS DBIO: The War on Cancer: Physics Enters the Fray** Hilton Baltimore Holiday Ballroom  
6 - Arian Pregoner, Sandia National Laboratories

**8:00AM R55.00001 Why is Physics Important to Cancer Research?** , ANNA D. BARKER, Director, Transformative Healthcare Networks — Cancer is increasingly described as a "disease of the genes", and while the genome (in fact all of the omes) are important information molecules that drive aspects of the initiation and progression of cancer, they are far from the whole story. Cancer is an extraordinarily complex system (in fact a complex of systems) that occurs in three-dimensional space, across multiple scales and often over extended periods of time. The most challenging issues that plague the cancer field such as metastasis, cellular heterogeneity and resistance to therapy are in large part more rationally explained in the context of the physics of these systems vs. genomics. For example, the biology of metastasis has been studied extensively for decades with little progress. Metastatic disease depends on cells acquiring (or expressing innate information) new properties that enable and sustain their ability to migrate to distant sites. Developing a fundamental understanding of key cancer processes ranging from metastasis to immunotherapeutic responses requires that physicists (and mathematicians and engineers) be integrated into a new generation of cancer research period! The presentation will focus on those areas where physics is essential and the hows and whos of achieving the integration required.

**8:36AM R55.00002 Evolution, Physics, and Cancer: Disrupting Traditional Approaches** , ROBERT AUSTIN, Princeton University — Physicists who were recruited to try and assist with the stubbornly constant mortality rates of cancer world-wide over the past 100 years have basically had the invitation withdrawn by the oncology community. The oncologists became annoyed with the independence of thought and the skepticism of some physicists with continuation of the present paradigm of the cancer genome as the rosette stone as the key to cancer. To quote a recent letter in Physics Today: "Curing cancer is a complex biological problem to be solved by biologists". Apparently our mission as minions is to be high-level technicians. But I think that is wrong and will lead to continuation of the string of failures and deceptions foisted on the public at large by the Medical Industrial Complex. I think we really need to re-think cancer as a phenomena which is driven by evolution and may be desired by the organism and be a product of both the aging of the proteome and the genome. Further, searching for mutations (The Cancer Genome) may be completely the wrong direction, searching for protected genes may be as important as looking for mutated genes. I'll try to present the case that physicists should not have been kicked out of the Medical Industrial Complex that keeps the cancer business humming and profitable.

**9:12AM R55.00003 Theoretical Physics and Cancer Research** , KRISTIAN B. BLAGOEV, Physics Div., National Science Foundation, Arlington, VA and Dept., of Biophysics, Johns Hopkins University, Baltimore, MD — Cancer is a multifaceted disease which involves profound disruptions to biological mechanisms and structures that have evolved since the beginning of life. The most dramatic change is the failure of multicellularity and organ homeostasis. Time and time again, this complex disease has evaded the silver bullet cure attempts that rely on simple strategies including targeting dividing cells with broad acting chemotherapies, using radiation to cause DNA damage, and using molecular targeting agents. Even the most recent efforts, such as using immune stimulating agents and activated immune cells, are missing the mark. Against all these efforts, the cancer, even if it retreats, usually returns and often then does not respond to any of our available arsenal. The origin of this persistence is the robustness of life itself. During the past 4 billion years, life has survived many dramatic events and living organisms can be found in the most hostile places on Earth. Based on my research and on analysis of outcomes from several meetings between physicists and cancer researchers, organized by the National Science Foundation, I will argue that we need to integrate theoretical physics approaches to understand the emergence of resistance to treatment and to develop robust and curative interventions in cancer. The adaptive response of living systems to external and internal changes involve many interacting parts and networks. Phenomenological and reductionist approaches must be used synergistically to understand the phenomena at the appropriate spatial and temporal scales. This approach has been successful in understanding inanimate matter in the Universe and should be used in understanding animate matter as well and in particular cancer. I will also argue that public-private partnerships can speed up the process and bring innovation to transform the field.

**9:48AM R55.00004 Information, Physics, and Cancer** , CHRIS ADAMI, Michigan State University — Many researchers have doubts that a "theory of cancer" can exist, given the fact that there are so many different cancer phenotypes. However, such a situation—many significantly different manifestations of an underlying law—is not at all uncommon in physics. I argue that a unified cause for all forms of cancer is possible, but that such a theory must be cast in terms of information and communication theory. I briefly revisit key concepts of that theory, then discuss possible applications to communication in game theory that could lead us to view cancer as a disease that, at its root, is a cellular failure to properly communicate.

**10:24AM R55.00005 The National Cancer Institute's Physical Sciences - Oncology Network** , MICHAEL GRAHAM ESPEY, National Cancer Institute — In 2009, the NCI launched the Physical Sciences - Oncology Centers (PS-OC) initiative with 12 Centers (U54) funded through 2014. The current phase of the Program includes U54 funded Centers with the added feature of soliciting new Physical Science - Oncology Projects (PS-OP) U01 grant applications through 2017; see NCI PAR-15-021. The PS-OPs, individually and along with other PS-OPs and the Physical Sciences-Oncology Centers (PS-OCs), comprise the Physical Sciences-Oncology Network (PS-ON). The foundation of the Physical Sciences-Oncology initiative is a high-risk, high-reward program that promotes a 'physical sciences perspective' of cancer and fosters the convergence of physical science and cancer research by forming transdisciplinary teams of physical scientists (e.g., physicists, mathematicians, chemists, engineers, computer scientists) and cancer researchers (e.g., cancer biologists, oncologists, pathologists) who work closely together to advance our understanding of cancer. The collaborative PS-ON structure catalyzes transformative science through increased exchange of people, ideas, and approaches. PS-ON resources are leveraged to fund Trans-Network pilot projects to enable synergy and cross-testing of experimental and/or theoretical concepts. This session will include a brief PS-ON overview followed by a strategic discussion with the APS community to exchange perspectives on the progression of trans-disciplinary physical sciences in cancer research.

**Thursday, March 17, 2016 11:15AM - 2:15PM —**  
**Session S1 DCMP: Topological Mysteries in Kondo Insulating SmB<sub>6</sub>** Ballroom I - Lu Li, University of Michigan

**11:15AM S1.00001 Topologically protected surface states in SmB<sub>6</sub>** , JING XIA, University of California, Irvine — No abstract available.

**11:51AM S1.00002 Two-dimensional Fermi surfaces in Kondo insulating SmB<sub>6</sub>** , GANG LI, University of Michigan — There has been renewed interest in Samarium Hexaboride, which is a strongly correlated heavy Fermion material. Hybridization between itinerant electrons and localized orbitals lead to an opening of charge gap at low temperature. However, the resistivity of SmB<sub>6</sub> does not diverge at low temperature. Former studies suggested that this residual conductance is contributed by various origins. Recent theoretical developments suggest that the particular symmetry of energy bands of SmB<sub>6</sub> may host a topologically non-trivial surface state, i.e., a topological Kondo insulator. To probe the Fermiology of the possible metallic surface state, we use sensitive torque magnetometry to detect the de Haas van Alphen (dHvA) effect due to Landau level quantization on flux-grown crystals, down to He-3 temperature and up to 45 Tesla. Our angular and temperature dependent data suggest two-dimensional Fermi Surfaces lie in both crystalline (001) and (101) surface planes of SmB<sub>6</sub>.

**12:27PM S1.00003 Unconventional bulk three-dimensional Fermi surface in Kondo insulating SmB<sub>6</sub>** , BENG TAN, University of Cambridge — We report the observation of a paradoxical insulator with a bulk state which is electrically insulating and simultaneously yields quantum oscillations typical of good metals. We present high field measurements of conductivity and magnetic torque in high purity single crystals of the Kondo insulator SmB<sub>6</sub> which reveal an activated behavior characteristics of an insulator with an energy gap at the Fermi energy in the former and quantum oscillation of frequencies characteristics of a large three-dimensional conduction electron Fermi surface similar to the metallic rare earth hexaborides such as PrB<sub>6</sub> and LaB<sub>6</sub> in the latter. The quantum oscillations observed in the magnetic torque measurements are characteristic of an unconventional Fermi liquid – the amplitude strongly increases at low temperatures in a stark contrast to the saturating Lifshitz-Kosevich behavior in conventional metallic states.

**1:03PM S1.00004 Neutron scattering from the Kondo Insulator SmB<sub>6</sub>**<sup>1</sup> , COLLIN BROHOLM, Johns Hopkins University — A review of neutron scattering work probing the Kondo insulator SmB<sub>6</sub> is presented with special emphasis on assessing the topology of the underlying strongly renormalized band structure. A 14 meV excitation dominates the spectrum and is evidence of strong electron correlations [1]. Though the data generally supports the proposal that SmB<sub>6</sub> is a topological Kondo insulator, specific heat and high-resolution neutron scattering data show a continuum of states well below the bulk transport gap, which enrich the problem and may connect to the recent surprising de Haas van Alphen results.

[1] Interaction Driven Subgap Spin Exciton in the Kondo Insulator SmB<sub>6</sub>, W.?T. Fuhrman, J. Leiner, P. Nikolic, G.?E. Granroth, M.?B. Stone, M.?D. Lumsden, L. DeBeer-Schmitt, P.?A. Alekseev, J.-M. Mignot, S.?M. Koohpayeh, P. Cottingham, W. Adam Phelan, L. Schoop, T.?M. McQueen, and C. Broholm, Phys. Rev. Lett. **114**, 036401 (2015).

<sup>1</sup>Supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Material Sciences and Engineering, under Grant No. DEFG02-08ER46544 and the Gordon and Betty Moore Foundation.

**1:39PM S1.00005 Kondo Breakdown and Quantum Oscillations in SmB<sub>6</sub>**<sup>1</sup> , ONUR ERTEN, Rutgers University — Motivated by the observation of light surface states of SmB<sub>6</sub>, I will discuss the effects of surface Kondo breakdown in topological Kondo insulators, in particular SmB<sub>6</sub>. I will present both numerical and analytic results which show that the decoupling of the localized moments at the surface disturbs the compensation between light and heavy electrons and dopes the Dirac cone. Dispersion of these uncompensated surface states are dominated by inter-site hopping, which leads to much lighter quasiparticles in accordance with ARPES experiments [1]. Another tantalizing result about SmB<sub>6</sub> comes from the recent quantum oscillation experiments which lead to completely controversial interpretations. I will discuss a general theoretical viewpoint considering both bulk and surface scenarios and our new interpretation in terms of Kondo breakdown in topological surface states [2]. [1] V. Alexandrov, P. Coleman, O. Erten, Phys. Rev. Lett. **114**, 177202 (2015) [2] O. Erten, P. Ghaemi, P. Coleman arXiv: 1510.02313 (2015)

<sup>1</sup>Work supported by Department of Energy grant DE-FG02- 99ER45790

**Thursday, March 17, 2016 11:15AM - 2:15PM —**  
**Session S2 GSOFD DFD: Rheology of Dense Particulate Media** Ballroom II - Ted Brzinski, North Carolina State University

**11:15AM S2.00001 Flow of colloidal suspensions and gels<sup>1</sup>**, ROSEANNA ZIA, Cornell University — Our recent studies of yield of colloidal gels under shear show that yield in such gels occurs in distinct stages. Under fixed stress, yield follows a finite delay period of slow solid-like creep. Post yield, the gel fluidizes and may undergo long-time viscous flow or, in some cases, may re-solidify. Under imposed strain rate, the transition from equilibrium to long-time flow is characterized by one or more stress overshoots, signifying a yield process here as well. These rheological changes are accompanied by evolution in morphology and dynamics of the gel network. Similar regimes have been observed in gels subjected to gravitational forcing; the gel initially supports its own weight, or perhaps undergoes slow, weak compaction. This may be followed by a sudden transition to rapid compaction or sedimentation. Various models have been put forth to explain these behaviors based on structural evolution, but this detail is difficult to observe in experiment. Here we examine the detailed microstructural evolution and rheology of reversible colloidal gels as they deform under gravity, identifying the critical buoyant force at which yield occurs, the role played by ongoing gel coarsening, and similarities and differences compared to yield under shear.

<sup>1</sup>We gratefully acknowledge the support of the NSF XSEDE Computational Resource, the NSF Early CAREER Program, and the Office of Naval Research Young Investigator Program.

**11:51AM S2.00002 A unified description of the rheology of hard particles**, MICHEL HERMES, University of Edinburgh — No abstract available.

**12:27PM S2.00003 Linking Microstructural Changes to Bulk Behavior in Shear Disordered Matter<sup>1</sup>**, DANIEL BLAIR, Georgetown University — Soft and biological materials often exhibit disordered and heterogeneous microstructure. In most cases, the transmission and distribution of stresses through these complex materials reflects their inherent heterogeneity. Through the combination of rheology and 4D imaging we can directly alter and quantify the connection between microstructure and local stresses. We subject soft and biological materials to precise shear deformations while measuring real space information about the distribution and redistribution of the applied stress. In this talk, I will focus on the flow behavior of two distinct but related disordered materials; a flowing compressed emulsion above its yield stress and a strained collagen network. In the emulsion system, I will present experimental and computational results on the dynamical response, at the level of individual droplets, that directly links the particle motion and deformation to the rheology. I will also present results that utilize boundary stress microscopy to quantify the spatial distribution of surface stresses that arise from sheared in-vitro collagen networks. I will outline our main conclusions which is that the strain stiffening behavior observed in collagen networks can be parameterized by a single characteristic strain and associated stress. This characteristic rheological signature seems to describe both the strain stiffening regime and network yielding.

<sup>1</sup>NSF DMR: 0847490

**1:03PM S2.00004 Nonlinear and nonlocal rheology of jammed matter**, BRIAN TIGHE, TU Delft — Emulsions, foams, and grains all jam into a weakly elastic state when confined by pressure. By now the mechanics of jammed matter is well understood in the case of slow, weak, and homogeneous forcing – but in reality, it is rare for all three of these assumptions to hold. Here we demonstrate the complex rheology that results when jammed materials are forced at finite rate, finite amplitude, and finite wavelength. Using computer simulations, we subject dense soft sphere packings to a host of rheological tests, including stress relaxation, flow start-up, oscillatory shear, and standing wave forcing. These allow us to tease apart the influence of viscous, nonlinear, and nonlocal effects, and also to probe the link between particle dynamics and bulk response. We identify strain, time, and length scales that depend critically on the distance to the jamming transition, and which govern the onset of shear thinning, strain softening, and gradient elasticity.

**1:39PM S2.00005 Effects of confinement on nanoparticle flows<sup>1</sup>**, JACINTA CONRAD, University of Houston — The transport properties of nanoparticles that are dispersed in complex fluids and flowed through narrow confining geometries affect a wide range of materials shaping and forming processes, including three-dimensional printing and nanocomposite processing. Here, I will describe two sets of experiments in which we use optical microscopy to probe the structure and transport properties of suspensions of particles that are confined geometrically. First, we investigate the structure and flow properties of dense suspensions of submicron particles, in which the particles interact via an entropic depletion attraction, that are confined in thin films and microchannels. Second, we characterize the transport properties of nanoparticles, dispersed at low concentration in water or in aqueous solutions of high-molecular weight polymers, that are confined in regular arrays of nanoposts or in disordered porous media. I will discuss our results and their practical implications for materials processing as well as for other applications that require confined transport of nanomaterials through complex media.

<sup>1</sup>Welch Foundation (E-1869) and NSF (CBET-1438204)

**Thursday, March 17, 2016 11:15AM - 2:15PM –**  
**Session S3 DMP: Towards Design of Correlated Electron Materials** Ballroom III - Laura H. Greene, Florida State University, NHMFL

**11:15AM S3.00001 Spin-Orbit Coupling, Strong Interactions, and Topological Character<sup>1</sup>**, WARREN E. PICKETT, University of California Davis — In recent years the electronic structure of crystalline solids has come under close scrutiny because of the various types of topological characters that may arise. Most of the work is done at the one-electron (non-interacting) level, and most innovations have arisen from model tight-binding Hamiltonians and their eigenvectors. This talk will focus on a few examples of *discoveries made computationally* through DFT studies of actual materials, thus providing a physical realization as the discovery was made. Competition and partnership between strong interactions and spin-orbit coupling will be emphasized. Examples will include (1) the 'semi-Dirac' point Fermi surface phase in VO<sub>2</sub> thin films, the first member of a class now called *multi Weyl*: massive in some direction, massless in other direction; (2) a nodal loop semimetal phase found in computational studies of thin SrVO<sub>3</sub> films, realized more recently in NbP etc.; (3) the buckled honeycomb lattice of a (111) bilayer of LaMnO<sub>3</sub> encased on LaAlO<sub>3</sub>, which is a Chern insulator and may be a realization of the Weyl-Mott insulator proposed recently by Morimoto and Nagaosa. Acknowledgments: R. Pentcheva, V. Pardo, K.-W. Lee, S. Gangopadhyay.

<sup>1</sup>DOE Grant DE-FG02-04ER46111

**11:51AM S3.00002 Towards prediction of correlated material properties using quantum Monte Carlo methods**, LUCAS WAGNER, Univ of Illinois - Urbana — Correlated electron systems offer a richness of physics far beyond noninteracting systems. If we would like to pursue the dream of designer correlated materials, or, even to set a more modest goal, to explain in detail the properties and effective physics of known materials, then accurate simulation methods are required. Using modern computational resources, quantum Monte Carlo (QMC) techniques offer a way to directly simulate electron correlations. I will show some recent results on a few extremely challenging materials including the metal-insulator transition of VO<sub>2</sub>, the ground state of the doped cuprates, and the pressure dependence of magnetic properties in FeSe. By using a relatively simple implementation of QMC, at least some properties of these materials can be described truly from first principles, without any adjustable parameters. Using the QMC platform, we have developed a way of systematically deriving effective lattice models from the simulation. This procedure is particularly attractive for correlated electron systems because the QMC methods treat the one-body and many-body components of the wave function and Hamiltonian on completely equal footing. I will show some examples of using this downfolding technique and the high accuracy of QMC to connect our intuitive ideas about interacting electron systems with high fidelity simulations. The work in this presentation was supported in part by NSF DMR 1206242, the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research, Scientific Discovery through Advanced Computing (SciDAC) program under Award Number FG02-12ER46875, and the Center for Emergent Superconductivity, Department of Energy Frontier Research Center under Grant No. DEAC0298CH1088. Computing resources were provided by a Blue Waters Illinois grant and INCITE PhotSuper and SuperMatSim allocations.

**12:27PM S3.00003 Towards the design of novel cuprate-based superconductors**, CHUCK-HOU YEE, Rutgers Univ — The rapid maturation of materials databases combined with recent development of theories seeking to quantitatively link chemical properties to superconductivity in the cuprates provide the context to design novel superconductors. In this talk, we describe a framework designed to search for new superconductors, which combines chemical rules-of-thumb, insights of transition temperatures from dynamical mean-field theory, first-principles electronic structure tools, materials databases and structure prediction via evolutionary algorithms. We apply the framework to design a family of copper oxysulfides and evaluate the prospects of superconductivity.

**1:03PM S3.00004 Itinerant magnetism without magnetic elements<sup>1</sup>**, EMILIA MOROSAN, Rice University — The origin of magnetism in metals has been traditionally discussed in two diametrically opposite limits: itinerant and local moments. Surprisingly, there are very few known examples of materials that are close to the itinerant limit, and their properties are not universally understood. In the case of the two such examples discovered several decades ago, both itinerant ferromagnets (IFMs) ZrZn<sub>2</sub> and Sc<sub>3</sub>In, the understanding of their magnetic ground states draws on the existence of 3d electrons subject to strong spin fluctuations. In this talk I will contrast the physical properties of these two IFMs without magnetic elements with those of the recently discovered first itinerant antiferromagnetic (IAFM) metal with no magnetic constituents, TiAu. The IFMs have surprisingly different properties, with ZrZn<sub>2</sub> showing signatures of mean field, Fermi liquid behavior, while the Sc<sub>3</sub>In compound is characterized by non-mean field magnetization exponents, and displays non fermi liquid behavior in both the FM and the paramagnetic states. The IAFM TiAu orders below a Neel temperature  $T_N \approx K$ , about an order of magnitude smaller than in the IAFM Cr, rendering the spin fluctuations in TiAu more important at low temperatures. Like in the two IFMs, doping induces a quantum phase transition in TiAu, and the quantum critical behavior in all three systems is discussed and compared.

<sup>1</sup>This work is supported by NSF DMR-1506704.

**1:39PM S3.00005 In situ measurements of high temperature growth of correlated systems: a materials by design scheme<sup>1</sup>**, HUA HE<sup>2</sup>, Department of Physics & Astronomy, Texas A & M University — There is great interest in developing new ways to use predictive theory to accelerate materials synthesis. We have previously shown that DFT+DMFT electronic structure calculations are successful at predicting gaps and ordered moments, even when correlations are very strong.<sup>[1,2]</sup> Building on these results, we set out to explore an even closer integration of theory and synthesis, aiming to discover new routes for doping Mott insulators and producing new superconductors. In situ high temperature high energy X-ray diffraction is used to determine the crystal structures of compounds just as they form from the growths, and the structural information is used as input for DFT+DMFT calculations that predict functionality, closing the synthesis loop by suggesting productive new directions. Using this approach, we have investigated the transition metal oxysulfide system Ba-Co-S-O and successfully discovered the new compound BaCoSO, and identified it as an interesting small gap Mott insulator by DFT+DMFT calculations even before any traditional crystal growth is attempted in the lab. [1] J. W. Simonson, et al. Proc. Nat. Acad. Sci. 109 (2012) E1815 [2] J. Guo, et al. Nat. Sci. Rep. 3 (2013) 2555

<sup>1</sup>We acknowledge the Office of Assistant Secretary of Defense for Research and Engineering for providing the NSSEFF funds that supported this research.  
<sup>2</sup>Work performed in collaboration with D. E. McNally (Stony Brook Univ.), J. Simonson (Farmingdale State College), G. Kotliar (Rutgers Univ.), S. Ghose, E. Doorhyee (BNL), K. W. Post, D. N. Basov (UCSD), M. C. Aronson (TAMU)

## Thursday, March 17, 2016 11:15AM - 2:15PM —

Session S4 GQI DCMP: Quantum Dot-Cavity Hybrid Systems Ballroom IV - Guido Burkard, University of Konstanz

**11:15AM S4.00001 Probing light-matter interactions at the level of single photons and electrons<sup>1</sup>**, JASON R. PETTA, Department of Physics, Princeton University — Pioneering experiments by Fujisawa *et al.* examined the detuning dependence of the current in semiconductor double quantum dots (DQDs) and highlighted the important role of electron-phonon coupling in inelastic transport.<sup>1</sup> Later experiments by the same group directly measured orbital relaxations rates, which were consistent with a phonon-mediated relaxation process.<sup>2</sup> By placing semiconductor DQDs inside of high quality factor microwave cavities it is now feasible to achieve charge-cavity coupling rates that are comparable to the phonon emission rate. I will describe recent experiments that examine masing in cavity-coupled semiconductor DQDs. The application of a source-drain bias results in single electron tunneling and population inversion. The interdot tunneling process generates photons and leads to gain in the cavity transmission. We measure the detuning dependence of the gain and find that the gain feature is very broad compared to the cavity linewidth. Recent theory accounts for the broad gain feature by considering a second-order process that involves the simultaneous emission of a cavity photon and a phonon.<sup>3</sup> With sufficient cavity driving, it is feasible to achieve above-threshold maser action, which is verified by comparing the statistics of the emitted microwave field above and below the maser threshold.<sup>4</sup>

### References

1. T. Fujisawa *et al.*, Science **282**, 932 (1998).
2. T. Fujisawa *et al.*, Nature **419**, 278 (2002).
3. M. J. Gullans *et al.*, Phys. Rev. Lett. **114**, 196802 (2015).
4. Y.-Y. Liu *et al.*, Science **347**, 285 (2015).

<sup>1</sup>In collaboration with Y.-Y. Liu, J. Stehlik, C. Eichler, M. J. Gullans, and J. M. Taylor. Supported by the Packard Foundation, the NSF (DMR-1409556 and DMR-1420541), and the Gordon and Betty Moore Foundation's EPiQS Initiative through Grant No. GBMF4535.

**11:51AM S4.00002 Strongly Coupled Quantum Dot-Nanocavity Systems** , JELENA VUCKOVIC, Stanford University — No abstract available.

**12:27PM S4.00003 Theory of strongly driven cavity coupled quantum dots: from micromasers to BECs of light** , MICHAEL GULLANS, NIST - Natl Inst of Stds & Tech — Embedding a double quantum dot (DQD) in a low loss microwave resonator results in a large electric dipole interaction between the charge states of the DQD and single microwave photons in the resonator. In the regime of a few electrons and photons, this system is reminiscent of well-known models of cavity quantum electrodynamics from atomic physics; however, there are important deviations due to the strong coupling of the DQD to the electronic reservoirs in the leads, as well as phonons in the lattice. In this talk, we explore how external control and driving of this unique hybrid system can be used to induce non-equilibrium states of light in the resonator.

**1:03PM S4.00004 Cavity quantum electrodynamics with carbon nanotube quantum dots** , TAKIS KONTOS, Laboratoire Pierre Aigrain, Ecole Normale Supérieure, CNRS — Cavity quantum electrodynamics techniques have turned out to be instrumental to probe or manipulate the electronic states of nanoscale circuits. Recently, cavity QED architectures have been extended to quantum dot circuits. These circuits are appealing since other degrees of freedom than the traditional ones (e.g. those of superconducting circuits) can be investigated. I will show how one can use carbon nanotube based quantum dots in that context. In particular, I will focus on the coherent coupling of a single spin [1] or non-local Cooper pairs to cavity photons. Quantum dots also exhibit a wide variety of many body phenomena. The cQED architecture could also be instrumental for understanding them. One of the most paradigmatic phenomenon is the Kondo effect which is at the heart of many electron correlation effects. I will show that a cQED architecture has allowed us to observe the decoupling of spin and charge excitations in a Kondo system. [1] J. J. Viennot, M.C. Dartailh, A. Cottet and T. Kontos Science 349 408 (2015).

**1:39PM S4.00005 Microwave emission from double quantum dots into cavities** , ANDREAS WALLRAFF, ETH - Zurich — No abstract available.

**Thursday, March 17, 2016 11:15AM - 2:15PM —**  
**Session S5 DMP: New Fe-based Superconductors and Related Materials I** 301 - Fazel Tafti, Princeton University

**11:15AM S5.00001 Coexistence of superconductivity and antiferromagnetism in  $(\text{Li}_{0.8}\text{Fe}_{0.2})\text{OHFeSe}$**  , XIANHUI CHEN, Hefei National Laboratory for Physical Sciences at Microscale and Department of Physics, University of Science and Technology of China, Hefei, Anhui — In this talk, we report the synthesis of an air-stable material,  $(\text{Li}_{0.8}\text{Fe}_{0.2})\text{OHFeSe}$ , which shows superconducting transition temperature up to  $T_c \sim 40$  K, by means of a novel hydrothermal method [1]. The crystal structure is unambiguously determined by a combination of X-ray and neutron powder diffraction and nuclear magnetic resonance. Moreover, antiferromagnetic order is found to coexist with superconductivity. We also grew single crystals of  $(\text{Li,Fe})\text{OHFeSe}$ , and observed a first-order transition from superconductor to AFM insulator with a strong charge doping induced by ionic gating in the thin flakes of single crystal [2].  $T_c$  is continuously enhanced with electron doping by ionic gating up to a maximum  $T_c$  of 43 K, and a striking superconductor-insulator transition occurs just at the verge of optimal doping with highest  $T_c$ . A novel phase diagram of temperature-gating voltage with the superconductor-insulator transition is mapped out, indicating that the superconductor-insulator transition is a common feature for unconventional superconductivity. References: [1] X. F. Lu, N. Z. Wang, H. Wu, Y. P. Wu, D. Zhao, X. Z. Zeng, X. G. Luo, T. Wu, W. Bao, G. H. Zhang, F. W. Huang, Q. Z. Huang, X. H. Chen, Nature Mater. **14**, 352 (2015). [2] B. Lei, Z. J. Xiang, X. F. Lu, N. Z. Wang, J. R. Chang, S. Chang, A. M. Zhang, Q. M. Zhang, X. G. Luo, T. Wu, Z. Sun, and X. H. Chen, arXiv: 1503.02457.

**11:51AM S5.00002 Atomic scale visualization of novel magnetic phase transitions in Fe-based superconductor  $\text{Sr}_4\text{V}_2\text{O}_6\text{Fe}_2\text{As}_2$**  , SEOKHWAN CHOI, Dept. of physics, KAIST, WON-JUN JANG, CAPP, IBS, JONG MOK OK, Dept. of physics, POSTECH, HYUN WOO CHOI, HYUN JUNG LEE, JIN OH JUNG, DONG HYUN SON, Dept. of physics, KAIST, HWAN SOO SUH, SAIT, JUN SUNG KIM, Dept. of physics, POSTECH, YANNIS K. SEMERTZIDIS, CAPP, IBS, JHINHWAN LEE, Dept. of physics, KAIST —  $\text{Sr}_4\text{V}_2\text{O}_6\text{Fe}_2\text{As}_2$  consists of superconducting FeAs layers and Mott insulating  $\text{Sr}_2\text{VO}_3$  layers, and exhibits superconductivity with  $T_c$  near 30 K despite being a parent compound material. Unlike normal Fe-based superconductors, the magnetism of  $\text{Sr}_4\text{V}_2\text{O}_6\text{Fe}_2\text{As}_2$  has complexity due to the presence of two magnetic atomic layers of V and Fe; therefore, the issue of magnetism has been actively debated. In this work, we studied the orbital and magnetic phase transitions in the range of 4 K to 180 K using spin-polarized scanning tunneling microscope. We directly observed the changes of charge density waves of V atomic layer related to the nematicity at 150 K, and spin density waves of V atomic layer resulting from spin ordering of underlying Fe atomic layer below 50 K. Moreover, controlling the sample bias voltage, the hysteresis of magnetic domain is observed at 4 K. Our results show key clues to solve controversy about the magnetism of  $\text{Sr}_4\text{V}_2\text{O}_6\text{Fe}_2\text{As}_2$ .

**12:03PM S5.00003 Observation of coexistence of itinerant electronic states and local moments in parents compound superconductor  $\text{Sr}_4\text{V}_2\text{O}_6\text{Fe}_2\text{As}_2$**  , WON-JUN JANG, Center for Axion and Precision Physics, IBS, SEOKHWAN CHOI, Dept. of physics, KAIST, JONG MOK OK, Dept. of physics, POSTECH, HYUN WOO CHOI, HYUN JUNG LEE, JIN OH JUNG, DONG HYUN SON, Dept. of physics, KAIST, HWAN SOO SUH, Samsung Advanced Institute of Technology, JUN SUNG KIM, Dept. of physics, POSTECH, YANNIS K. SEMERTZIDIS, Center for Axion and Precision Physics, IBS, JHINHWAN LEE, Dept. of physics, KAIST — Using variable temperature scanning tunneling spectroscopy (STS) and quasi-particle interference (QPI) analysis, we studied coexistence of itinerant electronic states and local moments in  $\text{Sr}_4\text{V}_2\text{O}_6\text{Fe}_2\text{As}_2$ . Temperature dependent STS measurements showed Fano resonances resulting from the hybridization between local moments (V) and itinerant electrons (Fe) below 100 K, and the formation of Fano lattice implying collective spin excitations between local moments of V atoms below 50 K. QPI analysis showed replica bands and kink features in Fe-itinerant band, implying the existence of Bosonic modes between  $\text{Sr}_2\text{VO}_3$  layers and FeAs layers. Our results show the collective behaviors of itinerant electrons and local moments, and the possibility of local moments contributing to superconductivity.

**12:15PM S5.00004 Bipartite bosonic modes and magnetic memory effects in superconducting  $\text{Sr}_4\text{V}_2\text{O}_6\text{Fe}_2\text{As}_2$** , JHINHWAN LEE, SEOKHWAN CHOI, HYUN JUNG LEE, KAIST, Physics Dept., WON-JUN JANG, KAIST, Physics Dept., IBS CAPP, JONG MOK OK, POSTECH, Physics Dept., HYUN WOO CHOI, JIN OH JUNG, DONG HYUN SON, KAIST, Physics Dept., HWAN SOO SUH, SAIT, YANNIS SEMERTZIDIS, KAIST, Physics Dept., IBS CAPP, JUN SUNG KIM, POSTECH, Physics Dept. — Using a homemade variable temperature high field spin-polarized STM, we have performed spectroscopic-imaging STM measurement on the parent-state superconductor  $\text{Sr}_4\text{V}_2\text{O}_6\text{Fe}_2\text{As}_2$  with each unit cell composed of superconducting FeAs layer sandwiched by two nearly Mott-insulating  $\text{Sr}_2\text{VO}_3$  layers. The hybridization between the localized V electrons and the itinerant Fe electrons causes electron transfer to the FeAs bands and generates a Gamma-centered electron pocket, as well as a Fano resonance at -18 meV with signature of Fano lattice. In the QPI measurement, we observed two distinct bosonic modes, i.e. the kinks and the partial replicas of the QPI dispersion with characteristic mode energies around 14 meV and 20 meV respectively, which agree with the self-energies due to two distinct electron-boson mode coupling functions in Migdal approximation. In spin-polarized STM mode, we observed atomic scale magnetic memory effect of the V atoms controlled with low energy (around 50 meV) spin-polarized tunneling current and used it to reveal underlying magnetic domains in the FeAs layer. Variable temperature spin-polarized STM measurements on some known antiferromagnetic materials will also be presented and discussed.

**12:27PM S5.00005 Unusual phase transition in a natural heterostructure of iron pnictides and vanadium oxides**, JONG MOK OK, POSTECH, S.-H. BAEK<sup>1</sup>, IFW Dresden, MAN JIN EOM, POSTECH, C. HOCH, R. K. KREMER, Max-Planck-Institut für Festkörperforschung, DONG-HWAN KIM, POSTECH, CHUN-FU CHANG, KYUNG-TAE KO, Max-Planck-Institut für Chemische Physik fester Stoffe, SANG-YOUN PARK, SUNG DAE JI, POSTECH, B. BÜCHNER, IFW Dresden, JAE-HOON PARK, J. H. SHIM, POSTECH, I. I. MAZIN, Naval Research Laboratory, JUN SUNG KIM<sup>2</sup>, POSTECH — We report the unusual phase transition in  $\text{Sr}_2\text{VO}_3\text{FeAs}$  single crystal, where the Mott-insulating vanadium oxides and the high- $T_c$  superconducting iron pnictides form a natural heterostructure. Clear evidence of the phase transition at  $T_0 = 155$  K was observed in the iron pnictide layer, not in the vanadium oxide layer, using bulk and NMR measurements. Neither magnetic ordering with sufficient spin moment nor symmetry change in the crystal structure has been detected at  $T_0$ . At  $T_{mag} \approx 45$  K, far below  $T_0$ , magnetic transition occurs in the iron pnictide layer, while the vanadium oxide layer remains nonmagnetic at low temperatures. The complex evolution of various phases in  $\text{Sr}_2\text{VO}_3\text{FeAs}$  is drastically distinct from the phase transitions found in other iron pnictides or vanadium oxides, highlighting the importance of the additional interlayer coupling between the layers.

<sup>1</sup>equal contribution, corresponding author

<sup>2</sup>corresponding author

**12:39PM S5.00006 Linear Magnetoresistance of  $\text{Ca}_{10}\text{Pt}_n\text{As}_8(\text{Fe}_2\text{As}_2)_5$  ( $n = 3$  and 4)**, JIAYUN PAN, AMAR KARKI, RONGYING JIN, Department of Physics and Astronomy, Louisiana State University — We report the normal-state magnetoresistance (MR) of superconducting  $\text{Ca}_{10}\text{Pt}_n\text{As}_8(\text{Fe}_2\text{As}_2)_5$  ( $n = 3$  and 4) as a function of temperature (50 – 300 K) and magnetic field (0 – 14 Tesla). It is found that MR is positive in a wide temperature range in both transverse ( $H \perp I$ ) and longitudinal ( $H \parallel I$ ) cases. At a fixed temperature and field, we observe MR ( $H \perp I$ ) > MR ( $H \parallel I$ ), suggesting spin-orbital coupling in addition to charge-spin interaction. Remarkably, MR shows linear field dependence between 0 and 14 Tesla in a wide temperature range for both  $n = 3$  and 4. The implication of such unusual field dependence of MR will be discussed.

**12:51PM S5.00007 Correlation induced self-doping in the iron-pnictide superconductor  $\text{Ba}_2\text{Ti}_2\text{Fe}_2\text{As}_4\text{O}$** , J.Z. MA<sup>1</sup>, P. RICHARD, G.F. CHEN, H. MIAO, L.K. ZENG, Institute of Physics, Chinese Academy of Sciences, A.VAN ROEKEGHEM, S. BIERMANN, Centre de Physique Thorique, Ecole Polytechnique, N. XU, M. SHI, Paul Scherrer Institute, Swiss Light Source, Z.H. LIU, J.B. HE, S.C. WANG, Department of Physics, Renmin University, C. CAO, Department of Physics, Hangzhou Normal University, Y.L. SUN, G.H. CAO, Department of Physics, Zhejiang University, T. QIAN, H. DING, Institute of Physics, Chinese Academy of Sciences — The electronic structure of the intercalated iron-based superconductor  $\text{Ba}_2\text{Ti}_2\text{Fe}_2\text{As}_4\text{O}$  ( $T_c \sim 21.5$  K) has been investigated by using ARPES and combined LDA + DMFT calculations. The electronic states near the Fermi level are dominated by both the Fe 3d and Ti 3d orbitals, indicating that the spacing layers separating different FeAs layers are also metallic. By counting the enclosed volumes of the Fermi surface sheets, we observe a large self-doping effect, i.e., 0.25 electrons per unit cell are transferred from the FeAs layer to the  $\text{Ti}_2\text{As}_2\text{O}$  layer, leaving the FeAs layer in a hole-doped state, which is in contrast with the LDA prediction of an electron-doped FeAs layer. This exotic behavior is successfully reproduced by the LDA + DMFT calculations, in which the self-doping effect is attributed to the electronic correlations in the Fe 3d shell. Our work provides an alternative route of effective doping without element substitution for iron-based superconductors.

<sup>1</sup>Beijing 100190, China

**1:03PM S5.00008 Numerical Study of a Multiorbital Hubbard Model for the Two-Leg Ladder  $\text{BaFe}_2\text{S}_3$  High- $T_c$  Superconductor Using the Density Matrix Renormalization Group**, NIRAVKUMAR PATEL, The University of Tennessee, Knoxville, Tennessee 37996, USA, ALBERTO NOCERA, GONZALO ALVAREZ, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, RYOTARO ARITA, RIKEN, 2-12-1 Hirasawa, Wako, Saitama 351-0198, Japan, ELBIO DAGOTTO, The University of Tennessee, Knoxville, Tennessee 37996, USA — Iron based high- $T_c$  superconductors have attracted considerable attention because of its unconventional superconducting properties. Here, we analyze the magnetic and pairing characteristics of the recently discovered two-leg ladder material  $\text{BaFe}_2\text{S}_3$  that becomes superconducting by applying pressure [1], using a two-orbital Hubbard model studied via the Density Matrix Renormalization Group technique. The hopping parameters, which spans up to the 2<sup>nd</sup> nearest-neighbor rungs, were obtained from the ab-initio downfolded band structure at ambient and high pressures [2]. The magnetic phase diagram at a realistic Hund coupling  $J/U = 0.25$  is presented varying the Hubbard  $U$ , at select values of the electronic fillings. At half-filling, we find a robust magnetic order in excellent agreement with experiments [1] i.e. antiferromagnetic (ferromagnetic) along the leg (rung) directions. We also discuss a possible tendency for this system to form a paired bound state of holes in a small but finite window of Hubbard  $U$ . The symmetries of this tentative paired ground state will be discussed.

[1] Hiroki Takahashi et al., *Nature Materials* **14**, 1008 (2015)

[2] Ryotaro Arita et al., *Phys. Rev. B* **92**, 054515 (2015)

**1:15PM S5.00009 Enhancement of Superconductivity Near a Structural Instability in  $\text{Ba}(\text{Ni}_{1-x}\text{Co}_x)_2\text{As}_2$** , CHRIS ECKBERG, HYUNSOO KIM, PETER ZAVALIJ, PHILIP PICCOLI, Univ of Maryland-College Park, JOHNPIERRE PAGLIONE, University of Maryland-College Park — We present a comprehensive study of single crystals of  $\text{Ba}(\text{Ni}_{1-x}\text{Co}_x)_2\text{As}_2$  synthesized using a flux method. With cobalt substitution, we track the evolution of the structural triclinic phase of  $\text{BaNi}_2\text{As}_2$  and the superconducting ground state with heat capacity and resistivity measurements. We will present our study of the systematic suppression of the low temperature triclinic state with increasing Co concentration as well as a more than threefold enhancement in the superconducting critical temperature, discussing its relation to iron-based superconductors.

**1:27PM S5.00010 Magnetism in  $LnMnSbO$  ( $Ln = La$  or  $Ce$ )<sup>1</sup>**, QIANG ZHANG, Iowa State University, NAVEEN KUMAR CHOGONDAHALI M., Jlich Centre for Neutron Science, KEVIN DENNIS, ALAN GOLDMAN, DAVID VAKNIN, Iowa State University — Neutron diffraction of polycrystalline (PND)  $LnMnSbO$  ( $Ln = La$  or  $Ce$ ) reveals differences between the magnetic ground state of the two compounds due to the strong Ce-Mn coupling compared to La-Mn. The two compounds adopt the  $P4/nmm$  space group down to 1.5 K and whereas magnetization measurements do not show any anomaly at high temperatures, PND reveals a C-type antiferromagnetic (AFM) order below  $T_N = 255$  K for  $LaMnSbO$  and 240 K for  $CeMnSbO$ . While the magnetic structure of  $LaMnSbO$  is preserved to base temperature, a sharp transition at  $T_{SR} = 5$  K in  $CeMnSbO$  due to a spin-reorientation (SR) transition of the  $Mn^{2+}$  from pointing along the  $c$ -axis to the  $ab$ -plane is found. The SR transition in  $CeMnSbO$  is accompanied by a simultaneous long-range AFM ordering of the Ce moments. This indicates that the Mn SR transition is driven by the Ce-Mn coupling similar to recent observation in the isostructural  $CeMnAsO$ . The ordered moments are found to be somewhat smaller than those expected for  $Mn^{2+}$  ( $S = 5/2$ ) in insulators, but large enough to suggest that these compounds belong to the class of local-moment antiferromagnets. The lower  $T_N$  found in this compound compared to the As-based counterpart ( $T_N = 347$  K for  $CeMnAsO$ ) indicates that the Mn- $Pn$  ( $Pn = As$  or  $Sb$ ) hybridization that mediates the exchange Mn-Mn coupling is weaker for the Sb-based compounds.

<sup>1</sup>Ames Laboratory is supported by U.S. DOE, BES, DMSE under contract DE-AC02-07CH11358. Oak Ridge National Laboratory's Spallation Neutron Source is sponsored by U.S. DOE, BES, SUFD.

**1:39PM S5.00011 Collinear antiferromagnetism in trigonal  $SrMn_2As_2$  revealed by single crystal neutron diffraction**, A. KREYSSIG\*, P. DAS\*, N. S. SANGEETHA\*, Z. A. BENSON\*, T. HEITMAN<sup>+</sup>, D. C. JOHNSTON\*, A. I. GOLDMAN\*, \*Ames Laboratory, Dept. of Phys. and Astro., Iowa State University, IA, USA; <sup>+</sup>University of Missouri Research Reactor, MO, USA — FeAs-based compounds and related materials have been an area of intense research in understanding the complex interplay between magnetism and superconductivity. Here we report on the magnetic structure of  $SrMn_2As_2$  that crystallizes in a trigonal structure ( $P\bar{3}m1$ ) and undergoes an antiferromagnetic (AFM) transition at  $T_N \approx 120$  K. The temperature dependence of the magnetic susceptibility remains nearly constant below  $T_N$  with  $H \parallel c$  while it decreases significantly with  $H \parallel ab$ . This shows that the local Mn moments order and lie in the  $ab$  plane instead of aligning along the  $c$  axis as in  $BaMn_2As_2$ . Single crystal neutron diffraction measurements on  $SrMn_2As_2$  determined that the Mn moments are collinearly aligned in a G-type AFM order with AFM alignments between a moment and all nearest neighbors in the basal plane and also perpendicular to it. This manifests that G-type AFM order is robust for Mn122 systems despite different symmetries, i.e. tetragonal for  $BaMn_2As_2$  and trigonal for  $SrMn_2As_2$ . Work at Ames Laboratory was supported by the DOE, BES, Division of Materials Sciences & Engineering, through DE-AC02-07CH11358. This research used resources at University of Missouri Research Reactor.

**1:51PM S5.00012 Anomalous frequency dependent diamagnetism in metal silicide<sup>1</sup>**, ASHUTOSH DAHAL, JAGAT GUNASEKERA, University of Missouri, Columbia, MO, LELAND HARRIGER, NIST Center For Neutron Research, Gaithersburg, MD, DAVID J. SINGH, DEEPAK K. SINGH, University of Missouri, Columbia, MO, LELAND HARRIGER COLLABORATION — Discovery of superconductivity in PbO-type FeSe has generated a lot of interest. Among the samples we synthesize with similar structure, NiSi has showed anomalous but very interesting results. Nickel silicides are important electronic materials that have been used as contacts for field effect transistors, as interconnects and in nanoelectronic devices. The magnetic properties of NiSi are not well known, however. In this presentation, we report a highly unusual magnetic phenomenon in NiSi. The ac susceptibility measurements on NiSi reveal strong frequency dependence of static and dynamic susceptibilities that are primarily diamagnetic at room temperature. The static susceptibility is found to exhibit a strong frequency dependence of the diamagnetic response below 100K, while dynamic susceptibility showed peak type feature at 10KHz frequency around 50K. Detailed neutron scattering measurements on high quality powder sample of NiSi on SPINS cold spectrometer further revealed an inelastic peak around 1.5meV, even though no magnetic order is detected. The inelastic peak dissipates above 100K, which is where the static susceptibility starts to diverge with frequency.

<sup>1</sup>Research is supported by U.S. Department of Energy, Office of Basic Energy Sciences under Grant No. DE-SC0014461.

**2:03PM S5.00013 The Long Forgotten Compound: CoTe, and its Epitaxial Film Growth and Properties<sup>1</sup>**, ZHIWEI ZHANG, ZHIHAI ZHU, WILLIAM A. HINES, JOSEPH I. BUDNICK, BARRETT O. WELLS, Physics Department, University of Connecticut — As part of our investigation of Co-doped, Fe-chalcogenide superconductors, we have synthesized films of CoTe, a long forgotten binary compound. Using pulsed laser deposition, we have grown epitaxial films on MgO, CaF<sub>2</sub>, and SrTiO<sub>3</sub> and have found that careful control of growth conditions allows for the synthesis of either (001) or (101) oriented films. X-ray diffraction shows the structure of the films is hexagonal. However, we also find the surprising presence of the nominally disallowed (001) peak. We also report temperature dependent transport and magnetic properties. This material may be of interest as a magnetic semiconductor and for its relationship to chemically doping Fe-based superconductors.

<sup>1</sup>DOE/BES contract DE-FG02-00ER45801

**Thursday, March 17, 2016 11:15AM - 2:15PM –**

**Session S6 GMAG DMP: Magneto-Optic/Electric and Strain/Shape Induced Magnetism** 302 - Anirudh Sharma, Flinders University

**11:15AM S6.00001 magnetoelectric switching and spin wave generation**, BART SOREE, DAVIDE TIerno, CHRISTOPH ADELMANN, ODYSSEAS ZOGRAFOS, ADRIEN VAYSET, FLORIN CIUBOTARU, imec, SPIN WAVE IMEC TEAM — We have investigated the dynamics of the magnetization in magnetoelectric elements for switching and generation of spin waves. The behavior of the magnetization in the magnetostrictive material coupled to the piezoelectric not only depends on the strain induced by the piezo, but also depends on the relative contribution of the different magnetic anisotropies (shape, magnetocrystalline, magnetoelastic) present in the magnetoelectric element which is coupled to a spin wave bus. Performing micromagnetic simulations allow us to draw several conclusions w.r.t. the switching behavior of magnetoelectric elements as well as conditions to generate spin waves in an effective manner.

**11:27AM S6.00002 Electric field controlled strain induced reversible switching of magnetization in Galfenol nanomagnets delineated on PMN-PT substrate<sup>1</sup>**, HASNAIN AHMAD, Department of Electrical and Computer Engineering, Virginia Commonwealth University, JAYASIMHA ATULASIMHA, Department of Mechanical and Nuclear Engineering, Virginia Commonwealth University, SUPRIYO BANDYOPADHYAY, Department of Electrical and Computer Engineering, Virginia Commonwealth University — We report a *non-volatile* converse magneto-electric effect in elliptical Galfenol (FeGa) nanomagnets of ~300 nm lateral dimensions and ~10nm thickness delineated on a PMN-PT substrate. This effect can be harnessed for energy-efficient non-volatile memory. The nanomagnets are fabricated with e-beam lithography and sputtering. Their major axes are aligned parallel to the direction in which the substrate is poled and they are magnetized in this direction with a magnetic field. An electric field in the opposite direction generates compressive strain in the piezoelectric substrate which is partially transferred to the nanomagnets and rotates their magnetization away from the major axes to metastable orientations. There they remain after the field is removed, resulting in non-volatility. Reversing the electric field generates tensile strain which returns the magnetization to the original state. The two states can encode two binary bits which can be written using the correct voltage polarity, resulting in non-toggle behavior. Scaled memory fashioned on this effect can exhibit write energy dissipation of only ~2 aJ.

<sup>1</sup>Work is supported by NSF under ECCS 1124714 and CCF- 1216614. Sputtering was carried out at NIST Gaithersburg.

**11:39AM S6.00003 Giant magnetoelectric effect in thin magnetic films utilizing inter-ferroelectric transitions.<sup>1</sup>**, PETER FINKEL, MARGO STARUCH, US Naval Research Laboratory — There has recently been much interest to multiferroic magnetoelectric composites based on relaxor ferroelectric single crystals as potential candidates for devices such as magnetic field sensors, energy harvesters, or transducers. Large magnetoelectric coupling coefficient is prerequisite for superior device performance in a broad range of frequencies and functioning conditions. In magnetoelectric heterostructures based on ternary relaxors  $\text{Pb}(\text{In}_{1/2}\text{Nb}_{1/2})\text{O}_3$ - $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$ - $\text{PbTiO}_3$  (PIN-PMN-PT) crystal better operational range and temperature stability as compared to binary relaxors can be achieved. Giant linear converse magnetoelectric coupling up to  $2 \times 10^{-6} \text{ s m}^{-1}$  were observed in heterostructural composites with multilayered FeCo/Ag deposited on (011) PIN-PMN-PT crystals. Further enhancement of magnetoelectric coupling is demonstrated by utilizing inter-ferroelectric rhombohedral – orthorhombic phase transitions in PIN-PMN-PT. Mechanical clamping was a precondition to utilize this inter-ferroelectric transition mode to bring the crystal to a point just below its transformation threshold when very small perturbations at the input will cause large swings at the output generating a sharp uniaxial increase in strain (~0.5 %) and polarization change, giving rise to nonlinear effects. Details of these results and their implications will be presented.

<sup>1</sup>Giant magnetoelectric effect in thin magnetic fillms utilizing inter-ferroelectric transitions

**11:51AM S6.00004 Exploring Strain Induced Magnetization Effects in Metamagnetic Artificial Multiferroics using Polarized Neutron Reflectometry**, STEVEN BENNETT, ANDREAS HERKLOTZ, ANTHONY WONG, THOMAS WARD, VALERIA LAUTER, Oak Ridge National Laboratory — There is currently a strong drive to realize a controllable magnetic ordering transition for use in next generation spintronic based memory and computation devices. One proposed method to gain such control is the use of a changing strain in a thin film metamagnetic artificial multiferroic system. While basic concepts using electric field actuated piezoelectric strain have been recently demonstrated<sup>1</sup>, there is very little understanding of the details of strains effect on such magnetic phase transitions. Using the depth sensitive method of polarized neutron reflectometry we have been able to probe the fine details of strains contribution to the metamagnetic transition in thin films of metamagnetic  $\text{FeRh}$ <sup>2</sup>. Here we explore the effects of changing lattice strain as a function of depth using both a barium titanate substrate's structural phase transitions<sup>3</sup> and He ion implantation. These studies have discovered a remarkably large coupling between the systems strain state and the switching behavior across the magnetostructural metamagnetic transition. <sup>1</sup> Cherifi, R. O. et al. Nat. Mater. 31, 345–351 (2014), <sup>2</sup> Bennett, S. P. et al. Sci. Rep. 5, 9142 (2015), <sup>3</sup> Bennett, S. P. et al. submitted (2015)

**12:03PM S6.00005 Writing magnetic phase and domain structure in  $\text{FeRh}$  by controlling lattice symmetry with strain doping**, T. ZAC WARD, ANDREAS HERKLOTZ, Oak Ridge National Lab, ANTHONY WONG, Univ. of Tennessee, STEVEN BENNETT, VALERIA LAUTER, Oak Ridge National Lab — Low energy helium ion implantation is an effective approach to strain doping materials which allows one to expand the out-of-plane lattice parameter in epitaxial films without vacancy generation or electron/hole doping the system [1]. The ability to control crystal anisotropy and overcome Poisson's drive to conserve volume can thus offer huge dividends in controlling magnetic properties due to magnetostrictive phenomena. We present recent studies on epitaxial  $\text{FeRh}$  films which demonstrate how controlling crystal symmetry in this important intermetallic material can be used to finely control magnetic properties. We find that the first order magneto-structural phase transition from antiferromagnetic to ferromagnetic can be directly controlled through single axis lattice expansion; this effectively allows us to dictate the transition temperature anywhere between 400K and 150K. Polarized Neutron Reflectometry (PNR) data and scanning Magneto-optic Kerr effect (MOKE) measurements will be presented which demonstrate that this phase control can be confined to a specific region of the film both in depth and/or lateral position. While this holds great promise for magnetocaloric applications, many possibilities remain for devising new functionalities and gaining a deeper understanding of material properties using this technique. [1]H.W. Guo, S. Dong, P.D. Rack, J.D. Budai, A.T. Wong, A. Herklotz, P.C. Snijders, E. Dagotto, and T.Z. Ward, Phys. Rev. Lett. 114, 256801 (2015). Funded by DOE-BES-MSED.

**12:15PM S6.00006 Current Control of Magnetic Anisotropy via Strain in a  $\text{CoFeB}$  Waveguide<sup>1</sup>**, KYONGMO AN, XIN MA, Department of Physics, University of Texas, Austin, Texas 78712, USA, CHI-FENG PAI, Cornell University, Ithaca, New york 14853, USA, JUSANG YANG, KEVIN OLSSON, JAMES ERSKINE, ALLAN MACDONALD, Department of Physics, University of Texas, Austin, Texas 78712, USA, DANIEL RALPH, ROBERT BUHRMAN, Cornell University, Ithaca, New york 14853, USA, XIAOQIN LI, Department of Physics, University of Texas, Austin, Texas 78712, USA — We demonstrate that in-plane charge current can effectively control the spin precession resonance in an  $\text{Al}_2\text{O}_3/\text{CoFeB}/\text{Ta}$  heterostructure. Brillouin Light Scattering (BLS) was used to detect the ferromagnetic resonance field under microwave excitation of spin waves at fixed frequencies. Such control originates from the modified in-plane uniaxial magnetic anisotropy field  $H_K$ , which changes symmetrically with respect to the current direction. Numerical simulation suggests that the anisotropic stress introduced by Joule heating plays an important role in controlling  $H_K$ . The results provide new insights into current manipulation of magnetic properties and have broad implications on spintronic devices.

<sup>1</sup>This work is supported by SHINES, an Energy Frontier Research Center funded by the U.S. Department of Energy (DoE), Office of Science, Basic Energy Science (BES) under award DE-SC0012670

**12:27PM S6.00007 Incoherent stress-mediated magnetization reversal in shape anisotropic multiferroic nanomagnets<sup>1</sup>**, DHIRITIMAN BHATTACHARYA, MD MAMUN AL-RASHID, VIMAL SAMPATH, NOEL D'SOUZA, SUPRIYO BANDYOPADHYAY, JAYASIMHA ATULASIMHA, Virginia Commonwealth Univ — Strain mediated switching of multiferroic nanomagnets promises to be extremely energy efficient with dissipation per switching event of  $\sim 1$  aJ<sup>[1,2,3]</sup>. Most theoretical approaches to studying the switching dynamics use the macrospin approximation in which all the spins in the nanomagnet are assumed to rotate coherently. However, recent experiments show that while initial and final states are well approximated by this single domain assumption, intermediate states visited during the magnetization rotation process cannot be described by it. In such cases, an interplay between the exchange, magnetostatic and stress anisotropy energies can introduce incoherent magnetization dynamics. Hence, intermediate micromagnetic configurations such as vortex states can be stabilized, particularly in nanomagnets of larger dimensions. In this work, we present rigorous micromagnetic simulations to study the peculiarities of the incoherent switching process in the context of shape anisotropic nanomagnets subjected to stress. 1.Appl. Phys. Lett., 97, 173105, 2010. 2.Appl. Phys. Lett., 99, 063108, 2011. 3.Nanotechnology, 23, 105201, 2012.

<sup>1</sup>This work is supported by NSF under grant CAREER grant CCF-1253370.

**12:39PM S6.00008 Experimental manipulation of magnetic states of magnetostrictive nanomagnets using surface acoustic waves<sup>1</sup>**, VIMAL SAMPATH, DHIRITIMAN BHATTACHARYA, NOEL D'SOUZA, SUPRIYO BANDYOPADHYAY, JAYASIMHA ATULASIMHA, Virginia Commonwealth University — The use of Surface Acoustic Waves (SAW) to assist magnetization switching in magnetostrictive nanomagnets has been theoretically studied [1] and SAW-induced magnetization rotation in micron size magnets has been experimentally demonstrated [2]. We report recent experiments on manipulation of magnetic states of Co nanoscale magnets shaped like elliptical disks ( $\sim 300$  nm major axis, 240 nm minor axis and 10 nm thickness) delineated on bulk 128 Y-cut lithium niobate using SAW. Specifically, isolated nanomagnets that are initially in single domain states with magnetization pointing along the major axis of the ellipse are driven into a vortex state by SAW waves. However, SAW waves can trigger complete magnetization reversal in nanomagnets of moderate shape anisotropy that are dipole coupled to a highly shape anisotropic neighboring nanomagnet. [1] A.K. Biswas, S. Bandyopadhyay & J. Atulasimha, Appl. Phys. Lett., 105, 072408 (2014). [2] S. Davis, A. Baruth & S. Adenwalla, App. Phys. Lett., 97, 232507 (2010). The authors acknowledge the use of high voltage and high frequency pulse generator from Prof. Umit Ozgur's lab and the help of Prof. Gary Atkinson in fabrication of the IDTs for generating the SAW.

<sup>1</sup>We acknowledge SHF-Small CCF-1216614 and CAREER CCF-1253370 grants; and use of CNST Nanofab facility at NIST, Gaithersburg.

**12:51PM S6.00009 Magnetic domain response to strain generated by focused surface acoustic waves<sup>1</sup>**, UDAY SINGH, SHIREEN ADENWALLA, University of Nebraska - Lincoln — The effects of strain on magnetostrictive ferromagnets include changes in the magnetization, anisotropy and domain wall velocities. A ferromagnet (FM) on the surface of a surface acoustic wave (SAW) is subjected to periodic compressive and tensile strain that has resulted in coherent rotation of the magnetization, as well as inducing ferromagnetic resonance in FM films. We describe the response of magnetic domains in Co/Pt multilayers when subjected to the high strains generated by a focused SAW. Annular interdigital transducers (AIDT) patterned on LiNbO<sub>3</sub> form a SAW standing wave pattern with large strain amplitude at the focal center. Domains in [Co(3Å)/Pt(8Å)]<sub>x</sub>5 with perpendicular magnetic anisotropy were observed using a MOKE microscope within this focal region. Controlled magnetic pulses steered a magnetic domain boundary to the large strain region after nucleation. Excitation of the AIDT resulted in a reversible change in the domain wall boundary in the high strain region. We attribute this to magnetic anisotropy changes in the presence of RF strain, which results in changes in the domain configuration to minimize the free energy. We will present results showing both slow and fast magnetization changes in Co/Pt occurring in the presence of high frequency strain. This work is supported by NSF (DMR 1409622) and Nebraska MRSEC (DMR-1420645).

<sup>1</sup>This work is supported by NSF (DMR 1409622) and Nebraska MRSEC (DMR-1420645).

**1:03PM S6.00010 Orientation dependences of surface morphologies and energies of iron-gallium alloys<sup>1</sup>**, MARCIO COSTA, HUI WANG, JUN HU, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine, SUOK-MIN NA, HYUNSUK CHUN, ALISON B FLATAU, Department of Aerospace Engineering, University of Maryland, College Park, MD, UNIVERSITY OF CALIFORNIA, IRVINE COLLABORATION, UNIVERSITY OF MARYLAND COLLABORATION — Magnetostrictive Fe-Ga alloys (Galfenol) are very promising rare-earth free materials for applications in sensors, actuators, energy-harvesters and spintronic devices. Investigation on surface energies of Galfenol based on density functional calculations (DFT) and contact angle measurements may provide fundamental understandings and guidance to further optimize the performance of Galfenol. DFT calculations predict that Ga-covered (110) surface of Galfenol is more stable in Ga-rich condition, while Ga-covered (001) surface of Galfenol surface become more favorable in Ga-poor condition. Moreover, a full Ga overlayer tends to form on top of Galfenol surfaces regardless their orientation, both in agreement with the experimental observation. Further studies on Ga segregation in the Fe bcc matrix demonstrate that the Fe-Ga separation is unlikely to occur since Ga diffusion toward the surface is effectively self-stopped once the Ga overlayers form on the facets.

<sup>1</sup>This work was supported by the National Science Foundation through the SUSCHEM-Collaborative Research program (grant numbers: DMR- 1310494 at UCI and DMR-1310447 at UMD). Work at UCI was also supported by the ONR (grant number: N00014-13-1-0445).

**1:15PM S6.00011 Fingerprinting Morphology of Magnetic Shape Memory Alloys Using First Order Reversal Curves (FORC) and Neutron Scattering<sup>1</sup>**, IGOR V. ROSHCHIN, Texas A&M Univ., PAVEL N. LAPA, Texas A&M Univ., Argonne Nat. Lab., KATHRYN L. KRYCKA, BRIAN B. MARANVILLE, CNR, NIST, JAMES A. MONROE, BRIAN E. FRANCO, IBRAHIM KARAMAN, Texas A&M Univ. — In Ni-Mn-In- and Ni-Mn-Sn-based alloys, two magnetic phases with ferromagnetic and antiferromagnetic exchange couplings between two nearest Mn atoms can coexist. The interaction between these phases results in exchange bias (EB). The EB field depends on the cluster sizes. Using the first order reversal curve (FORC) analysis of magnetization for Ni-Co-Mn-Sn and Ni-Co-Mn-In samples with different heat treatment, we can obtain information about cluster sizes of the structural phases in these alloys. This is especially important for polycrystalline alloy samples where dark-field images showing different phases are hard to obtain. Such a Ni-Co-Mn-Sn polycrystalline sample was characterized with small angle neutron scattering (SANS). Analyses of the scattering as a function of wavevector transfer in 50 Oe and 15 kOe applied field yield the average magnetic domain size of  $21.2 \pm 6.6$  nm and a polydispersity of  $0.32 \pm 0.02$  at 300 K, in good agreement with our prediction. The temperature evolution of the domain size will be discussed. Using an off-specular reflectometer in transmission geometry, the same sample was measured at a field of 270 Oe and 5.15 kOe. The fit of the 270 Oe data yields grain sizes of approximately  $0.11$ – $0.12$   $\mu\text{m}$  with polydispersities between 0.98 and 1.27.

<sup>1</sup>Supported by Texas A&M University, US-DOE, and US NSF-DMR.

**1:27PM S6.00012 Detecting an in-plane rotation of magnetization in GdFeCo films<sup>1</sup>**, FARZANEH HOVEYDA, SERBAN SMADICI, University of Louisville — It is often important to distinguish between magnetization reversal by coherent rotation in different planes and domain wall motion. Magnetization curves were measured at different temperatures with magneto-optical Kerr Effect in longitudinal (L-MOKE) and polar (P-MOKE) geometries on sputter-deposited  $\text{Gd}_x\text{Fe}_y\text{Co}_{1-x-y}$  (GFC) films of variable thickness. Depending on the probed region, the L-MOKE signal measured with decreasing external field  $H_{\text{ext}}$  was found to be lower than the signal observed with increasing  $H_{\text{ext}}$  (negative remanence magnetization). We show that this is due to a contribution to the signal of  $M_{\perp}$ , the magnetization component perpendicular to the scattering plane. This identifies the type of reversal in these GFC films as in-plane coherent rotation of magnetization.  $M_{\perp}$  is also proportional to the torque. Azimuthal measurements on  $\text{Co}_2\text{FeAl}$  samples showed a regular variation of the MOKE signal, in one possible application of these observations to torque measurements.

<sup>1</sup>Work supported by the University of Louisville Research Foundation.

**1:39PM S6.00013 Nanoscale Confinement of All-Optical Magnetic Switching in TbFeCo<sup>1</sup>**, TIANMIN LIU, TIANHAN WANG, Stanford University, ALEXANDER REID, SLAC National Accelerator Laboratory, MATTEO SAVOINI, Radboud University Nijmegen, XIAOFEI WU, Universität Würzburg, BENNY KONENE, Radboud University Nijmegen, PATRICK GRANITZKA, University of Amsterdam, CATHERINE GRAVES, DANIEL HIGLEY, ZHAO CHEN, Stanford University, GARY RAZINSKAS, Universität Würzburg, MARKUS HANTSCHMANN, Institute Methods and Instrumentation for Synchrotron Radiation Research, ANDREAS SCHERZ, JOACHIM STOHR, SLAC National Accelerator Laboratory, ARATA TSUKAMOTO, College of Science and Technology, BERT HECHT, Universität Würzburg, ALEXEY KIMEL, ANDREI KIRILYUK, THEO RASING, Radboud University Nijmegen, HERMANN DURR, SLAC National Accelerator Laboratory, DURR/STOHR TEAM, THEO RASING TEAM, ARATA TSUKAMOTO TEAM, BERT HECHT TEAM — Gold two-wire antennas structures are placed upon the surface of the all-optical switching film TbFeCo. They resonate with the optical field and create a field enhancement in its vicinity, which is used to confine the area where optical switching can occur. It is demonstrated that single femtosecond optical laser pulses can reverse magnetization in a controllable fashion by such confinement. The magnetic states are imaged using resonant X-ray holography and magnetic circular dichroism. The results not only show the feasibility of controllable switching with antenna assistance but also demonstrate the highly inhomogeneous nature of the switching process, which is attributed to the material's heterogeneity.

<sup>1</sup>Research is supported by U.S. DOE, Office of Basic Energy Sciences, Materials Sciences and Engineering Division

**1:51PM S6.00014 Measurements of the Domain Magnetization Direction and its Effects on the Sensitivity of Magneto-optic Field Sensors.**, MANNIX SHINN, ANTHONY GARZARELLA, DONG HO WU, United States Naval Research Laboratory, RONGJIA TAO, Temple University — Bismuth doped, rare earth iron garnet (Bi:RIG) thick films exhibit a large magneto-optic response to external magnetic fields while exhibiting low optical insertion loss, making them ideal candidates for polarimetric magnetic field sensors. It was generally found that the Faraday rotation and overall sensitivity of the sensors depends on the orientation of the local domain magnetization relative to the direction of laser propagation. In arrayed Bi:RIG sensors, it is critical that the optical path of the laser is perpendicular to the easy-axis of each film of the array, in order to avoid magnetically-induced optical incoherence (MIOI). Therefore a precise, localized measurement of the magnetization vector within the films is necessary. Since traditional magnetization measurement techniques do not provide adequate resolution, several new approaches to precisely measure the easy axis were developed and will be described in this presentation. These approaches involve measurements of the directionality of the Faraday response, incoherence in the Malus curves, and damping in the domain wall motion. Such measurements have been instrumental in constructing and optimizing arrayed Bi:RIG sensors, which currently have a sensitivity of  $6 \text{ pT/Hz}^{1/2}$ .

**2:03PM S6.00015 Dynamic Interplay of Coherent Rotations and Domain Wall Motion in Faraday Rotators based on Ferromagnetic Crystals.**, ANTHONY GARZARELLA, DONG WU, MANNIX SHINN, Naval Research Laboratory — Under small, externally-applied magnetic fields, the Faraday rotation in magneto-optic material containing ferromagnetic domains is driven primarily by two principal mechanisms: domain wall motion and coherent domain rotations. Domain wall motion yields a larger Faraday responsivity but is limited by magnetically induced optical incoherence and by damping effects. Coherent domain rotation yields smaller Faraday rotations, but exhibits a flatter and broader frequency response. The two mechanisms occur along orthogonal principal axes and may be probed independently. However, when probed along an oblique angle to the principal axes, the relationship between the Faraday rotation and the external field changes from linear to tensorial. Although this may lead to more complicated phenomena (e.g. a sensitivity axis that depends on RF frequency), the interplay of domain rotation and domain wall motion can be exploited to improve responsivity or bandwidth. The detailed experimental data can be understood in terms of a quantitative model for the magnitude and direction of the responsivity vector. Applications to magnetic field sensors based on arrayed bismuth doped iron garnet films will be emphasized in this presentation.

## Thursday, March 17, 2016 11:15AM - 2:15PM — Session S7 FEd: Physics Education 303 - Robin Selinger, Kent State University

**11:15AM S7.00001 The Impact of Network Embeddedness on Student Persistence**, JUSTYNA ZWOLAK, ERIC BREWE, Florida International University, INSPIRE TEAM — Society is constantly in flux, which demands the continuous development of our educational system to meet new challenges and impart the appropriate knowledge/skills to students. In particular, in order to improve student learning (among other things), the way we are teaching has significantly changed over the past few decades. We are moving away from traditional, lecture-based teaching towards a more interactive approach using, e.g., clicker questions, modeling instruction (MI), and other engagement strategies. A current, major challenge for universities is to increase student retention. I am examining the use of network analysis to investigate academic and social experiences of students in and beyond the classroom. There is a compelling case that transformed physics classes, such as ones that use MI, promote persistence by the creation of learning communities that support the integration of students into the university. I will discuss recent results connecting the MI approach to network structures in the students' interactions and how students' position impacts persistence in taking a subsequent MI vs. traditional lecture-based course.

**11:27AM S7.00002 Using Video Analysis and Biomechanics to Engage Life Science Majors in Introductory Physics**, JEFF STEPHENS, Misericordia University — There is an interest in Introductory Physics for the Life Sciences (IPLS) as a way to better engage students in what may be their only physical science course. In this talk I will present some low cost and readily available technologies for video analysis and how they have been implemented in classes and in student research projects. The technologies include software like Tracker and LoggerPro for video analysis and low cost high speed cameras for capturing real world events. The focus of the talk will be on content created by students including two biomechanics research projects performed over the summer by pre-physical therapy majors. One project involved assessing medial knee displacement (MKD), a situation where the subject's knee becomes misaligned during a squatting motion and is a contributing factor in ACL and other knee injuries. The other project looks at the difference in landing forces experienced by gymnasts and cheer-leaders while performing on foam mats versus spring floors. The goal of this talk is to demonstrate how easy it can be to engage life science majors through the use of video analysis and topics like biomechanics and encourage others to try it for themselves.

**11:39AM S7.00003 Development of a Hands-On Survey Course in the Physics of Living Systems** , MEGAN MATTHEWS, DANIEL I. GOLDMAN, Georgia Institute of Technology — Due to the widespread availability and technological capabilities of modern smartphones, many biophysical systems can be investigated using easily accessible, low-cost, and/or “homemade” equipment. Our survey course is structured to provide students with an overview of research in the physics of living systems, emphasizing the interplay between measurement, mechanism, and modeling required to understand principles at the intersection of physics and biology. The course proceeds through seven modules each consisting of one week of lectures and one week of hands-on experiments, called “microlabs”. Using smartphones, Arduinos, and 3D printed materials students create their own laboratory equipment, including a 150X van Leeuwenhoek microscope, a shaking incubator, and an oscilloscope, and then use them to study biological systems ranging in length scales from nanometers to meters. These systems include population dynamics of rotifer/algae cultures, experimental evolution of multicellularity in budding yeast, and the bio- & neuromechanics involved in animal locomotion, among others. In each module, students are introduced to fundamental biological and physical concepts as well as theoretical and computational tools (nonlinear dynamics, molecular dynamics simulation, and statistical mechanics). At the end of the course, students apply these concepts and tools to the creation of their own microlab that integrates hands-on experimentation and modeling in the study of their chosen biophysical system.

**11:51AM S7.00004 Physics of Health Sciences** , MILLARD BAUBLITZ, BENNETT GOLDBERG, Boston University — A one-semester algebra-based physics course is being offered to Boston University students whose major fields of study are in allied health sciences: physical therapy, athletic training, and speech, language, and hearing sciences. The classroom instruction incorporates high-engagement learning techniques including worksheets, student response devices, small group discussions, and physics demonstrations instead of traditional lectures. The use of pre-session exercises and quizzes has been implemented. The course also requires weekly laboratory experiments in mechanics or electricity. We are using standard pre- and post-course concept inventories to compare this one-semester introductory physics course to ten years of pre- and post-course data collected on students in the same majors but who completed a two-semester course.

**12:03PM S7.00005 Promoting Active Learning: The Use of Computational Software Programs** , TOM DICKINSON, Washington State University — The increased emphasis on active learning in essentially all disciplines is proving beneficial in terms of a student's depth of learning, retention, and completion of challenging courses. Formats labeled flipped, hybrid and blended facilitate face-to-face active learning. To be effective, students need to absorb a significant fraction of the course material prior to class, e.g., using online lectures and reading assignments. Getting students to assimilate and at least partially understand this material prior to class can be extremely difficult. As an aid to achieving this preparation as well as enhancing depth of understanding, we find the use of software programs such as Mathematica® or MatLab®, very helpful. We have written several Mathematica® applications and student exercises for use in a blended format two semester E&M course. Formats include tutorials, simulations, graded and non-graded quizzes, walk-through problems, exploration and interpretation exercises, and numerical solutions of complex problems. A good portion of this activity involves student-written code. We will discuss the efficacy of these applications, their role in promoting active learning, and the range of possible uses of this basic scheme in other classes.

**12:15PM S7.00006 Student Responses to a Flipped Introductory Physics Class with built-in Post-Video Feedback Quizzes** , ROBERTO RAMOS, University of the Sciences — We present and analyze student responses to multiple Introductory physics classes in a university setting, taught in a “flipped” class format. The classes included algebra- and calculus-based introductory physics. Outside class, students viewed over 100 online video lectures on Classical Mechanics, Electricity and Magnetism, and Modern Physics prepared by this author and in some cases, by a third-party lecture package available over YouTube. Inside the class, students solved and discussed problems and conceptual issues in greater detail. A pre-class online quiz was deployed as an important source of feedback. I will report on the student reactions to the feedback mechanism, student responses using data based on anonymous surveys, as well as on learning gains from pre-/post- physics diagnostic tests. The results indicate a broad mixture of responses to different lecture video packages that depend on learning styles and perceptions. Students preferred the online quizzes as a mechanism to validate their understanding. The learning gains based on FCI and CSEM surveys were significant.

**12:27PM S7.00007 Teaching Electrostatics and Entropy in Introductory Physics** , MARK REEVES, George Washington University — Entropy changes underlie the physics that dominates biological interactions. Indeed, introductory biology courses often begin with an exploration of the qualities of water that are important to living systems. However, one idea that is not explicitly addressed in most introductory physics or biology courses is important contribution of the entropy in driving fundamental biological processes towards equilibrium. I will present material developed to teach electrostatic screening in solutions and the function of nerve cells where entropic effects act to counterbalance electrostatic attraction. These ideas are taught in an introductory, calculus-based physics course to biomedical engineers using SCALEUP pedagogy. Results of student mastering of complex problems that cross disciplinary boundaries between biology and physics, as well as the challenges that they face in learning this material will be presented.

**12:39PM S7.00008 ABSTRACT WITHDRAWN —**

**12:51PM S7.00009 High speed video analysis study of elastic and inelastic collisions<sup>1</sup>** , ANDREW BAKER, JACOB BECKEY, VASUDEVA ARAVIND, Clarion University, CLARION TEAM — We study inelastic and elastic collisions with a high frame rate video capture to study the process of deformation and other energy transformations during collision. Snapshots are acquired before and after collision and the dynamics of collision are analyzed using Tracker software. By observing the rapid changes (over few milliseconds) and slower changes (over few seconds) in momentum and kinetic energy during the process of collision, we study the loss of momentum and kinetic energy over time. Using this data, it could be possible to design experiments that reduce error involved in these experiments, helping students build better and more robust models to understand the physical world.

<sup>1</sup>We thank Clarion University undergraduate student grant for financial support involving this project.

**1:03PM S7.00010 Hurricane Balls: A rigid-body-motion student project** , DAVID JACKSON, DAVID MERTENS, BRETT PEARSON, Dickinson College — Hurricane Balls is a spinning-top toy that consists of two metal spheres that are welded (or glued) together. The motion of Hurricane Balls provides a beautiful example of rotational motion in which the angular velocity and angular momentum point in different directions. Because the motion is both captivating to students and extremely reproducible, this system is an ideal example to include in a classical mechanics course. Moreover, the excellent agreement between theory and experiment makes a detailed analysis of Hurricane Balls a perfect topic for an independent student project. This talk will give an overview of the system and will provide some tips on how to make such a project a successful student experience.

**1:15PM S7.00011 First order error corrections in common introductory physics experiments<sup>1</sup>**, JACOB BECKEY, ANDREW BAKER, VASUDEVA ARAVIND, Clarion University, CLARION TEAM — As a part of introductory physics courses, students perform different standard lab experiments. Almost all of these experiments are prone to errors owing to factors like friction, misalignment of equipment, air drag, etc. Usually these types of errors are ignored by students and not much thought is paid to the source of these errors. However, paying attention to these factors that give rise to errors help students make better physics models and understand physical phenomena behind experiments in more detail. In this work, we explore common causes of errors in introductory physics experiment and suggest changes that will mitigate the errors, or suggest models that take the sources of these errors into consideration. This work helps students build better and refined physical models and understand physics concepts in greater detail.

<sup>1</sup>We thank Clarion University undergraduate student grant for financial support involving this project.

**1:27PM S7.00012 Are our textbooks too good to be good? Let students own their textbooks to own the skills**, XIUPING TAO, Winston-Salem State University — The two new yearlong high school courses, AP Physics 1 and 2, are equivalent to the two-semester algebra-based introductory Physics college course. The AP courses have more than 300 instruction hours, while the college course less than 100. This partially explains why college instructors always struggle to cover the important topics to not necessarily prepared students. To make it worse, many college students are not buying or reading textbooks and rely on instructors to get the course content. The fragmented reception is preventing students from getting a complete picture of the course. Not that there is a shortage of textbooks. There are many 1000-page tomes costing \$200 or more, too good to be good. All the struggles contribute to U.S. students' relatively low STEM skills. I propose to let students own their books to own the skills. Students need much shorter (thus manageable) and much more affordable books, and they need to own it for good. Cross-culture comparison reveals that students learn better when they truly own their books (without planning to resell).

**1:39PM S7.00013 Physics and Physics Education at Clarion University**, VASUDEVA ARAVIND, Clarion University — Clarion University is located in the rolling hills of western Pennsylvania. We are a primarily undergraduate public institution serving about 6000 students. We graduate students who take different career paths, one of them being teaching physics at high schools. Since educating teachers of tomorrow requires us to introduce currently trending, research proven pedagogical methods, we incorporate several aspects of physics pedagogies such as peer instruction, flipped classroom and hands on experimentation in a studio physics lab format. In this talk, I discuss some of our projects on physics education, and seek to find potential collaborators interested in working along similar lines.

**1:51PM S7.00014 Learning Through Doing: Teaching Advanced Physics Concepts Through Freshmen Research Immersion**, MATTHEW WAHILA, LOUIS PIPER, Dept. of Physics, Binghamton University, JENNIFER AMEY, WAYNE JONES, Dept. of Chemistry, Binghamton University, MEGAN FEGLEY, NANCY STAMP, Freshmen Research Immersion Program, Binghamton University — Often undergraduates have difficulty grasping advanced concepts in physics due to the seemingly abstract and foreign nature of the time and length scales involved. The Smart Energy Freshmen Research Immersion (FRI) program at Binghamton University was created as a way to address this issue and, in turn, improve undergraduate performance and retention in physics and chemistry. Using real-world research problems as a wider context to frame their understanding, we have developed a course sequence providing a more intuitive and comprehensive understanding of core physics and chemistry concepts over the course of the program. Advanced condensed matter topics, such as optical band gaps, crystal and electronic structure, and electron/hole conduction are introduced to students through hands-on, authentic research activities incorporating materials for real-world device applications. I will discuss how employing p-n junctions as a model device can allow for a natural and intuitive progression from basic to advanced physics and chemistry concepts. This approach illustrates how shifting exotic concepts into a more relatable form through the use of analogy is important for fostering a more intuitive understanding of physical phenomena.

**2:03PM S7.00015 Transferring a Flipped Class in Algebra-based Physics to New Faculty<sup>1</sup>**, LEIGH SMITH, ALEXANDRE SOUSA, Department of Physics, University of Cincinnati — Transferring existing active classroom educational efforts to new faculty is a challenge that must be met to ensure sustainability of changes. We describe a flipped class approach to teaching algebra-based Physics being transferred to a new faculty member. This flipped class includes extensive video and reading-based preparation materials outside of class, and the use of Learning Catalytics for in-class work is developed and tested by one of the authors. These materials are of course idiosyncratic to the style of the developer. Student results using the new materials are compared with students in more standard classes which suggest significant positive benefit over several years. A faculty member decided to use these materials in his own section of the same course. Our experience shows that it takes some time for the new faculty member to use and adapt the materials in a way which matches his own style, which in the end results in equivalently enhanced results. Lessons learned from this transfer process will be discussed.

<sup>1</sup>We acknowledge the financial support of the NSF through DUE 1544001 and 1431350.

**Thursday, March 17, 2016 11:15AM - 2:15PM –**  
**Session S8 DMP: Electrical Transport and Photoexcitations in Organic/Inorganic Perovskites**  
304 - Jisong Huang, University of Nebraska Lincoln

**11:15AM S8.00001 Charge Transport in Hybrid Halide Perovskite Field-Effect Transistors<sup>1</sup>**, OANA JURCHESCU, Wake Forest University, Department of Physics — Hybrid organic-inorganic trihalide perovskite (HTP) materials exhibit a strong optical absorption, tunable band gap, long carrier lifetimes and fast charge carrier transport. These remarkable properties, coupled with their reduced complexity processing, make the HTPs promising contenders for large scale, low-cost thin film optoelectronic applications. But in spite of the remarkable demonstrations of high performance solar cells, light-emitting diodes and field-effect transistor devices, all of which took place in a very short time period, numerous questions related to the nature and dynamics of the charge carriers and their relation to device performance, stability and reliability still remain. This presentation describes the electrical properties of HTPs evaluated from field-effect transistor measurements. The electrostatic gating of provides a unique platform for the study of intrinsic charge transport in these materials, and, at the same time, expand the use of HTPs towards switching electronic devices, which have not been explored previously. We fabricated FETs on SiO<sub>2</sub> and polymer dielectrics from spin coating, thermal evaporation and spray deposition and compare their properties. CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3-x</sub>Cl<sub>x</sub> can reach balanced electron and hole mobilities of 10 cm<sup>2</sup>/Vs upon tuning the thin-film microstructure, injection and the defect density at the semiconductor/dielectric interface. The work was performed in collaboration with Yaochuan Mei (Wake Forest University), Chuang Zhang, and Z. Valy Vardeny (University of Utah).

<sup>1</sup>The work is supported by ONR grant N00014-15-1-2943.

**11:51AM S8.00002 Understanding charge transport in organometal halide field effect transistors.**<sup>1</sup>, SATYAPRASAD P SENANAYAK, BINGYAN YANG, ADITYA SADHANALA, PROF. SIR RICHARD FRIEND, PROF. HENNING SIRRNIGHAUS, Optoelectronics Group, Cavendish Laboratory, University of Cambridge — Organometal halide based perovskite are emerging materials for wide range of electronic applications. A range of optoelectronic applications like high efficiency solar cells, color pure LEDs and optical pumped lasers have been demonstrated. Here, we report the demonstration of a high performance field effect transistor fabricated from iodide perovskite material at room temperature. The devices exhibit clean saturation behavior with electron  $\mu_{\text{FET}} > 3 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1}$  and current modulation in the range of  $10^6 - 10^7$  which are till date the best performance achieved with these class of materials. This high performance is attributed to a combination of novel film fabrication technique and device engineering strategies. Detailed understanding of the observed band-like transport phenomenon is developed by tuning the different sources of dynamic and static disorder prevalent in the system. These finding are expected to pave way for developing next generation electronic application from perovskite materials.

<sup>1</sup>Authors acknowledge EPSRC for funding and SPS acknowledges Royal Society Newton Fellowship

**12:03PM S8.00003 Charge carrier transport properties of methyl-ammonium-lead-trihalide perovskites investigated by the time-of-flight method**<sup>1</sup>, EVAN LAFALCE, CHUANG ZHANG, Z. VALY VARDENY, University of Utah, UNIVERSITY OF UTAH TEAM — We studied the charge transport properties of methyl-ammonium-lead-trihalide perovskites using the photocurrent transient time-of-flight method. Various morphologies that include single-crystals and thin films with different crystalline grain sizes and surface roughness were investigated. The photocurrent transients were recorded as a function of excitation wavelength, intensity, and applied electric field as well as the sample temperature. We found that surface recombination leads to a photocurrent response that is sharply peaked at the band edge. While the carrier mobility depends on the sample preparation and sample temperature, typical values are on the order of  $1 \text{ cm}^2/\text{Vs}$ , consistent with previous reports using similar methods. This value is high compared to other solution-processed semiconductors such as pi-conjugated polymers and quantum dots; however it is relatively low compared to inorganic semiconductors. Therefore determining the mobility limiting factors in hybrid perovskite devices is important for progress in their optoelectronic device performance.

<sup>1</sup>This work was funded by ONR grant N00014-15-1-2524 at the Un. of Utah.

**12:15PM S8.00004 ABSTRACT WITHDRAWN —**

**12:27PM S8.00005 Electronic Structure Approach to Tunable Electronic Properties of Hybrid Organic-Inorganic Perovskites**, GARNETT LIU, Department of Chemistry, Duke University, Durham, NC 27708, WILLIAM HUHN, DAVID B. MITZI, MEMS Department, Duke University, Durham, NC 27708, YOSUKE KANAI, Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599, VOLKER BLUM, MEMS Department, Duke University, Durham, NC 27708 — We present a study of the electronic structure of layered hybrid organic-inorganic perovskite (HOIP) materials using all-electron density-functional theory. Varying the nature of the organic and inorganic layers should enable systematically fine-tuning the carrier properties of each component. Using the HSE06 hybrid density functional including spin-orbit coupling (SOC), we validate the principle of tuning subsystem-specific parts of the electron band structures and densities of states in  $\text{CH}_3\text{NH}_3\text{PbX}_3$  ( $\text{X}=\text{Cl}, \text{Br}, \text{I}$ ) compared to a modified organic component in layered  $(\text{C}_6\text{H}_5\text{C}_2\text{H}_4\text{NH}_3)_2\text{PbX}_4$  ( $\text{X}=\text{Cl}, \text{Br}, \text{I}$ ) and  $\text{C}_{20}\text{H}_{22}\text{S}_4\text{N}_2\text{PbX}_4$  ( $\text{X}=\text{Cl}, \text{Br}, \text{I}$ ). We show that tunable shifts of electronic levels indeed arise by varying  $\text{Cl}, \text{Br}, \text{I}$  as the inorganic components, and  $\text{CH}_3\text{NH}_3^+$ ,  $\text{C}_6\text{H}_5\text{C}_2\text{H}_4\text{NH}_3^+$ ,  $\text{C}_{20}\text{H}_{22}\text{S}_4\text{N}_2^+$  as the organic components. SOC is found to play an important role in splitting the conduction bands of the HOIP compounds investigated here. The frontier orbitals of the halide shift, increasing the gap, when  $\text{Cl}$  is substituted for  $\text{Br}$  and  $\text{I}$ .

**12:39PM S8.00006 Electronic properties of  $\text{CH}_3\text{NH}_3\text{PbBr}_3$  (001) surface**, XIN HUANG, TULA PAUDEL, University of Nebraska-Lincoln, SHUAI DONG, Southeast University, China, EVGENY TSYMBAL, University of Nebraska-Lincoln — The energetics and electronic properties of cubic  $\text{CH}_3\text{NH}_3\text{PbBr}_3$  (001) surfaces are studied using a first-principles method. We find that the uncompensated intrinsic dipole moment of a  $\text{CH}_3\text{NH}_3$  molecule induces a band bending, being larger for the  $\text{PbBr}_2$ -terminated surface than for the  $\text{CH}_3\text{NH}_3\text{Br}$ -terminated surface. When the intrinsic dipole are fully compensated, the surface electronic structure shows new states near band edges for both  $\text{MABr}$  and  $\text{PBB}_2$  terminations. We find that for the  $\text{PbBr}_2$ -terminated surface, less dispersive surface states appear just above the bulk valence bands at the center of Brillouin zone ( $\Gamma$  point), while for the  $\text{CH}_3\text{NH}_3\text{Br}$ -terminated surface, more dispersive surface states appear below the conduction bands at the  $\text{M}$  point. These states effectively reduce the band gap and improve optical absorption properties. The  $\text{PbBr}_2$ -terminated surface states are of the  $\text{Pb-p}$  character, and hence are strongly affected by spin-orbit coupling, whereas the  $\text{CH}_3\text{NH}_3\text{Br}$ -terminated surface states are of the  $\text{Pb-s}$  character and hence are not affected by the spin-orbit coupling effect. Our study suggests a way to tune the spin-orbit coupling by selecting an appropriate surface.

**12:51PM S8.00007 Phase stability, electronic structure and phonons in  $\text{CsGeI}_3$** <sup>1</sup>, LING-YI HUANG, WALTER LAMBRECHT, Case Western Reserve Univ — Because  $\text{Ge}$  is smaller than  $\text{Sn}$  and  $\text{Pb}$ ,  $\text{CsGeI}_3$  is promising to overcome the stability problems of the perovskite forms of  $\text{CsSnI}_3$  and  $\text{CsPbI}_3$  halides toward the denser yellow phase in which octahedra are edge as well as cornersharing in one dimensional chains. This phase has higher gaps and is unsuitable for photovoltaics.  $\text{CsGeI}_3$  and other trihalide germanates are found to exist in the cubic perovskite phase at high temperature but in a rhombohedral phase in which the  $\text{Ge}$  is displaced toward three of the halogen neighbors in its surrounding octahedron, accompanied by a rhombohedral distortion of the lattice vectors. We will present density functional total energy calculations and band structures obtained within the quasi-particle self-consistent  $\text{GW}$  method for both the cubic and rhombohedral phase of  $\text{CsGeI}_3$ . For the latter, we find a gap of 1.6 eV in excellent agreement with recent experiments on its absorption edge. We will also present optical dielectric function and effective mass results for this material and discuss the trends for different types of distortions in halides depending on the chemical composition. The phonons at the Brillouin zone center are calculated and compared to experimental Raman spectra.

<sup>1</sup>NSF and DOE

**1:03PM S8.00008 Interface Engineering in Metal Halides Perovskites: from molecules to devices.**, ANNAMARIA PETROZZA, Istituto Italiano di Tecnologia — In this talk we review our recent studies which aim to clarify the relationship between structural and electronic properties from a molecular to mesoscopic level. First we identify the markers for local disorder at molecular level by using Raman Spectroscopy as a probe. Then, we exploit such a tool to explore the role of microstructure on the absorption and emission properties of the semiconductor looking both at polycrystalline thin films and single crystals. We address the controversy surrounding electron hole interactions and excitonic effects. We show that in hybrid lead-halide perovskites dielectric screening also depends on the local microstructure of the hybrid crystals and not only on its chemical composition. This leads to the possibility of band gap engineering and the consequent control of the elementary photo-excitation dynamics that determine the perovskites performances in different optoelectronic devices. Finally, the role of interface engineering, the effect of ion migration, and interface doping on charge extraction will be elucidated to provide a guideline for the design of hysteresis free solar cells. 1)G. Grancini & AR Srimath Kandada et al, Nature Photonics, 9 (10), 695-701, 2015 2) C. Tao et al, Energy Environ. Sci., 8, 2365-2370, 2015

**1:39PM S8.00009 Transient Spectroscopy of Photoexcitations and Morphology Control of Organometal Trihalide Perovskites<sup>1</sup>**, YAXIN ZHAI, EVAN LAFALCE, Univ of Utah, CHUAN-XIANG SHENG, Nanjing University of Science and Technology, CHUANG ZHANG, DALI SUN, ZEEV VALY VARDENY, Univ of Utah — We studied the photoexcitation dynamics in various hybrid perovskites by using broadband ps transient photomodulation (PM) spectroscopy and variable stripe length (VSL) technique. We observed both excitonic and free carriers spectral features in MAPbI<sub>3</sub> but mainly excitonic transition in MAPbI<sub>1.1</sub>Br<sub>1.9</sub> and MAPbI<sub>3-x</sub>Cl<sub>x</sub> films. We also fabricated MAPbBr<sub>3</sub> films with nano-crystal pinning (NCP) treatment, which allows for smaller crystalline grain size. The transient spectra show a narrower and longer-lived photobleaching band in NCP treated films consistent with the increase in the photoluminescence efficiency. In addition the net optical gain measured by VSL is markedly increased up to 300 cm<sup>-1</sup>, and the lasing threshold is concurrently reduced. Measurement of the waveguide losses in the NCP films shows that the improvement in lasing properties can partly be attributed to the reduced optical scattering.

<sup>1</sup>Work supported by the AFOSR through a MURI grant RA 9550-14-1-0037

**1:51PM S8.00010 Photoluminescence and lasing properties of MAPbBr<sub>3</sub> single crystals grown from solution<sup>1</sup>**, SANDIP ARYAL, EVAN LAFALCE, CHUANG ZHANG, YAXIN ZHAI, Z. VALY VARDENY, University of Utah — Recent studies of solution-grown single crystals of inorganic-organic hybrid lead-trihalide perovskites have suggested that surface traps may play a significant role in their photophysics. We study electron-hole recombination in single crystal MAPbBr<sub>3</sub> through such trap states using cw photoluminescence (PL) and ps transient photoinduced absorption (PA) spectroscopies. By varying the depth of the collecting optics we examined the contributions from surface and bulk radiative recombination. We found a surface dominated PL band at the band-edge that is similar to that observed from polycrystalline thin films, as well as a weaker red-shifted emission band that originates from the bulk crystal. The two PL bands are distinguished in their temperature, excitation intensity and polarization dependencies, as well as their ps dynamics. Additionally, amplified spontaneous emission and crystal-related cavity lasing modes were observed in the same spectral range as the PL band assigned to the surface recombination.

<sup>1</sup>This work was funded by AFOSR through MURI grant RA 9550-14-1-0037.

**2:03PM S8.00011 Ultrafast Extreme Ultraviolet Spectroscopy of Lead Iodide and Methylammonium Lead Iodide**, MAX VERKAMP, MING-FU LIN, ELIZABETH RYLAND, JOSH VURA-WEIS, University of Illinois at Urbana-Champaign — Methylammonium lead iodide (perovskite) is a leading candidate for use in next-generation solar cell devices. However, the photophysics of perovskite responsible for its strong photovoltaic qualities are not fully understood. Ultrafast extreme ultraviolet (XUV) spectroscopy was used to investigate relaxation dynamics in perovskite and its precursor, lead iodide, with carrier-specific signals arising from transitions from a common inner-shell level (I 4d) to the valence and conduction bands. Ultrashort (30 fs) pulses of XUV radiation in a broad spectrum (40-70 eV) were obtained using high-harmonic generation in a tabletop instrument. Transient absorption measurements with visible pump (3.1 eV) and XUV probe directly observed the relaxation of charge carriers after above band excitation for both perovskite and lead iodide in the femtosecond and picosecond time ranges.

## Thursday, March 17, 2016 11:15AM - 2:15PM –

Session S11 GMAG DMP: Thin Film Skyrmions 307 - Wanjun Jiang, Argonne National Laboratory

**11:15AM S11.00001 Synthesizing Skyrmion Molecules in Fe-Gd Thin Films<sup>1</sup>**, J. C. T LEE, Materials Sciences Division, Lawrence Berkeley National Laboratory, J. CHESS, Dept. of Physics, University of Oregon, Eugene, S. A. MONTROYA, Center for Magnetic Recording Research, UC San Diego, X. W. SHI, Dept. of Physics, University of Oregon, Eugene, NOBUMICHI TAMURA, S. K. MISHRA, Advanced Light Source, LBNL, D. H. PARKS, Dept. of Physics, University of Oregon, Eugene, P. FISCHER, MSD, LBNL; and Dept. of Physics, UC Santa Cruz, B. MCMORRAN, Dept. of Physics, University of Oregon, Eugene, S. K. SINHA, Dept. of Physics, UC San Diego, E. FULLERTON, Center for Magnetic Recording Research, UC San Diego, S. D. KEVAN, Dept. of Physics, University of Oregon, Eugene; ALS and MSD, LBNL, S. ROY, Advanced Light Source, LBNL — Controlled creation of tunable skyrmion phases at room temperature holds the promise of advanced spintronics applications using these topological entities. By varying the composition and thickness of an amorphous Fe-Gd thin film and optimizing the applied field protocol, we produced at room temperature an ordered, achiral phase of skyrmion molecules, that is, bound pairs of magnetic skyrmions having the same polarity but opposite helicity. This phase appears between stripe and uniform magnetization phase and its origin lies in the existence of mirror planes in the stripe domain structure. Dipolar, exchange, and anisotropy forces are the dominant interactions in these materials, while the role of bulk and surface chiral exchange interactions is small.

<sup>1</sup>Supported by the Basic Energy Sciences, US DOE: DE-AC02-05CH11231; DE- FG02-11ER46831; and DE-SC0003678

**11:27AM S11.00002 Chirality evaluation of spin spiral in Mn thin film on W(110)**, MASAHIRO HAZE, YASUO YOSHIDA, YUKIO HASEGAWA, The Institute for Solid State Physics, The University of Tokyo — In crystal fields with broken inversion symmetry such as surfaces or interfaces, the Dzyaloshinskii-Moriya interaction (DMI), which is induced by the spin orbit interaction, may have a significant contribution to the formation of spin structures. Because of DMI, magnetic thin films formed on a heavy-elemental substrate such as W often exhibit peculiar spin spiral structures whose chirality is fixed and determined by the polarity of DMI. Investigating the chirality of spin structures is thus important to reveal the formation mechanism of spin structures and, more specifically, to determine whether DMI plays a decisive role on it. Monolayer (ML) Mn thin films formed on W(110), the first surface spin spiral structures, show a cycloidal spin spiral structure propagating along to [1-10] axis. Spin-polarized scanning tunneling microscopy (SP-STM) and theoretical analysis based on density functional calculation revealed left-handed chirality of the structure and concluded that it is driven by DMI. A SP-STM recent study revealed that double layer (DL) Mn thin films on W(110) show a conical spin spiral structure whose propagation direction is along [001]. The chirality and its driving interaction, however, have not been revealed yet. Here in this study, we have investigated the chirality of DL Mn by SP-STM. Our experimental results revealed that the spin spiral structure of DL Mn is homochiral but right-handed, which is opposite to that of ML Mn. In the presentation we will discuss different roles of DMI exerted on the two Mn thin films.

**11:39AM S11.00003 Determination of interfacial Dzyaloshinskii-Moriya exchange interaction from static domain size imaging**, PARNIKA AGRAWAL, IVAN LEMESH, MIT, SARAH SCHLOTTER, Harvard University, GEOFFREY BEACH, MIT — Dzyaloshinskii-Moriya interaction (DMI) has been identified [1-2] as a necessary ingredient for the formation of chiral spin structures such as skyrmions and Néel domain walls in perpendicularly magnetized thin films. Various simulation and experimental studies have tried to quantify DMI from domain wall [2] and skyrmion [3-4] motion with applied currents and magnetic fields. Here, a means to quantify DMI in multilayer films using only static magnetic characterizations is proposed. Static domain structure is observed using magnetic force microscopy (MFM) in multilayer stacks of [Pt(2.5-7.5nm)/CoFeB(0.8nm)/MgO(1.5nm)]<sub>15</sub> where the thickness  $t_{pt}$  of the Pt layer is systematically varied from 2.5 nm to 7.5 nm. A variation of domain size from ~300 nm to ~70 nm is seen in the labyrinthine demagnetized state as  $t_{pt}$  is decreased. It is shown that the domain size as a function of  $t_{pt}$  can be well-fitted analytically by a model in which the domain wall energy is the sole free parameter. Additional measurements of magnetic anisotropy of the film reveal the significant contribution of interfacial DMI (~1.4 mJ/m<sup>2</sup>) to the domain wall energy. Ref: 1.Fert et al., *Nat. Nanotech.*, 8, 152-156 (2013); 2. S. Emori et al., *Nature Materials* 12,611–616 (2013); 3. S. Woo et al., arXiv:1502.07376; 4.W. Jiang et al., arXiv:1502.08028v1

**11:51AM S11.00004 Interface-induced skyrmions in magnetic films and multilayers**, ALBERT FERT, CNRS/THALES and Universit Paris Saclay, Palaiseau, France — The talk is on individual skyrmions induced by interface Dzyaloshinskii-Moriya Interactions (DMI) in thin magnetic films or multilayers. I will present:

1. Ab-initio calculations of the characteristic features of interface DMI [1]: extension of the DMI away from the interface in the magnetic film, thickness dependence, influence of the existence of proximity-induced magnetism in neighbor layers, influence of interface roughness, perspective with new materials. . .
2. Experimental results on small skyrmions at room temperature in (Ir/Co/Pt) $\times$ 10 multilayers [2].
3. Towards applied devices: micromagnetic simulations of the nucleation and current-induced motion of skyrmions [3].

[1] H. Yang et al, arXiv:1501.055112. [2] C. Moreau-Luchaire et al, arXiv: 1502.07853. [3] J. Sampaio et al. Nat. Nanotech. 8, 839-844 (2013).

**12:27PM S11.00005 Observation of sub-100 nm Néel skyrmions at room temperature**<sup>1</sup>, S.G.E. TE VELTHUIS, W. JIANG, S. ZHANG, C. PHATAK, W. ZHANG, M.B. JUNGFLIECH, J.E. PEARSON, A. PETFORD-LONG, A. HOFFMANN, Argonne National Laboratory — Magnetic skyrmions are topologically stable spin textures that have attracted tremendous attention in the field of spintronics. As compared to Bloch skyrmions, which are typical for only few bulk chiral magnets, Néel skyrmions in magnetic multilayers [1, 2, 3] may be more ubiquitous and have the advantage that included layers of heavy metals provide efficient current induced spin-orbit torques. By optimizing the stacking structure, we present an experimental strategy towards nanometer-scale skyrmions at room temperature in the absence of a magnetic field. Furthermore, we discuss the experimental challenge of identifying the chiral nature of Néel skyrmions by using Lorentz transmission electron microscopy. Our results constitute an important step for enabling skyrmion based ultra-high density data storage, and for probing topological physics at room temperature. [1] W. Jiang, et al., Science, 349, 283 (2015). [2] S. Woo, et al., arXiv:1502.07376 (2015). [3] C. Moreau-Luchaire, et al., arXiv:1502.07853 (2015).

<sup>1</sup>Work supported by the Department of Energy, Office of Science, Basic Energy Science, Materials Sciences and Engineering Division.

**12:39PM S11.00006 Skyrmions in thin-film multilayers with interfacially-induced Dzyaloshinskii-Moriya interaction observed by MFM**, MIRKO BACANI, MIGUEL A. MARIONI, JOHANNES SCHWENK, SARA ROMER, XUE ZHAO, ALEXANDRE GUILLER, Empa, Duebendorf, Switzerland, HANS J. HUG, Empa, Duebendorf, Switzerland and Department of Physics, University of Basel, Basel, Switzerland — By proper selection of interfaces in thin-film multilayers one can separately engineer the anisotropy, magnetization and Dzyaloshinskii-Moriya interaction (DMI), which is useful in the design of skyrmion materials. We use high-sensitivity, high-resolution magnetic force microscopy (MFM) in various applied magnetic fields to image the micromagnetic structures in multilayers based on symmetric-interface stacks of Pt/Co/Pt and asymmetric ones of Pt/Co/Ir. The former have domain sizes of several microns, whereas the latter show considerably smaller domain sizes. These are (246 $\pm$ 40) nm independently of the demagnetization process used. We attribute the lower domain size to a net DMI. The calculated DMI in the asymmetric case is too small to support a skyrmion phase, but isolated skyrmions can exist. MFM experiments reveal skyrmions with a diameter below 50 nm, when the field is reduced from positive saturation. In negative fields these skyrmions are either incorporated into expanding domains or burst into a larger domain. Local DMI constants estimated from the bursting fields agree well with the average DMI constant. Our work demonstrates that MFM can detect skyrmions in thin films, and can help accelerate research in this field.

**12:51PM S11.00007 Engineering of the anisotropy and Dzyaloshinskii-Moriya interaction energies in Pt-Co and Pt-Co-Cu heterostructures**, SARAH SCHLOTTER, Harvard University SEAS, GEOFFREY BEACH, Massachusetts Inst of Tech-MIT — It has previously been shown that perpendicular magnetic anisotropy is increased in Pt-Co-Pt structures by placing a Cu spacer between the top, diffuse Co-Pt interface.<sup>1</sup> However, including a spacer layer increases interfacial asymmetry in the system: a prerequisite for a strong Dzyaloshinskii-Moriya interaction (DMI) which governs helical spin structures such as skyrmions and chiral domain walls.<sup>2</sup> We show that the increased asymmetry significantly enhances DMI strength in Pt-Co-Cu-Pt heterostructures as compared to corresponding Pt-Co-Pt systems. We further show that one can control the characteristic length scales governing domain width by engineering the magnetostatic, anisotropy, and DMI energies in heavy-metal/ferromagnet heterostructures. These structures may provide insight into engineering the size of skyrmions in spintronic devices.

<sup>1</sup>S. Bandiera et al, **Appl. Phys. Lett.** 100, 142410 (2012)

<sup>2</sup>S. Emori et al, **Nature Mater.** 12, 611-616 (2013)

**1:03PM S11.00008 Skyrmion bubble stability in thin films with strong Dzyaloshinskii-Moriya interaction**, LUCAS CARETTA, UWE BAUER, ALEXANDRA CHURIKOVA, MAXWELL MANN, GEOFFREY BEACH, Massachusetts Inst of Tech-MIT — The Dzyaloshinskii-Moriya interaction (DMI) at heavy-metal/FM interfaces stabilizes chiral spin textures, such as magnetic skyrmions [1]. Magnetic skyrmions are applicable to energy efficient spintronics [2,3]. However, room temperature stability of skyrmion bubbles (SBs) has not been quantified experimentally. We show when the ratio of the DMI effective field to the perpendicular anisotropy field is large, expanding bubble domains leave behind fine-scale dendritic structure, consisting of coupled 360 degree domain walls (DW). Dendritic structures are manipulated to form stable SBs. We imaged SBs in Pt(3nm)/Co(0.9nm)/Gd(1nm)/GdOx(30nm) films using Kerr microscopy to characterize the stability of SBs. We show that the field stability of SBs is a strong function of the applied in-plane field. Increasing in-plane field reduces the annihilation threshold of the skyrmions. The SB annihilation field becomes deterministic at in-plane fields near the DMI effective field. Simulations show Bloch points are formed in the SB DW at high in-plane fields, leading to the deterministic collapse of the bubbles.[1] A. Fert et al., Nat. Nano., 8, 152-156 (2013) [2] S. Woo et al., arXiv:1502.07376 (2015) [3] A. Fert et al., arXiv:1502.07853 (2015)

**1:15PM S11.00009 Skyrmion-induced bound states on the surface of 3D Topological Insulators**, DIMITRIOS ANDRIKOPOULOS<sup>1</sup>, BART SOREE<sup>2</sup>, Katholieke Univ Leuven — In this work, we study the interaction between the surface state of a 3D Topological Insulator and a skyrmion magnetic texture. The skyrmion texture couples to the spin of the surface state electron with strength  $\Delta_S$ . Vortex and hedgehog skyrmion and anti-skyrmion structures are considered and their interaction is compared. Due to the vortex structure, the interaction of the in-plane components can be neglected and a step function is used to describe the skyrmion magnetization profile. In the hedgehog case, it is shown that the in-plane components cannot be disregarded and thus a realistic description for the skyrmion is required. Working in the micromagnetic framework, we derive a macrospin description for the skyrmion using the variational principle and then numerically solve for the bound states. It is shown that the existence and properties of these states as a function of skyrmion size, strongly depend on the skyrmion type. Both vortex and hedgehog skyrmions or anti-skyrmions can induce bound states with energies  $|E| < \Delta_S$ . For the hedgehog skyrmion case however, bound state appearance depends on the chirality. Finally, the probability densities in these states are computed and it is demonstrated that the electrons are localized throughout the skyrmion region.

<sup>1</sup>Also affiliated with imec, Belgium

<sup>2</sup>Also affiliated with imec, Belgium

**1:27PM S11.00010 Skyrmion-induced bound states in a superconductor<sup>1</sup>**, SERGEY S. PERSHOGUBA, Nordita, Center for Quantum Materials, KTH Royal Institute of Technology, and Stockholm University, Roslagstullsbacken 23, S-106 91 Stockholm, Sweden, SHO NAKOSAI, Condensed Matter Theory Laboratory, RIKEN, Wako, Saitama, 351-0198, Japan, ALEXANDER V. BALATSKY, Institute for Materials Science, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — We consider a superconductor proximity coupled to a two-dimensional ferromagnetic film with a skyrmion texture. We predict the skyrmion bound states (SBS) that are induced in the superconductor, similar to the well-known Yu-Shiba-Rusinov (YSR) states. Using the T-matrix calculations and numerical modeling we calculate the spin-polarized local density of states in the superconductor in the vicinity of the skyrmion. The SBS wavefunctions have spatial power-law decay. Presence of the SBS suggests the mechanism by which superconductivity could facilitate an effective long-range interaction between skyrmions when their SBS wavefunctions overlap. arXiv:1511.01842

<sup>1</sup>S.S.P. and A.V.B are supported by US DOE BES E304. S.N. is supported by the Grant-in-Aid for Research Activity Start-up (No. 15H06858).

**1:39PM S11.00011 Stability of skyrmion lattices and symmetries of Dzyaloshinskii-Moriya magnets<sup>1</sup>**, UTKAN GÜNGÖRDÜ, RABINDRA NEPAL, Univ of Nebraska - Lincoln, OLEG A. TRETIKOV, Tohoku Univ, KIRILL BELASHCHENKO, ALEXEY A. KOVALEV, Univ of Nebraska - Lincoln — Recently, there has been substantial interest in realizations of skyrmions, in particular in 2D systems due to increased stability resulting from reduced dimensionality. A stable skyrmion, representing the smallest realizable magnetic texture, could be an ideal element for ultra-dense magnetic memories. Here, we use the most general form of the 2D free energy with Dzyaloshinskii-Moriya interactions constructed from general symmetry considerations reflecting the underlying system. We predict that skyrmion phase is robust and it is present even when the system lacks the in-plane rotational symmetry. In fact, the lowered symmetry leads to increased stability of vortex-antivortex lattices with four-fold symmetry and in-plane spirals, in some instances even in the absence of an external magnetic field. Our results relate different hexagonal and square cell phases to the symmetries of materials used for realizations of skyrmions. This will give clear directions for experimental realizations of hexagonal and square cell phases, and will allow engineering of skyrmions with unusual properties. We also predict striking differences in gyro-dynamics induced by spin currents for isolated skyrmions and for crystals where spin currents can be induced by charge carriers or by thermal magnons.

<sup>1</sup>DOE Early Career Award DE-SC0014189, NSF Grants Nos. Phy-1415600, PHY11-25915, DMR-1420645, and DMR-1308751; Grants-in-Aid from MEXT and SpinNet (Nos. 25800184, 25247056, and 15H01009)

**1:51PM S11.00012 Increasing skyrmion lattice stability: theory and experiment**, ALEX KRUCHKOV, Ecole Polytechnique Federale de Lausanne (EPFL), JONATHAN WHITE, Paul Scherrer Institut (PSI), HENRIK RONNOW, IVICA ZIVKOVIC, Ecole Polytechnique Federale de Lausanne (EPFL) — Magnetic skyrmions are vortices of spins, considered to be topologically protected against perturbations, and envisaged as very possible next-generation information carriers due to their nanoscale size. In chiral ferromagnets they form a two-dimensional hexagonal array - the skyrmion lattice. A key challenge is that bulk skyrmions have been restricted so far to a tiny region in the temperature-field phase diagram. In this work we address theoretically the stability of the skyrmion lattice. We demonstrate that tuning anisotropy can lead to dramatic (20 times) enhancement of the skyrmion phase volume, which has been recently revealed in our experiment.

**2:03PM S11.00013 Enhanced stability of skyrmions in magnets with broken mirror symmetry<sup>1</sup>**, JAMES ROWLAND, Ohio State University, SUMILAN BANERJEE, Weizmann Institute of Science, MOHIT RANDEIRA, Ohio State University — Most previous work on skyrmion phases in chiral magnets with Dzyaloshinskii-Moriya interactions (DMI) focuses on the case of broken bulk inversion symmetry. The skyrmion crystal is then stable only in a limited range of parameter space with easy-axis anisotropy. In this talk I will describe the effects [1] of including broken mirror or surface inversion symmetry which leads to a Rashba DMI, in addition to the Dresselhaus DMI arising from broken bulk inversion. I will show that increasing Rashba DMI leads to a progressively larger domain of stability for skyrmions, especially in the easy-plane anisotropy regime. In the latter regime the topological charge density shows an unusual internal structure, and isolated skyrmions cannot be embedded in a ferromagnetic background. Thus the homotopy group  $\pi_2(S^2)$  method of classifying skyrmions fails. I will discuss a Chern number classification of these non-trivial skyrmions using maps from the 2-torus (the unit cell for skyrmion crystals) to the 2-sphere in spin space. Finally, I will discuss the elliptic cone phase, a new state that emerges for easy-axis anisotropy and broken mirror symmetry. [1] J. Rowland, S. Banerjee, and M. Randeria, arXiv:1509.07508v2.

<sup>1</sup>We acknowledge support by the National Science Foundation by the NSF Graduate Research Fellowship Program Grant No. DGE-1343012 (JR), by an NSF grant DMR-1410364 (MR), and by the CEM, an NSF MRSEC, under grant DMR-1420451.

**Thursday, March 17, 2016 11:15AM - 2:15PM –**  
**Session S12 FIAP GIMS: Prospects and Challenges in Medical Physics and Imaging** 308 - Larry Nagahara, Johns Hopkins University

**11:15AM S12.00001 Future Directions in Medical Physics**, ROBERT JERAJ, University of Wisconsin — Medical Physics is a highly interdisciplinary field at the intersection between physics and medicine and biology. Medical Physics is aiming at development of novel applications of physical processes and techniques in various areas of medicine and biology. Medical Physics had and continues to have profound impact by developing improved imaging and treatment technologies, and helping to advance our understanding of the complexity of the disease. The general trend in medicine towards personalized therapy, and emphasis on accelerated translational research is having a profound impact on medical physics as well. In the traditional stronghold for medical physicists – radiation therapy – the new reality is shaping in the form of biologically conformal and combination therapies, as well as advanced particle therapy approaches, such as proton and ion therapies. Rapid increase in faster and more informative multi-modality medical imaging is bringing a wealth of information that is being complemented with data obtained from genomic profiling and other biomarkers. Novel data analysis and data mining approaches are proving grounds for employment of various artificial intelligence methods that will help further improving clinical decision making for optimization of various therapies as well as better understanding of the disease properties and disease evolution, ultimately leading to improved clinical outcomes.

**11:51AM S12.00002 Opportunities of using Stimulated Emission from Biological Tissue**, S. H. ANDY YUN, Harvard Medical School and Massachusetts General Hospital — Fluorescence or spontaneous emission has been a powerful tool in biomedical applications ranging from biochemical assays and cytometry to microscopy and medical imaging. Here I present the opportunities in the generation and applications of coherent stimulated emission within biological samples.

**12:27PM S12.00003 Future Directions in Medical Physics: Models, Technology, and Translation to Medicine<sup>1</sup>** , JEFFREY SIEWERDSEN, Johns Hopkins University — The application of physics in medicine has been integral to major advances in diagnostic and therapeutic medicine. Two primary areas represent the mainstay of medical physics research in the last century: in radiation therapy, physicists have propelled advances in conformal radiation treatment and high-precision image guidance; and in diagnostic imaging, physicists have advanced an arsenal of multi-modality imaging that includes CT, MRI, ultrasound, and PET as indispensable tools for noninvasive screening, diagnosis, and assessment of treatment response. In addition to their role in building such technologically rich fields of medicine, physicists have also become integral to daily clinical practice in these areas. The future suggests new opportunities for multi-disciplinary research bridging physics, biology, engineering, and computer science, and collaboration in medical physics carries a strong capacity for identification of significant clinical needs, access to clinical data, and translation of technologies to clinical studies. In radiation therapy, for example, the extraction of knowledge from large datasets on treatment delivery, image-based phenotypes, genomic profile, and treatment outcome will require innovation in computational modeling and connection with medical physics for the curation of large datasets. Similarly in imaging physics, the demand for new imaging technology capable of measuring physical and biological processes over orders of magnitude in scale (from molecules to whole organ systems) and exploiting new contrast mechanisms for greater sensitivity to molecular agents and subtle functional / morphological change will benefit from multi-disciplinary collaboration in physics, biology, and engineering. Also in surgery and interventional radiology, where needs for increased precision and patient safety meet constraints in cost and workflow, development of new technologies for imaging, image registration, and robotic assistance can leverage collaboration in physics, biomedical engineering, and computer science. In each area, there is major opportunity for multi-disciplinary collaboration with medical physics to accelerate the translation of such technologies to clinical use.

<sup>1</sup>Research supported by the National Institutes of Health, Siemens Healthcare, and Carestream Health

**1:03PM S12.00004 Imaging and Analytics: The changing face of Medical Imaging** , THOMAS FOO, GE Global Research — There have been significant technological advances in imaging capability over the past 40 years. Medical imaging capabilities have developed rapidly, along with technology development in computational processing speed and miniaturization. Moving to all-digital, the number of images that are acquired in a routine clinical examination has increased dramatically from under 50 images in the early days of CT and MRI to more than 500-1000 images today. The staggering number of images that are routinely acquired poses significant challenges for clinicians to interpret the data and to correctly identify the clinical problem. Although the time provided to render a clinical finding has not substantially changed, the amount of data available for interpretation has grown exponentially. In addition, the image quality (spatial resolution) and information content (physiologically-dependent image contrast) has also increased significantly with advances in medical imaging technology. On its current trajectory, medical imaging in the traditional sense is unsustainable. To assist in filtering and extracting the most relevant data elements from medical imaging, image analytics will have a much larger role. Automated image segmentation, generation of parametric image maps, and clinical decision support tools will be needed and developed apace to allow the clinician to manage, extract and utilize only the information that will help improve diagnostic accuracy and sensitivity. As medical imaging devices continue to improve in spatial resolution, functional and anatomical information content, image/data analytics will be more ubiquitous and integral to medical imaging capability.

**1:39PM S12.00005 NIH Funding for Biomedical Imaging<sup>1</sup>** , RICHARD CONROY, National Institute of Biomedical Imaging and Bioengineering — Biomedical imaging, and in particular MRI and CT, is often identified as among the top 10 most significant advances in healthcare in the 20th century. This presentation will describe some of the recent advances in medical physics and imaging being funded by NIH in this century and current funding opportunities. The presentation will also highlight the role of multidisciplinary research in bringing concepts from the physical sciences and applying them to challenges in biological and biomedical research..

<sup>1</sup>NIH Funding for Biomedical Imaging

## Thursday, March 17, 2016 11:15AM - 2:15PM – Session S13 DMP: 2D Materials: Semimetals 309 - Xuan Gao, Case Western Reserve University

**11:15AM S13.00001 Dirac Semimetals in Two Dimensions** , STEVE YOUNG, US Naval Research Laboratory — Graphene is well-known for its unusual band structure, which features a pair of two dimensional Dirac points – band degeneracies with linear dispersion – at the Fermi level, and has served as the canonical platform for exploring the novel physics that arises near such points. However, spin-orbit interaction breaks the degeneracy at the Dirac points, so that graphene is formally a quantum spin Hall insulator. In this talk I will discuss the theory of two dimensional materials with Dirac points that *persist* in the presence of spin-orbit interaction. These Dirac points are preserved by nonsymmorphic symmetries, which describe lattice invariance under a combined point group operation and fractional translation. This is the only means of protecting Dirac points against spin-orbit coupling in two dimensions, and such Dirac points are unique in marking the transition between topological and trivial insulating states. I will describe the general properties of these Dirac points and the nature of their protection by nonsymmorphic symmetry operations, and contrast them with Dirac points protected by symmorphic symmetries in both the three dimensional case and the spin-orbit-free two dimensional case. I will then delineate the possible configurations of two dimensional Dirac materials, classifying them by protective symmetries. The role of 2D Dirac materials as transition phases will be described in detail, and the topological and trivial phases that result from various modes of symmetry breaking will be explored. Finally, I will discuss the potential for realization of both Dirac materials and their derivative phases, paying special attention to relevant chemical considerations.

**11:51AM S13.00002 Bosonization of Weyl Fermions** , EDUARDO MARINO, UFRJ — The electron, discovered by Thomson by the end of the nineteenth century, was the first experimentally observed particle. The Weyl fermion, though theoretically predicted since a long time, was observed in a condensed matter environment in an experiment reported only a few weeks ago. Is there any linking thread connecting the first and the last observed fermion (quasi)particles? The answer is positive. By generalizing the method known as bosonization, the first time in its full complete form, for a spacetime with 3+1 dimensions, we are able to show that both electrons and Weyl fermions can be expressed in terms of the same boson field, namely the Kalb-Ramond anti-symmetric tensor gauge field. The bosonized form of the Weyl chiral currents lead to the angle-dependent magneto-conductance behavior observed in these systems.

**12:03PM S13.00003 Coulomb interaction effect in tilted Weyl fermion in two dimensions** , HIROKI ISOBE, Massachusetts Institute of Technology, NAOTO NAGAOSA, RIKEN and University of Tokyo — Weyl fermions with tilted linear dispersions characterized by several different velocities appear in some systems including the quasi-two-dimensional organic semiconductor  $\alpha$ -(BEDT-TTF)<sub>2</sub>I<sub>3</sub> and three-dimensional WTe<sub>2</sub>. The Coulomb interaction between electrons modifies the velocities in an essential way in the low energy limit, where the logarithmic corrections dominate. Taking into account the coupling to both the transverse and longitudinal electromagnetic fields, we derive the renormalization group equations for the velocities of the tilted Weyl fermions in two dimensions, and found that they increase as the energy decreases and eventually hit the velocity of light  $c$  to result in the Cherenkov radiation. Especially, the system restores the isotropic Weyl cone even when the bare Weyl cone is strongly tilted and the velocity of electrons becomes negative in certain directions.

**12:15PM S13.00004 Strong Correlation and Topological States in Orbital-Active Dirac Materials**, SHENGLONG XU, CONGJUN WU, University of California, San Diego — Two dimensional Dirac materials, starting with graphene, have drawn tremendous research interests in the past decade. Instead of focusing on the  $p_z$  orbital as in graphene, we go a step further and study its two orbitals counterpart, namely the  $p_x$  and  $p_y$  orbitals on a honeycomb lattice. The model applies to both optical lattices and several solid state systems including organic material, fluoridated tin film, BiX/SBX (X=H.F.Cl.Br). In the band structure, besides the well known Dirac points in the graphene band structure, the orbital degrees of freedom give rise to flat bands as well as quadratic band touching points. These new features provide an even wider playground for searching exotic states of matter. With help of mean field theory and functional renormalization group (FRG) method, we explore the effects of interaction on the system and investigate the consequential interesting states such as ferromagnetism, Wigner crystallization, quantum anomalous Hall states and f-wave superconductivity.

**12:27PM S13.00005 Three-dimensional Anisotropy and Kohler's Rule Scaling of the Magnetoresistance in  $\text{WTe}_2$** <sup>1</sup>, YONG-LEI WANG, Materials Science Division, Argonne National Laboratory & Department of Physics, University of Notre Dame — Tungsten ditelluride ( $\text{WTe}_2$ ) was recently discovered to have extremely large magnetoresistance (XMR) at low temperatures and exhibits a transformative 'turn-on' temperature behavior: when the applied magnetic field  $H$  is above a certain value, the resistivity versus temperature  $\rho(T)$  curve shows a minimum at a field dependent temperature  $T^*(H)$ . Since  $\text{WTe}_2$  is a layered compound with metal layers sandwiched between adjacent insulating chalcogenide layers, it is typically considered to be a two dimensional (2D) material, whereby the anisotropic magnetoresistance is attributed only to the perpendicular component of the magnetic field. Moreover, the 'turn-on' temperature behavior has been interpreted as a magnetic-field-driven metal-insulator transition or attributed to an electronic structure change. In this talk I will report on two scaling behaviors of the magnetoresistance in  $\text{WTe}_2$ . The first shows that the angle dependence of the magnetoresistance follows a conventional 3D anisotropy scaling and hence reveals the electrical 3D nature of  $\text{WTe}_2$  [1]. The second demonstrates that the  $\rho(T, H)$  curves, including those with 'turn-on' temperature behavior, can be scaled with Kohler's rule [2]. The observed Kohler's rule scaling excludes the possible existence of a magnetic-field-driven metal-insulator transition or significant contribution of an electronic structure change to the low-temperature XMR in  $\text{WTe}_2$ . It indicates that both the XMR and the 'turn-on' behavior originate from the high mobilities of the charge carriers, which are strongly temperature dependent in  $\text{WTe}_2$ . We also derived quantitative expressions for the magnetic field dependence of the 'turn-on' temperature  $T^*(H)$  and for the temperature dependence of the resistivity  $\rho(T^*, H)$  at the onset of the XMR behavior.

In collaboration with L. R. Thoutam, Z. L. Xiao, J. Hu, S. Das, Z. Q. Mao, J. Wei, R. Divan, A. Luican-Mayer, G. W. Crabtree, and W. K. Kwok

References:

[1] L. R. Thoutam, Y. L. Wang et al., Phys. Rev. Lett. 115, 046602 (2015)

[2] Y. L. Wang et al. Phys. Rev. B 92, 180402(R) (2015)

<sup>1</sup>This work was supported by the U.S. DOE, Office of Science, BES, Materials Sciences and Engineering Division.

**1:03PM S13.00006 Electronic Transport in Ultra-Thin  $1\text{T}'\text{-WTe}_2$** , VALLA FATEMI, SARANESH PREMBABU, MIT, MAZHAR N. ALI, Princeton, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, Tsukuba, Japan, ROBERT J. CAVA, Princeton, PABLO JARILLO-HERRERO, MIT — We report low-temperature electronic transport measurements of  $1\text{T}'\text{-WTe}_2$  in the few-layer limit. Thin layers of  $\text{WTe}_2$  are obtained by the mechanical exfoliation technique and are subsequently encapsulated between thin hexagonal Boron Nitride crystals via a dry crystal transfer technique. These devices are fabricated entirely inside an inert-atmosphere glove box to avoid degradation. We report on the temperature, magnetic field, and electrostatic gate voltage dependence of these devices for several different thicknesses.

**1:15PM S13.00007 Spin Orbit Induced Electronic Structure and Magnetotransport in  $\text{WTe}_2$** <sup>1</sup>, DAVID J. SINGH, University of Missouri, MINGHU PAN, Huazhong University of Science and Technology, JIAQIANG YAN, University of Tennessee, BIAO YANG, Soochow University, YUNYI ZANG, Tsinghua University, JUNJIE ZHANG, Soochow University, KE HE, Tsinghua University, MENGHAO WU, Huazhong University of Science and Technology, YANFEI ZHAO, Peking University, DAVID MANDRUS, University of Tennessee, JIAN WANG, Peking University, QIKUN XUE, Tsinghua University, LIFENG CHI, QING LI, Soochow University — We report electronic structure studies of  $\text{WTe}_2$ , which shows an XMR behavior and is non-centrosymmetric. We find a spin-orbit split semimetallic band structure with a different Fermi surface topology than that initially reported, including Rashba split bands with Fermi surface around the zone center. The metallic properties are not one dimensional and are best described in terms of an anisotropic 3D metal with compensating low carrier density Fermi surfaces. The spin texture and transport is discussed as the origin of the XMR effect and in particular is consistent with the geometry in which the XMR effect is observed and its angle dependence.

<sup>1</sup>Work supported by DOE through the Computational Synthesis of Materials Software Project

**1:27PM S13.00008 Electronic and Magnetic Anisotropy of Layered  $\text{IrTe}_2$  Single Crystals**<sup>1</sup>, GUIXIN CAO, RONGYING JIN, Louisiana State University, Baton Rouge — Layered  $\text{IrTe}_2$  is known to exhibit extremely rich physical properties with two successive phase transitions at  $T_1 \sim 280$  K and  $T_2 \sim 180$  K. We have grown  $\text{IrTe}_2$  single crystals with typical sizes of  $451.2 \text{ mm}^3$ . This allows us to experimentally investigate physical properties along different directions. While the lattice parameter ratio  $c/a$  is small, both electrical resistivity and magnetic susceptibility show much higher anisotropy. In particular, we only observe resistivity and susceptibility anomaly along the  $ab$  plane at  $T_2$ , indicating the 2D character of electronic and magnetic properties at low temperatures.

<sup>1</sup>This material is based upon work supported by the U.S. Department of Energy under EPSCoR Grant No. DE-SC0012432.

**1:39PM S13.00009 Magnetoresistance Anisotropy in  $\text{WTe}_2$** , LAXMAN RAJU THOUTAM, Northern Illinois University, Argonne National Laboratory, YONGLEI WANG, Argonne National Laboratory, ZHILI XIAO, Northern Illinois University, Argonne National Laboratory, SAPTARSHI DAS, ADINA LUICAN MAYER, RALU DIVAN, Argonne National Laboratory, GEORGE W CRABTREE, Argonne National Laboratory, University of Illinois at Chicago, WAI KWONG KWOK, Argonne National Laboratory — We report the angle dependence of the magnetoresistance in  $\text{WTe}_2$ . Being a layered material,  $\text{WTe}_2$  is considered to be electronically two-dimensional (2D). Our results demonstrate that it is in fact 3D with an anisotropy of effective mass as small as 2. We measured the magnetic field dependence of the sample resistance  $R(H)$  at various angles between the applied magnetic field with respect to the  $c$ -axis of the crystal and found that they can be scaled based on the mass anisotropy, which changes from  $\sim 2$  to  $\sim 5$  with decreasing temperature in the Fermi liquid state. We will also discuss the origin of the turn-on temperature behavior in this material.

**1:51PM S13.00010 Magnetotransport Measurements of Thin Layered WTe<sub>2</sub>** , BOSONG SUN, ZAIYAO FEI, SANFENG WU, JOE FINNEY, PAUL NGUYEN, University of Washington, JIAQIANG YAN, Oak Ridge National Laboratory, TAUNO PALOMAKI, XIAODONG XU, DAVID COBDEN, University of Washington — Tungsten Telluride, a semimetallic layered transition-metal dichalcogenide, was recently found to have extremely large magnetoresistance at helium temperatures. The unconventional non-saturating behavior may be related to near-perfect charge compensation between electron and hole pockets, but this is still debated. Since that discovery there have been several studies of angle-resolved photoemission and quantum transport on the bulk material which found the Fermi surface to be rather complex. It is clear that insights stand to be gained from the variation of the properties on thinning down to a single monolayer. Measurements of thin exfoliated crystals have indicated that the carriers become increasingly localized on approaching the monolayer limit. This may be an intrinsic feature or it may be a result of the disorder produced by oxidation of the surface layers. We report transport measurements on few-layer and monolayer WTe<sub>2</sub> with and without encapsulation in hBN, including the dependence on thickness, crystal axis, temperature, gate voltage and magnetoresistance, which resolve this question.

**2:03PM S13.00011 Magnetotransport properties of nearly-free electrons in two-dimensional hexagonal metals and application to the Mn+1AX<sub>n</sub> phases** , LU SHI, Univ Catholique de Louvain, THIERRY OUISSE, LMGP/INPG, Grenoble, France, BENJAMIN PIOT, LNCMI/CNRS, Grenoble, France, DIDIER CHAUSSSENDE, LMGP/INPG, Grenoble, France, BENOIT HACKENS, Univ Catholique de Louvain — We propose a general model for explaining the weak field magneto-transport properties of the Mn+1AX<sub>n</sub> phases in their crystalline form. By using this model to describe the magnetotransport properties of nearly-free electrons in two-dimensional hexagonal metals, we modify it so as to be applicable for Mn+1AX<sub>n</sub> phases. It is demonstrated that the values of the in-plane Hall coefficient and magnetoresistance are due to the specific shape of the Fermi surface of almost two-dimensional hole and electron bands. If the contribution of the electron pockets to in-plane resistivity can be predicted to be a minor one, in contrast, both holes and electrons should substantially contribute to the overall value of the in-plane Hall coefficient. The relevance of this model is then supported by elementary considerations, analytical computations and a set of experimental data obtained from single crystals of V<sub>2</sub>AlC and Cr<sub>2</sub>AlC as a function of temperature and magnetic field, both in the basal plane and along the c-axis.

**Thursday, March 17, 2016 11:15AM - 1:15PM –**

**Session S14 FPS FHP: The Iran Nuclear Deal: Physics, Physicists and the Historic Agreement**

310 - Micah Lowenthal, National Academy of Science

**11:15AM S14.00001 TBD** , R. SCOTT KEMP, Assistant Professor of Nuclear Science and Engineering, MIT — No abstract available.

**11:51AM S14.00002 ABSTRACT WITHDRAWN –**

**12:03PM S14.00003 Beller Lecture: Dialogue Across Divides - Physicists and the Iran Dossier** , GTZ NEUNECK, Deputy Director IFSH and Chair WG Physics and Disarmament at DPG — For over a decade, the nuclear activities of the Islamic Republic of Iran have been at the center of international concerns and subsequent track II talks. NGOs, think tanks and analysts played a role to help to find technical solutions in a highly political setting. The talk will give an overview about the role of physicists to understand the Iranian sensitive nuclear fuel-cycle and to prepare the ground for the JCPOA. Furthermore, the experience of the work of the Pugwash Conferences on Science and World Affairs will be elaborated.

**12:39PM S14.00004 Marshak Lectureship Talk** , ANTON V. KHLOPKOV, Director, Center for Energy and Security Studies (CENESS) — .

**Thursday, March 17, 2016 11:15AM - 2:15PM –**

**Session S15 DMP: 2D Materials: Superconductivity and Correlations II** 314 - James Eckstein, UIUC

**11:15AM S15.00001 2D superconductivity by ionic gating<sup>1</sup>** , YOSHI IWASA, The University of Tokyo AND RIKEN CEMS — 2D superconductivity is attracting a renewed interest due to the discoveries of new highly crystalline 2D superconductors in the past decade. Superconductivity at the oxide interfaces triggered by LaAlO<sub>3</sub>/SrTiO<sub>3</sub> has become one of the promising routes for creation of new 2D superconductors. Also, the MBE grown metallic monolayers including FeSe are also offering a new platform of 2D superconductors. In the last two years, there appear a variety of monolayer/bilayer superconductors fabricated by CVD or mechanical exfoliation. Among these, electric field induced superconductivity by electric double layer transistor (EDLT) is a unique platform of 2D superconductivity, because of its ability of high density charge accumulation, and also because of the versatility in terms of materials, stemming from oxides to organics and layered chalcogenides. In this presentation, the following issues of electric field induced superconductivity will be addressed; (1) Tunable carrier density, (2) Weak pinning, (3) Absence of inversion symmetry. (1) Since the sheet carrier density is quasi-continuously tunable from 0 to the order of 10<sup>14</sup> cm<sup>-2</sup>, one is able to establish an electronic phase diagram of superconductivity, which will be compared with that of bulk superconductors. (2) The thickness of superconductivity can be estimated as 2 – 10 nm, dependent on materials, and is much smaller than the in-plane coherence length. Such a thin but low resistance at normal state results in extremely weak pinning beyond the dirty Boson model in the amorphous metallic films. (3) Due to the electric field, the inversion symmetry is inherently broken in EDLT. This feature appears in the enhancement of Pauli limit of the upper critical field for the in-plane magnetic fields. In transition metal dichalcogenide with a substantial spin-orbit interactions, we were able to confirm the stabilization of Cooper pair due to its spin-valley locking.

<sup>1</sup>This work has been supported by Grant-in-Aid for Specially Promoted Research (No. 25000003) from JSPS.

**11:51AM S15.00002 Electrochemical manipulation of two-dimensional materials** , YIJUN YU, FANGYUAN YANG, Fudan University, XIU FANG LU, YA JUN YAN, University of Science and Technology of China, YONG-HEUM CHO, Rutgers University, LIGUO MA, XIAOHAI NIU, Fudan University, SEJOONG KIM, YOUNG-WOO SON, Korea Institute for Advanced Study, DONGLAI FENG, SHIYAN LI, Fudan University, SANG-WOOK CHEONG, Rutgers University, XIAN HUI CHEN, University of Science and Technology of China, YUANBO ZHANG, Fudan University — The electronic properties of a variety of two-dimensional (2D) materials can be modulated by electrochemical modifications on mesoscopic scale. Here we demonstrate a proof-of-concept ionic field-effect transistor (iFET), which is based on reversible modifications of the electronic properties of a wide range of layered materials (e.g. 1T-TaS<sub>2</sub> and 2H-TaS<sub>2</sub>) through gate-controlled electrochemical reactions with mobile ions in the electrolyte. By fine-tuning the electrochemical reactions, we can switch between Mott phase, superconducting phase, metallic phase and insulating phase in a single 1T-TaS<sub>2</sub> iFET device. Such technique opens up new possibilities in searching for the novel state of matter in 2D materials.

**12:03PM S15.00003 Griffiths singularity of quantum phase transition in ion-gated ZrNCl**, YU SAITO, The University of Tokyo, TSUTOMU NOJIMA, Tohoku University, YOSHIHIRO IWASA, The University of Tokyo — Recent technological advances of thin films fabrication, especially mechanical exfoliation, led to discoveries of less-disordered highly-crystalline two-dimensional (2D) superconductors; atomically thin NbSe<sub>2</sub> and ion-gated 2D materials, which show intrinsic properties of 2D superconductors with minimal disorder; for example, metallic ground state [1,2], and unconventional 2D Ising superconductivity due to pure spin-valley locking effect [3-5]. In this talk, we focus on magnetotransport properties of an ionic-liquid gated ZrNCl, which exhibited Griffiths singularity-like behavior in superconductor-metal-insulator transition induced by magnetic fields at low carrier concentrations. The overall behavior is quite similar to the recent results of superconducting Ga thin films, in which quantum Griffiths singularity was observed in vortex-glass state [6]. We will discuss the relationship between Griffiths singularity and quantum tunneling or flux flow of vortices phase (vortex liquid) in our system. [1] Y. Saito et al. Science 350, 409 (2015). [2] A. W. Tsen et al. arXiv 1507.08639 [3] Y. Saito et al. Nature Phys. doi: 10.1038/nphys3580. (arXiv:1506.04146). [4] X. Xi et al. arXiv:1507.08731. [5] J. M. Lu et al. arXiv:1506.07620. [6] Y. Xing et al. Science 350, 542 (2015).

**12:15PM S15.00004 Spin-valley locking of the bulk transition-metal dichalcogenide superconductor NbSe<sub>2</sub>**, L. BAWDEN, Univ of St Andrews, S. COOIL, F. MAZZOLA, Norwegian Univ of Science & Tech., J.M. RILEY, Univ of St Andrews & Diamond Light Source, L. COLLINS-MCINTYRE, Univ of St Andrews, V. SUNKO, Univ of St Andrews & Max Planck Inst. for Chemical Physics of Solids, J. WELLS, Norwegian Univ of Science & Tech., G. BALAKRISHNAN, Univ of Warwick, S. BAHRAMY, Univ of Tokyo & RIKEN, P.D.C. KING, Univ of St Andrews — 2H-NbSe<sub>2</sub> is a metallic transition metal dichalcogenide, which hosts instabilities to a charge density wave phase, and a superconducting phase at low temperatures [1]. To date, it has been assumed that these phases are largely unaffected by the spin degree of freedom. In contrast, from spin- and angle-resolved photoemission measurements, supported by first principles calculations, we reveal that the normal state Fermi surface hosts a complex spin texture. We uncover a rich spin-valley locking of the form also observed in the semiconducting materials of the same family [2], consistent with the recent observation of Ising pairing in the superconducting state of monolayer NbSe<sub>2</sub> [3]. We find that in the normal state of the bulk compound there is persistent spin polarisation which becomes intrinsically linked to the electronic dimensionality, showing a significant dependence on the out-of-plane momentum. This prompts a reinterpretation of the complex phases that emerge in this, and related materials. [1] Wilson JA et al, Phys. Rev. Lett. 32, 882 (1974). [2] Xiao D et al, Phys. Rev. Lett. 108, 196802 (2012); Xu X et al, Nature Phys. 10, 343350 (2014); Riley JM et al, Nature Phys. 10, 835 (2014). [3] Xi X et al, arXiv:1507.08731.

**12:27PM S15.00005 Superconductivity in few-layer NbS<sub>2</sub> and TaS<sub>2</sub> prepared by mechanical exfoliation**, YUESHEN WU, HAILONG LIAN, SHUJIE FAN, MUYAO FAN, HUI XING, SHUN WANG, Shanghai Jiao Tong Univ, YING LIU, Shanghai Jiao Tong Univ; Pennsylvania State Univ — 2D materials with novel physical properties are useful for scientific inquiries and technological applications. The superconducting 2D materials provide an opportunity to explore the superconductivity in the 2D limit. In this work, the superconductivity in few layer 2H-NbS<sub>2</sub> and 2H-TaS<sub>2</sub> are studied. Single crystals are obtained by vapor transport method and flakes are obtained by mechanical exfoliation. In NbS<sub>2</sub> flakes, the superconducting transition temperature (T<sub>c</sub>) monotonically decreases with decreasing thickness. On the other hand, T<sub>c</sub> of TaS<sub>2</sub> flakes appears to monotonically increase as the flake gets thinner and the signature of CDW transition in R vs. T curves eventually disappear. The electric double layer transistors (EDLTs) of NbS<sub>2</sub> and TaS<sub>2</sub> flakes are also being fabricated to tune superconductivity in these 2D crystals. The results on these experiments will be presented.

**12:39PM S15.00006 Characterizing the electronic ground states of single-layer NbSe<sub>2</sub> via STM/STS**, YI CHEN, MIGUEL UGEDA, AARON BRADLEY, UC Berkeley, YI ZHANG, LBNL, SEITA ONISHI, WEI RUAN, CLAUDIA OJEDA-ARISTIZABAL, UC Berkeley, HYEJIN RYU, LBNL, MARK EDMONDS, HSIN-ZON TSAI, ALEXANDER RISS, UC Berkeley, SUNG-KWAN MO, LBNL, DUNGHA LEE, ALEX ZETTL, UC Berkeley, ZAHID HUSSAIN, LBNL, ZHI-XUN SHEN, Stanford University, MICHAEL CROMMIE, UC Berkeley — Layered transition metal dichalcogenides (TMDs) are ideal systems for exploring collective electronic phases such as charge density wave (CDW) order and superconductivity. In bulk NbSe<sub>2</sub> the CDW sets in at TCDW = 33K and superconductivity sets in at T<sub>c</sub> = 7.2K. Below T<sub>c</sub> these electronic states coexist but their microscopic formation mechanisms remain controversial. Here we present an electronic characterization study of a single 2D layer of NbSe<sub>2</sub> by means of low temperature scanning tunneling microscopy/spectroscopy (STM/STS), angle-resolved photoemission spectroscopy (ARPES), and electrical transport measurements. We demonstrate that the CDW order remains intact in 2D and exhibits a robust 3 × 3 superlattice. Superconductivity also still occurs but its onset is depressed to 1.6K. Our STS measurements at 5K reveal a CDW gap of Δ = 4 meV at the Fermi energy, which is accessible via STS due to the removal of bands crossing the Fermi surface in the 2D limit. Our observations are consistent with the predicted simplified (compared to bulk) electronic structure of single-layer NbSe<sub>2</sub>, thus providing new insight into CDW formation and superconductivity in this model strongly-correlated system.

**12:51PM S15.00007 Studies of the epitaxial monolayer NbSe<sub>2</sub> by ultra-low-temperature scanning tunnelling microscope**, SHUAI-HUA JI, State Key Laboratory of Low-Dimensional Quantum Physics, Department of Physics, Tsinghua University, Beijing 100084, China. — Monolayer NbSe<sub>2</sub> has been successfully synthesized by molecular beam epitaxy on the graphitized SiC(0001) surface. Wide substrate temperature window from 200°C to 650°C for the epitaxial growth has been observed. The polycrystalline nature of the epitaxial sheet, which is caused by the weak Van der Waals interaction with substrate, has been evidenced by reflection high-energy electron diffraction and locally by scanning tunnelling microscope. Under the high temperature growth condition, grain size could reach as large as hundreds of nanometers. The shape of grain boundary is strongly depended on the misaligned angle between adjacent grains. Mainly, three type grain boundaries have been identified at the atomic scale by the local scanning probe. The BCS-like superconducting gap and the spatial fluctuation of order parameter have been revealed by ultra-low temperature scanning tunnelling microscope in the sub-Kelvin range.

**1:03PM S15.00008 A New Platform for Engineering Topological Superconductors: Superlattices on Rashba Superconductors.**, YAO LU, KAM TUEN LAW, The Hong Kong University of Science and Technology — The search for topological superconductors which support Majorana fermion excitations has been an important topic in condensed matter physics. In this work, we propose a new experimental scheme for engineering topological superconductors. In this scheme, by manipulating the superlattice structure of organic molecules placed on top of a superconductor with Rashba spin-orbit coupling, topological superconducting phases can be achieved without fine-tuning the chemical potential. Moreover, superconductors with different Chern numbers can be obtained by changing the superlattice structure of the organic molecules.

**1:15PM S15.00009 Trion formation in monolayer transition metal dichalcogenides**, ROMAN YA. KEZERASHVILI, New York City College of Technology, City University of New York, SHALVA M. TSIKLARI, Borough of Manhattan Community College, The City University of New York — We present three-body calculations for trions binding energy in monolayer transition metal dichalcogenides using the method of hyperspherical harmonics (HH). In numerical calculations for a proper treatment of Coulomb screening in two dimensions we assume that electrons and holes are interacted via Keldysh potential [1]. The convergences of binding energy calculations for the ground state of the trion as a function of the grand angular momentum are studied. For the trion binding energy in MoS<sub>2</sub> we obtain 19.2 meV. This value is remarkably close to the experimental one of 18 meV. A comparison with results of other calculations are presented. We also study solutions of a hyperradial equation in a minimal approximation for the ground angular momentum to examine two regimes: a long range and a short range cases when the inter particle distance is much greater and much less than the screening length. For these cases, we find analytical expressions for the energy and wave function for trion states. [1] L. V. Keldysh, JETP Lett. 29, 658 (1979)

**1:27PM S15.00010 Effects of the environment on the switching current in graphene-based Josephson Junctions.** , IVAN BORZENETS, The University of Tokyo, CHUNG-TING KE, FRANCOIS AMET, MING TSO WEI, Duke University, MICHIIHISA YAMAMOTO, The University of Tokyo, YURIY BOMZE, Duke University, SEIGO TARUCHA, The University of Tokyo, GLEB FINKELSTEIN, Duke University — The nature of the switching current and hysteresis (difference between switching and retrapping currents) in graphene-based Josephson junctions depends greatly on the interaction with the environment. Conventional devices result in underdamped Josephson junctions making the true critical current inaccessible. On the other hand, heavily isolating the Josephson junctions places them in the microscopic quantum tunneling regime even at high temperatures, also masking the critical current. We study the critical current, and the switching statistics in graphene Josephson junctions while varying the effects of the environment. Proper isolation of graphene Josephson junctions is necessary to measure the true critical current, especially so for the cases of small currents around the Dirac point. This is true for the case of conventional diffusive as well as the novel ballistic Josephson junctions.

**1:39PM S15.00011 Sub-Kelvin lateral thermal transport in graphene with superconducting contacts** , ANNE DRAELOS, AVERY SILVERMAN, JIYINGMEI WANG, CHUNG-TING KE, MING-TSO WEI, Duke University, IVAN VLASSIOUK, Oak Ridge National Laboratory, FRANCOIS AMET, Appalachian State University, GLEB FINKELSTEIN, Duke University — We studied thermal transport in graphene with superconducting contacts at low temperatures,  $\sim 0.1$  to 3 K, below the Bloch-Grüneisen temperature. The lead (Pb) superconducting electrodes placed along the length of the graphene form a thermal barrier by preventing the outflow of hot electrons, thus allowing us to isolate and study other cooling pathways. We were able to observe a lateral thermal gradient by studying strips ( $5 \times 50 \mu\text{m}$ ) of CVD-grown graphene transferred onto a  $\text{SiO}_2$  substrate. The characteristic length scale of the temperature profile is determined by the competition of the lateral heat flow within the electron system versus the local cooling of electrons by phonon emission. We anticipate extending this measurement in the near future to examine the outstanding question of electron-phonon cooling close to the Dirac point.

**1:51PM S15.00012 Transport properties of high quality heterostructures from unstable 2D crystals prepared in inert atmosphere** , GELIANG YU, School of Physics and Astronomy, University of Manchester, CAO YANG, Centre for Mesoscience and Nanotechnology, University of Manchester, EKATERINA KHESTANOVA, ARTEM MISHCHENKO, School of Physics and Astronomy, University of Manchester, ANDY KRETININ, ROMAN GORBACHEV, Centre for Mesoscience and Nanotechnology, University of Manchester, KONSTANTIN NOVOSELOV, GEIM ANDRE, School of Physics and Astronomy, University of Manchester, MANCHESTER GROUP TEAM — Many layered materials can be cleaved down to individual atomic planes, similar to graphene, but only a small minority of them are stable under ambient conditions. The rest reacts and decomposes in air, which has severely hindered their investigation and possible uses. Here we introduce a remedial approach based on cleavage, transfer, alignment and encapsulation of air-sensitive crystals, all inside a controlled inert atmosphere. To illustrate the technology, we choose two archetypal two-dimensional crystals unstable in air: black phosphorus and niobium diselenide. Our field-effect devices made from their monolayers are conductive and fully stable under ambient conditions, in contrast to the counterparts processed in air.  $\text{NbSe}_2$  remains superconducting down to the monolayer thickness. Starting with a trilayer, phosphorene devices reach sufficiently high mobilities to exhibit Landau quantization. The approach offers a venue to significantly expand the range of experimentally accessible two-dimensional crystals and their heterostructures.

**2:03PM S15.00013 Spin-orbit coupling induced by band hybridization in Graphene/WS2 heterostructures**<sup>1</sup> , BOWEN YANG, UCR, MIN-FENG TU, Caltech, JEONGWOO KIM, UCI, YONG WU, UCR, JASON ALICEA, Caltech, RUQIAN WU, UCI, MARC BOCKRATH, JING SHI, UCR — Graphene are known to have a negligibly small intrinsic spin-orbit coupling (SOC), however, many novel physical phenomena such as the quantum spin Hall effect and the quantum anomalous Hall effect have been predicted if strong SOC exists in graphene. Despite that many theoretical studies have been carried out on the enhancement of the SOC strength in graphene, few experiments have been conducted to confirm the existence of and investigate the physical origin of the enhanced SOC in graphene. Here we demonstrated the introduction of SOC into graphene through the proximity effect by stacking WS2 onto graphene. We studied the magnetoconductance of graphene and found weak antilocalization emerges when graphene is covered by WS2. This is in a clear contrast with the weak localization behavior observed in bare graphene and thus provides an unambiguous evidence of the induced Rashba SOC. By focusing on a high carrier density region, we showed that it is possible to reliably extract the strength of Rashba SOC. Furthermore, via investigating the electric field dependence of the Rashba SOC with a dual-gate device, we found that the origin of this enhanced SOC is the band hybridization between graphene and WS2, in agreement with our theoretical calculations.

<sup>1</sup>The work was supported by the grant DE-FG02-07ER4635 funded by the U.S. Department of Energy, Office of Science.

## Thursday, March 17, 2016 11:15AM - 2:15PM –

Session S16 DMP: 2D Devices: Mechanical metamaterials 315 - Charlie Johnson, University of Pennsylvania

**11:15AM S16.00001 Hard and Soft Physics with 2D Materials.** , PAUL MCEUEN, Cornell University — With their remarkable structural, thermal, mechanical, optical, chemical, and electronic properties, 2D materials are truly special. For example, a graphene sheet can be made into a high-performance transistor, but it is also the ultimate realization of a thin mechanical sheet. Such sheets, first studied in detail by August Föppl over a hundred years ago, are notoriously complex, since they can bend, buckle, and crumple in a variety of ways. In this talk, I will discuss a number of experiments to probe these unusual materials, from the effects of ripples on the mechanical properties of a graphene sheet, to folding with atomically thin bimorphs, to the electronic properties of bilayer graphene solitons. Finally, I discuss how the Japanese paper art of kirigami (kiru = 'to cut', kami = 'paper') applied to 2D materials offers a route to mechanical metamaterials and the construction of nanoscale machines.

**11:51AM S16.00002 Band Gap Engineering of  $\text{PbI}_2$  by Incommensurate Van der Waals Epitaxy** , YIPING WANG, JIAN SHI, Department of Material Science and Engineering, Rensselaer Polytechnic Institute — Van der Waals epitaxial growth had been thought to have trivial contribution on inducing substantial epitaxial strain in thin films due to its weak nature of Van der Waals interfacial energy. Due to this, electrical and optical structure engineering via Van der Waals epitaxial strain has been rarely studied. However, by appropriate film-substrate selection, we show that significant band structure engineering could be achieved in a soft thin film material  $\text{PbI}_2$  via Van der Waals epitaxy. The thickness dependent photoluminescence of single crystal  $\text{PbI}_2$  flakes was studied and attributed to the substrate-film coupling effect via incommensurate Van der Waals epitaxy. It is proposed that the Van der Waals strain is resulted from the soft nature of  $\text{PbI}_2$  and large Van der Waals interaction due to the involvement of heavy elements. Such strain plays vital roles in modifying the band gap of  $\text{PbI}_2$ . The deformation potential theory is used to quantitatively unveil the correlation between thickness, strain and band gap change. Our hypothesis is confirmed by the subsequent mechanical bending test and Raman characterization.

**12:03PM S16.00003 Introducing lattice strain to graphene encapsulated in hBN** , HIKARI TOMORI, University of Tsukuba and PRESTO-JST, RINEKA HIRAIDE, YOUTI OOTUKA, University of Tsukuba, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science (NIMS), AKINOBU KANDA, University of Tsukuba — Due to the characteristic lattice structure, lattice strain in graphene produces an effective gauge field. Theories tell that by controlling spatial variation of lattice strain, one can tailor the electronic state and transport properties of graphene. For example, under uniaxial local strain, graphene exhibits a transport gap at low energies, which is attractive for a graphene application to field effect devices. Here, we develop a method for encapsulating a strained graphene film in hexagonal boron-nitride (hBN). It is known that the graphene carrier mobility is significantly improved by the encapsulation of graphene in hBN, which has never been applied to strained graphene. We encapsulate graphene in hBN using the van der Waals assembly method. Strain is induced by sandwiching a graphene film between patterned hBN sheets. Spatial variation of strain is confirmed with micro Raman spectroscopy. Transport measurement of encapsulated strained graphene is in progress.

**12:15PM S16.00004 Probing Mechanics of Crumpled Two-Dimensional Membranes and Cantilevers** , RYAN NICHOLL, HIRAM CONLEY, Vanderbilt University, NICKOLAY LAVRIK, IVAN VLASSIOUK, Oak Ridge National Laboratory, YEVGENIY PUZYREV, VIJAYASHREE PARSI SREENIVAS, SOKRATES PANTELIDES, Vanderbilt University, KIRILL BOLOTIN, Vanderbilt University, Freie Universität — Two-dimensional materials (2DMs) are inevitably crumpled in the out-of-plane direction due to both static wrinkling associated with uneven stresses and dynamic wrinkling resulting from flexural phonons. Here, we investigate the effect of this crumpling on mechanical properties of 2DMs – in-plane stiffness and bending rigidity. To carry out these measurements, we developed techniques to fabricate graphene membranes and singly clamped graphene cantilevers that are stable in vacuum and air. The measurements are performed by actuating these devices electrostatically and monitoring their displacement via sensitive interferometric profilometry both at room and low temperatures. We find that crumpling lowers the in-plane stiffness and strongly increases the bending rigidity of 2DMs. Furthermore, we unravel the relative contribution of static and dynamic wrinkling to observed renormalization of the effective mechanical constants.

**12:27PM S16.00005 Electromechanical coupling in atomically thin MoS<sub>2</sub> and graphene** , SAJEDEH MANZELI, MUHAMMED MALIK BENAMEUR, ADRIEN ALLAIN, AMIRHOSSEIN GHADIMI, MAHMUT TOSUN, ANDRAS KIS, Electrical Engineering Institute, Ecole Polytechnique Federale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland, FERNANDO GARGIULO, GABRIEL AUTS, OLEG V. YAZYEV, Institute of Theoretical Physics, Ecole Polytechnique Federale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland — Nanoelectromechanical systems (NEMS) based on novel materials such as graphene and MoS<sub>2</sub> allow studying their electromechanical characteristics. Here, we incorporate single and bilayer MoS<sub>2</sub> and graphene into NEMS and investigated their electromechanical behavior. We observe a Strain-induced bandgap modulation in atomically thin MoS<sub>2</sub> membranes with a thickness dependent modulation rate. Finite element modeling is used to extract the piezoresistive gauge factor for MoS<sub>2</sub>. In the case of graphene, deflection of monolayer graphene nanoribbons results in a linear increase in their electrical resistance where an upper limit is estimated for the gauge factor. Surprisingly, we observe oscillations in the electromechanical response of bilayer graphene. Our numerical simulations indicate that these oscillations arise from quantum mechanical interference in the transition region induced by sliding of individual graphene layers with respect to each other. Our results reveal that atomically thin MoS<sub>2</sub> membranes show strong piezoresistive effect, comparable to the state-of-the-art silicon sensors. Moreover, bilayer graphene conceals unexpectedly novel physics allowing the rare observation of room temperature electronic interference phenomena.

**12:39PM S16.00006 Effect of strain on the electronic transport properties of mono- and bilayer graphene** , FEN GUAN, XU DU, Stony Brook University - SUNY — It has been theoretically proposed that strain can have a significant impact on the electronic and charge transport properties of mono- and bilayer graphene. Experimental study of such "strain engineering" in field effect devices has been limited, mainly due to the challenge in creating an effective tuning knob of strain. Here we report the fabrication and characterization of suspended graphene field effect transistor (FET) on a Polyimide substrate, where uniaxial strain is applied by bending the substrate. Magnetotransport measurement of both mono- and bilayer graphene FETs are carried out with variable strain, from compressive to tensile, over wide range of temperature (4.2-300K). The impact of the strain on the conductivity of graphene will be discussed and compared to the theoretical predictions on strain-induced gauge field and flexural phonon scatterings.

**12:51PM S16.00007 Simulating MEMS Chevron Actuator for Strain Engineering 2D Materials<sup>1</sup>** , MOUNIKA VUTUKURU, JASON CHRISTOPHER, DAVID BISHOP, ANNA SWAN, Boston Univ — 2D materials pose an exciting paradigm shift in the world of electronics. These crystalline materials have demonstrated high electric and thermal conductivities and tensile strength, showing great potential as the new building blocks of basic electronic circuits. However, strain engineering 2D materials for novel devices remains a difficult experimental feat. We propose the integration of 2D materials with MEMS devices to investigate the strain dependence on material properties such as electrical and thermal conductivity, refractive index, mechanical elasticity, and band gap. MEMS Chevron actuators, provides the most accessible framework to study strain in 2D materials due to their high output force displacements for low input power. Here, we simulate Chevron actuators on COMSOL to optimize actuator design parameters and accurately capture the behavior of the devices while under the external force of a 2D material. Through stationary state analysis, we analyze the response of the device through IV characteristics, displacement and temperature curves. We conclude that the simulation precisely models the real-world device through experimental confirmation, proving that the integration of 2D materials with MEMS is a viable option for constructing novel strain engineered devices.

<sup>1</sup>The authors acknowledge support from NSF DMR1411008

**1:03PM S16.00008 Mechanically tunable strain fields in suspended graphene by micro electromechanical systems** , TYMOFIY KHODKOV, MATTHIAS GOLDSCHKE, JENS SONNTAG, 2A Physik Institut, RWTH, Aachen, SVEN REICHARDT, Facult des Sciences, de la Technologie et de la Communication, Universit du Luxembourg, GERARD VERBIEST, 2A Physik Institut, RWTH, Aachen, STEPHAN TRELLENKAMP, Peter Grnberg Institute 9, FZ, Jlich, CHRISTOPH STAMPFER, 2A Physik Institut, RWTH, Aachen — The discovery of graphene triggered an enormous interest on the class of two-dimensional (2D) materials. 2D materials manifested high sensitivity of their thermal, optical or electric response to applied tensile stress. Therefore, a rigorous and systematic investigation of their mechanical properties is extremely important. On the example of graphene – a top candidate for future flexible electronic devices and sensors – we demonstrate fully controlled and restorable realization of various strain fields in 2D membranes by coupling them to Si-based electrostatic micro-actuators (comb-drives). The comb-drive actuators are capable to provide significant forces and they are made of highly-doped silicon, i.e. they can be operated down to cryogenic temperatures allowing the investigation of quantum effects in electromechanical systems. Using confocal Raman spectroscopy we characterize strain distribution in suspended mono- and bilayer graphene sheets under induced tension (up to 0.5%). A detailed analysis clearly show that graphene samples reproducibly experience strain in different directions only while applying voltages to the micro-actuator. This approach empowers accurate tuning of applied tension in any isolated 2D materials independent on other crucial parameters.

**1:15PM S16.00009 ABSTRACT WITHDRAWN —**

**1:27PM S16.00010 Low dissipative mechanical resonators based on WSe<sub>2</sub> monolayers**, NICOLAS MORELL, ANTOINE RESERBAT-PLANTEY, IOANNIS TSIOUTSIOS, KEVIN SCHADLER, ICFO The Institute of Photonic Sciences, FRANCOIS DUBIN, Institut des NanoSciences de Paris, FRANK KOPPEN, ADRIAN BACHTOLD, ICFO The Institute of Photonic Sciences, QUANTUMNANOMECHANICS TEAM, NANOOPTOELECTRONICS TEAM, NANOSTRUCTURES ET SYSTMES QUANTIQUES TEAM — Atomically thin nano-electromechanical systems (2D-NEMS) combine low mass resonators having resonant frequencies in the MHz-GHz range, wide tunability and low damping. Atomically thin 2D semiconductors, such as transition metal dichalcogenides (TMD), have rich optical properties (direct band gap, spin valley, embedded quantum emitters. . . ), which are linked to their low dimensionality. While optical and electronic properties of WSe<sub>2</sub> have been intensively investigated, there have not been any studies on WSe<sub>2</sub> mechanical resonators. Although TMD NEMs have been fabricated, they have not been measured at cryogenic temperature so far. I will present a new semiconductor 2D-NEMS made of a single layer of WSe<sub>2</sub>. We measured mechanical and photoluminescence spectra of WSe<sub>2</sub> suspended drums at cryogenic temperatures. Our results demonstrate an extremely low damping at low temperature with a quality factor  $Q > 47000$  at  $T=3K$ , which is higher than what can be achieved with graphene NEMs. In addition, we investigated photothermal and optoelectronic effects on the mechanical degree of freedom, revealing the high potential of semiconductor 2D-NEMS for optomechanics experiments.

**1:39PM S16.00011 Folded graphene nanochannels via pulsed patterning of graphene**<sup>1</sup>, RODRIGO G. LACERDA, IVE SILVESTRE, Dept. Física, Universidade Federal de Minas Gerais, CP 702, Belo Horizonte, MG, Brazil, ARTHUR W. BARNARD, School of Applied Eng. Physics, Cornell University, Ithaca, NY 14853, USA, SAMANTHA P. ROBERTS, PAUL MCEUEN, Dept. of Physics, Cornell University, Ithaca, NY 14853, USA — We present a resist-free patterning technique to form electrically contacted graphene nanochannels via localized burning by a pulsed white light source. The technique uses end-point detection to stop the burning process at a fixed resistance. By this method folded graphene nanochannels down to 30 nm in width with controllable resistance ranging from 10 k $\Omega$  to 100 k $\Omega$  is achieved [1]. Folding of the graphene sheet takes place during patterning, which provides very straight edges (zigzag/armchair) as identified by AFM, SEM and TEM. Electrical transport measurements for the nanochannels show a non-linear behavior of the current vs source-drain voltage as the resistance goes above 20 k $\Omega$  indicating conduction tunneling effects. The method described can be interesting not only for fundamental studies correlating edge folded structures with electrical transport but also as a promising path for fabricating graphene devices in situ. This method might also be extended to create nanochannels in other 2D materials. [1] I. Silvestre et al., APL, 106, 153105, 2015.

<sup>1</sup>Acknowledgments: Fapemig, CAPES, CNPQ, NSF, Cornell/CNF.

**1:51PM S16.00012 Shear elastic constants of thin films of the misfit layered compound [(SnSe)<sub>1.05</sub>]<sub>n</sub>[MoSe<sub>2</sub>]<sub>n</sub>**<sup>1</sup>, DONGYAO LI, University of Illinois, GAVIN MITCHSON, DAVID JOHNSON, University of Oregon, ANDRE SCHLEIFE, DAVID CAHILL, University of Illinois — Crystalline materials with interlayer van der Waals bonding typically have low stiffness for shear deformation that reduces the through-plane thermal conductivity and facilitates the use of layered materials as solid-state lubricants. In graphite and MoS<sub>2</sub>,  $c_{44} = 5\text{GPa}$  and  $18\text{GPa}$  respectively. The shear modulus of incommensurate layered materials is expected to be strongly reduced relative to ordered crystals but the magnitude of the suppression is currently unknown. We have recently developed an approach for measuring the shear modulus of thin layers using GHz surface acoustic waves (SAW). [(SnSe)<sub>1.05</sub>]<sub>n</sub>[MoSe<sub>2</sub>]<sub>n</sub> with  $n=1-4$  were prepared as thin films (60 nm) on Si substrates using the modulated elemental reactants technique. The SAW velocity  $v_{SAW}$  of Al/[(SnSe)(MoSe<sub>2</sub>)]/Si structures was measured using a polydimethylsiloxane (PDMS) phase-shift optical mask in a pump-probe system.  $c_{44}$  was determined by fitting the measured  $v_{SAW}$  to the calculated SAW velocity using multi-layer SAW model.  $c_{33}$  was measured by picosecond acoustics.  $c_{11}$ ,  $c_{12}$  and  $c_{13}$  were calculated using density functional theory (DFT) with van der Waals correction. The measured  $c_{33}$  and  $c_{44}$  are compared with the DFT prediction. Experimentally we obtain  $c_{44} = 1.9\text{GPa}$ ,  $1.2\text{GPa}$ , and smaller than  $0.05\text{GPa}$  for  $n=1, 2$  and  $4$ .

<sup>1</sup>The author acknowledge the support of International Institute for Carbon Neutral Energy Research

**2:03PM S16.00013 Realization of Ripple Induced Pseudomagnetic Fields in Graphene.**<sup>1</sup>, YUHANG JIANG, JINHAI MAO, GUOHONG LI, Rutgers University, DAIARA FARIA, UERJ, Nova Friburgo, RJ-Brazil, ANDREA LATGE, Universidade Federal Fluminense, Niteroi, RJ-Brazil, RAMON CARRILLO-BASTOS, UABC, Ensenada, Baja California, Mexico, NANCY SANDLER, Ohio University, Athens, Ohio, USA, EVA Y. ANDREI, Rutgers University, Piscataway, NJ USA — Strain induced distortions of the honeycomb lattice in graphene produce pseudo-magnetic (PM) fields which change the low energy electronic structure by introducing pseudo Landau levels (LLs), similar to real magnetic fields. The spatial distribution of the PM field is a sensitive function of the strain geometry providing new opportunities for engineering the band structure and transport properties. Here we report on scanning tunneling microscopy (STM), spectroscopy (STS), and numerical simulations on strain-induced PM field generated by quasi 1D ripples in graphene supported by flat substrates, such as hBN or SiO<sub>2</sub>. The ripples are typically  $\sim 1\ \mu\text{m}$  long,  $\sim 20\text{ nm}$  wide and several nm high. Their height profile, which is measured by STM, is compared to numerical simulations from which the local strain and the spatial distribution of the PM field is calculated. An independent measure of the local PM field, obtained from the LLs sequence in STS measurements, gives values comparable to those calculated from the height profile. We further show that the ripple geometry produces regions of alternating PM fields which may be associated with ballistic valley filter channels.

<sup>1</sup>Work supported by DOE-FG02-99ER45742, NSF DMR 1207108 and NSF grant DMR 1508325.

**Thursday, March 17, 2016 11:15AM - 2:15PM —**

**Session S17 DMP: 2D Semiconductor Physics II** 316 - Jeanie Lau, University of California, Riverside

**11:15AM S17.00001 Novel exciton systems in 2D TMD monolayers and heterobilayers<sup>1</sup>**, HONGYI YU, Department of Physics and Center of Theoretical and Computational Physics, The University of Hong Kong — In this talk, two exciton systems in transition metal dichalcogenides (TMDs) monolayer and heterobilayer will be discussed. In TMD monolayers, the strong e-h Coulomb exchange interaction splits the exciton and trion dispersions into two branches with zero and finite gap, respectively<sup>2 3</sup>. Each branch is a center-of-mass wave vector dependent coherent superposition of the two valleys, which leads to a valley-orbit coupling and possibly a trion valley Hall effect. The exchange interaction also eliminates the linear polarization of the negative trion PL emission<sup>4</sup>. In TMD heterobilayers with a type-II band alignment, the low energy exciton has an interlayer configuration with the e and h localized in opposite layers. Because of the inevitable twist or/and lattice mismatch between the two layers, the bright interlayer excitons are located at finite center-of-mass velocities with a six-fold degeneracy<sup>5</sup>. The corresponding photon emission is elliptically polarized, with the major axis locked to the direction of exciton velocity, and helicity determined by the valley indices of the e and h. Some experimental results on the interlayer excitons in the WSe<sub>2</sub>-MoSe<sub>2</sub> heterobilayers will also be presented. The interlayer exciton exhibits a long lifetime as well as a long depolarization time, which facilitate the observation of a PL polarization ring pattern due to the valley dependent exciton-exciton interaction induced expansion<sup>6</sup>.

<sup>1</sup>The works were supported by the Research Grant Council of Hong Kong (HKU17305914P, HKU705513P), the Croucher Foundation, and the HKU OYRA and ROP.

<sup>2</sup>H. Yu, G.-B. Liu, P. Gong, X. Xu, and W. Yao, Nat. Commun. **5**, 3876 (2014).

<sup>3</sup>H. Yu, X. Cui, X. Xu, and W. Yao, Natl Sci Rev **2**, 57 (2015).

<sup>4</sup>A. Jones, H. Yu, N. Ghimire, S. Wu, G. Aivazian, J. Ross, B. Zhao, J. Yan, D. Mandrus, D. Xiao, W. Yao, and X. Xu, Nature Nanotech. **8**, 634 (2013).

<sup>5</sup>H. Yu, Y. Wang, Q. Tong, X. Xu, and W. Yao, Phys. Rev. Lett. **115**, 187002 (2015).

<sup>6</sup>P. Rivera, K. L. Seyler, H. Yu, J. R. Schaibley, J. Yan, D. G. Mandrus, W. Yao, and X. Xu, to be published.

**11:51AM S17.00002 Engineering topological band with superlattice.<sup>1</sup>**, XIAOOU ZHANG, WENYU SHAN, DI XIAO, Carnegie Mellon Univ — Since the discovery of the quantum Hall effect, the search for topological states has been a major subject of interest in condensed matter physics. Here we propose a general scheme to create nontrivial Chern band by fabricating superlattice structure on a system with non-zero Berry curvature. We analyze the topological band structure by deriving an effective Hamiltonian that incorporates the Berry curvature effect. The Chern number is tunable by the superlattice configurations that are realizable with existing experimental technology.

<sup>1</sup>This work is supported by DOE Basic Energy Sciences Grant No. DE-SC0012509 (D.X. and W.S.) and by AFOSR Grant No. FA9550-14-1-0277 (X.Z.)

**12:03PM S17.00003 Optical properties of quantum dots in buckled graphene-like materials**, THAKSHILA HERATH, VADYM APALKOV, Georgia State University — The band gap of buckled graphene-like materials, such as silicene and germanene, depends on external perpendicular electric field. A specially design profile of electric field produces a quantum dot, i.e., trapping potential for electrons in such materials. We theoretically study the optical properties of such silicene/germanene quantum dots. There are two types of absorption spectra in the quantum dot: interband (optical transitions between the states of the valence and conduction bands) and intraband (transitions between the states of conduction/valence band). The interband absorption spectra have triple-peak structure with peak separation around 10 meV, while intraband absorption spectra, which depend on the number of electrons in the dot, have double-peak structure with separation between the peaks around 15meV. The interband optical spectra as a whole are red-shifted with increasing electric field in the internal region of the quantum dot, while the energy separation between the peaks depends weakly on the electric field. With increasing the size of the quantum dot, the interband and intraband absorption spectra become red shifted as well.

**12:15PM S17.00004 Charge density wave transition in single-layer titanium diselenide**, PENG CHEN, University of Illinois at Urbana-Champaign, YANG-HAO CHAN, Academia Sinica, XINYUE FANG, University of Illinois at Urbana-Champaign, YI ZHANG, Nanjing University, MEI-YIN CHOU, Academia Sinica, SUNG-KWAN MO, ZAHID HUSSAIN, ALEXEI FEDOROV, Lawrence Berkeley National Laboratory, TAI-CHANG CHIANG, University of Illinois at Urbana-Champaign — A single molecular layer of titanium diselenide (TiSe<sub>2</sub>) is a promising material for advanced electronics beyond graphene-a strong focus of current exploration. Such molecular layers are at the quantum limit of device miniaturization and can show enhanced electronic effects not realizable in thick films. We show that single-layer TiSe<sub>2</sub> exhibits a charge density wave (CDW) transition at critical temperature T<sub>C</sub> = 232 K, which is higher than the bulk T<sub>C</sub> = 200 K. Angle-resolved photoemission spectroscopy measurements reveal a small absolute bandgap at room temperature, which grows wider with decreasing temperature T below T<sub>C</sub> in conjunction with the emergence of (2x2) ordering. The results are rationalized in terms of first-principles calculations, symmetry breaking and phonon entropy effects. The observed BCS behaviour of the gap implies a mean-field CDW order in the single layer and an anisotropic CDW order in the bulk.

**12:27PM S17.00005 Spatially Indirect Exciton Condensates in Double Bilayer Graphene**, JUNG-JUNG SU, Department of Electrophysics, National Chiao Tung University, ALLAN H. MACDONALD, Department of Physics, University of Texas at Austin — Many-body interaction effects have a strong influence on the low-energy electronic properties of graphene bilayers because of the nearly quadratic dispersion at the K/K' band-crossing points. In the single graphene bilayer systems, the ground state has an energy gap thought to be a consequence of spin-density wave order and other competing ordered states are believed to be nearby in energy. In systems with two closely spacing bilayer, spatially indirect exciton states are expected in neutral systems with inter-bilayer charge transfer. This transfer can be achieved by applying either a vertical electrical displacement fields or an interbilayer potential bias. Here we report that the different combinations of displacement field and potential bias can give rise to different types of indirect exciton condensate states that are distinguished by the two-dimensional momentum dependence of the spontaneous inter-bilayer coherence. In general a displacement field prefers an excitonic condensate in which the phase coherence between the inner two layers of the four layer system, while the potential bias prefers momentum-independent coherence between remote layers. The complete phase diagram reported exhibits excitonic coherence states mentioned above, and more interestingly, their mixtures.

**12:39PM S17.00006 Exciton-polariton condensation in transition metal dichalcogenide bilayer heterostructure<sup>1</sup>**, KI HOON LEE, JAE-SEUNG JEONG, HONGKI MIN, SUK BUM CHUNG, Seoul Natl Univ — For the bilayer heterostructure system in an optical microcavity, the interplay of the Coulomb interaction and the electron-photon coupling can lead to the emergence of quasiparticles consisting of the spatially indirect exciton and cavity photons known as *dipolariton*, which can form the Bose-Einstein condensate above a threshold density. Additional physics comes into play when each layer of the bilayer system consists of the transition metal dichalcogenide (TMD) monolayer. The TMD monolayer band structure in the low energy spectrum has two valley components with nontrivial Berry phase, which gives rise to a selection rule in the exciton-polariton coupling, e.g. the exciton from one (the other) valley can couple only to the clockwise (counter-clockwise) polarized photon. We investigate possible condensate phases of exciton-polariton in the bilayer TMD microcavity changing relevant parameters such as detuning, excitation density and interlayer distance.

<sup>1</sup>This work was supported in part by the Institute for Basic Science of Korea (IBS) under Grant IBS-R009-Y1 and by the National Research Foundation of Korea (NRF) under the Basic Science Research Program Grant No. 2015R1D1A1A01058071.

**12:51PM S17.00007 Berry Phase Modification to the Energy Spectrum of Excitons<sup>1</sup>**, DI XIAO, JIANHUI ZHOU, WENYU SHAN, Carnegie Mellon Univ, WANG YAO, University of Hong Kong — By quantizing the semiclassical motion of excitons, we show that the Berry curvature can cause an energy splitting between exciton states with opposite angular momentum. This splitting is determined by the Berry curvature flux through the k-space area spanned by the relative motion of the electron-hole pair in the exciton wave function. Using the gapped two-dimensional Dirac equation as a model, we show that this splitting can be understood as an effective spin-orbit coupling effect. In addition, there is also an energy shift caused by other relativistic terms. Our result reveals the limitation of the venerable hydrogenic model of excitons, and it highlights the importance of the Berry curvature in the effective mass approximation.

<sup>1</sup>This work is supported by DOE Basic Energy Sciences Grant No. DE-SC0012509 (D. X. and W. S.) and by AFOSR Grant No. FA9550-14-1-0277 (J. Z.).

**1:03PM S17.00008 Optical and Electronic Properties of doped-MoS<sub>2</sub>: Joint Theoretical/Experimental Study**, MILLER EATON, HANSIKA SIRIKUMARA, HASSANA SAMASSEKOU, DIPANJAN MAZUMDAR, THUSHARI JAYASEKERA, Southern Illinois University Carbondale, LAALITHA LIYANAGE, MARCO BUONGIORNO NARDELLI, University of North Texas — Substitutional doping of transition metal dichalcogenides (TMDs) is an attractive way of engineering their electronic properties. The dependence of optoelectronic properties of TMDs on the dopant is largely under-explored. In this work, we will discuss how different species affect the optical properties of MoS<sub>2</sub>. The electronic structure calculations of doped TMDs are carried out using Density Functional Theory with the recently developed ACBN0 functional, a pseudo-hybrid Hubbard density functional that is a fast, accurate and parameter-free alternative to traditional DFT+U and hybrid exact exchange methods [L.A. Agapito, S. Curtarolo, and M. Buongiorno Nardelli, Phys. Rev. X 5, 011006 (2015)]. We compare our ACBN0 predictions with measurement of the electronic and optical properties of pristine and niobium doped MoS<sub>2</sub> films synthesized via physical vapor deposition and characterized using spectroscopic ellipsometry and optical spectroscopy.

**1:15PM S17.00009 Storing excitons in transition-metal dichalcogenides using dark states<sup>1</sup>**, DANIEL GUNLYCKE, Naval Research Laboratory, FRANK TSENG, NRL/NRC Research Associate, ERGUN SIMSEK, The George Washington University — Monolayer transition-metal dichalcogenides exhibit strongly bound excitons confined to two dimensions. One challenge in exploiting these excitons is that they have a finite life time and collapse through electron-hole recombination. We propose that the exciton life time could be extended by transitioning the exciton population into dark states. The symmetry of these dark states require the electron and hole to be spatially separated, which not only causes these states to be optically inactive but also inhibits electron-hole recombination. Based on an atomistic model we call the Triangular Lattice Exciton (3ALE) model, we derive transition matrix elements and approximate selection rules showing that excitons could be transitioned into and out of dark states using a pulsed infrared laser. For illustration, we also present exciton population scenarios based on different recombination decay constants. Longer exciton lifetimes could make these materials candidates for applications in energy management and quantum information processing.

<sup>1</sup>This work was supported by the Office of Naval Research, directly and through the Naval Research Laboratory.

**1:27PM S17.00010 Excitonic effects in 2D semiconductors: Path Integral Monte Carlo approach**, KIRILL VELIZHANIN, AVADH SAXENA, Los Alamos National Laboratory — One of the most striking features of novel 2D semiconductors (e.g., transition metal dichalcogenide monolayers or phosphorene) is a strong Coulomb interaction between charge carriers resulting in large excitonic effects. In particular, this leads to the formation of multi-carrier bound states (e.g., excitons, trions and biexcitons), which could remain stable at near-room temperatures and contribute significantly to optical properties of such materials. In my talk, I will report on our recent progress in using the Path Integral Monte Carlo methodology to numerically study properties of multi-carrier bound states in 2D semiconductors. Incorporating the effect of the dielectric confinement (via Keldysh potential), we have investigated and tabulated the dependence of single exciton, trion and biexciton binding energies on the strength of dielectric screening, including the limiting cases of very strong and very weak screening. The implications of the obtained results and the possible limitations of the used model will be discussed. The results of this work are potentially useful in the analysis of experimental data and benchmarking of theoretical and computational models.

**1:39PM S17.00011 Theoretical ultra-fast spectroscopy in transition metal dichalcogenides**, ALEJANDRO MOLINA-SANCHEZ, Physics and Materials Science Research Unit, University of Luxembourg, DAVIDE SANGALLI, ANDREA MARINI, ISM-CNR, Monterotondo, Rome, Italy, LUDGER WIRTZ, Physics and Materials Science Research Unit, University of Luxembourg — Semiconducting 2D-materials like the transition metal dichalcogenides (TMDs) MoS<sub>2</sub>, MoSe<sub>2</sub>, WS<sub>2</sub>, WSe<sub>2</sub> are promising alternatives to graphene for designing novel opto-electronic devices. The strong spin-orbit interaction along with the breaking of inversion symmetry in single-layer TMDs allow using the valley-index as a new quantum number [1]. The practical use of valley physics depends on the lifetimes of valley-polarized excitons which are affected by scattering at phonons, impurities and by carrier-carrier interactions. The carrier dynamics can be monitored using ultra-fast spectroscopies such as pump-probe experiments. The carrier dynamics is simulated using non-equilibrium Greens function theory in an ab-initio framework. We include carrier relaxation through electron-phonon interaction. We obtain the transient absorption spectra of single-layer TMD and compare our simulations with recent pump-probe experiments [2]. [1] D. Xiao et. al., Phys. Rev. Lett. **108**, 196802 (2012). X. Xu et. al., Nature Physics **10**, 343 (2014). [2] Y. T. Wang, et. al., Scientific Reports **5**, 8289 (2015).

**1:51PM S17.00012 Interaction Induced Quantum Valley Hall Effect in Graphene<sup>1</sup>**, CRISTIANE MORAIS SMITH<sup>2</sup>, Institute for Theoretical Physics, Utrecht University, Netherlands, EDUARDO C. MARINO, LEANDRO O. NASCIMENTO, Instituto de Física, Universidade Federal do Rio de Janeiro, Brazil, A VAN SERGIO, Departamento de Física, Universidade Federal do Para, Brazil — We use Pseudo Quantum Electrodynamics (PQED) in order to describe the full electromagnetic interaction of the electrons in graphene in a consistent 2D formulation. We first consider the effect of this interaction in the vacuum polarization tensor or, equivalently, in the current correlator to evaluate the Kubo's formula. Thereby, we obtain the usual expression for the minimal conductivity plus corrections due to the interaction. We then predict the onset of an interaction-driven spontaneous Quantum Valley Hall effect by solving the Schwinger-Dyson equation. The obtained Valley-Hall conductivity is exact and universal [1]. [1] E. C. Marino, Leandro O. Nascimento, V. S. Alves, and C. Morais Smith, Phys. Rev. X **5**, 011040 (2015).

<sup>1</sup>We acknowledge the Science Without Borders Program for financial support.

<sup>2</sup>first abstract submitted too large

**2:03PM S17.00013 Lateral Heterostructures of Monolayer Transition Metal Dichalcogenides: a First-principles Study<sup>1</sup>**, MENG WU, TING CAO, STEVEN G. LOUIE, Physics Department, UC Berkeley and Lawrence Berkeley National Lab — Using first-principles calculations, we investigate the electronic structure and optical properties of lateral heterostructures consisting of different monolayer transition metal dichalcogenides (TMDs). We find that the spin-orbital coupling effect plays an important role in modifying the ground-state electronic structure and excited-state properties such as optical responses. The anisotropy of optical absorption is investigated including local-field effects.

<sup>1</sup>This work was supported by NSF Grant No. DMR15-1508412, the U.S. DOE under Contract No. DE-AC02-05CH11231. Computational resources have been provided by DOE at Lawrence Berkeley National Laboratory's NERSC facility.

**Thursday, March 17, 2016 11:15AM - 2:03PM —**  
**Session S18 GMAG DMP FIAP: Magnetic Thin Films** 317 - Burm Baek, NIST

**11:15AM S18.00001 Imaging of precessional phase variations in spin Hall devices using picosecond heat pulses**, FENG GUO, JASON BARTELL, GREGORY FUCHS, Cornell University — We introduce a new approach of studying the spin Hall effect in patterned magnetic multilayers by imaging ferromagnetic resonance (FMR) precession phase. Using time-resolved anomalous Nernst effect (TRANE) microscopy, we quantify the amplitude and phase of local magnetic precession, which allows us to image the total driving field vector orientation. In a 5  $\mu\text{m}$  wide channel, we observe a substantial variation of the driving field vector as a function of lateral position that we attribute to variations in the total Oersted field angle and the demagnetization field. Next, using the same device, we compare TRANE phase imaging measurements to all-electrical spin-transfer torque ferromagnetic resonance (STFMR) measurements that sense the spatially averaged precession phase. We find that spatial phase variations introduce a systematic error in the spin Hall efficiency measured using conventional STFMR analysis in our devices. These results underscore the importance of phase-sensitive dynamic imaging to augment all-electrical FMR techniques in quantifying the spin Hall efficiencies of devices.

**11:27AM S18.00002 Magnon excitation and transport in Ferromagnetic Insulator/metal multilayers<sup>1</sup>**, TAO LIU, JIE REN, JIANWEI ZHANG, School of Physics, Tongji University — We studied magnon excitation and transport in a Ferromagnetic Insulator(FI) layer(such as YIG), which connected with Ferromagnetic/normal metal multilayers in two sides. In our modeling, we adopted self-consistent spin dependent Boltzmann equations in metal layers and magnon Boltzmann equation in FI layer. When applying an in-plane current in FM layer, a transverse spin current was generated due to Anomalous Hall effect, after crossing normal metal layer, it will produce magnon excitation at N/FI interface. With carrying spin information, magnon excitation in FI can eventually excite a new spin current at second F/N interface. This is so call magnon-drag effect [1]. In our work, we focused on magnon propagation in FI, with all two-magnon, three magnon, and four magnon scattering. Associated with spin dependent Boltzmann equation, we can investigate magnon excitation and transport properties in FI layer from the interface to bulk scale. The magnon excitation in FI layer is dominated not only by the interface interaction at Normal/FI boundary, but also by the bulk scattering in FI. Our results show the magnon in FI layer has decay behaviors to low energy model. We also showed a new way to manipulate magnon transport in FI. [1] S.L. Zhang and S. Zhang, PRL,109,096603(2012)

<sup>1</sup>This work was supported by NSFC grant No.11274240 and 51471119

**11:39AM S18.00003 Parity-Time Symmetry Breaking in Non-Equilibrium Magnetic Systems**, ALEXEY GALDA, VALERII VINOKUR, Argonne National Laboratory — We introduce generalized non-Hermitian Hamiltonian approach for description of out-of-equilibrium phase transitions in the exemplary context of dissipative non-equilibrium dynamics of an open quantum spin system. The imaginary part of the proposed Hamiltonian describes effects of damping and the applied Slonczewski spin-transfer torque (STT). In the classical limit, our approach reproduces Landau-Lifshitz-Slonczewski dynamics of a large macrospin. We reveal the STT-driven parity-time (PT) symmetry-breaking transition corresponding to a phase transition from precessional magnetization dynamics to controlled switching. Micromagnetic simulations for nanoscale ferromagnetic disks demonstrate the predicted effect. Our findings break ground for a general quantitative description of out-of-equilibrium phase transitions.

**11:51AM S18.00004 Unveiling magnetic Hysteresis**, PAULA MELLADO, ANDRES CONCHA, DAVID AGUAYO, Adolfo Ibez University — Hysteresis manifests as the lack of retraceability of the magnetization curve in magnetic systems. It has been associated with rotation of magnetization and changes of magnetic domains. However, up to date there has been no realization that allows to separate these coupled mechanisms. We introduce a minimal magnetic system where hysteresis is realized in a simple and minimal fashion. The basic units are a few U(1) ferromagnetic altitudinal rotors placed along a one dimensional chain. They exhibit a dissipative dynamics, interacting via magnetic coupling among them and via Zeeman interaction with the external magnetic field. The system displays a hysteretic behavior starting with N=2 rotors which remains qualitatively invariant as more magnets are added to the chain. We explain this irreversibility by using a model that includes Coulombic interactions between magnetic charges located at the ends of the magnets, zeeman coupling and viscous dissipation. We show that interactions between the unit components is the key element responsible for hysteresis and find that the ability to perceive hysteresis, depends on how the time frequencies of damping and interactions inherent to the system compare with the time frequency set by the external field ramping rate.

**12:03PM S18.00005 Combined Molecular Dynamics-Spin Dynamics Simulation of  $\alpha$ -Iron in an External Magnetic Field**, MARK MUDRICK, DILINA PERERA, DAVID P. LANDAU, Univ of Georgia — Using an atomistic model that treats both translational and spin degrees of freedom, combined molecular and spin dynamics simulations have been performed to study dynamic properties of  $\alpha$ -iron. Atomic interactions are described by an empirical many-body potential<sup>1</sup> while spin-spin interactions are handled with a Heisenberg-like Hamiltonian with a coordinate dependent exchange interaction<sup>2</sup>. Each of these interactions are parameterized by first-principles calculations. These simulations numerically solve equations of motion using an algorithm based on the second-order Suzuki-Trotter decomposition for the time evolution operator<sup>3</sup>. Through calculation of the Fourier transform of space-displaced time-displaced correlation functions, vibrational and magnetic excitations have been studied. The application of an external magnetic field up to 10-T has now been included and has been shown to increase the characteristic frequencies of the single-spin-wave excitations. Two-spin-wave interactions have also been investigated.

<sup>1</sup>Dudarev S L, Derlet P M 2005 *J. Phys.: Cond. Matter* **17** 7097

<sup>2</sup>Ma P W, Woo C H, Dudarev S L 2008 *Phys. Rev. B* **78** 024434

<sup>3</sup>Perera D, et al. 2014 *J. Phys.: Conf. Ser.* **487** 012007

## 12:15PM S18.00006 Magnetic dynamics studied by high-resolution electron spectroscopy and time-resolved electron microscopy.

, RAJESWARI JAYARAMAN, EPFL - Lausanne — Future information technology requires an increased magnetically encoded data density and novel electromagnetic modes of data transfer. While to date magnetic properties are observed and characterized mostly statically, the need emerges to monitor and capture their fast dynamics. In this talk, I will focus on the spin dynamics i.e. spin wave excitations and the dynamics of a new topological distribution of spins termed “skyrmions”. Wave packets of spin waves offer the unique capability to transport a quantum bit, the spin, without the transport of charge or mass. Here, large wave-vector spin waves are of particular interest as they admit spin localization within a few nanometers. By using our recently developed electron energy loss spectrometer, we could study such spin waves in ultrathin films with an unprecedented energy resolution of 4 meV. By virtue of the finite penetration depth of low energy electrons, spin waves localized at interfaces between a substrate and a thin capping layer can be studied yielding information about the exchange coupling between atoms at the interface. The quantization of spin waves with wave vectors perpendicular to the film gives rise to standing modes to which EELS has likewise access. Such studies when carried out as function of the film thickness again yield information on the layer dependence of the exchange coupling. Magnetic skyrmions are promising candidates as information carriers in logic or storage devices. Currently, little is known about the influence of disorder, defects, or external stimuli on the spatial distribution and temporal evolution of the skyrmion lattice. In this talk, I will describe the dynamical role of disorder in a large and flat thin film of  $\text{Cu}_2\text{OSeO}_3$ , exhibiting a skyrmion phase in an insulating material. We image up to 70,000 skyrmions by means of cryo-Lorentz Transmission Electron Microscopy as a function of the applied magnetic field. In the skyrmion phase, dislocations are shown to cause the emergence and switching between domains with different lattice orientations, and the temporal fluctuation of these domains is filmed. These observations pave the way to the control of a large 2D array of skyrmions.

## 12:51PM S18.00007 Collective Mode Splitting in Coupled Ferromagnet/Oxide Heterostructures<sup>1</sup>

, JUAN G. RAMIREZ, Department of Physics, Universidad de los Andes, Bogotá 111711, Colombia, J. DE LA VENTA, Dep. of Physics, Colorado State University, Fort Collins, CO 80523, USA, SIMING WANG, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA, THOMAS SAERBECK, Institut Laue-Langevin, 71 avenue des Martyrs, 38000 Grenoble, France, ALI C. BASARAN, Department of Physics, Gebze Technical University, Gebze, Kocaeli 41400, Turkey, X. BATLLE, Departament de Física Fonamental Universitat de Barcelona, 08028 Barcelona, Catalonia, Spain, IVAN K. SCHULLER, Department of Physics, University of California San Diego, La Jolla, CA 92093 USA — The coupling of electronic, magnetic, and structural properties between two dissimilar materials in contact can induce novel functionalities. Here we report on a drastic modification of the magnetization dynamics of thin Nickel films in  $\text{Ni}/\text{V}_2\text{O}_3$  bilayers. We performed temperature-dependent ferromagnetic resonance measurements across the first-order structural phase transition (SPT) of  $\text{V}_2\text{O}_3$ . The results show a strong coupling of the  $\text{V}_2\text{O}_3$  lattice dynamics to the magnon spectra of the Ni film in proximity. We have performed similar measurements across the second-order SPT in  $\text{Ni}/\text{SrTiO}_3$  hybrids. In this later case, only a slight change of the static magnetization was found with no modification of the magnetization dynamics. Our results suggest that the phase coexistence across the first-order SPT of  $\text{V}_2\text{O}_3$  is responsible for the effects observed in the  $\text{Ni}/\text{V}_2\text{O}_3$  hybrids. This suggests the existence of similar effects in other hybrid materials with first-order structural phase transitions.

<sup>1</sup>Supported by DOE grant No DE FG02-87ER-45332 and AFOSR grant No. FA9550-12-1-0381.

## 1:03PM S18.00008 Localized spin wave modes in parabolic field wells

, ROBERT MCMICHAEL, Center for Nanoscale Science and Technology, NIST, ELENA TARTAKOVSKAYA, Institute of Magnetism, NAS of Ukraine and Institute of High Technologies, Taras Shevchenko National University of Kiev, MARTHA PARDAVI-HORVATH, School of Engineering and Applied Science, The George Washington University — We describe spin wave modes trapped in parabolic-profile field wells. Trapped spin waves can be used as local probes of magnetic properties with resolution down to 100 nm in ferromagnetic resonance force microscopy.[1,2] Localized modes have been shown to form around field minima from a number of sources, including stray fields from magnetic probe tips [1,3-4] and inhomogeneous magnetostatic fields near film edges.[2] Here, we address the most basic trap, which is a parabolic minimum in the applied field. The magnetic eigenmodes in this trap are tractable enough to serve as approximations in more realistic situations. For a parabolic field, we select basis mode profiles proportional to Hermite functions because they are eigenfunctions of the applied field and exchange parts of the equations of motion. Additionally, we find that these Hermite modes are approximate eigenfunctions of magnetostatic interactions, showing good agreement with micromagnetic calculations. More precise agreement is achieved by diagonalizing the equations of motion using only a few modes. 1. I. Lee et al., Nature 466, 845 (2010). 2. F. Guo et al. Phys. Rev. Lett, 110, 017601 (2013) 3. H.-J. Chia, et al., Phys. Rev. Lett. 108, 087206 (2012). 4. R. Adur et al, Phys. Rev. Lett. 113, 176601 (2014).

## 1:15PM S18.00009 Cavity mediated coherent coupling between yttrium iron garnet magnets

, NICHOLAS LAMBERT, University of Cambridge, JAMES HAIGH, Hitachi Cambridge Laboratory, STEFAN LANGENFELD, University of Cambridge, ANDREW DOHERTY, University of Sydney, ANDREW FERGUSON, University of Cambridge — Strong coupling between the magnetostatic modes of an yttrium iron garnet (YIG) magnet and a microwave frequency electromagnetic cavity is now readily achievable[1,2,3]. Recently, coupling between a magnon and a superconducting qubit mediated by a cavity has also been demonstrated[4]. In this talk, we describe dispersive measurement[5] of the cavity-mediated coupling of magnetostatic modes in two YIG magnets. We find they are strongly coupled even when detuned from the cavity modes. We study the strength of the coupling as a function of the detuning, and find a  $1/\Delta$  dependence when close to individual cavity modes. Dark states of the coupled magnets are observed, in which the symmetry of the microwave drive does not match that of the new eigenstates. Our results are described well within the framework of circuit QED. Such an approach to coupling magnets might be used to phase-lock many spatially separated magnetic oscillators, such as those in spin-torque nano-oscillators or magnetic metamaterials. [1] Huebl et al., Phys. Rev. Lett., 111, 127003 (2013) [2] Zhang et al., Phys. Rev. Lett., 113, 156401 (2014) [3] Lambert et al., J. Appl. Phys., 117, 053910 (2015) [4] Tabuchi et al., Science, 349(6246), 405408 (2015) [5] Haigh et al., Phys. Rev. B, 91, 104410 104410 (2015)

## 1:27PM S18.00010 Rabi nutations in a ferromagnetic film

, AMIR CAPUA, CHARLES RETTNER, IBM Almaden Res Ctr, STUART PARKIN, IBM Almaden Res Ctr, Max Plank Inst. Halle — When electromagnetic radiation interacts with a two-level system, energy is transferred back and forth between the quantum system and the electromagnetic radiation at a rate defined by the Rabi frequency. This process takes place as long as coherence prevails, until steady state is reached. Rabi nutations have been observed in a variety of quantum systems (atomic vapors, semiconductors, superconducting qubits, etc.). Here, we observe Rabi nutations in an ultrathin  $\sim 10$  Å perpendicularly magnetized CoFeB film. A hybrid ferromagnetic resonance (FMR) – time resolved magneto optical Kerr effect (TRMOKE) system is used for this observation. Namely, a strong optical pump pulse perturbs the precessing spin system after which a weak optical probe pulse is sent at different times to map its recovery until steady precessional motion is reached again. The responses at the different detunings of magnetic field away from resonance conditions readily indicate the occurrence of the Rabi nutations which are initiated by the pump arriving at  $t=0$ . Excellent agreement with the prediction given by the Rabi formula is found. The method we report presents a new approach to study dynamical phenomena in magnetic materials.

## 1:39PM S18.00011 Propagation of pulsed surface spin-wave signals at millikelvin temperatures<sup>1</sup>

, ARJAN VAN LOO, RICHARD MORRIS, ALEXY KARENOWSKA, Clarendon Laboratory, Department of Physics, University of Oxford — Propagating microwave-frequency magnons in magnetic films attract increasing attention on account of their potential interface with superconducting quantum circuit and qubit systems. Their rich dynamics and slow speeds make magnons an interesting addition to the circuit quantum electrodynamics toolbox and, at the same time, superconducting circuit technology promises to be a powerful tool in the investigation of their quantum properties. We have studied the propagation of pulsed surface spin-wave signals over millimeter distances in yttrium iron garnet waveguides at  $\sim 10$  mK. Input microwave pulses and pulse trains with various envelope shapes were applied to an inductive input antenna, and the resulting magnons were detected by an output antenna of identical design. The shape of the output signal was observed to depend on the frequency content (carrier and pulse shape) of the input pulse. By performing measurements at varying frequencies and magnetic fields we have been able to map out the dispersion relation for surface magnon modes. These experiments were undertaken as a first step towards coupling propagating magnons in thin films to other quantum systems with microwave-frequency transition energies, and superconducting qubits in particular.

<sup>1</sup>The authors acknowledge support from the EPSRC (EP/K032690/1).

## 1:51PM S18.00012 Spin waves of ferromagnetic films<sup>1</sup>

, RODRIGO ARIAS, Universidad de Chile — The spin wave modes of ferromagnetic films have been studied for a long time experimentally as well as theoretically: initially magnetostatic and later dipole-exchange modes. Theoretically dipole-exchange modes have been solved exactly numerically for some configurations and boundary conditions, and there are approximations of their frequency dispersion relations based on infinite series solutions and perturbation theory, valid for arbitrary orientations of an applied magnetic field, and for boundary conditions that allow varying degrees of pinning. A theoretical method that allows to determine with ease the exact frequency dispersion relations of the dipole-exchange modes is presented: it is required to solve numerically a 6x6 linear eigenvalue problem at each wavevector of interest; the spin wave modes inside or outside the sample may be plotted. Analogous calculations may be done to determine magnetostatic modes in detail. The method corresponds to a generalization of Green's theorem to the problem of determining the dipole-exchange modes of a ferromagnetic film: convolution integral equations for the magnetization and magnetostatic potential are derived on the surfaces of the film that become simple local algebraic equations in Fourier space, or for specific wavevectors.

<sup>1</sup>This work was supported by Project ICM FP10-061-F-FIC, Chile, and Center for the Development of Nanoscience and Nanotechnology CEDENNA FB0807 (Chile).

## Thursday, March 17, 2016 11:15AM - 2:15PM —

Session S19 GMAG DMP FIAP: Cooperative Phenomena: Spin-Orbit Coupling and Antiferromagnetism 318 - Ian Gilbert, NIST

## 11:15AM S19.00001 Electron correlation, spin-orbit coupling, intersite effects and the metal-insulator transition in pyrochlore iridates<sup>1</sup>

, RUNZHI WANG, ARA GO, ANDREW MILLIS, Columbia University — We perform density functional theory (DFT) plus single-site and cluster dynamical mean-field theory (DMFT/CDMFT) calculations to study the metal-insulator transition in the pyrochlore iridates  $\text{Lu}_2\text{Ir}_2\text{O}_7$ ,  $\text{Y}_2\text{Ir}_2\text{O}_7$  and  $\text{Eu}_2\text{Ir}_2\text{O}_7$ . The calculations include spin-orbit coupling. Single-site DMFT calculations indicate that the Lu compound is much more insulating than the Y or Eu materials but predict that the critical interaction strength is almost exactly the same for the Eu and Y compounds, although experimentally the metal-insulator transition temperatures are quite different. We further carry out the cluster DMFT (CDMFT) and observe much larger differences, consistent with experiments, demonstrating the crucial role played by spatial correlations.

<sup>1</sup>This work is supported by NSF DMR 1308236

## 11:27AM S19.00002 Magnetization and transport properties of single $\text{RPd}_2\text{P}_2$ (R=Y, La-Nd, Sm-Ho, Yb)<sup>1</sup>

, GIL DRACHUCK, ANNA BOEHMER, SERGEY L. BUD'KO, PAUL CANFIELD, Iowa State University/Ames Lab — Single crystals of  $\text{RPd}_2\text{P}_2$  (R=Y, La-Nd, Sm-Ho, Yb) were grown using a self-flux method and were characterized by room-temperature powder X-ray diffraction, anisotropic temperature and field dependent magnetization and temperature dependent in-plane resistivity. Anisotropic magnetic properties, arising mostly from crystal electric field (CEF) effects, were observed for most magnetic rare earths. The experimentally estimated CEF parameters  $B_0^2$  were calculated from the anisotropic paramagnetic  $\theta_{ab}$  and  $\theta_c$  values. Ordering temperatures, as well as the polycrystalline averaged paramagnetic Curie-Weiss temperature,  $\theta_{ave}$ , were extracted from magnetization and resistivity measurements.

<sup>1</sup>Work done at Ames Laboratory was supported by US Department of Energy, Basic Energy Sciences, Division of Materials Sciences and Engineering under Contract NO. DE-AC02-07CH111358.

## 11:39AM S19.00003 Dynamic scaling invariance at low temperatures

, VLADIMIR UDODOV, Katanov Khakas State University, KATANOV KHAKAS STATE UNIVERSITY TEAM — Using thermodynamic arguments we prove that the conventional consequences of the dynamic scale hypothesis change their character in the limit as the critical temperature  $T_c$  approaches zero. In particular, for liquid helium-4, the critical exponent  $\alpha$  associated with the heat capacity ( $\alpha < 0$ ) and other exponents related by the following new relation

$$\nu(z-1) = (1 + S_I - \alpha)/6, \quad T_C = T_\lambda \geq 0, \quad (3)$$

$$S_I = \left(\frac{T_C}{T}\right)^n, \quad T \geq T_C, \quad (4)$$

where  $n$  is a positive constant [1] and  $z$  is the dynamic critical exponent,  $\nu$  – the critical exponent of the correlation length. It is important that now the exponent  $z$  depends on  $T$  and  $T_\lambda$ . If  $T_\lambda = 0$  and  $T > 0$ , then the  $S_I$ -function [1] is zero and Eq. (??) becomes

$$\nu(z-1) = (1 - \alpha)/6, \quad T_C = 0, \quad (T > 0, \alpha < 0). \quad (5)$$

Eq. (??) can be applied, for example, to a mixture of liquid  $\text{He}^3$  and  $\text{He}^4$ . The results are valid for multi-component order parameter. 1. Udodov V. Violating of the Essam-Fisher and Rushbrooke Relationships at Low Temperatures// World Journal of Condensed Matter Physics. — 2015. — .5. — 2. — . 55-59. <http://dx.doi.org/10.4236/wjcmp.2015.52008>.

## 11:51AM S19.00004 Application of Novel Molecular Field Theory to Helical Antiferromagnetic Ordering in $\text{EuCo}_2\text{P}_2$ <sup>\*</sup>, D. C. JOHNSTON, N. S. SANGEETHA, Iowa State Univ — A formulation of Weiss molecular field theory (MFT) was recently advanced for antiferromagnetic (AFM) systems of identical crystallographically-equivalent local moments interacting by Heisenberg exchange that does not utilize the concept of magnetic sublattices.<sup>1</sup> This formulation has the attractive feature that the magnetic and thermal properties in magnetic fields $H \rightarrow 0$ depend only on the interactions of a representative spin with its neighbors, and thus allows the properties of collinear and coplanar noncollinear AFM structures to be understood and modeled on the same footing. Neutron diffraction measurements showed that $\text{EuCo}_2\text{P}_2$ with the bct $\text{ThCr}_2\text{Si}_2$ -type structure undergoes an AFM transition to a coplanar noncollinear $c$ -axis helical AFM structure below the ordering temperature $T_N = 66.5$ K.<sup>2</sup> Here we report the properties and apply our MFT to model the anisotropic magnetic susceptibility of single-crystal $\text{EuCo}_2\text{P}_2$ below $T_N$ .

1. D. C. Johnston, PRL **109**, 077201 (2012); PRB **91**, 064427 (2015).  
2. M. Reehuis et al., J. Phys. Chem. Solids **53**, 687 (1992).

\*Research supported by U.S. Department of Energy, Division of Materials Science and Engineering, under Contract No. DE-AC02-07CH11358.

## 12:03PM S19.00005 Investigation of Quantum Phase Transitions of Spin-3/2 AKLT Systems On the Hexagonal Lattice via the Tensor-Network Method<sup>1</sup>, TZU-CHIEH WEI, CHING-YU HUANG, C.N. Yang Institute for Theoretical Physics, Stony Brook University — The spin-3/2 Affleck-Kennedy-Lieb-Tasaki (AKLT) state on the hexagonal lattice is an example of valence-bond solid state (VBS), which is recently shown to provide resource for quantum computation and is also a nontrivial symmetry protected topologically ordered state if the translation invariance is imposed in addition to the rotation symmetry. Niggemann et al. previously studied a deformation of the AKLT model and derived a one-parameter family of ground states (parametrized by $a$ ) that are deformed from the AKLT point ( $a = \sqrt{3}$ ). By mapping to a free-fermion eight-vertex model, they identified a VBS to Néel transition at $a_{c2} \approx 2.5425$ . We employ the tensor-network method to directly compute the Néel order parameter and obtain results that agree with theirs. We also study the regime where the deformation parameter $a$ decreases close to zero. We find that there is a transition at $a_{c1} \approx 0.58$ to an XY phase, which is characterized by algebraically decaying correlations, rotation invariance of spins in the $x$ - $y$ plane and the induced magnetization being aligned with the direction of the extend field.

<sup>1</sup>This work was supported in part by the National Science Foundation.

## 12:15PM S19.00006 Inelastic neutron scattering study and magnetic excitations on the low-dimensional antiferromagnet $\alpha\text{-Cu}_2\text{V}_2\text{O}_7$ , GANATEE GITGEATPONG, Mahidol University, YANG ZHAO, University of Maryland, YIMING QIU, NIST Center for Neutron Research, KITTIWIT MATAN, Mahidol University — Magnetic excitations of the low-dimensional antiferromagnet $\alpha\text{-Cu}_2\text{V}_2\text{O}_7$ have been investigated using inelastic neutron scattering. The study reveals unusual commensurate splitting of magnetic excitation branches centered at a wave vector $(0, \pm\delta, 0)$ with $\delta = 0.25$ away from a magnetic zone center, where a magnetic Bragg peak is observed. The energy gap of 0.75 meV at $(0, \pm\delta, 0)$ was found to decrease as a function of temperature and the magnetic excitations become diffusive and disappear above 35 K coincident with $T_N = 33.4$ K. A recent experiment at the Multi Axis Crystal Spectrometer, MACS, to map the excitations over a large momentum space clearly shows the splitting of the dispersion at most of the allowed magnetic reflections. This commensurate splitting of the spin-wave-type excitations without the magnetic Bragg reflections at the same commensurate wave vectors has not yet been previously observed and remains unexplained. In the presentation, the experimental data will be shown and the possible explanation will also be discussed.

<sup>1</sup>This work was supported in part by the National Science Foundation.

## 12:27PM S19.00007 Tunable Collective Modes in the Dilute Ising Magnet $\text{LiHo}_{0.045}\text{Y}_{0.955}\text{F}_4$ , D.M. SILEVITCH, California Institute of Technology, G. AEPPLI, Paul Scherrer Institute, T.F. ROSENBAUM, California Institute of Technology — Collections of quantum mechanical spins with dipolar interactions exhibit a complex set of states and excitations due to the long range and alternating sign of the dipolar potential. We use nonlinear ac magnetic susceptibility on the dilute dipole Ising magnet $\text{LiHo}_{0.045}\text{Y}_{0.955}\text{F}_4$ to study the behavior of coupled clusters of spins. Pump-probe spectroscopy excites Fano resonance behavior between coherent, isolated spin clusters and a background spin bath. The evolution of these clusters exhibits universal behavior as a function of several different tuning parameters such as static transverse field, ac pump field, and thermal connectivity to a heat reservoir. We discuss our results within the framework of many-body localization.

<sup>1</sup>This work is supported by the US DOE, Basic Energy Sciences under Contract No. DE-AC02-07CH11358

## 12:39PM S19.00008 Physical properties of $\text{RMg}_2\text{Cu}_9$ ( $R = \text{Y, Ce-Nd, Gd-Dy}$ )<sup>1</sup>, TAI KONG, SERGEY BUD'KO, PAUL CANFIELD, Ames Laboratory/Iowa State University — $\text{RMg}_2\text{Cu}_9$ is a family of hexagonal compounds with a single rare earth site that has a $\bar{6}m2$ local symmetry. In this talk, magnetic, electric transport and specific heat data measured on single crystals of $\text{RMg}_2\text{Cu}_9$ synthesized using Ta crucible will be presented and discussed. Due to a strong CEF effect, all local moment bearing members (except for isotropic $\text{GdMg}_2\text{Cu}_9$ ) in the present study show a higher magnetic susceptibility when external field is applied along the $ab$ -plane than along the $c$ -axis. For $R = \text{Ce, Nd, Gd-Dy}$ , the compounds order antiferromagnetically above 2 K. The ordering temperature deviates from de Gennes scaling with $\text{GdMg}_2\text{Cu}_9$ ordering at a lower temperature than $\text{TbMg}_2\text{Cu}_9$ . $\text{PrMg}_2\text{Cu}_9$ does not order magnetically down to 2 K and might have a singlet ground state. This series of compounds offer an opportunity to study in-plane anisotropy of rare earth in a hexagonal CEF configuration, following our previous work on in-plane 4-state clock model in a tetragonal system, for example: $\text{HoNi}_2\text{B}_2\text{C}$ (P.C. Canfield et al. PRB 55, 970) and $\text{DyAgSb}_2$ (K.D. Myers et al. PRB 59, 1121).

<sup>1</sup>This work is supported by the US DOE, Basic Energy Sciences under Contract No. DE-AC02-07CH11358

## 12:51PM S19.00009 Multiplicative logarithmic corrections to quantum criticality in three-dimensional dimerized antiferromagnets, YANQI QIN, Institute of Physics, Chinese Academy of Sci (CAS), BRUCE NORMAND, Department of Physics, Renmin University of China, Beijing 100872, China, ANDERS SANDVIK, Department of Physics, Boston University, 590 Commonwealth Avenue, Boston, Massachusetts 02215, USA, ZI YANG MENG, Institute of Physics, Chinese Academy of Sci (CAS) — We investigate the quantum phase transition in an $S=1/2$ dimerized Heisenberg antiferromagnet in three spatial dimensions. By means of quantum Monte Carlo simulations and finite-size scaling analyses, we get high-precision results for the quantum critical properties at the transition from the magnetically disordered dimer-singlet phase to the ordered Neel phase. This transition breaks $O(N)$ symmetry with $N=3$ in $D=3+1$ dimensions. This is the upper critical dimension, where multiplicative logarithmic corrections to the leading mean-field critical properties are expected; we extract these corrections, establishing their precise forms for both the zero-temperature staggered magnetization, $m_s$ , and the Neel temperature, $T_N$ . We present a scaling ansatz for $T_N$ , including logarithmic corrections, which agrees with our data and indicates exact linearity with $m_s$ , implying a complete decoupling of quantum and thermal fluctuation effects close to the quantum critical point. These logarithmic scaling forms have not previously identified or verified by unbiased numerical methods and we discuss their relevance to experimental studies of dimerized quantum antiferromagnets such as $\text{TiCuCl}_3$ . Ref.: arXiv:1506.06073

<sup>1</sup>This work is supported by the US DOE, Basic Energy Sciences under Contract No. DE-AC02-07CH11358

**1:03PM S19.00010 Magnon-induced nonanalyticities in thermodynamic and transport properties of quantum ferromagnets<sup>1</sup>**, SRIPOORNA BHARADWAJ, DIETRICH BELITZ, Department of Physics and Institute of Theoretical Science, University of Oregon, Eugene, OR 97403, THEODORE R. KIRKPATRICK, Institute for Physical Science and Technology, and Department of Physics, University of Maryland, College Park, MD 20742 — Soft modes and their effects on thermodynamic and transport properties are of great interest. An example of a nonanalyticity induced by Goldstone modes is the divergence of the longitudinal susceptibility,  $\chi_L(k) \sim 1/k^{4-d}$ , in a classical isotropic Heisenberg ferromagnet in  $2 < d < 4$  dimensions everywhere in the ordered phase. Here we investigate the fate of this nonanalyticity in a quantum ferromagnet. Power counting at  $T = 0$  suggests a weaker singularity,  $\chi_L(k) \sim k^{d-2}$ , due to the additional frequency integration. We find that this term has a zero prefactor due to spin conservation. Consistent with this, a corresponding term in an antiferromagnet has a nonzero prefactor. A small but nonzero temperature restores the nonanalyticity in a ferromagnet, and the prefactor vanishes linearly with  $T$ . Similarly, magnetic impurities violate the spin conservation and lead to a nonanalytic term even at  $T = 0$ . We explore all of these effects by means of nonlinear sigma models for both ferromagnets and antiferromagnets, and by an effective field theory for itinerant ferromagnets, and discuss the crossover from the classical result to the  $T = 0$  limit in detail.

<sup>1</sup>Supported by the National Science Foundation under Grants No. DMR-140410 and DMR-140449

**1:15PM S19.00011 Magnetic phase transitions and magnetization reversal in MnRuP<sup>1</sup>**, P. LAMPEN-KELLEY, D. MANDRUS, University of Tennessee and Oak Ridge National Lab — The ternary phosphide MnRuP is an incommensurate antiferromagnetic metal crystallizing in the non-centrosymmetric Fe<sub>2</sub>P-type crystal structure. Below the Neel transition at 250 K, MnRuP exhibits hysteretic anomalies in resistivity and magnetic susceptibility curves as the propagation vectors of the spiral spin structure change discontinuously across  $T_1 = 180$  K and  $T_2 = 100$  K. Temperature-dependent X-ray diffraction data indicate that the first-order spin reorientation occurs in the absence of a structural transition. A strong magnetization reversal (MR) effect is observed upon cooling the system through  $T_N$  in moderate dc magnetic fields. Positive magnetization is recovered on further cooling through  $T_1$  and maintained in subsequent warming curves. The field dependence and training of the MR effect in MnRuP will be discussed in terms of the underlying magnetic structures and compared to anomalous MR observed in vanadate systems.

<sup>1</sup>This work is supported by the Gordon and Betty Moore Foundation GBMF4416 and U.S. DOE, Office of Science, BES, Materials Science and Engineering Division

**1:27PM S19.00012 ARPES study of the Kitaev Candidate RuCl<sub>3</sub>**, XIAOQING ZHOU, HAOXIANG LI, JUSTIN WAUGH, STEPHEN PARHAM, University of Colorado at Boulder, HEUNG-SIK KIM, HAE-YOUNG KEE, JENNIFER SEARS, YOUNG-JUNE KIM, University of Toronto, DANIEL DESSAU, University of Colorado at Boulder — RuCl<sub>3</sub> has been identified as a spin-orbital-assisted Mott insulator with possible Kitaev magnetic orders at low temperature by X-ray absorption, susceptibility, specific heat and Raman scattering[1-3]. Here we report high resolution ARPES spectroscopy measurements on single crystal RuCl<sub>3</sub>, and compare it with DFT calculations with and without magnetic order. Furthermore, the possible spin-orbital-assisted Mott transition is investigated through electron doping. [1] K.W.Plumb et al., Phys. Rev. B, 90, 041112 (2014). [2] J.A.Sears et al., Phys. Rev. B, 94, 144420 (2015). [3] L. J. Sandilands et al. Phys. Rev. Lett. 114, 147201 (2015).

**1:39PM S19.00013 Lifshitz-type metal-to-insulator transition via strong relativistic renormalization in NaOsO<sub>3</sub>**, BONGJAE KIM, PEITAO LIU, ZEYNEP ERGÖNENC, University of Vienna, Faculty of Physics, Computational Materials Physics, ALESSANDRO TOSCHI, Institut für Festkörperphysik, Technische Universität Wien, SERGI KHMELEVSKYI, University of Vienna, Faculty of Physics, Computational Materials Physics and Department of Physics, Budapest University of Technology and Economics, CESARE FRANCHINI, University of Vienna, Faculty of Physics, Computational Materials Physics — Using *ab initio* band structure methods in the framework of density functional theory (DFT), we study the mechanism responsible for the metal-to-insulator transition (MIT) in the 5d oxide NaOsO<sub>3</sub> and reinterpret its previously proposed Slater nature. We show that spin-orbit coupling (SOC) causes a strong relativistic renormalization of the electronic correlation that moves the system to a weakly interacting itinerant limit, where the physics of itinerant magnetism prevails. This is the opposite effect as compared to the widely studied iridates, where SOC drives the formation of a relativistic Mott state. By mapping the magnetically constrained non-collinear DFT calculation using spin-fluctuation theory, we explain the MIT of the system in connection with the anomalies observed in the experimental resistivity curve. We show that the continuous MIT is associated to the progressive disappearance of electron and hole pockets in the Fermi surface, typical of a Lifshitz-type MIT, and is mediated by spin-fluctuations. We discuss the inconsistencies of a pure Slater interpretation and propose that NaOsO<sub>3</sub> should be classified as a magnetically-driven relativistic Lifshitz insulator.

**1:51PM S19.00014 Spin-texture induced by oxygen vacancies in Strontium perovskites (001) surfaces: A theoretical comparison between SrTiO<sub>3</sub> and SrHfO<sub>3</sub>**, MAIA VERGNIO, Donostia International Physics Center, ANDRÉS-CAMILO GARCA-CASTRO, ERIC BOUSQUET, Physique Théorique des Matériaux, Université de Lige, B-4000 Sart-Tilman, Belgium, ALDO HUMBERTO ROMERO, Physics Department, West Virginia University, WV-26506-6315, Morgantown, USA — The electronic structure of SrTiO<sub>3</sub> and SrHfO<sub>3</sub> (001) surfaces with oxygen vacancies is studied by means of first-principles calculations. We reveal how oxygen vacancies within the first atomic layer of the SrTiO<sub>3</sub> surface (i) induce a large antiferrodistortive motion of the oxygen octahedra at the surface, (ii) drive localized magnetic moments on the Ti-3d orbitals close to the vacancies and (iii) form a two-dimensional electron gas localized within the first layers. The analysis of the spin-texture of this system exhibits a splitting of the energy bands according to the Zeeman interaction, lowering of the Ti-3d<sub>xy</sub> level in comparison with  $d_{xz}$  and  $d_{yz}$  and also an in-plane precession of the spins. No Rashba-like splitting for the ground state neither for *ab initio* molecular dynamics trajectory at 400K is recognized as suggested recently by A. F. Santander-Syro *et al.* [?]. Instead, a sizeable Rashba-like splitting is observed when the Ti atom is replaced by a heavier Hf atom with a much larger spin-orbit interaction. However, we observe the disappearance of the magnetism and the surface two-dimensional electron gas when full structural optimization of the SrHfO<sub>3</sub> surface is performed. Our results uncover

**2:03PM S19.00015 Quantum Impurities develop Fractional Local Moments in Spin-Orbit Coupled Systems<sup>1</sup>**, ADHIP AGARWALA, VIJAY B. SHENOY, Indian Institute of Science Bangalore — Systems with spin-orbit coupling have the potential to realize exotic quantum states which are interesting both from fundamental and technological perspectives. We investigate the new physics that arises when a correlated spin-1/2 quantum impurity hybridizes with a spin-orbit coupled Fermi system. The intriguing aspect uncovered is that, in contrast to unit local moment in conventional systems, the impurity here develops a *fractional local moment* of 2/3. The concomitant Kondo effect has a high Kondo temperature ( $T_K$ ). Our theory explains these novel features including the origins of the fractional local moment and provides a recipe to use spin-orbit coupling ( $\lambda$ ) to enhance Kondo temperature ( $T_K \sim \lambda^{4/3}$ ). These results will be useful in shedding light on a range of experiments, including those of magnetic impurities at oxide interfaces. Our predictions can also be directly tested in cold-atom systems where the spin-orbit coupling can be engendered via a uniform synthetic non-Abelian gauge field. In addition, this work opens up new directions of research in spin-orbit coupled Kondo lattice systems. Reference: arXiv:1509.07328

<sup>1</sup>Work supported by CSIR, DST and DAE

**Thursday, March 17, 2016 11:15AM - 2:15PM —**

**Session S20 DCOMP: Quantum Many-Body Systems and Methods I 319 - Brian Moritz, SLAC**

**11:15AM S20.00001 Tensor Network Algorithms for Braiding Anyons**, BABATUNDE AYENI, SUKHWINDER SINGH, Centre for Engineered Quantum Systems, Macquarie University, ROBERT PFEIFER, Dept. of Physics & Astronomy, GAVIN BRENNEN, Centre for Engineered Quantum Systems, Macquarie University — Anyons are point-like (quasi)particles which exist only in two-dimensional systems and have exchange statistics that are neither bosonic nor fermionic. These particles were first proposed as a mere theoretical curiosity, but it was later shown that they arise in topological states of matter and that certain species of non-Abelian anyons can be used for low error quantum computation. Despite the importance of anyons, fundamentally and technologically, comparatively little is understood about their many body behaviour especially when the non local effects of braiding are taken into account. This largely due to the lack of efficient numerical methods to study them. In order to circumvent this problem, and to broaden our understanding of the physics of anyons, the authors have developed several numerical methods based on tensor network algorithms including: anyonic Matrix Product States (MPS), anyonic Time Evolving Block Decimation (TEBD), anyonic Density Matrix Renormalization Group (DMRG), and Anyonic U(1) MPS. These can be used to simulate static interacting and itinerant braiding anyons on a finite or infinite lattice. We have used our methods to study the phase diagrams of some species, such as Abelian Z3 anyons and non-Abelian Fibonacci and Ising.

**11:27AM S20.00002 A Tensor Network Framework for Topological Order in Higher Dimensions**, BURAK SAHINOGLU, University of Vienna, MICHAEL WALTER, Stanford University, DOMINIC WILLIAMSON, University of Vienna — We present a general scheme for constructing topological lattice models in any space dimension using tensor networks. Our approach relies on finding "simplex tensors" that satisfy a finite set of tensor equations. Given any such tensor, we construct a discrete topological quantum field theory (TQFT) and local commuting projector Hamiltonians on any lattice. The ground space degeneracy of these models is a topological invariant that can be computed via the TQFT, and the ground states are locally indistinguishable when the ground space is nondegenerate on the sphere. Any ground state can be realized by a tensor network obtained by contracting simplex tensors. Our models are exact renormalization fixed points, covering a broad range of models in the literature. Lastly, we identify symmetries on the virtual level of the tensor networks of our models that generalize the topological invariance properties beyond fixed point models. This framework combined with recent tensor network techniques is convenient for studying excitations, their statistics, phase transitions, and ultimately for classification of gapped phases of many-body theories in 3+1 and higher dimensions.

**11:39AM S20.00003 Some tensor-network diagnostics for a class of 2D SPT states with internal symmetry**, ABHISHODH PRAKASH, TZU-CHIEH WEI, Stony Brook University — We demonstrate some diagnostic techniques to characterize certain 2D tensor network states with internal symmetries that are classified by the third group cohomology of the symmetry group. We use the discussions of Else et al. [Phys. Rev. B 90, 235137 (2014)] to extract data that determines the phase of matter from the tensors that make up a specific class of wave functions. This is possible because the symmetry transformation at the 'physical' level, which is of product form, translates to a symmetry in the 'virtual' level which may no longer be of product form. An appropriate analysis of the virtual-space symmetry helps us obtain the topological information (the 3-cocycle twist) that places the wave function in the classification scheme. This reproduces the results of Chen et al. [Phys. Rev. B 87, 155114 (2013)] without using projection operators in merging two 'Matrix Product Operators' of the symmetry representation of two group actions.

**11:51AM S20.00004 Weak-coupling instabilities of SU(N) fermions on the Bernal-stacked honeycomb bilayer in presence of on-site Hubbard Interactions<sup>1</sup>**, SUMIRAN PUJARI, University of Kentucky, THOMAS C. LANG, University of Innsbruck, RIBHU K. KAUL, University of Kentucky — Bernal-stacked bilayer graphene hosts an interesting 'non-relativistic' semi-metallic dispersion different from monolayer graphene. At this quadratic band touching, short-range interactions are marginal and hence cause instabilities to a variety of ground states. In this work we consider the instabilities of even  $N$  species of fermions on the Bernal bilayer with an  $SU(N)$ -symmetric contact interaction. For  $SU(2)$  fermions with an on-site Hubbard interaction the ground state has been found to be to a magnetic Nél state for all strengths of the interaction. In contrast, the leading weak coupling instability for  $N > 2$  is a non-magnetic ground state, which is gapped and odd under time reversal. On the other hand, at strong coupling we expect Nél or VBS ground states of the effective self-conjugate  $SU(N)$  spin models. Motivated by this observation, we investigate the phase diagram for even  $N > 2$  using determinantal quantum Monte Carlo computations.

<sup>1</sup>Support from NSF grant DMR-1056536 and XSEDE grant DMR-150037.

**12:03PM S20.00005 A many-body interpretation of Majorana bound states, and conditions for their localisation**, THOMAS O'BRIEN, Lorentz Institute, ANTHONY WRIGHT, University of Queensland — We derive a condition for the existence of completely or exponentially localised Majorana bound states (with the potential for non-Abelian statistics) in a generic many-body system. We discuss the relationship between the existence of these operators and the protection of the ground state degeneracy from local perturbations. We use our methods to study the exponential decay of the Majorana bound states in the non-interacting Kitaev chain, finding complete agreement between our many-body calculation and single-particle results. We then apply these results to various interacting systems which have previous evidence for Majorana bound states.

**12:15PM S20.00006 Hybrid-Space Density Matrix Renormalization Group Study of the Two-Dimensional Hubbard Model**, GEORG EHLERS, REINHARD M. NOACK, Philipps-University Marburg — We investigate the ground state of the two-dimensional Hubbard model on a cylinder geometry at intermediate coupling and weak doping. We study properties such as the behavior of the ground-state energy, pair-field correlations, and the appearance of stripes. We find striped ground states generically, with the width of the stripes depending on the filling, the boundary conditions, and the circumference of the cylinder. Furthermore, we analyse the interplay between the different stripe configurations and the decay of the pairing correlations. Our analysis is based on a hybrid-space density matrix renormalization group (DMRG) approach, which uses a momentum-space representation in the transverse and a real-space representation in the longitudinal direction. Exploiting the transverse momentum quantum number makes significant speedup and memory savings compared to the real-space DMRG possible. In particular, we obtain computational costs that are independent of the cylinder width for fixed size of the truncated Hilbert space.

**12:27PM S20.00007 Improving the efficiency of the Finite Temperature Density Matrix Renormalization Group method<sup>1</sup>**, ALBERTO NOCERA, GONZALO ALVAREZ, Oak Ridge National Laboratory — I review the basics of the finite temperature DMRG method, and then show how its efficiency can be improved by working on reduced Hilbert spaces and by using canonical approaches. My talk explains the applicability of the ancilla DMRG method beyond spins systems to t-J and Hubbard models, and addresses the computation of static and dynamical observables at finite temperature. Finally, I discuss the features of and roadmap for our DMRG++ codebase.

<sup>1</sup>Work done at CNMS, sponsored by the SUF Division, BES, U.S. DOE under contract with UT-Battelle. Support by the early career research program, DSUF, BES, DOE.

**12:39PM S20.00008 Geometric stability of the many-body localized phase in two and higher dimensions** , ANUSHYA CHANDRAN, Perimeter Institute, ARIJEET PAL, Oxford University, CHRIS LAUMANN, University of Washington, ANTONELLO SCARDICCHIO, Abdus Salam ICTP — Isolated disordered quantum systems need not equilibrate and be described by statistical mechanics; this is the phenomenon of many-body localization (MBL). In higher dimensions, the existence of MBL is a delicate question due to the possibility of inclusions of lower dimensional "thermal" regions. In this talk, I will argue that MBL is stable in higher dimensions by analyzing the geometry of a MBL insulator coupled to a thermal edge and develop a phenomenology of such systems.

**12:51PM S20.00009 Many-body localization characterized from a one-particle perspective** , SOUMYA BERA, MPI-PKS Dresden, HENNING SCHÖMERUS, Lancaster, UK, FABIAN HEIDRICH-MEISNER, LMU, Munich, JENS BARDARSON, MPI-PKS Dresden — We show that the one-particle density matrix can be used to characterize the interaction-driven many-body localization transition in closed fermionic systems. The eigenstates of density matrix are localized in the many-body localized phase and spread out when one enters the delocalized phase, while the eigenvalues reveals the distinctive Fock-space structure of the many-body eigenstates, exhibiting a step-like discontinuity in the localized phase. The associated one-particle occupation entropy is small in the localized phase and large in the delocalized phase, with diverging fluctuations at the transition. We analyze the inverse participation ratio of the natural orbitals and found that it is independent of system size in the localized phase.

**1:03PM S20.00010 Characterizing gapped phases of a 1D spin chain with on-site and spatial symmetries<sup>1</sup>** , COLIN WEST, ABHISHODH PRAKASH, TZU-CHIEH WEI, State Univ of NY- Stony Brook — We investigate the phase diagram of a spin-1 chain whose Hamiltonian is invariant under translation, lattice inversion and a global  $A_4$  symmetry in the spin degrees of freedom. The classification scheme by Chen, Gu, and Wen allows us to enumerate all possible phases under the given symmetry. Then, we determine which of these phases actually occur in the two-parameter Hamiltonian. Using numerical methods proposed by Pollmann and Turner (2012) we determine the characteristic projective parameters for the Symmetry Protected Topological (SPT) phases. In addition, we present a method for determining the projective commutation parameter in these phases. The resulting phase diagram is rich and contains at least nine different SPT phases.

<sup>1</sup>This work was supported in part by the National Science Foundation.

**1:15PM S20.00011 Continuous Matrix Product States for Spin-1/2 Fermions with Mass- and Spin-Imbalance** , SANGWOO S. CHUNG, C. J. BOLECH, Univ of Cincinnati — Recently, we have proposed a continuous matrix product states (cMPS) ansatz that can approximate ground states of interacting spin-1/2 fermions with spin-imbalance in 1D. We now extend that effort to describe a more general system, having both spin- and mass-imbalance. With mass-imbalance, there is no exact solution for the Gaudin-Yang Hamiltonian, and this is one of the first applications of the fermionic cMPS on non-integrable systems.

**1:27PM S20.00012 Controlled quantum transport in a disordered one-dimensional lattice** , SAHEL ASHHAB, Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, Qatar Foundation, Doha, Qatar — We investigate the effect of disorder on the transfer of quantum states across a one-dimensional lattice with varying levels of control resources. We find that the application of properly designed control signals, even when applied only to the two ends of the lattice, allows perfect state transfer up to disorder strengths that would not allow a generic quantum state to propagate the length of the lattice. At sufficiently large disorder strengths, however, the local control signals fail to send the quantum state from one end of the system to the other end. Our results shed light on the interplay between disorder and controlled transport in one-dimensional systems.

**1:39PM S20.00013 Inhomogeneous CDMFT and nonmagnetic impurities in graphene<sup>1</sup>** , M. CHARLEBOIS, D. SÉNÉCHAL, A.-M. GAGNON, A.-M.S. TREMBLAY, Université de Sherbrooke — In cluster dynamical mean-field theory (CDMFT), we usually apply the self-consistency condition on an infinite super-lattice of identical clusters. However, in some problems a large unit cell is required, for instance in the presence of a periodically repeated impurity. Since the impurity solver (exact diagonalization) can only treat small clusters, we break the unit cell into multiple small clusters that can be solved individually. This new technique is called inhomogeneous CDMFT (1) and is analogous to inhomogeneous DMFT (2). In this presentation, we will explain both the CDMFT and inhomogeneous CDMFT self-consistency loops within a unified, simple picture. We then apply this technique to a nonmagnetic impurity in graphene and study the emerging magnetism. Our results take into account dynamical correlations; nevertheless they qualitatively agree with previous mean-field and density functional theory studies.  
(1) Charlebois, M. et al., Phys. Rev. B 91, 035132 (2015).  
(2) Snoek, M. et al., New J. Phys. 10, 093008 (2008).

<sup>1</sup>Supported by NSERC, CIFAR and the Tier I Canada Research Chair Program

**1:51PM S20.00014 Spin selective localization transition in disordered interacting system in two dimensions: A quantum Monte-Carlo study** , SHASHI KUNWAR, Indian Inst of Tech-Madras, PRABUDDHA CHAKRABORTY, Indian Statistical Institute Chennai, RAJESH NARAYANAN, Indian Inst of Tech-Madras — The phenomenon of Anderson localization wherein non-interacting electrons are localized by quenched impurities is a subject matter that has been extremely well studied. However, localization transition under the combined influence of interaction and quenched disorder is less well understood. In this context we study the localization transition in a two-dimensional Hubbard model under the influence of a spin-selective disorder i.e, disorder which is operational on just one of the spin-species. The model is analyzed by laying recourse to a Quantum Monte Carlo based scheme. Using this approach we show the possibility of a metal-insulator transition. However, we will show that this metal-insulator transition is extremely sensitive to the filling-fraction inherent in the system. Our results will be encapsulated in a phase diagram.

**2:03PM S20.00015 Real space study of current flow through nanoscopic Kondo lattices** , JOHN VAN DYKE, DIRK MORR, University of Illinois at Chicago — We study current flow through a nanoscopic Kondo lattice in real space and with finite applied voltage. We show how the presence of a defect, such as an f-electron vacancy, modifies the current flow in its vicinity, depending on lead geometry and coupling to phonons. Finally, we report a self-consistent calculation of the change in the hybridization between the conduction and f-electrons caused by the applied bias.

**Thursday, March 17, 2016 11:15AM - 2:15PM –**

**Session S21 GSCCM DCOMP DMP: Materials at Extremes: Kinetics of Phase Transitions** 320

- Ricky Chau, LLNL

**11:15AM S21.00001 Coupling phase transition kinetics and hydrodynamics: Models for solid-solid and liquid-solid transformation in dynamically driven materials<sup>1</sup>**, JONATHAN BELOF, LORIN BENEDICT, ALEXANDER CHERNOV, BURL HALL, SEBASTIEN HAMEL, TOMORR HAXHIMALI, BABAK SADIGH, LUIS ZEPEDA-RUIZ, Lawrence Livermore National Laboratory — High pressure and high strain-rate experiments are opening a new frontier toward the study of material science under extreme conditions. As the energy density of experimental platforms is increased, the timescale for observation is typically decreased to the point where the time dependence of phase transitions is now a subject of direct study. We will present new phase transition kinetics models that have been developed with unique considerations that arise in shock-wave driven phase transformation, highlighting applications of the methodology to the simulation of recent experiments of iron and water.

<sup>1</sup>This work is performed under the auspices of the U. S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

**11:27AM S21.00002 Construction of a kinetics model for liquid-solid transitions built from atomistic simulations<sup>1</sup>**, LORIN BENEDICT, LUIS ZEPEDA-RUIZ, TOMORR HAXHIMALI, SEBASTIEN HAMEL, BABAK SADIGH, ALEXANDER CHERNOV, JONATHAN BELOF, Lawrence Livermore National Laboratory — We discuss work in progress towards a kinetics model for dynamically-driven liquid-solid transitions built from MD simulations. The growth of solid particles within a liquid is studied for a range of conditions, and careful attention is paid to the construction of an accurate multi-phase (equilibrium) equation of state for the system under consideration, in order to provide a framework upon which the non-equilibrium physics is based.

<sup>1</sup>his work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC.

**11:39AM S21.00003 A mean-field thermodynamic description of the kinetics of overdriven interfaces.<sup>1</sup>**, TOMORR HAXHIMALI, JONATHAN BELOF, BABAK SADIGH, Lawrence Livermore National Laboratory — A key aspect of an accurate description of shock-induced structural phase transitions is the rigorous computation of the dynamics of the interfaces between coexisting phases. In the wake of the shock, the system will be exposed to strong gradient fields that give rise to overdriven interfaces during the induced phase transformation. In this work we take a mean-field approach using a time-dependent Ginzburg-Landau formalism to describe the dynamics of such overdriven interfaces. We make a connection of the mean-field result to a quasi-Langevin description, the Kardar-Parisi-Zhang (KPZ) equation, of the kinetics of the interface. Further, larger coarse-grained descriptions of the phase transition such as the Kolmogorov-Johnson-Mehl-Avrami (KJMA) model, which are commonly coupled to hydrodynamic equations that describe the evolution of the temperature and pressure during the shock propagation, ignore the details of the dynamics and structure of the interfacial regions. Overlaying the KPZ description of the interface evolution to these coarse-grained methods will result in physically more accurate multiscale models for shock propagation. We will present results from our efforts in this regard.

<sup>1</sup>This work is performed under the auspices of the U. S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

**11:51AM S21.00004 Dynamic materials response at multiscales: Experiments and simulations<sup>1</sup>**, SHENG-NIAN LUO, The Peac Institute of Multiscale Sciences, Chengdu, Sichuan, 630031, P. R. China — One of the grand challenges in materials physics is dynamic responses to impulsive loading, including shock waves, radiation, and pulsed fields, due to their highly transient nature and extremely complex microstructure effects. Dynamic responses, such as plasticity, damage, cavitation, phase changes, and chemical reactions, are inherently multiscale and heavily dependent on microstructure. One has to resort to a suite of tools, including experiments, modeling and simulations, and theory. However, the gaps in spatial or temporal scales between experiments and simulations are still wide, while cross-scale theories are still in early development. To this end, we exploit large-scale molecular dynamics simulations, electron microscopy, and ultrafast synchrotron X-ray imaging and scattering, to probe materials response at length scales ranging from lattice to micron, and time scales, from picosecond to second. For examples, simultaneous, high-speed, X-ray imaging (mesoscale strain-field mapping) and diffraction measurements along with macroscopic measurements have been achieved. Based on classical nucleation theory and large-scale molecular dynamics simulations, we demonstrate the equivalence between length and time scales for nucleation events, which provides a framework to bridge different scales. Certainly, advancing multiscale science requires sustained, concerted, experimental, modeling and theoretical efforts.

<sup>1</sup>We have benefited from the colleagues at the Advanced Photon Source, and the Peac Institute of Multiscales Sciences.

**12:27PM S21.00005 Accelerating Molecular Dynamics Simulations to Investigate Shock Response at the Mesoscales.**, AVINASH DONGARE, GARVIT AGARWAL, University of Connecticut, RAMAKRISHNA VALISETTY, RAJU NAMBURU, US Army Research Laboratory, ARUNACHALAM RAJENDRAN, University of Mississippi — The capability of large-scale molecular dynamics (MD) simulations to model dynamic response of materials is limited to system sizes at the nanoscales and the nanosecond timescales. A new method called quasi-coarse-grained dynamics (QCGD) is developed to expand the capabilities of MD simulations to the mesoscales. The QCGD method is based on solving the equations of motion for a chosen set of representative atoms from an atomistic microstructure and retaining the energetics of these atoms as would be predicted in MD simulations. The QCGD method allows the modeling of larger size systems and larger time-steps for simulations and thus is able to extend the capabilities of MD simulations to model materials behavior at mesoscales. The success of the QCGD method is demonstrated by reproducing the shock propagation and failure behavior of single crystal and nanocrystalline Al microstructures as predicted using MD simulations and also modeling the shock response and failure behavior of Al microstructures at the micron length scales. The scaling relationships, the hugoniot behavior, and the predicted spall strengths using the MD and the QCGD simulations will be presented. This work is sponsored by the US Army Research Office under Contract# W911NF-14-1-0257.

**12:39PM S21.00006 Corrections of Hayes Equation of State for Phase Transform under Dynamic Loading.**, TAO CHONG<sup>1</sup>, USTC — **Abstract:** The experimental results of iron under ramp wave and shock compression are simulated with Hayes equation of state (EOS) for phase transition. The calculated results are consistent with the experimental data under shock, and don't agree well with the data under ramp wave loading. The reason for the problem is that the bulk modulus in Hayes model is constant (i.e., Bulk sound speed is constant). The sound speed corresponds to the slope of the Rayleigh line when materials leap from the initial state to the final state under shock loading, therefore, the bulk modulus can be considered as a constant. However, under ramp loading, material from initial to the final state is consecutive, and the bulk modulus is not a constant any more but a function of pressure and temperature. The bulk modulus of Hayes EOS is corrected with Murnaghan EOS, and the corrected Hayes EOS is applies to simulate the experimental results. The results show that the calculated data agree well with the experimental data under both shock and ramp wave loadings. .

<sup>1</sup>I hope you give me an oral presentation, otherwise I might not be able to attend the meeting

**12:51PM S21.00007 Mercury Induced by Pressure to act as a Transition Metal in Mercury Fluorides**, JORGE BOTANA, Beijing CSRC, XIAOLI WANG, Institute of Condensed Matter Physics, Linyi University, CHUNJU HOU, School of Science, Jiangxi University of Science and Technology, DADONG YAN, Department of Physics, Beijing Normal University, HAIQING LIN, Beijing CSRC, YANMING MA, State Key Lab of Superhard Materials, Jilin University, MAO-SHENG MIAO, Department of Chemistry and Biochemistry, California State University — The question of whether Hg is a transition metal remains open for stable solids. In our work we propose that high-pressure techniques will help prepare unusual oxidation states[1] of Hg in Hg-F compounds. By means of *ab initio* calculations and an advanced structure-search algorithm we find that under high pressure charge is transferred from the Hg d orbitals to the F, and becomes a transition metal.[2] HgF<sub>3</sub> and HgF<sub>4</sub> have been found to be stable compounds at high pressure. HgF<sub>4</sub> consists of planar molecules, a typical geometry for d<sup>8</sup> metallic centers. HgF<sub>3</sub> is an example of metallic and ferromagnetic compound, with an electronic structure analogous to transparent conductors due to the Hg d<sup>9</sup> configuration.

## References

[1] M.-S. Miao, Nat. Chem. **5**, 846 (2013)

[2] J. Botana, X. Wang, C. Hou, D. Yang, H. Lin, Y. Ma, M.-S. Miao, Angew. Chem. Int. Edit. **54**, 9280 (2015).

**1:03PM S21.00008 Can high pressure I-II transitions in semiconductors be affected by plastic flow and nanocrystal precipitation in phase I?**, B. A. WEINSTEIN, SUNY at Buffalo, Physics Dept., Buffalo, NY 14260 USA, G. P. LINDBERG, Rochester Precision Optics, W. Henrietta, NY 14586 USA — Pressure-Raman spectroscopy in ZnSe and ZnTe single crystals reveals that Se and Te nano-crystals (NCs) precipitate in these II-VI hosts for pressures far below their I-II phase transitions.[1] The inclusions are evident from the appearance and negative pressure-shift of the A<sub>1</sub> Raman peaks of Se and Te (trigonal phase). The Se and Te NCs nucleate at dislocations and grain boundaries that arise from pressure-induced plastic flow. This produces chemical and structural inhomogeneities in the zincblende phase of the host. At substantially higher pressures, the I-II transition proceeds in the presence of these inhomogeneities. This can affect the transition's onset pressure  $P_t$  and width  $\Delta P_t$ , and the occurrence of metastable phases along the transition path. Precipitation models in metals show that nucleation of inclusions depends on the Peierls stress  $\tau_p$  and a parameter  $\alpha$  related to the net free energy gained on nucleation. For favorable values of  $\tau_p$  and  $\alpha$ , NC precipitation at pressures below the I-II transition could occur in other compounds. We propose criteria to judge whether this is likely based on the observed ranges of  $\tau_p$  in the hosts, and estimates of  $\alpha$  derived from the cohesive energy densities of the NC materials. One finds trends that can serve as a useful guide, both to test the proposed criteria, and to decide when closer scrutiny of phase transition experiments is warranted, e.g., in powders where high dislocation densities are initially created. [1] G. P. Lindberg, et. al., Phys. Status Solidi B 250, 711 (2013)

**1:15PM S21.00009 Tin phase transition in terapascal pressure range described accurately with Quantum Monte Carlo.**, ROMAN NAZAROV, RANDOLPH HOOD, MIGUEL MORALES, Lawrence Livermore Natl Lab — The accurate prediction of phase transitions is one of the most important research areas in modern materials science. The main workhorse for such calculations, Density functional theory (DFT), employs different forms of approximate exchange-correlation functionals which may lead to overstabilization of one phase compared to another, therefore, predict incorrectly phase transition pressures. A recent example of such deficiency has been demonstrated in Sn: no bcc to hcp phase transition has been observed in Sn when dynamically compressed to 1.2 TPa while DFT predicts a transition to occur at 0.16-0.2 TPa [1]. To overcome the limitations of DFT, we have employed diffusion quantum Monte Carlo (DMC) method which treats the many body electron problem directly. In order to get highly accurate results we systematically assess the effect of controllable approximations of DMC such as fixed node approximation, finite-size effects and the use of pseudopotentials. Based on metrologically accurate DMC equation of states we construct the pressure-temperature phase diagram and demonstrate its good agreement with experiment in contrast to DFT calculations. [1] A. Lazicki et al., X-Ray Diffraction of Solid Tin to 1.2 TPa. Phys. Rev. Lett. 115, 075502 (2015).

**1:27PM S21.00010 Phase conversion in silicon and carbon nanomaterials at extreme pressure**, MATTHEW CRANE, BENNETT SMITH, EVAN ABRAMSON, PETER PAUZAUSKIE, University of Washington — The high pressures and temperatures accessible in laser-heated diamond anvil cells (LH-DAC) have produced fundamental insights by identifying metastable states with extraordinary properties. However, the actual conditions necessary to access a metastable state depend on the kinetics of phase transformation. The explosion of research in nanomaterials has generated interest in exploring how phase transformations occur in materials with high radii of curvature, and how we can leverage these effects. We present work investigating phase transformations in Si- and C-based nanomaterials with high radii of curvature. We have loaded a LH-DAC with Si nanowires (NWs) and examined the phase at a range of pressures to discover a recoverable phase transition to a wurtzite crystal structure. For C materials, we have synthesized a pyrolyzed carbon aerogel, an amorphous carbon sol gel with size features of ~10 nm and incredibly low density and thermal conductivity (~10<sup>-2</sup> W/m-K). We investigate spatial resolution of heating under pressure and the effect of temperature on resulting material electronic structure. Finally, we model heating with Mie theory to provide insights into the phase transformations of nanomaterials.

**1:39PM S21.00011 ABSTRACT WITHDRAWN —**

**1:51PM S21.00012 Equilibrium phase boundary between hcp-cobalt and fcc-cobalt**, HYUNCHAE CYNN, MAGNUS J. LIPP, WILLIAM J. EVANS, BRUCE J. BAER, Lawrence Livermore Natl Lab — In 2000 (Yoo et al., PRL), fcc-cobalt was reported as a new high pressure phase transforming from ambient hcp-cobalt starting at around 105 GPa and 300 K. Both cobalts coexist up to 150 GPa and thereafter only fcc-cobalt was found to be the only stable phase to 200 GPa. Our recent synchrotron x-ray diffraction data on cobalt are at odds with the previous interpretation. We will present our new finding and elaborate on our understanding in terms of the equilibrium phase boundary of cobalt. We will also compare our previous work on xenon (Cynn et al., 2001, PRL) with our new results on cobalt. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. Portions of this work were performed at HPCAT (Sector 16), APS, Argonne National Laboratory. HPCAT operations are supported by DOE-NNSA under Award No. DENA0001974 and DOE-BES under Award No. DE-FG02-99ER45775. The Advanced Photon Source is a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

**2:03PM S21.00013 Atomistic simulation of Shock Induced Structural Phase Transition of Single Crystal Copper**, NILANJAN MITRA, ANUPAM NEOGI, Indian Institute of Technology Kharagpur — It is well known that pure Single crystal copper subjected to shock wave loading of different intensities results in development of different types of plasticity mechanisms. Beyond that regime of shock wave intensity it has also been shown in several literature that single crystal Cu shows melting. A regime of shock loading has been identified in this research in which single crystal Cu undergoes a structural phase transition. Identification of this structural phase transition mechanism as well as the resulting phase has not only been done using radial distribution functions and structure factor but also with virtual X-Ray diffraction. Phonon dispersion at these high temperatures and pressures have also been investigated. The effect of crystallographic orientation and initial temperature of the sample has been investigated in this simulation study.

**Thursday, March 17, 2016 11:15AM - 2:15PM –**  
**Session S22 DCOMP: Revealing New Physics With Petascale and Beyond Computational Resources** 321 - Bogdan Mihalia, National Science Foundation

**11:15AM S22.00001 Scalable real space pseudopotential density functional codes for materials in the exascale regime<sup>1</sup>**, CHARLES LENA, JAMES CHELIKOWSKY, GRADY SCHOFIELD, University of Texas at Austin, ARIEL BILLER, LEEOR KRONIK, Weizmann Institute of Science, YOUSEF SAAD, University of Minnesota, JACK DESLIPPE, National Energy Research Scientific Computing Center — Real-space pseudopotential density functional theory has proven to be an efficient method for computing the properties of matter in many different states and geometries, including liquids, wires, slabs, and clusters with and without spin polarization. Fully self-consistent solutions using this approach have been routinely obtained for systems with thousands of atoms. Yet, there are many systems of notable larger sizes where quantum mechanical accuracy is desired, but scalability proves to be a hindrance. Such systems include large biological molecules, complex nanostructures, or mismatched interfaces. We will present an overview of our new massively parallel algorithms, which offer improved scalability in preparation for exascale supercomputing. We will illustrate these algorithms by considering the electronic structure of a Si nanocrystal exceeding  $10^4$  atoms.

<sup>1</sup>Support provided by the SciDAC program, Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Sciences. Grant Numbers DE-SC0008877 (Austin) and DE-FG02-12ER4 (Berkeley)

**11:27AM S22.00002 Large DFT: to 100K atoms and beyond.**, JONATHAN MULLIN, Army Research Laboratory — A quantum mechanical (QM) approach to materials science provides a gold standard atomistic picture of the mechanisms responsible for a range of phenomena seen in macroscopic and experimental situations. The need to understand materials science problems from atomistic to macroscale was the impetus for ARL to initiate the Enterprise for Multiscale Material Research. This long term project attempts to redefine how materials science questions are posed, and solved. To support this goal, current state-of-the-art QM capabilities need to be extended in the number of atoms which can be treated and the length scale of the dynamics which can be simulated. This extension is referred to as large scale QM, both large spatially and temporally. This will enable fundamental advances in the understanding of materials science problems.

**11:39AM S22.00003 Real Space Multigrid (RMG) Open Source Software Suite for Multi-Petaflops Electronic Structure Calculations**, EMIL BRIGGS, MIROSLAV HODAK, WENCHANG LU, JERRY BERNHOLC, YAN LI, North Carolina State University — RMG is a cross platform open source package for ab initio electronic structure calculations that uses real-space grids, multigrid pre-conditioning, and subspace diagonalization to solve the Kohn-Sham equations. The code has been successfully used for a wide range of problems ranging from complex bulk materials to multifunctional electronic devices and biological systems. RMG makes efficient use of GPU accelerators, if present, but does not require them. Recent work has extended GPU support to systems with multiple GPU's per computational node, as well as optimized both CPU and GPU memory usage to enable large problem sizes, which are no longer limited by the memory of the GPU board. Additional enhancements include increased portability, scalability and performance. New versions of the code are regularly released at [sourceforge.net/projects/rmgdft/](http://sourceforge.net/projects/rmgdft/). The releases include binaries for Linux, Windows and Macintosh systems, automated builds for clusters using cmake, as well as versions adapted to the major supercomputing installations and platforms.

**11:51AM S22.00004 Understanding Strongly Correlated Materials thru Theory Algorithms and High Performance Computers**, GABRIEL KOTLIAR, Rutgers University and Brookhaven National Laboratories — A long standing challenge in condensed matter physics is the prediction of physical properties of materials starting from first principles. In the past two decades, substantial advances have taken place in this area. The combination of modern implementations of electronic structure methods in conjunction with Dynamical Mean Field Theory (DMFT), in combination with advanced impurity solvers, modern computer codes and massively parallel computers, are giving new system specific insights into the properties of strongly correlated electron systems enable the calculations of experimentally measurable correlation functions. The predictions of this "theoretical spectroscopy" can be directly compared with experimental results. In this talk I will briefly outline the state of the art of the methodology, and illustrate it with an example the origin of the solid state anomalies of elemental Plutonium.

**12:27PM S22.00005 Large-scale quantum transport calculations for electronic devices with over ten thousand atoms**, WENCHANG LU, YAN LU, ZHONGCAN XIAO, MIROSLAV HODAK, EMIL BRIGGS, JERRY BERNHOLC, North Carolina State University — The non-equilibrium Greens function method (NEGF) has been implemented in our massively parallel DFT software, the real space multigrid (RMG) code suite. Our implementation employs multi-level parallelization strategies and fully utilizes both multi-core CPUs and GPU accelerators. Since the cost of the calculations increases dramatically with the number of orbitals, an optimal basis set is crucial for including a large number of atoms in the active device part of the simulations. In our implementation, the localized orbitals are separately optimized for each principal layer of the device region, in order to obtain an accurate and optimal basis set. As a large example, we calculated the transmission characteristics of a Si nanowire p-n junction. The nanowire is along (110) direction in order to minimize the number dangling bonds that are saturated by H atoms. Its diameter is 3 nm. The length of 24 nm is necessary because of the long-range screening length in Si. Our calculations clearly show the I-V characteristics of a diode, i.e., the current increases exponentially with forward bias and is near zero with backward bias. Other examples will also be presented, including three-terminal transistors and large sensor structures.

**12:39PM S22.00006 Implementing Parquet equations using HPX<sup>1</sup>**, SAMUEL KELLAR, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana, BIBEK WAGLE, Department of Computer Science and Engineering, Louisiana State University, Baton Rouge, Louisiana, SHUXIANG YANG, KA-MING TAM, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana, HARTMUT KAISER, Center of Computation and Technology, Louisiana State University, Baton Rouge, Louisiana, JUANA MORENO, MARK JARRELL, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana — A new C++ runtime system (HPX) enables simulations of complex systems to run more efficiently on parallel and heterogeneous systems. This increased efficiency allows for solutions to larger simulations of the parquet approximation for a system with impurities. The relevancy of the parquet equations depends upon the ability to solve systems which require long runs and large amounts of memory. These limitations, in addition to numerical complications arising from stability of the solutions, necessitate running on large distributed systems. As the computational resources trend towards the exascale and the limitations arising from computational resources vanish efficiency of large scale simulations becomes a focus. HPX facilitates efficient simulations through intelligent overlapping of computation and communication. Simulations such as the parquet equations which require the transfer of large amounts of data should benefit from HPX implementations.

<sup>1</sup>Supported by the the NSF EPSCoR Cooperative Agreement No. EPS-1003897 with additional support from the Louisiana Board of Regents

**12:51PM S22.00007 Asperities, Crack Front Waves and Crack Self Healing**, PANKAJ RAJAK, RAJIV KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, Univ of Southern California — We have performed petascale simulations to study nanomaterial systems capable of sensing and repairing damage in high temperature/high pressure operating conditions. The system we have studied is a ceramic nanocomposite consisting of silicon carbide/silicon dioxide core/shell nanoparticles embedded in alumina. We observe that the interaction of the crack with core/shell asperities gives rise to crack-front waves. We also study crack healing by diffusion of silica into the crack as a function of nanoparticle size and inter-particle distance. Our results are well supported by experimental observations.

**1:03PM S22.00008 Biophysical Discovery through the Lens of a Computational Microscope**, ROMMIE AMARO, University of California, San Diego — With exascale computing power on the horizon, improvements in the underlying algorithms and available structural experimental data are enabling new paradigms for chemical discovery. My work has provided key insights for the systematic incorporation of structural information resulting from state-of-the-art biophysical simulations into protocols for inhibitor and drug discovery. We have shown that many disease targets have druggable pockets that are otherwise “hidden” in high resolution x-ray structures, and that this is a common theme across a wide range of targets in different disease areas. We continue to push the limits of computational biophysical modeling by expanding the time and length scales accessible to molecular simulation. My sights are set on, ultimately, the development of detailed physical models of cells, as the fundamental unit of life, and two recent achievements highlight our efforts in this arena. First is the development of a molecular and Brownian dynamics multi-scale modeling framework, which allows us to investigate drug binding kinetics in addition to thermodynamics. In parallel, we have made significant progress developing new tools to extend molecular structure to cellular environments. Collectively, these achievements are enabling the investigation of the chemical and biophysical nature of cells at unprecedented scales.

**1:39PM S22.00009 Multiscale Dynamics in Soft-Matter Systems: Enzyme Catalysis, Sec-Facilitated Protein Translocation, and Ion-Conduction in Polymers.**, THOMAS MILLER, California Institute of Technology — Nature exhibits dynamics that span extraordinary ranges of space and time. In some cases, these dynamical hierarchies are well separated, simplifying their understanding and description. But chemistry and biology are replete with examples of dynamically coupled scales. In this talk, we will discuss the use of high-performance computing and new simulation methods that enable the inclusion of nuclear quantum effects, such as zero point energy and tunneling, in the reaction dynamics of enzymes, as well as coarse-graining strategies to enable minute-timescale simulations of protein targeting to cell membranes and ion-conduction in polymer electrolytes for lithium-ion battery applications.

**Thursday, March 17, 2016 11:15AM - 2:15PM –**

**Session S23 DMP GERA FIAP: Thermoelectrics Theory I** 322 - Joseph Feser, University of Delaware

**11:15AM S23.00001 Phonon Heat Conduction In Nanostructures: Ballistic, Coherent, Localized, Hydrodynamic, and Divergent Modes<sup>1</sup>**, GANG CHEN, Massachusetts Institute of Technology — In this talk, we will discuss different modes of heat conduction in nanostructures. Ballistic transport happens when phonon mean free path is longer than the characteristic size of the structure. We will discuss how we compute phonon mean free path distributions based on first-principles and measure the distributions with optical pump-probe techniques by exploring ballistic phonon transport processes. In superlattice structures, ballistic phonon transport across the whole thickness of the superlattices implies phase coherence. We observed this coherent transport in GaAs/AlAs superlattices with fixed periodic thickness and varying number of periods. Simulations show that although high frequency phonons are scattering by roughness, remaining long wavelength phonons maintain their phase and traverse the superlattices ballistically. Accessing the coherent heat conduction regime opens a new venue for phonon engineering. We show further that phonon heat conduction localization happens in GaAs/AlAs superlattice by placing ErAs nanodots at interfaces. This heat-conduction localization phenomenon is confirmed by nonequilibrium atomic Green's function simulation. These ballistic and localization effects can be exploited to improve thermoelectric energy conversion materials via reducing their thermal conductivity. In another opposite, we will discuss phonon hydrodynamic transport mode in graphene via first-principle simulations. In this mode, phonons drift with an average velocity under a temperature gradient, similar to fluid flow in a pipe. Conditions for observing such phonon hydrodynamic modes will be discussed. Finally, we will talk about the one-dimensional nature of heat conduction in polymer chains. Such 1D nature can lead to divergent thermal conductivity. Inspired by simulation, we have experimentally demonstrated high thermal conductivity in ultra-drawn polyethylene nanofibers and sheets.

<sup>1</sup>Work supported by DOE Office of Basic Energy Sciences under Award Number: DE-SC0001299/DE-FG02-09ER46577.

**11:51AM S23.00002 Green-Kubo Modal Analysis**, ASEGUN HENRY, Georgia Institute of Technology — A new method for direct calculation of the modal contributions to thermal conductivity, which is termed Green-Kubo modal analysis (GKMA) will be presented. The GKMA method combines the lattice dynamics formalism with the Green-Kubo formula for thermal conductivity, such that the thermal conductivity becomes a direct summation of modal contributions, where one need not define the phonon velocity. As a result, the GKMA method can be applied to any material/group of atoms, where the atoms vibrate around stable equilibrium positions, which includes crystalline line compounds, non-stoichiometric compounds, random alloys, amorphous materials and even rigid molecules. By using molecular dynamics simulations to obtain the time history of each mode's contribution to the heat current, one naturally includes anharmonicity to full order and can obtain insight into the interactions between different modes through the cross-correlations. Several example materials will be discussed and the specific attention will be devoted to new fundamental questions that arise from the changes in mode character that occur in disordered systems. The GKMA method provides new insight into the nature of phonon transport, as it casts the problem in terms of mode-mode correlation instead of scattering, and provides a general unified formalism that can be used to understand phonon-phonon interactions in essentially any class of materials or structures where the atoms vibrate around stable equilibrium sites.

**12:03PM S23.00003 On The Solenoidal Heat Flux in Quasi-Ballistic Thermal Conduction<sup>1</sup>**, ASHOK RAMU, JOHN BOWERS, UC Santa Barbara — The Boltzmann transport equation for phonons is recast directly in terms of the heat-flux by means of iteration followed by truncation at the second order in the spherical harmonic expansion of the distribution function. This procedure displays the heat-flux in an explicitly coordinate-invariant form, and leads to a natural decomposition into two components, namely the solenoidal component in addition to the usual irrotational component. The solenoidal heat-flux is explicitly shown to arise in a right-circular cylinder when the transport is in the quasi-ballistic regime. These findings are important in the context of phonon resonators that utilize the strong quasi-ballistic thermal transport reported recently in silicon membranes at room temperature. Effects due to circulating heat fluxes are noted in the effective thermal conductivity of silicon discs.

<sup>1</sup>This work was funded by the National Science Foundation, USA under project number CMMI-1363207.

**12:15PM S23.00004 Active Extraction of Near-field Thermal Radiation** , DING DING, TAEYONG KIM, AUSTIN MINNICH, Caltech — Radiative heat transport between materials supporting surface-phonon polaritons is greatly enhanced when the materials are placed at sub-wavelength separation as a result of the contribution of near-field surface modes. However, the enhancement is limited to small separations due to the evanescent decay of the surface waves. In this work, we propose and numerically demonstrate an active radiative cooling (ARC) scheme to extract these modes to the far-field. Our approach exploits the monochromatic nature of near-field thermal radiation to drive a transition in a laser gain medium, which, when coupled with external optical pumping, allows the resonant surface mode to be emitted into the far-field. We also provide further insights into our ARC scheme by applying the theoretical framework used for laser cooling of solids (LCS) to ARC. We show that LCS and ARC can be described with the same mathematical formalism by replacing the electron-phonon coupling parameter in LCS with the electron-photon coupling parameter in ARC. Using this framework, we examine the predictions of the formalism for LCS and ARC using realistic parameters and find that ARC can achieve higher efficiency and extracted power over a wide range of conditions. Our study demonstrates a new approach to manipulate near-field thermal radiation for thermal management.

**12:27PM S23.00005 Spectral Analysis of Surface Controlled Phonon Transport in Nanophononic Metamaterials<sup>1</sup>** , SANGHAMITRA NEOGI, University of Colorado at Boulder, DAVIDE DONADIO, University of California Davis — Phonon engineering in nanostructured semiconductors has shown promises to further advance the performance of energy applications beyond the state-of-the-art limit. In nanostructured materials, phonon transport is greatly affected by the surface nanoscale character[1]. The concept of nanophononic metamaterial (NPM) was introduced recently [2] to affect nanoscale thermal transport with the inclusion of local surface resonators. We carried out a systematic investigation of phonon transport in locally resonant silicon-based NPMs. We used classical equilibrium molecular dynamics and a Boltzmann transport equation approach with the relaxation time approximation to investigate the nature of phononic thermal transport in nanopatterned silicon membranes with thicknesses of the order of 10 nm and below. We find the presence of local surface resonators has a significant effect on the phonon dispersion and has a direct consequence of suppression of group velocities of phonons in the NPMs. We completed the investigation by relating nanoscale resonant character (geometry and material composition) with phonon scattering, and consequently, phonon transport in the locally resonant silicon membrane NPMs. [1] Neogi et al, ACS nano, 9(4), 3820-3828 (2015) [2] Davis & Hussein, PRL, 12, 055505 (2014)

<sup>1</sup>This project is funded by the program FP7-ENERGY-2012-1-2STAGE under contract number 309150.

**12:39PM S23.00006 Nanophononic metamaterial: Thermal conductivity reduction by full-spectrum resonance hybridizations.** , MAHMOUD HUSSEIN, HOSSEIN HONARVAR, LINA YANG, University of Colorado Boulder — Engineered manipulation of phonons can yield beneficial thermal properties in semiconducting materials. One pivotal application relates to thermoelectric materials, or the concept of converting energy in the form of heat into electricity and vice-versa. The ability to use nanostructuring to reduce the thermal conductivity without negatively impacting the power factor provides a promising avenue for achieving high values of the thermoelectric energy conversion figure-of-merit, ZT. Here, we propose a novel nanostructured material configuration that seeks to achieve this goal. Termed “nanophononic metamaterial,” the configuration is based on a freestanding silicon membrane with a periodic array, or random forest, of nanopillars erected on the surface. The nanopillars qualitatively alter the base membrane phonon spectrum due to a hybridization mechanism between their local resonances and the underlying atomic lattice dispersion. Using equilibrium molecular dynamics simulations, we predict a factor of 10 drop in the thermal conductivity compared to the corresponding uniform membrane value despite the fact that the nanopillars add more phonon modes to the spectrum.

**12:51PM S23.00007 Design principles of interfacial thermal conductance** , CARLOS POLANCO, ROUZBEH RASTGARKAFSHGARKOLAEI, JINGJIE ZHANG, NAM LE, PAMELA NORRIS, AVIK GHOSH, Univ of Virginia — We explore fundamental principles to design the thermal conductance across solid interfaces by changing the composition and disorder of an intermediate matching layer. In absence of phonon-phonon interactions, the layer addition involves two competing effects that influence the conductance. The layer can act as an impedance matching bridge to increase the mode-averaged phonon transmission. However, it also reduces the relevant modes that conserve their momenta transverse to the interface, so that the net result depends on features such as the overlap of conserving modes and the dispersivity of the transverse subbands. Moving into the interacting anharmonic regime, we find that the added layer aids conductance when the decreased resistances at the contact-layer boundaries compensate for the layer resistance. In fact, we show that the maximum conductance corresponds to an exact matching of the two separate contact-layer resistances. For instance, if we vary just the atomic mass across layers, then maximum conductance happens when the intervening layer mass is the geometric mean of the contact masses. We conjecture that the best interfacial layer is one that is compositionally graded into many geometric means in other words, an exponential variation in thermal impedance.

**1:03PM S23.00008 Modal Contributions to Heat Conduction across Crystalline and Amorphous Si/Ge Interfaces** , KIARASH GORDIZ, ASEGUN HENRY, Georgia Institute of Technology — Until now, our entire understanding of interfacial heat transfer has been based on the phonon gas model and Landauer formalism. Based on this framework, it is difficult to offer any intuition on heat transfer between two solid materials if one side of the interface is an amorphous structure. Here, using the interface conductance modal analysis (ICMA) method, we investigate the modal contributions to thermal interface conductance (TIC) through crystalline (c) and amorphous (a) Si/Ge interfaces. It is revealed that around 15% of the conductance through the cSi/cGe interface arises from less than 0.1% of the modes of vibration in the structure that exist between 12-13THz and because of their large eigenvectors around the interface are classified as interfacial modes. Correlation maps show that these interfacial modes exhibit strong correlations with all the other modes. The physics behind this strong coupling ability is studied by calculating the mode-level harmonic and anharmonic energy distribution among all the atoms in the system. It is found that these interfacial modes are enabled by the large degree of anharmonicity near the interface, which is higher than the bulk and ultimately allows this small group of modes to couple to other modes of vibration. In addition, unlike the cSi/cGe, correlation maps for aSi/cGe, cSi/aGe, and aSi/aGe interfaces show that the majority of contributions to TIC arise from auto-correlations instead of cross-correlations. The provided analysis sheds light on the nature of localized vibrations at interfaces and can be enlightening for other investigations of localization.

**1:15PM S23.00009 SiC-Si interfacial thermal and mechanical properties of reaction bonded SiC/Si ceramic composites** , CHUN-YEN HSU, FEI DENG, PRASHANT KARANDIKAR, CHAOYING NI, University of Delaware — Reaction bonded SiC/Si (RBSC) ceramic composites are broadly utilized in military, semiconductor and aerospace industries. RBSC affords advanced specific stiffness, hardness and thermal. Interface is a key region that has to be considered when working with any composites. Both thermal and mechanical behaviors of the RBSC are highly dependent on the SiC-Si interface. The SiC-Si interface had been found to act as a thermal barrier in restricting heat transferring at room temperature and to govern the energy absorption ability of the RBSC. However, up to present, the role of the SiC-Si interface to transport heat at higher temperatures and the interfacial properties in the nanoscale have not been established. This study focuses on these critically important subjects to explore scientific phenomena and underlying mechanisms. The RBSC thermal conductivity with volume percentages of SiC at 80 and 90 vol% was measured up to 1,200 C, and was found to decrease for both samples with increasing environmental temperature. The RBSC with 90 vol% SiC has a higher thermal conductivity than that of the 80 vol%; however, is still significantly lower than that of the SiC. The interfacial thermal barrier effect was found to decrease at higher temperatures close 1200 C. A custom-made *in-situ* tensile testing device which can be accommodated inside a ZEISS Auriga 60 FIB/SEM has been setup successfully. The SiC-Si interfacial bonding strength was measured at 98 MPa. The observation and analysis of crack propagation along the SiC-Si interface was achieved with *in-situ* TEM.

**1:27PM S23.00010 Kapitza resistance at segregated boundaries in  $\beta$ -SiC**, NIPUN GOEL, EDMUND WEBB III, ALPARSLAN OZTEKIN, JEFFREY RICKMAN, SUDHAKAR NETI, Lehigh University — Silicon Carbide is a candidate material for high-temperature thermoelectric applications for harvesting waste heat associated with exhaust from automotive and furnaces as well hot surfaces in solar towers and power electronics. However, for SiC to be a viable thermoelectric material, its thermoelectric figure of merit must be improved significantly. In this talk we examine the role of grain-boundary segregation on phononic thermal transport, an important factor in determining the figure of merit, via non-equilibrium molecular dynamics simulations. In particular, we consider the role of dopant concentration and dopant/matrix interactions on the enhancement of the Kapitza resistance of symmetric tilt grain boundaries. We find that the calculated resistance depends on the segregation profile, with increases of more than a factor of 50 (relative to an unsegregated boundary) at the highest dopant concentrations. Finally, we relate the calculated phonon density of states to changes in the Kapitza resistance.

**1:39PM S23.00011 Heat current characteristics in nanojunctions: The effect of external magnetic fields<sup>1</sup>**, D. MELISA DOMINGUEZ, Universidad de Antioquia, JULIANA RESTREPO, Universidad Antonio Nario, BORIS A. RODRIGUEZ, Universidad de Antioquia, R CHITRA, Institute of Theoretical Physics ETH — We study the heat current in the simplest hybrid device of a two level system weakly coupled to two heat baths. We consider both metallic and semiconducting baths with external magnetic fields applied on the central spin and the baths. By using a reduced density matrix approach together with a simple Born-Markov approximation we calculate the heat current. Our goal is to investigate the effect of the applied fields in the transient and steady state heat current, the ensuing rectification and the possibility of using our setup as a building block for a quantum thermal diode.

<sup>1</sup>This work was supported by the Vicerrectoria de Investigacion of the Universidad Antonio Nario, Colombia under project number 20141031 and by COLCIENCIAS under grant number 111556934912

**1:51PM S23.00012 Estimating thermal conductivity and thermoelectricity in PbTiO<sub>3</sub> from first principles**, ANINDYA ROY, Johns Hopkins University — A combination of density functional theory and Boltzmann transport equation is used in this study to calculate the lattice thermal conductivity ( $\kappa_L$ ) of PbTiO<sub>3</sub> (PTO). We cannot apply this procedure to determine  $\kappa_L$  in presence of imaginary phonon modes ("soft modes"). Hence the tetragonal structure of PTO is used in these calculations, and the predicted  $\kappa_L$  is extrapolated to higher temperature using insights from experiments. The computed  $\kappa_L$  of PTO is low, possibly due to the anharmonicity associated with the ferroelectric/paraelectric transition. Electronic transport parameters such as the Seebeck coefficient and the electrical conductivity are also determined (under constant scattering time approximation in semiclassical Boltzmann theory) for PTO. The low  $\kappa_L$  and the electronic transport parameters together indicate excellent thermoelectric properties of PTO ( $zT > 1.5$  at 1000 K). As a technologically important ferroelectric/piezoelectric material, PTO is used in alloys and in layered structures. These morphologies could bring down the  $\kappa_L$  further, improving its thermoelectric performance. Synthesis of electrically conducting samples of PTO would allow us to verify the above predictions.

**2:03PM S23.00013 Rayleigh surface waves, phonon mode conversion, and thermal transport in nanostructures**, LEON MAURER, IRENA KNEZEVIC, University of Wisconsin-Madison — We study the effects of phonon mode conversion and Rayleigh (surface) waves on thermal transport in nanostructures. We present a technique to calculate thermal conductivity in the elastic-solid approximation: a finite-difference time-domain (FDTD) solution of the elastic or scalar wave equations combined with the Green-Kubo formula. The technique is similar to an equilibrium molecular dynamics simulation, captures phonon wave behavior, and scales well to nanostructures that are too large to simulate with many other techniques. By imposing fixed or free boundary conditions, we can selectively turn off mode conversion and Rayleigh waves to study their effects. In the example case of graphenelike nanoribbons with rough edges, we find that mode conversion among bulk modes has little effect on thermal transport, but that conversion between bulk and Rayleigh waves can significantly reduce thermal conductivity. With increasing surface disorder, Rayleigh waves readily become trapped by the disorder and draw energy away from the propagating bulk modes, which lowers thermal conductivity. We discuss the implications on the accuracy of popular phonon-surface scattering models that stem from scalar wave equations and cannot capture mode conversion to Rayleigh waves.

**Thursday, March 17, 2016 11:15AM - 2:15PM —**

**Session S24 DMP: Mesoscopic Materials and Devices II** 323 - David Lederman, West Virginia University

**11:15AM S24.00001 Using charged defects in BN to create rewritable graphene quantum dots and visualize quantum interference**, JAIRO VELASCO JR., University of California, Santa Cruz — Heterostructures of graphene and hexagonal boron nitride (BN) are highly tunable platforms that enable the study of novel physical phenomena and technologically promising nanoelectronic devices. Common control schemes employed in these studies are electrostatic gating and chemical doping. However, these methods have significant drawbacks, such as complicated fabrication processes that introduce contamination and irreversible changes to material properties, as well as a lack of flexible control. To address these problems we have developed a new method that employs light and/or electric field excitation to control defect charge (from the single impurity level to ensembles) in the underlying BN. We have used optoelectronic and scanning tunneling spectroscopy measurements to characterize these BN defects. We find that by manipulating defect charge in BN it is possible to create rewritable tip-induced doping patterns such as gate-tunable graphene pn junctions and quantum dots. This creates new opportunities for mapping the electronic states of confined electrons in graphene and to visualize their quantum interference behavior.

**11:51AM S24.00002 Quantum Imaging of Interaction-Induced Spontaneous Broken-Symmetry Phases in Molecular Graphene**, DOMINIK RASTAWICKI, YAN SUN, YANG LIU, YI-TING CHEN, HARI C. MANOHARAN, Stanford University — We present a survey of quantum states with interaction-induced broken symmetries observed in molecular graphene, assembled with atomic manipulation. These materials are assembled with atomic precision by patterning the Cu(111) two-dimensional electron gas surface state by single molecules; the molecules function as local potentials which form a coherently coupled system of electron quantum dots in a honeycomb lattice embedding massless Dirac fermions and tunable graphene properties. By crafting different local molecular arrangements together with varying lattice constants, we are able to probe a large parameter space of the strength of the intersite hopping parameter (bond strength), the doping level, and the interaction strength. The assembled nanomaterials are probed through STM/STS measurement, differential conductance maps, and quasiparticle interference with Fourier-transform STS. We observe both spontaneous nematic states and sublattice symmetry breaking in molecular graphene at very low band filling factors, and a nematic state in graphene variants where kinetic energy is effectively quenched. We show it is possible to modify and enhance the symmetry breaking effects by controlling certain boundary conditions and lattice geometry.

**12:03PM S24.00003 Vertical gating of sketched nanodevices<sup>1</sup>**, YUN-YI PAI, University of Pittsburgh, DONG-WOOK PARK, University of Wisconsin at Madison, MENGCHEN HUANG, ANIL ANNADI, University of Pittsburgh, HYUNGWOO LEE, ZHENQIANG MA, CHANG-BEOM EOM, University of Wisconsin at Madison, PATRICK IRVIN, JEREMY LEVY, University of Pittsburgh — Conductive-atomic force microscope (c-AFM) lithography at the  $\text{LaAlO}_3/\text{SrTiO}_3$  interface has enabled the creation of various classes of nanostructures, such as nanoscale transistors<sup>2</sup>, single-electron transistors<sup>3</sup> and has proven to be a promising testbed for mesoscopic physics<sup>4</sup>. To date, these devices have used lithographically-defined side gates, which are limited by leakage currents. To reduce leakage and improve the electric field effect, we have investigated nanostructures with in-situ grown gold top gate. We will discuss designs of logic devices such as inverters, NAND, and NOR gates. In the quantum regime, we compare the performance of in-situ vertical top gates and that of written coplanar side gates with Quantum Dot devices.

<sup>1</sup>We gratefully acknowledge financial support from the following agencies and grants: AFOSR (FA9550-10-1-0524(JL), FA9550-12-1-0342(CBE)), NSF (DMR1124131 (JL, CBE) and DMR1234096 (CBE)), ONR (N00014-15-1-2847 (JL)).

<sup>2</sup>C. Cen, *et al.*, Science **323**, 1026 (2009).

<sup>3</sup>G. L. Cheng, *et al.*, Nature Nanotechnology **6**, 343 (2011).

<sup>4</sup>G. L. Cheng, *et al.*, Nature **521**, 196 (2015).

**12:15PM S24.00004 Fabrication of Ultralow Density Interconnected Pure Metal Foams<sup>1</sup>**, EDWARD C. BURKS, DUSTIN A. GILBERT, KAI LIU, University of California, Davis, SERGEI O. KUCHEYEV, JEFFREY D. COLVIN, Lawrence Livermore National Laboratory, THOMAS E. FELTER, Sandia National Laboratory — Ultra-low density metallic nanostructures have been shown to possess interesting thermal, electrical, magnetic, chemical and mechanical properties due to their extremely high surface areas, nanoscale geometries and high porosities. Here we report the synthesis of pure metal foams using interconnected metallic nanowires with densities as low as 0.1% of their bulk density that are still mechanically stable. The highly porous monoliths are macroscopic in size (several mm) and can be created in a wide variety of shapes for application-specific needs. Preliminary studies of such metal foams have already revealed fascinating mechanical and magnetic properties, since the physical dimensions of the foams are below some of the basic length scales that govern the material properties. These foams have been used as targets for ultrabright x-ray sources. They also have a wide variety of other potential applications such as photovoltaic devices, supercapacitors, catalysts, coatings, fuel cells, etc.

<sup>1</sup>This work has been supported by DTRA BRCALL08-Per3-C-2-0006, and in part by NSF DMR-1008791 and DMR-1543582. Work at LLNL was performed under the auspices of the U.S. DOE by LLNL under Contract DE-AC52-07NA27344.

**12:27PM S24.00005 Attraction by Repulsion: Pairing Electrons using Electrons.**, SHAHAL ILANI, Weizmann Institute of Science — One of the fundamental properties of electrons is their mutual Coulombic repulsion. If electrons are placed in a solid, however, this basic property may change. A famous example is that of superconductors, where coupling to lattice vibrations makes electrons attractive and leads to the formation of bound pairs. But what if all the degrees of freedom in the solid are electronic? Is it possible to make electrons attract each other only by their repulsion to other electrons? Such an 'excitonic' mechanism for attraction was proposed fifty years ago by W. A. Little, with the hope that it could lead to better and more exotic superconductivity. Yet, despite many efforts to synthesize materials that possess this unique property, to date there is still no evidence for electronic-based attraction. In this talk I will present our recent experiments that observe this unusual electronic attraction using a different, bottom-up approach. Our experiments are based on a new generation of quantum devices made from pristine carbon nanotubes, combined with precision cryogenic manipulation. Using this setup we can now assemble the fundamental building block of the excitonic attraction and demonstrate that two electrons that naturally repel each other can be made attractive using an independent electronic system as the binding glue. I will discuss the lessons learned from these experiments on what is achievable with plain electrostatics, and on the possibility to use the observed mechanism for creating exotic states of matter.

**1:03PM S24.00006 ABSTRACT WITHDRAWN —**

**1:15PM S24.00007 Universality of Non-equilibrium Fluctuations in Strongly Correlated Quantum Liquids.**, MEYDI FERRIER, Univ. Paris sud, TOMONORI ARAKAWA, TOKURO HATA, RYO FUJIWARA, Univ. Osaka, RAPHAELLE DELAGRANGE, RICHARD DEBLOCK, Univ. Paris sud, RUI SAKANO, ISSP, Univ. Tokyo, AKIRA OGURI, Univ. Osaka city, KENSUKE KOBAYASHI, Univ. Osaka — In a quantum dot, Kondo effect occurs when the spin of the confined electron is entangled with the electrons of the leads forming locally a strongly correlated Fermi-liquid. Our experiments were performed in such a dot formed in a single carbon nanotube, where Kondo effect with different symmetry groups, namely SU(2) and SU(4), shows up. In the latter case, as spin and orbital degrees of freedom are degenerate, two channels contribute to transport and Kondo resonance emerges for odd and even number of electrons. With our sample it was possible to investigate both symmetries near the unitary limit. In the Kondo regime, strong interaction creates a peculiar two-particle scattering which appears as an effective charge  $e^*$  for the quasi-particles. We have extracted the signature of this effective charge in the shot noise for both symmetry in good agreement with theory<sup>1</sup>. This result demonstrates that theory of the Kondo effect can be safely extended out of equilibrium even in the unconventional SU(4) symmetry.

<sup>1</sup>M. Ferrier *et al.*, accepted in Nature Physics

**1:27PM S24.00008 In-plane electrical transport across cavity-quantum well system in Bose-Einstein condensate phase**, MING XIE, ALLAN MACDONALD, University of Texas at Austin — Cavity polaritons are coupled states of quantum well excitons and vertical cavity photons which can undergo Bose-Einstein condensation under appropriate circumstances. The macroscopic condensate state can be described by two coupled order parameters - the coherent exciton field and the coherent photon field. When the dominant process for electron transfer between conduction and valence bands is by scattering off the photon condensate, electrical bias voltages can be used to control the condensate. We study the in-plane transport properties of electrical current through the cavity-quantum well system, and show how the coherent photon fields respond to the current flow. The possibility of tailoring light via electrical current and vice versa simultaneously might lead to interesting new applications.

**1:39PM S24.00009 Fano Resonance in an Electrically Driven Plasmonic Device**, YUVAL VARDI, EYAL COHEN-HOSHEN, GUY SHALEM, ISRAEL BAR-JOSEPH, Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 76100, Israel — Electrically driven plasmonic devices offer unique opportunities as a research tool and for practical applications. In such devices, current that flows across a metallic tunnel junction excites a plasmon, which gives rise to light emission. This local nature of the excitation allows access into "dark" modes, which are not easily excited by far field illumination. We present an electrically driven plasmonic device, based on a gold nanoparticle single-electron-transistor, and investigate the light emission due to the tunneling current. The applied voltage determines the emitted spectral lineshape, enables an excellent control of the plasmonic spectrum. We show that the use of this structure allows us to characterize the electrical properties of the two tunnel barriers, and determine their role in the light emission process. Furthermore, we find a Fano resonance, resulting from interference between the nanoparticle and electrodes dipoles. This resonance is seen due to the local nature of the excitation, and is manifested as a sharp asymmetrical spectral dip. We show that the spectral position of this resonance can be conveniently controlled by the design of the structural parameters. Such devices may be a step toward the realization of an on-chip nano-optical emitters and sensors.

**1:51PM S24.00010 Classical decoherence in a nanomechanical resonator** , OLIVIER MAILLET, ANDREW FEFERMAN, RASUL GAZIZULIN, HENRI GODFRIN, OLIVIER BOURGEOIS, EDDY COLLIN, CNRS/Neel Inst, ULT GRENOBLE TEAM — Decoherence can be viewed either in its quantum picture, where it stands for the loss of phase coherence of a superposition state, or as its classical equivalent, where the phase of an oscillating signal is smeared due to frequency fluctuations. Little is known about quantum coherence of mechanical systems, as opposed to electromagnetic degrees of freedom. Indeed the bridge between quantum and classical physics is under intense investigation, using in particular classical nanomechanical analogues of quantum phenomena. Here we report on a model experiment in which the coherence of a high quality silicon-nitride mechanical resonator is defined in the classical picture. Its intrinsic properties are characterized over an unprecedentedly large dynamic range. By engineering frequency fluctuations, we can create artificial pure dephasing and study its effects on the dynamics of the system. Finally, we develop the methods to characterize pure dephasing that can be applied to a wide range of mechanical devices.

**2:03PM S24.00011 A self-saturating mechanical oscillator with linear feedback** , CHANGYAO CHEN, Argonne National Lab, DAMIAN ZANETTE, Centro Atmico Bariloche, DAVID CZAPLEWSKI, JEFFREY GUEST, DANIEL LOPEZ, Argonne National Lab — Oscillators, opposed to resonators, produce a prescribed periodic signal without any external frequency reference. In order to maintain stable oscillations, there needs to be an amplitude limiting mechanism, which is usually realized by saturating at least one of the sustaining amplifiers. Here we demonstrate a simple oscillator structure that solely relies on the nonlinearity inherent to the constituent mechanical resonator to limit the oscillating amplitude, while the performance of the feedback loop remains in the linear regime. To validate the model, we experimentally demonstrate the principle using a non-linear silicon microelectromechanical (MEMS) resonator, and perform comprehensive characterizations that agree well with the theoretical predictions.

**Thursday, March 17, 2016 11:15AM - 2:15PM –**  
**Session S25 DCMP: Superconductivity: Less Common Materials II** 324 - Roser Valenti, Institut fr  
Theoretische Physik, Goethe-Universitt Frankfurt am Main

**11:15AM S25.00001 Instability of three-band Luttinger liquids: renormalization group analysis and possible application to  $K_2Cr_3As_3$**  , JIAN-JIAN MIAO, FU-CHUN ZHANG, YI ZHOU, Zhejiang Univ — Motivated by recently discovered quasi-one-dimensional superconductor  $K_2Cr_3As_3$  with  $D_{3h}$  lattice symmetry, we study one-dimensional three-orbital Hubbard models with generic electron repulsive interaction described by intra-orbital repulsion  $U$ , inter-orbital repulsion  $U'$ , and Hund's coupling  $J$ . As extracted from density functional theory calculation, two of the three atomic orbitals are degenerate and the third one is non-degenerate, and the system is presumed to be at incommensurate filling. With the help of bosonization, we have usual three-band Luttinger liquids in the normal state. Possible charge density wave (CDW), spin density wave (SDW) and superconducting instabilities are analyzed by one-loop renormalization group. The ground state depends on the ratio  $J/U$ . For the physical relevant parameter region,  $0 < J/U < 1/2$ , the ground states are superconducting states. When  $0 < J/U < 1/3$ , spin singlet superconducting state is favored. While spin triplet superconductor will be favored when  $1/3 < J/U < 1/2$ . The spin density wave state can be achieved only in the unphysical parameter region  $J/U > 1/2$ .

**11:27AM S25.00002 Evaluations of  $MgB_2$  Coatings on 2" Copper Discs for Superconducting Radio Frequency Applications.** , WENURA WITHANAGE, TENG TAN, NAMHOON LEE, HUTA BANJADE, Temple University, GRIGORY EREMEEV, Thomas Jefferson National Accelerator Facility, PAUL WELANDER, SLAC National Accelerator Laboratory, ANNE-MARIE VALENTE-FELICIANO, Thomas Jefferson National Accelerator Facility, ROBERT KUSTOM, Argonne National Laboratory, MATTHUS WOLAK, Temple University, ALIREZA NASSIRI, Argonne National Laboratory, XIAOXING XI, Temple University — We propose that coating the inner walls of copper RF cavities with superconducting  $MgB_2$  ( $T_c = 39$  K) can result in a viable alternative to the already established niobium-based SRF technology. This approach improves the thermal conductivity, allows for operation at higher temperatures, and reduces the need for large helium refrigeration, thereby resulting in lower operational costs. For our studies, we grew  $MgB_2$  films via hybrid physical chemical vapor deposition (HPCVD) on 2" Cu substrates. Since Mg and Cu readily form an alloy at higher temperatures, the HPCVD setup was modified in order to achieve lower deposition temperatures, minimize alloy formation, and provide high quality  $MgB_2$  films. This method yielded  $MgB_2$  coatings on 2" Cu discs with transition temperatures around 38 K. The samples were characterized with regards to their RF attributes and showed similar performance in comparison to Nb reference samples. The presented results show that  $MgB_2$  coated copper can be a suitable alternative for use in SRF cavities.

**11:39AM S25.00003 Electronic Pair-Binding and Hund's Rule Violations in Doped  $C_{60}$** <sup>1</sup> , HONG-CHEN JIANG, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, STEVEN KIVELSON, Department of Physics, Stanford University — We calculate the electronic properties of the t-J model on a  $C_{60}$  molecule using the density-matrix renormalization group and show that Hund's first rule is violated and that for an average of three added electron per molecule, an effective attraction (pair-binding) arises for intermediate values of  $t=J$ . Specifically, it is energetically favorable to put four electrons on one  $C_{60}$  and two on a second rather than putting three on each. Our results show that a dominantly electronic mechanism of superconductivity is possible in doped  $C_{60}$ .

<sup>1</sup>HCH and SAK were supported by the Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract DE-AC02-76SF00515.

**11:51AM S25.00004 The Role of Halogen Bonding in Metal Free phosphors** , HOSSEIN HASHEMI, JAEHUN JUNG, AVI BREGMAN, JOHN KIEFFER, JINSANG KIM, University of Michigan — Metal-organic phosphors can achieve theoretical efficiencies four times greater than their fluorescent analogues in Electroluminescence device, but they still have stability issue in case of blue emitting heavy-metal complexes and the price of transition metal like iridium has skyrocketed which discourages commercialization of OLEDs for solid-state lighting. By minimizing radiative loss due to vibrational effects and enhancing spin-orbit coupling via halogen bonding between aldehyde and heavy halide in an organic crystal, efficient room-temperature phosphorescence has been achieved. Therefore, the enhanced spin-orbit coupling necessary for phosphorescence is thought to be due to the halogen bonding that is present in the crystalline form. Here, the electronic and optical properties of purely organic phosphor candidates are explored using density functional theory (DFT), time-dependent density functional theory (TDDFT), GW and BSE methods. These calculations are compared with the absorption, fluorescence, and phosphorescence experimental spectra in their crystals as well as solution forms to elucidate the underlying the role of halogen bonding for phosphorescence mechanism. These results are used to guide future metal-free organic phosphors.

**12:03PM S25.00005 Camelback-shaped band reconciles heavy-electron behavior with weak electronic Coulomb correlations in superconducting  $\text{TiNi}_2\text{Se}_2$** , CHRISTIAN MATT, NAN XU, Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland, A. VAN ROEKEGHEM, S. BIERMANN, École Polytechnique, CNRS-UMR7644, 91128 Palaiseau, France, P. RICHARD, X. SHI, S.-F. WU, H. W. LIU, D. CHEN, T. QIAN, H. DING, Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, H. WANG, Q. MAO, J. DU, M. FANG, Department of Physics, Zhejiang University, Hangzhou 310027, China, N. PLUMB, M. RADOVIC, J. MESOT, M. SHI, Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland — Combining photoemission spectroscopy, Raman spectroscopy, and first-principles calculations, we characterize superconducting  $\text{TiNi}_2\text{Se}_2$  as a material with weak electronic Coulomb correlations leading to a bandwidth renormalization of 1.4. We identify a camelback-shaped band, whose energetic position strongly depends on the selenium height. While this feature is universal in transition metal pnictides, in  $\text{TiNi}_2\text{Se}_2$  it lies in the immediate vicinity of the Fermi level, giving rise to a pronounced van Hove singularity (VHS). The resulting heavy band mass resolves the apparent puzzle of a large normal-state Sommerfeld coefficient in this weakly correlated compound. The correlation effect evolution in pnictides upon d-shell filling in the presence of significant Hund's exchange coupling will also be discussed.

**12:15PM S25.00006 The happy marriage between electron-phonon superconductivity and Mott physics in  $\text{Cs}_3\text{C}_{60}$ : A first-principle phase diagram**, MASSIMO CAPONE, International School for Advanced Studies (SISSA) and CNR-IOM, YUSUKE NOMURA, École Polytechnique, SHIRO SAKAI, Riken Center for Emergent Matter Science, Japan, GIANLUCA GIOVANNETTI, CNR-IOM and International School for Advanced Studies (SISSA), RYOTARO ARITA, Riken Center for Emergent Matter Science, Japan — The phase diagram of doped fullerides like  $\text{Cs}_3\text{C}_{60}$  as a function of the spacing between fullerene molecules is characterized by a first-order transition between a Mott insulator and an s-wave superconductor with a dome-shaped behavior of the critical temperature. By means of an ab-initio modeling of the bandstructure, the electron-phonon interaction and the interaction parameter and a Dynamical Mean-Field Theory solution, we reproduce the phase diagram and demonstrate that phonon superconductivity benefits from strong correlations [1] confirming earlier model predictions [2]. The role of correlations is manifest also in infrared measurements carried out by L. Baldassarre [3]. The superconducting phase shares many similarities with "exotic" superconductors with electronic pairing, suggesting that the anomalies in the "normal" state, rather than the pairing glue, can be the real common element unifying a wide family of strongly correlated superconductors including cuprates and iron superconductors. [1] Y. Nomura, S. Sakai, K. Nakamura, M. Capone, and R. Arita, Science Advances 1, e1500568 (2015) [2] M. Capone et al., Science 296, 2364 (2002); M. Capone et al., Rev. Mod. Phys. 81, 943 (2009) [3] L. Baldassarre et al. Sci. Rep. 5, 15240 (2015)

**12:27PM S25.00007 Optimal High- $T_C$  Superconductivity in  $\text{Cs}_3\text{C}_{60}$** , DALE HARSHMAN, College of William and Mary, ANTHONY FIORY, New Jersey Institute of Technology — The highest superconducting transition temperatures in the  $(A_{1-x}B_x)_3\text{C}_{60}$  superconducting family are seen in the A15 and FCC structural phases of  $\text{Cs}_3\text{C}_{60}$  (optimized under hydrostatic pressure), exhibiting measured values for near-stoichiometric samples of  $T_C^{\text{meas.}} = 37.8$  K and 35.7 K, respectively. It is argued these two Cs-intercalated  $\text{C}_{60}$  compounds represent the optimal materials of their respective structures, with superconductivity originating from Coulombic  $e$ - $h$  interactions between the  $\text{C}_{60}$  molecules, which host the  $n$ -type superconductivity, and mediating holes associated with the Cs cations. A variation of the interlayer Coulombic pairing model [Harshman and Fiory, J. Supercond. Nov. Magn. 28, 2967 (2015), and references therein] is introduced in which  $T_C^{\text{calc.}} \propto 1/\ell\zeta$ , where  $\ell$  relates to the mean spacing between interacting charges on surfaces of the  $\text{C}_{60}$  molecules, and  $\zeta$  is the average radial distance between the surface of the  $\text{C}_{60}$  molecules and the neighboring Cs cations. For stoichiometric  $\text{Cs}_3\text{C}_{60}$ ,  $T_C^{\text{calc.}} = 38.08$  K and 35.67 K for the A15 and FCC macrostructures, respectively; the dichotomy is attributable to differences in  $\zeta$ .

**12:39PM S25.00008 Electrical transport properties of  $\text{C}_{60}$  superconductors in the vicinity of Mott metal-insulator transition**, YUKI MATSUDA, Department of Physics, Tohoku Univ., SATOSHI HEGURI, WPI-AIMR, Tohoku Univ., YUKI MATSUDA, Department of Physics, Tohoku Univ., KATSUMI TANIGAKI, WPI-AIMR, Tohoku Univ., Department of Physics, Tohoku Univ. — It was revealed in 2008 that  $\text{Cs}_3\text{C}_{60}$  showed superconductivity up to 38K under high pressure [1]. As the lattice constant is increased, the superconducting critical temperature ( $T_C$ ) decreases after experiencing the maximum  $T_C$  and finally  $\text{Cs}_3\text{C}_{60}$  becomes a Mott insulator [2]. This result suggests that  $\text{C}_{60}$  superconductors cannot be simply explained by the BCS theory [1-4]. There are strong electron correlations in the vicinity of Mott metal-insulator transition. Electrical transport properties are required because they provide us importantly intrinsic information on the electronic states, but the systematical electrical transport measurements have not been made due to the experimental difficulties. It will be reported that we have successfully obtained the electrical transport properties of expanded  $\text{C}_{60}$  superconductors in pellet form by using a specially designed pressure cell. [1] A. Y. Ganin et al., Nat. Mater. 7, 367 (2008). [2] A. Y. Ganin et al., Nature 466, 221 (2010). [3] Y. Takabayashi et al., Science, 323, 1585 (2009). [4] R. H. Zadic et al., Sci. Adv. 1, e1500059 (2015).

**12:51PM S25.00009 Isotope Effect on Electron-Phonon Coupling in Multiband Superconductor  $\text{MgB}_2$** , DAIXIANG MOU, VALENTIN TAUFOR, YUN WU, LUNAN HUANG, SERGUEI BUD'KO, PAUL CANFIELD, ADAM KAMINSKI, Division of Materials Science and Engineering, Ames Laboratory — We systematically investigate the isotope effect of electron-phonon coupling in multi-band superconductor  $\text{MgB}_2$  by laser based Angle Resolved Photoemission Spectroscopy. The kink structure around 70 meV on two  $\sigma$  bands, which is caused by electron coupling to  $E_{2g}$  phonon mode, is shifted to higher binding energy in  $\text{Mg}^{10}\text{B}_2$  than that in  $\text{Mg}^{11}\text{B}_2$ . The measured shifting energy of 3.5 meV is consistent with theoretical calculation based on harmonic phonon in  $\text{MgB}_2$ . Our temperature dependent measurement also indicates the isotope effect of kink structure is not dependent on superconducting transition.

**1:03PM S25.00010 Momentum-resolved electronic structure of the superconductor parent compound  $\text{BaBiO}_3$** , N.C. PLUMB, Z. RISTIC, J. PARK, Z. WANG, C.E. MATT, N. XU, Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland, B.Q. LV, Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, D. GAWRYLUK, E. POMJAKUSHINA, K. CONDER, Laboratory for Developments and Methods, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland, Y. WANG, S. JOHNSTON, Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996-1200, USA, J. MESOT, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland, M. SHI, M. RADOVIC, Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland — We use *in situ* angle-resolved photoemission to study thin films of  $\text{BaBiO}_3$ , a parent compound of bismuthate superconductors with  $T_c$  up to 30 K. By simple electron counting,  $\text{BaBiO}_3$  should be metallic. However, in analogy with many unconventional and high- $T_c$  superconductor families, it is instead insulating, and superconductivity emerges with doping. Our experiments reveal a folded band structure consistent with known  $\text{BiO}_6$  breathing distortions. However, charge ordering often thought to accompany the distortions is virtually nonexistent. The data combined with DFT calculations indicate that states near  $E_F$  are primarily oxygen-derived. Hence  $\text{BaBiO}_3$  appears to be characterized by negative charge transfer energy. This can account for the seeming discrepancy between the atomic structure and "missing" charge order. It should also be relevant for understanding the doping evolution and superconductivity in bismuthates.

**1:15PM S25.00011 Comparison of Tunneling in Fe-based Superconductors with Multi-band  $\text{MgB}_2$** , JOHN ZASADZINSKI, Physics Department, Illinois Institute of Technology, Chicago, IL, USA, MARIA IAVARONE, Physics Department, Temple University, Philadelphia, PA, USA —  $\text{MgB}_2$  is an s-wave, phonon coupled, multiband superconductor that exhibits novel tunneling spectra including a subtle dip feature due to quasiparticle transfer between bands. Since this feature mimics the above-gap spectral dip feature observed in Fe-based superconductors, typically attributed to a strong coupling boson, it is worthwhile to consider whether quasiparticle transfer is relevant. We first show that the dip in  $\text{MgB}_2$  appears in the  $\pi$ -band, DOS ( $\Delta = 2.4$  meV) and is due to quasiparticle transfer to the  $\sigma$ -band with  $\Delta = 7.2$  meV. Reviewing the spectral dip in Fe-based superconductors, including new data on FeSe crystals, there are inconsistencies with quasiparticle transfer as the origin. The conclusion is that the spectral dip is more likely due to a boson, the resonance spin excitation, as found in cuprate superconductors.

**1:27PM S25.00012 Robust Resistive Critical Field in Noncentrosymmetric B20 AuBe**, DJ REBAR, JF DITUSA, P ADAMS, J BALL, D BROWNE, I VEKHTER, D YOUNG, J PRESTIGIACOMO, Louisiana State University, JY CHAN, The University of Texas at Dallas — AuBe is a chiral-structured (B20 structure) superconductor. The B20 structure in magnetic systems was discovered to host a magnetic topological structure, the Skyrmin lattice, and our research focused on what behavior the same structure would effect in a superconducting system. Samples were arc-melted in an Ar atmosphere and characterized via powder XRD. Specific heat measurement revealed bulk superconductivity with an exponential form below  $T_c$  while magnetization showed Type I behavior near the  $T_c$  of 3.2 K and a crossover to Type II behavior at approximately 1.2 K. Resistance measurement revealed a critical field that deviates from that found in magnetization measurements at approximately 2.4 K linearly rising with decreasing T to approximately  $3.5 \times H_{c2}$  at  $T=0.3K$ . The resistive critical field was also found to be robust against a Cr film deposited on the surface of AuBe. We find similarity between this superconductivity crossover behavior and robust low temperature critical field with other noncentrosymmetric superconductors in literature. Additionally, we measured the de Haas-van Alphen effect in polycrystalline samples and derived an effective electron mass of 0.16 $m_0$  for a small spherical piece of Fermi surface.

**1:39PM S25.00013 ABSTRACT WITHDRAWN —**

**1:51PM S25.00014 Angle Resolved Thermal Conductivity of Superconducting CeCoIn<sub>5</sub> along the Nodal Direction<sup>1</sup>**, ROMAN MOVSHOVICH, DUK Y. KIM, SHIZENG LIN, FRANZISKA WEICKERT, ERIC D. BAUER, FILIP RONNING, JOE D. THOMPSON, Los Alamos National Laboratory — The thermal conductivity measurement in a rotating magnetic field is a powerful probe of the structure of the superconducting energy gap. The four-fold oscillation in thermal conductivity of CeCoIn<sub>5</sub>, with the heat current in the anti-nodal direction, has revealed the d-wave nature of its order parameter. We have measured the thermal conductivity with the heat current along the [110] (nodal) direction and the magnetic field rotating in the *ab*-plane. In contrast to the smooth oscillation found with the heat current along the anti-nodal direction, a sharp increase of thermal conductivity was observed when the magnetic field is also in the [110] direction, parallel to the heat current. This suggests that the scattering of the nodal quasiparticle is strongly suppressed along the magnetic field direction. In addition, a smaller increase of the thermal conductivity was observed when the magnetic field is approximately 30 degree away from the nodal direction, perhaps due to a Fermi surface anomaly.

<sup>1</sup>Work at Los Alamos was performed under the auspices of the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering.

**2:03PM S25.00015 electric dipole superconductor in bilayer exciton system<sup>1</sup>**, QING-FENG SUN, QING-DONG JIANG, ZHI-QIANG BAO, X.C. XIE, ICQM, School of Physics, Peking University, Beijing, 100871, China — Recently, it was reported that the bilayer exciton systems could exhibit many new phenomena, including the large bilayer counterflow conductivity, the Coulomb drag, etc. These phenomena imply the formation of exciton condensate superfluid state. On the other hand, it is now well known that the superconductor is the condensate superfluid state of the Cooper pairs, which can be viewed as electric monopoles. In other words, the superconductor state is the electric monopole condensate superfluid state. Thus, one may wonder whether there exists electric dipole superfluid state. In this talk, we point out that the exciton in a bilayer system can be considered as a charge neutral electric dipole. And we derive the London-type and Ginzburg-Landau-type equations of electric dipole superconductivity. From these equations, we discover the Meissner-type effect (against spatial variation of magnetic fields), and the dipole current Josephson effect. The frequency in the AC Josephson effect of the dipole current is equal to that in the normal (monopole) superconductor. These results can provide direct evidence for the formation of exciton superfluid state in the bilayer systems and pave new ways to obtain the electric dipole current.

<sup>1</sup>We gratefully acknowledge the financial support by NBRP of China (2012CB921303 and 2015CB921102) and NSF-China under Grants Nos. 11274364 and 11574007.

**Thursday, March 17, 2016 11:15AM - 2:03PM —**

**Session S26 DMP: 2D Materials Beyond Graphene** 325 - Chris Hinkle, University of Texas at Dallas

**11:15AM S26.00001 Two Dimensional Transition Metal Dichalcogenide and Their Heterostructures Through Chemical Vapor Deposition Synthesis**, JING KONG, Massachusetts Institute of Technology — In recent years tremendous efforts have been devoted to the research on two dimensional materials. Among them transition metal dichalcogenides (TMDs) have attracted significant attention owing to their unique structures, remarkable properties, and great potential for a wide range of applications in electronics, [ENREF.1](#) optoelectronics, valleytronics, catalysis, etc. The synthesis of high quality large area mono- and few-layer TMD materials is highly desirable for their applications. In this talk I will present the chemical vapor deposition (CVD) approach we have developed to synthesis these TMD materials and their heterostructures.

**11:51AM S26.00002 2D Crystal heterostructures properties and growth by molecular beam epitaxy<sup>1</sup>**, GRACE HUILI XING<sup>2</sup>, Cornell University — Two-dimensional (2D) crystals such as transition metal dichalcogenides (TMDs) along with other families of layered materials including graphene, SnSe<sub>2</sub>, GaSe, BN etc, has attracted intense attention from the scientific community. One monolayer of such materials represent the thinnest “quantum wells”. These layered materials typically possess an in-plane hexagonal crystal structure, and can be stacked together by interlayer van der Waals interactions. Therefore, it is possible to create novel heterostructures by stacking materials with large lattice mismatches and different properties, for instance, superconductors (NbSe<sub>2</sub>), metals, semi-metals (graphene), semiconductors (MoS<sub>2</sub>) and insulators (BN). Numerous novel material properties and device concepts have been discovered, proposed and demonstrated lately. However, the low internal photoluminescence efficiency (IPE, <1%) and low carrier mobility observed in the 2D semiconductors suggest strongly that the materials under investigation today most likely suffer from a high concentration of defects. In this talk, I will share our progress and the challenges we face in terms of preparing, characterizing these 2D crystals as well as pursuing their applications.

<sup>1</sup>This work has been supported in part by NSF, AFOSR and LEAST, one of the STARnet centers.

<sup>2</sup>co-authors: Suresh Vishwanath, Debdeep Jena, both from Cornell University

**12:27PM S26.00003 Quantum emission from hexagonal boron nitride monolayers**, IGOR AHARONOVICH, TOANTRONG TRAN, KEREM BRAY, MICHAEL J. FORD, MILOS TOTH, University of Technology Sydney, MTEE COLLABORATION — Artificial atomic systems in solids are widely considered the leading physical system for a variety of quantum technologies, including quantum communications, computing and metrology. To date, however, room-temperature quantum emitters have only been observed in wide-bandgap semiconductors such as diamond and silicon carbide, nanocrystal quantum dots, and most recently in carbon nanotubes. Here, we demonstrate room-temperature, polarized single-photon emission from a colour centre in two-dimensional hexagonal boron nitride. The emitters emit at the red and the near infrared spectral range and exhibit narrowband ultra bright emission (~full width at half maximum of below 10 nm with more than three million counts/s). Density functional theory calculations indicate that vacancy-related defects are a probable source of the emission. Our results demonstrate the unprecedented potential of van der Waals crystals for large-scale nanophotonics and quantum information processing.

**12:39PM S26.00004 Synthesis and Oxidation Resistance of h-BN Thin Films<sup>1</sup>**, DAVID STEWART, ROBERT MEULENBERG, ROBERT LAD, Univ of Maine — Hexagonal boron nitride (h-BN) is an exciting 2D material for use in sensors and other electronic devices that operate in harsh, high temperature environments. Not only is h-BN a wide band gap material with excellent wear resistance and high temperature stability, but recent reports indicate that h-BN can prevent metallic substrates from oxidizing above 600°C in low O<sub>2</sub> pressures. However, the PVD of highly crystalline h-BN films required for this oxidation protection has proven challenging. In this work, we have explored the growth of h-BN thin films by reactive RF magnetron sputtering from an elemental B target in an Ar/N<sub>2</sub> atmosphere. The film growth rate is extremely slow and the resulting films are atomically smooth and homogeneous. Using DC biasing during deposition and high temperature annealing treatments, the degree of film crystallinity can be controlled. The oxidation resistance of h-BN films deposited on inert sapphire and reactive metal substrates such as Zr and ZrB<sub>2</sub> has been examined by techniques such as XPS, XRD, and SEM after oxidation between 600 and 1200°C under varying oxygen pressures. The success of h-BN as a passivation layer for metallic substrates in harsh environments is shown to depend greatly on its crystalline quality and defects.

<sup>1</sup>Supported by the NSF SusChEM program

**12:51PM S26.00005 Surface Analysis of Hexagonal Boron Nitride Grown by Chemical Vapor Deposition**, ZACHARY ROBINSON, State Univ of NY - Brockport, J.K. HITE, C.R. EDDY JR., V.M. BERMUDEZ, B.N. FEIGELSON, U.S. Naval Research Laboratory — Hexagonal boron nitride (hBN) is an important material for development of 2-dimensional heterostructures. Chemical vapor deposition of hBN on Cu-foil substrates is one possible route towards large-scale production of hBN films with low defect density. Therefore, studying the growth kinetics of hBN on different orientations of Cu is an important first step towards understanding and controlling the growth process. In this work, hBN was simultaneously grown on Cu(111), Cu(100), Cu(110), and Cu-foil in order to investigate how the different substrate orientations affect the hBN overlayer. The post-growth crystallographic orientations were measured with electron backscatter diffraction (EBSD), and film coverages we measured with XPS. In addition, a grazing-incidence infrared reflection absorption spectroscopy (IRRAS) technique was developed to quickly characterize each hBN film. It was found that the growth rate was inversely proportional to the surface free energy of the Cu surface, with Cu(111) having the most h-BN surface coverage. The Cu foil predominately crystallized with a (100) surface orientation, and had a film coverage very close to the Cu(100).

**1:03PM S26.00006 Two-dimensional boron based nanomaterials: electronic, vibrational, Raman, and STM signatures**, DANIEL V. P. MASSOTE, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, New York 12180, LIANGBO LIANG, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, NEERAV KHARCHE, VINCENT MEUNIER, Department of Physics, Rensselaer Polytechnic Institute — Because boron has only three electrons on its outer shell, planar mono-elemental boron nanostructures are expected to be much more challenging to assemble than their carbon counterparts. Several studies proposed schemes in which boron is stabilized to form flat semiconducting sheets consisting of a hexagonal lattice of boron atoms with partial hexagon filling (PRL 99 115501, ACSNano 6 7443-7453). Other structures were proposed based on results from an evolutionary algorithm (PRL 112 085502). These structures are metallic and one even features a distorted Dirac cone near the Fermi level. Experimental evidence for 2D boron is still lacking but the recently proposed molecular synthesis of a flat all-boron molecule is a promising route to achieve this goal (Nat.Comms. 5 3113). Our research aims at providing a first-principles based description of these materials' properties to help in their identification. DFT is used to calculate phonon dispersion and associated Raman scattering spectra. We report some marked discrepancy between our findings and results from the recent literature and address the deviation using two methods for phonon dispersion. We also simulated STM images at various bias potentials to reveal the electronic symmetry of each material.

**1:15PM S26.00007 Observation of Dirac electrons in germanene on diboride thin films**, ANTOINE FLEURENCE, RAINER FRIEDLEIN, Japan Advanced Institute of Science and Technology, HIROYUKI YAMANE, Institute for Molecular Science, HOWON KIM, Institute for Solid State Physics, YUUTO AWATANI, Japan Advanced Institute of Science and Technology, SHINYA YOSHIMOTO, KOZO MUKAI, TAKANORI KOITAYA, YUKIO HASEGAWA, JUN YOSHINOBU, Institute for Solid State Physics, NOBUHIRO KOSUGI, Institute for Molecular Science, YUKIKO YAMADA-TAKAMURA, Japan Advanced Institute of Science and Technology — Germanene is a single atom thick honeycomb lattice of Ge atoms. Just like silicene, free-standing germanene is predicted to feature  $\pi$  bands forming graphene-like Dirac cones [1]. Epitaxial germanene was already claimed to form on number of substrates [2-4], but no evidence for the existence of a  $\pi$  electronic system has been reported yet. In the present work, we demonstrate experimentally that Ge atoms segregated on the (0001) surface of zirconium diboride (ZrB<sub>2</sub>) thin films grown on Ge(111) form a germanene layer. ZrB<sub>2</sub>(0001) with germanene is ( $\sqrt{3}\times\sqrt{3}$ )-reconstructed at low-temperature and ( $\sqrt{3}\times\sqrt{3}$ )-reconstructed at room temperature. The ( $\sqrt{3}\times\sqrt{3}$ ) reconstruction originates from the matching of this unit cell with the (4X4) unit cell of a Ge honeycomb lattice. Evidence for its germanene nature stems from the observation of the Dirac cone-like dispersion at the K point of its Brillouin zone. [1] S. Cahangirov et al., Phys. Rev. Lett. 102, 236804 (2009). [2] L. Li et al., Adv. Mater. 26, 4820 (2014). [3] M. E. Dávila et al., New J. Phys. 16, 095002 (2014). [4] M. Derivaz et al., Nano Lett. 15, 2510 (2015).

**1:27PM S26.00008 Silicene Evolution from Silicon Herringbones on Ru(0001)**, YANFANG ZHANG, Institute of Physics, Chinese Academy of Sciences, China, LI HUANG, Institute of Chemistry, and Institute of Physics, Chinese Academy of Sciences, China, WENYAN XU, YANDE QUE, EN LI, JINBO PAN, SHIXUAN DU, Institute of Physics, Chinese Academy of Sciences, China, YUNQI LIU, Institute of Chemistry, Chinese Academy of Sciences, China, YUYANG ZHANG, SOKRATES T. PANTELIDES, Vanderbilt University, United States, HONGJUN GAO, Institute of Chemistry, Chinese Academy of Sciences, China — Silicon-based 2D materials can potentially be integrated into Si-based electronics. Buckled silicene, an analog of graphene, was recently fabricated on a Ag (111) substrate and used to make a field effect transistor. Here, we report that, when Ru (0001) is used as a substrate, low Si coverage produces a herringbone structure, a new silicon phase. With increasing Si coverage, the elbow sites of the herringbone develop into nucleation sites of silicene. At even higher coverage, narrow Si ribbons with honeycomb structure develop between herringbones. Finally, with even higher Si coverage, a ( $\sqrt{3}\times\sqrt{3}$ ) silicene monolayer forms in registry on ( $\sqrt{7}\times\sqrt{7}$ ) Ru(0001). Scanning tunneling microscopy (STM) was used to image the structures. The growth process was confirmed by density functional theory (DFT) calculations. This work may contribute to precise control of growth of silicene and other silicon structures.

**1:39PM S26.00009 Phosphorenes with Non-Honeycomb Structures: A Much Extended Family<sup>1</sup>**, MENGHAO WU, HUAHUA FU, Huazhong University of Science and Technology, LING ZHOU, Miami University, KAILUN YAO, Huazhong University of Science and Technology, XIAO CHENG ZENG, University of Nebraska-Lincoln, HUAZHONG UNIVERSITY OF SCIENCE AND TECHNOLOGY TEAM, UNIVERSITY OF NEBRASKA-LINCOLN TEAM — We predict a new class of monolayer phosphorous allotropes, namely,  $\varepsilon$ -P,  $\zeta$ -P,  $\eta$ -P and  $\theta$ -P. Distinctly different from the monolayer  $\alpha$ -P (black) and previously predicted  $\beta$ -P (Phys. Rev. Lett. 112, 176802 (2014)),  $\gamma$ -P and  $\delta$ -P (Phys. Rev. Lett. 113, 046804 (2014)) with buckled honeycomb lattice, the new allotropes are composed of P<sub>4</sub> square or P<sub>5</sub> pentagon units that favor tricoordination for P atoms. The new four phases, together with 5 hybrid phases, are confirmed stable by first-principles calculations. In particular, the  $\theta$ -P is shown to be equally stable as the  $\alpha$ -P (black) and more stable than all previously reported phosphorene allotropes. Prediction of nonvolatile ferroelastic switching and structural transformation among different phases under strains points out their potential applications via strain engineering.

<sup>1</sup> MHW was supported by start-up fund from Huazhong University of Science and Technology.

**1:51PM S26.00010 Synthesis and characterizations of heterojunction of monolayer semiconductors.** , YI-HSIEN LEE, XIN-QUAN ZHANG, YU-WEN TSENG, KUANG-HUA HUANG, CHUN-AN CHEN , BO-HAN CHEN, National Tsing-Hua University — Monolayers of van der Waals materials, including graphene, and MoS<sub>2</sub>, offered a burgeoning field in fundamental physics, and optoelectronics.[1-5] Recently, atomically thin heterostructures of monolayer TMDc with various geometrical and energy band alignments are expected to be the key materials for next generation flexible optoelectronics. The individual TMDc monolayers can be adjoined vertically or laterally to construct diverse heterostructures which are difficult to reach with the laborious pick up-and-transfer method of the exfoliated flakes. The ability to produce copious amounts of high quality layered heterostructures on diverse surfaces is highly desirable but it has remained a challenging issue. Here, we have achieved a direct synthesis of various heterostructures of monolayer TMDc.[6] The synthesis was performed using CVD with aromatic molecules as seeding promoters. We will discuss possible growth behaviors, and we examine the symmetry and the interface of these heterostructures using optical analysis and scanning TEM. Reference: [1] Xiaozhe Liu et al, Nature Photonics, 9, p.30 (2015) [2] Yi-Hsien Lee, et al, Adv. Mater., 24, p.2320 (2012) [3] Yi-Hsien Lee, et al., Nano Lett., 13, 1852 (2013) [4] Xi-Ling et al, Nano Lett., 14, p.464 (2014) [5] Lili Yu et al, Nano Lett, 14, p.3055 (2014) [6] Xin-Quan Zhang et al, Nano Lett, 15, p.410 (2015)

**Thursday, March 17, 2016 11:15AM - 2:15PM –**  
**Session S27 DMP: Carbon Nanotube & Related Materials: Thermal, Mechanical & other Properties** 326 - Michael Schroeter, Technical University Dresden

**11:15AM S27.00001 Thermal Conductivity of 3D CNT-Polymer Composites with Controlled Dispersion** , MENA KLITTICH, XUE WANG, ALI DHINOJWALA, University of Akron — The high thermal conductivity of isolated carbon nanotubes (CNTs) has inspired its use as a thermal filler for insulative polymers. However, the performance of these composites has consistently been sub par. Extensive analyses of these complex systems have resulted in the conclusion that resistance at the CNT/polymer interface due to phonon mismatch and poor physical binding, as well as the weakly bonded tube-tube interactions restrict the effectiveness of CNTs in practice. Experimental comparisons of CNT treatments, coatings, functionalization, and interactions with various polymers have proved challenging, due to the interconnected nature of the composite properties. Here, we have reversed the paradigm and used a constant CNT structure that is then modified post-growth to allow for direct comparisons of polymer composites.

**11:27AM S27.00002 Multiscale Modeling of Heat Conduction in Carbon Nanotube Aerogels** , FENG GONG, DIMITRIOS PAPAVALASSIOU, University of Oklahoma, HAI DUONG, National University of Singapore — Carbon nanotube (CNT) aerogels have attracted a lot of interest due to their ultrahigh strength/weight and surface area/weight ratios. They are promising advanced materials used in energy storage systems, hydrogen storage media and weight-conscious devices such as satellites, because of their ultralight and highly porous quality. CNT aerogels can have excellent electrical conductivity and mechanical strength. However, the thermal conductivity of CNT aerogels are as low as 0.01-0.1 W/mK, which is five orders of magnitude lower than that of CNT (2000-5000 W/mK). To investigate the mechanisms for the low thermal conductivity of CNT aerogels, multiscale models are built in this study. Molecular dynamic (MD) simulations are first carried out to investigate the heat transfer between CNT and different gases (e.g. nitrogen and hydrogen), and the thermal conductance at CNT-CNT interface. The interfacial thermal resistances of CNT-gas and CNT-CNT are estimated from the MD simulations. Mesoscopic modeling of CNT aerogels are then built using an off-lattice Monte Carlo (MC) simulations to replicate the realistic CNT aerogels. The interfacial thermal resistances estimated from MD simulations are used as inputs in the MC models to predict the thermal conductivity of CNT aerogels. The volume fractions and the complex morphologies of CNTs are also quantified to study their effects on the thermal conductivity of CNT aerogels. The quantitative findings may help researchers to obtain the CNT aerogels with expected thermal conductivity.

**11:39AM S27.00003 Thermal conductivity of a film of single walled carbon nanotubes measured with infrared thermal imager<sup>1</sup>** , YA FENG, TAIKI INOUE, RONG XIANG, SHOHEI CHIASHI, Department of Mechanical Engineering, The University of Tokyo, SHIGEO MARUYAMA, Department of Mechanical Engineering, The University of Tokyo; Energy NanoEngineering Lab. AIST — Heat dissipation has restricted the modern miniaturization trend with the development of electronic devices. Theoretically proven to be with high axial thermal conductivity, single walled carbon nanotubes (SWNT) have long been expected to cool down the nanoscale world. Even though the tube-tube contact resistance limits the capability of heat transfer of the bulk film, the high intrinsic thermal conductivity of SWNT still glorify the application of films of SWNT network as a thermal interface material. In this work, we proposed a new method to straightly measure the thermal conductivity of SWNT film. We bridged two cantilevered Si thin plate with SWNT film, and kept a steady state heat flow in between. With the infrared camera to record the temperature distribution, the Si plates with known thermal conductivity can work as a reference to calculate the heat flux going through the SWNT film. Further, the thermal conductivity of the SWNT film can be obtained through Fourier's law after deducting the effect of thermal radiation. The sizes of the structure, the heating temperature, the vacuum degree and other crucial impact factors are carefully considered and analyzed.

<sup>1</sup>The author Y. F. was supported through the Advanced Integration Science Innovation Education and Research Consortium Program by the Ministry of Education, Culture, Sport, Science and Technology

**11:51AM S27.00004 Investigation of the Thermal Behavior of Single-Walled Carbon Nanotubes and Tungsten Oxide Nanostructures Using Raman Spectroscopy<sup>1</sup>** , PRABHAKAR MISRA, DANIEL CASIMIR, RAUL F. SANCHEZ, Howard Univ, CHRISTINA CRAIG, University of Dallas, Irving, SARAH BARTLEY, Agnes Scott College, SHANKAR BALIGA, General Monitors, Inc — Thermal conductivity measurements of a variety of Single-Walled Carbon Nanotube (SWCNT) samples via Raman shifts of the G<sup>+</sup> band frequency around 1592 cm<sup>-1</sup> recorded with a 780 nm laser as a function of laser power (0 – 25 mW) have allowed quantitative estimates of the purity levels of the SWCNTs. In addition, Raman spectra of a variety of tungsten oxide (WO<sub>3</sub>) nanomaterial samples, namely WO<sub>3</sub> on silicon substrate, as well as nanopowder and nanowires, exhibited clear variation in O-H band features around 1550 cm<sup>-1</sup> due to effects of ambient humidity, as well as other spectral features due to gas (NO<sub>x</sub>) exposure have been documented, as a function of varying temperature (in the range 27 – 200C). Thermal characteristics of SWCNTs and WO<sub>3</sub> samples, along with the associated Molecular Dynamics simulations performed, will prove useful for thermal energy storage and gas sensing applications.

<sup>1</sup>Financial support from the National Science Foundation (NSF PHY-1358727) is gratefully acknowledged.

**12:03PM S27.00005 Tuning Thermoelectric Properties of Chirality Selected Single Wall Carbon Nanotubes**, KAZUHIRO YANAGI, YUKI OSHIMA, YOSHIMASA KITAMURA, YUTAKA MANIWA, Dept. of Physics, Tokyo Metropolitan University — Thermoelectrics are a very important technology for efficiently converting waste heat into electric power. Hicks and Dresselhaus proposed an important approach to innovate the performance of thermoelectric devices, which involves using one-dimensional materials and properly tuning their Fermi level (PRB 1993). Therefore, understanding the relationship between the thermoelectric performance and the Fermi level of one-dimensional materials is of great importance to maximize their thermoelectric performance. Single wall carbon nanotube (SWCNT) is an ideal model for one-dimensional materials. Previously we reported continuous p-type and n-type control over the Seebeck coefficients of semiconducting SWCNT networks with diameter of 1.4 nm through an electric double layer transistor setup using an ionic liquid as the electrolyte (Yanagi et al, Nano Lett. 14, 6437 2014). We clarified the thermoelectric properties of semiconducting SWCNTs with diameter of 1.4 nm as a function of Fermi level. In this study, we investigated how the chiralities or electronic structures of SWCNTs influence on the thermoelectric properties. We found the significant difference in the line-shape of Seebeck coefficient as a function of gate voltage between the different electronic structures of SWCNTs.

**12:15PM S27.00006 Insights into heat transfer mechanisms of biased CNTs**, NORVIK VOSKANIAN, EVA OLSSON, Chalmers University of Technology, Applied Physics, JOHN CUMINGS, University of Maryland, Department of Materials Science and Engineering — There has been considerable interest in studying carbon nanotubes for thermal management applications and as components of electronic devices. For typical conductors, the electrical current results in temperature increase, but for the case of carbon nanotubes (CNTs) supported on SiN membranes, it has been shown that the traditional joule heating mechanisms are supplemented by remote heating of the substrate [1]. Using a thermal imaging technique based on Transmission Electron Microscopy [2], we demonstrate further evidence of this remote heating mechanism which suggests a non-equilibrium state between the electron temperature and phonon temperature of the CNT. We quantify the amount of remote heating as a ratio,  $\beta$ , between the power dissipation directly in the SiN divide by the total power applied. We find that initially  $\beta$  is high, but at higher applied voltage bias,  $\beta$  decreases, presumably because more hot electrons are available to scatter off carbon optical phonons, producing an increasing amount of traditional Joule heating. 1. K. Baloch, et al. *Nature Nano.* 7(5), 316-319 (2012). 2. T. Brintlinger, et. al. *Nano Lett.* 8, 582-585 (2008).

**12:27PM S27.00007 Argon Adsorption on Open Carbon Nanohorns<sup>1</sup>**, BRICE RUSSELL, Southern Illinois University Carbondale, ANGEL CALVILLO, None, PRAVIN KHANAL, ALDO MIGONE, Southern Illinois University Carbondale, SUMIO IJIMA, MASAKO YUDASAKA, National Institute of Advanced Industrial Science and Technology — We have measured adsorption isotherms for argon adsorbed on a 0.1692 g sample of chemically-opened carbon nanohorns. Two clear substeps are visible in the adsorption data, corresponding to groups of stronger binding sites (lower pressure substep) and weaker binding sites (higher pressure substep). We have measured adsorption at eight different temperatures in the range between approximately 70 and 110 K. The space at the interior of the individual nanohorns is accessible to sorbates in these chemically opened nanohorns. Consequently, higher loadings are obtained on these samples when compared to those measured on unopened (as-produced) nanohorns. Results for the kinetics of adsorption, the effective specific surface area, and the isosteric heat of adsorption as a function of sorbent loading will be presented and compared to results from other gases adsorbed on nanohorns.

<sup>1</sup>This work was supported by the NSF through grant DMR-1006428

**12:39PM S27.00008 CF<sub>4</sub> Adsorption on Open Carbon Nanohorns<sup>1</sup>**, PRAVIN KHANAL, BRICE RUSSELL, ALDO MIGONE, Southern Illinois University Carbondale, SUMIO IJIMA, MASAKO YUDASAKA, National Institute of Advanced Industrial Science and Technology — We have measured adsorption isotherms at ten different temperatures between 90.4 K and 163.8 K for CF<sub>4</sub> on a sample of chemically-opened carbon nanohorns. The interior of the individual nanohorns is accessible to sorbates in these chemically-opened nanohorns. Two substeps are visible in the adsorption data, one corresponding to groups of stronger binding sites (lower pressure substep) and another corresponding to weaker binding sites (higher pressure substep). The stronger binding sites are interstitial pore-like spaces within the nanohorn aggregates and intra-nanohorns pores while the weaker binding sites are the outer surfaces of the individual and interior sites located away from the tips of the nanohorns. Results for the effective specific surface area, the kinetics of adsorption, and the isosteric heat of adsorption as a function of sorbent loading will be presented and compared to adsorption results with other sorbates on open carbon nanohorns.

<sup>1</sup>This work was supported by the NSF through grant DMR-1006428.

**12:51PM S27.00009 Pull out instability in double walled carbon nanocones**, ARINDAM RAJ, Material Science and Engineering, Indian Inst of Tech-Kanpur, SHAKTI S GUPTA, Mechanical Engineering, Indian Inst of Tech-Kanpur, DEEPTI VERMA, Department of Chemical Engineering and Materials Science, University of Minnesota — Here, we present a molecular mechanics (MM) based study to show sharp changes in the variation of potential energy and wall morphology in double walled carbon nanocones (DWCNCs), when the constituent cones are pulled away from each other. In the MM simulations, bonded and non-bonded interactions among carbon atoms are prescribed using MM3 potential. The process of pulling out is simulated by constraining the base atoms of an inner cone and incrementally moving the tip atoms of the outer cone in the coaxial direction. In the relaxed state DWCNCs, the wall to wall normal distance between the cones is found to be 3.4Å, consistent with that obtained in two-layered graphene sheets. For each incremental step of separation, the minimum energy configuration of the entire system is obtained and the associated potential energy recorded. The instability leads to loss of concentricity of the cross-sections of cones in the sense that the wall of the outer cone deforms, making a single-sided cam-lobe type structure. DWCNCs of two different apex angles show the pull-out instability at almost the same separation distance.

**1:03PM S27.00010 Boron Nitride Coated Carbon Nanotube Arrays with Enhanced Compressive Mechanical Property**, LIN JING, ROLAND YINGJIE TAY, HONGLING LI, Nanyang Tech Univ, SIU HON TSANG, Temasek Laboratory@NTU, DUNLIN TAN, BOWEI ZHANG, ALFRED IING YOONG TOK, EDWIN HANG TONG TEO, Nanyang Tech Univ — Vertically aligned carbon nanotube (CNT) array is one of the most promising energy dissipating materials due to its excellent temperature invariant mechanical property. However, the CNT arrays with desirable recoverability after compression is still a challenge. Here, we report on the mechanical enhancement of the CNT arrays reinforced by coating with boron nitride (BN) layers. These BN coated CNT (BN/CNT) arrays exhibit excellent compressive strength and recoverability as compared to those of the as-prepared CNT arrays which totally collapsed after compression. In addition, the BN coating also provides better resistance to oxidation due to its intrinsic thermal stability. This work presented here opens a new pathway towards tuning mechanical behavior of any arbitrary CNT arrays for promising potential such as damper, vibration isolator and shock absorber applications.

**1:15PM S27.00011 Microwave Induced Welding of Carbon Nanotube-Thermoplastic Interfaces for Enhanced Mechanical Strength of 3D Printed Parts**, CHARLES SWEENEY, BLAKE LACKEY, Texas AM University Department of Chemical Engineering, MOHAMMAD SAED, Texas Tech University, MICAH GREEN, Texas AM University Department of Chemical Engineering — Three-dimensional (3D) printed parts produced by fused-filament fabrication of a thermoplastic polymer have become increasingly popular at both the commercial and consumer level. The mechanical integrity of these rapid-prototyped parts however, is severely limited by the interfillament bond strength between adjacent extruded layers. In this report we propose for the first time a method for welding thermoplastic interfaces of 3D printed parts using the extreme heating response of carbon nanotubes (CNTs) to microwave energy. To achieve this, we developed a coaxial printer filament with a pure polylactide (PLA) core and a CNT composite sheath. This produces parts with a thin electrically percolating network of CNTs at the interfaces between adjacent extruded layers. These interfaces are then welded together upon microwave irradiation at 2.45GHz. Our patent-pending method has been shown to increase the tensile toughness by 1000% and tensile strength by 35%. We investigated the dielectric properties of the PLA/CNT composites at microwave frequencies and performed in-situ microwave thermometry using a forward-looking infrared (FLIR) camera to characterize the heating response of the PLA/CNT composites upon microwave irradiation.

**1:27PM S27.00012 Mechanical properties of aligned carbon nanotube architectures: origin from 3D morphology**, ITAI Y. STEIN, BRIAN L. WARDLE, MIT — The scale-dependent properties of carbon nanotubes (CNTs) continue to motivate their study for next-generation material architectures. While recent work has shown that aligned CNT arrays can be made on the cm-scale, such systems exhibit properties that are orders of magnitude below those predicted by existing theories. This deviation mainly stems from the rudimentary assumptions made about the CNT morphology: CNTs are either devoid of local curvature (i.e. waviness) or have waviness that is easy to model, e.g. using helices and sine waves. Here, we use a simulation framework comprised of  $10^5$  CNTs with realistic 3D stochastic morphologies to elucidate the role morphology plays in the orders of magnitude over-prediction of the effective stiffness of aligned CNT structures. Application to aligned CNT polymer and carbon matrix nanocomposites reveals that the elimination of the torsion deformation mechanism, which dominates the effective compliance of CNT arrays, through CNT interactions with the matrix is responsible for the stiffness enhancement in CNT nanocomposites. This work paves the way to more accurate property prediction of CNT nanocomposites, and further work to predict the transport properties of aligned CNT architectures is planned.

**1:39PM S27.00013 Nanoscale Analysis of Interwall Interaction in a Multiwalled Carbon Nanotube by Tip-Enhanced Raman Spectroscopy**, SONGPOL CHAUNCHAIYAKUL, TAKESHI YANO, KAMONCHANOK KHOK-LANG, PAWEŁ KRUKOWSKI, MEGUMI AKAI-KASAYA, AKIRA SAITO, YUJI KUWAHARA, Osaka University — Raman spectroscopy is a useful tool for the study of carbon materials, but its spatial resolution is limited by the optical diffraction limit. Recently, we constructed a scanning tunneling microscope-based tip-enhanced Raman spectroscopy (STM-TERS) system in ultrahigh vacuum, which overcomes the optical diffraction limit, and enables the investigation of single-molecular Raman spectra simultaneously with topographic imaging. We have investigated position-sensitive Raman spectra along the tube axis of an isolated multiwalled carbon nanotube, which is a result of the different number of nanotube walls at each location. We found that the intensity ratio between the 2D to the G band increases with the number of walls. This indicates that the quantum interference between Raman scattering pathways affects each Raman mode differently. The interaction between nanotube walls induces splitting of the  $\pi$  and  $\pi^*$  bands which increases the number of the 2D band scattering pathways owing to double resonance, eventually increasing the probability of scattering for the 2D band relative to the G band. These results provide a deeper understanding of the single-molecule interaction of carbon materials in the nanoscale.

**1:51PM S27.00014 Title: Experimental and analytical study of frictional anisotropy of nanotubes<sup>1</sup>**, ELISA RIEDO, YANG GAO, TAI-DE LI, CUNY Advanced Science Research Center, HSIANG-CHIH CHIU, National Taiwan Normal University, SUENNE KIM, Hanyang University, CHRISTIAN KLINKE, University of Hamburg, ERIO TOSATTI, International School for Advanced Studies (SISSA), and CNR-IOM Democritos and International Centre for Theoretical Physics (ICTP) — The frictional properties of Carbon and Boron Nitride nanotubes (NTs) are very important in a variety of applications, including composite materials, carbon fibers, and micro/nano-electromechanical systems. Atomic force microscopy (AFM) is a powerful tool to investigate with nanoscale resolution the frictional properties of individual NTs. Here, we report on an experimental study of the frictional properties of different types of supported nanotubes by AFM. We also propose a quantitative model to describe and then predict the frictional properties of nanotubes sliding on a substrate along (longitudinal friction) or perpendicular (transverse friction) their axis. This model provides a simple but general analytical relationship that well describes the acquired experimental data. As an example of potential applications, this experimental method combined with the proposed model can guide to design better NTs-ceramic composites, or to self-assemble the nanotubes on a surface in a given direction.

<sup>1</sup>M. Lucas et al., Nature Materials 8, 876-881 (2009)

**2:03PM S27.00015 Structure and Properties of HELICAL CARBON NANOTUBES through MD Simulations.**, AKSHAY DAHIYA, Department of Mechanical Engineering, Indian Institute of Technology Ropar, DEEPTI VERMA, Chemical Engineering and Materials Science Department, University of Minnesota, SHAKTI S GUPTA, Department of Mechanical Engineering, Indian Institute of Technology Kanpur — Helical Carbon Nanotubes (HCNTs) are coiled 3-valent carbon networks which represent pure carbon helix. Here we study the geometries of two classes: hexagonal helix containing purely polyhex networks and the second class with 5- and 7-membered rings besides hexagons. We followed a model of hexagonal, single wall HCNTs, and determined their relaxed configuration using MD simulations based on Tersoff potential. A race-track like structure is observed in the cross-section of HCNTs upon minimization. For generating class two helix, the adjacency matrix eigenvector's (AME) method is applied which utilizes 3-coordinated tiling of the plane by 5-, 6-, and 7-membered ring for the construction of helical structures. The application of the AME method to torusenes is crucial for class two helix generation as it is based on an appropriate choice of bi-lobial eigenvectors triplet which can be selected on the basis of their nodal properties as verified here. After 3-D transformations the final structure was obtained with the help of MM3-potential based MD simulations on Tinker commercial code. The spring constants of HCNTs are computed through MD simulations.

**Thursday, March 17, 2016 11:15AM - 2:15PM –**

**Session S28 DMP: Advances in Topological Materials II** 327 - Liang Wu, University of California, Berkeley

**11:15AM S28.00001 Recent results on materials aspects of the investigation of new topological states of matter<sup>1</sup>**, ROBERT CAVA, Department of Chemistry, Princeton University, Princeton NJ — Investigation of the electronic states of matter that are determined by topological physics has exploded in recent years through parallel progress in theory, experimental characterization, device fabrication and new materials development. In our group working in this area, the speaker has been responsible for the development of new materials to allow the experimentalists to probe the emergence of new topological properties, and to help embody the concepts of our theorists in real materials. The field is fast-moving, with particular thrusts at the present time toward Weyl and Dirac semimetals, and in this talk I will describe the materials aspects of our work in the past year in these areas, specifically as they are related to our strong collaborations with the groups of N.P. Ong, A. Yazdani, and B.A. Bernevig at Princeton, T. Valla and J. Tao at Brookhaven, and A. Vishwanath at Berkeley.

<sup>1</sup>The support of our work in this area by the NSF through its MRSEC program, grant DMR 1420541, and the ARO through its MURI on topological insulators, grant W911NF-12-1-0461, is gratefully acknowledged.

**11:51AM S28.00002 Observation of Weyl nodes and Fermi arcs in TaP** , MING SHI, N. XU, Paul Scherrer Institute, Switzerland, H. M. WENG, Institute of Physics, Chinese Academy of Sciences, B. Q. LV, C. E. MATT, J. PARK, F. BISTI, V. N. STROCOV, D. GAWRYLUK, E. POMJAKUSHINA, K. CONDER, N. C. PLUMB, M. RADOVIC, Paul Scherrer Institute, Switzerland, G. AUTS, O. V. YAZYEV, cole Polytechnique Fdrale de Lausanne, Switzerland, Z. FANG, X. DAI, T. QIAN, Institute of Physics, Chinese Academy of Sciences, J. MESOT, Paul Scherrer Institute, Switzerland, H. DING, Institute of Physics, Chinese Academy of Sciences — A Weyl semimetal possesses topologically unavoidable crossings of spin-polarized bands dispersing linearly along all momentum directions, called Weyl nodes, connected by topological surface arcs. The crossing points have fixed chirality and behave the same as massless Weyl fermions, leading to exotic properties like chiral anomaly. To have the transport and other novel properties dominated by Weyl fermions, it is required that Weyl nodes (1) locate nearly at the chemical potential and (2) are well separated in momentum space and enclosed by pairs of individual Fermi surfaces with nonzero Fermi Chern numbers. By investigating the electronic structure of TaP using angle-resolved photoemission spectroscopy and first-principles calculation, we establish that TaP is a Weyl semimetal with only single type of Weyl fermions with well-separated Weyl nodes locating at the chemical potential, distinguished from TaAs where there are two types of Weyl fermions contributing to the low-energy physical properties. We have also observed Fermi arcs on the Ta-terminated surface, which appear in a different pattern from that on the As-terminated surface observed in TaAs and NbAs.

**12:03PM S28.00003 Fermiology in the Weyl semimetals (Nb,Ta)(As,P)** , QIU RUN ZHANG, SHAHRIAR MEMARAN, DANIEL RHODES, BIN ZENG, SUVADIP DAS, EFSTRATIOS MANOUSAKIS, RYAN BAUMBACH, LUIS BALICAS, National High Magnetic Field Laboratory, NASSER ALIDOUST, M. ZAHID HASAN, Princeton University — We present a detailed angular and temperature dependent study of the quantum oscillatory phenomena in the Weyl semimetals, (Ta,Nb)(As,P) under high magnetic fields. In general we find that the P compounds exhibit larger Fermi surfaces with lighter effective masses when compared to the As ones. We show that for (Nb,Ta)As we can reach the quantum limit with the currently available magnetic fields, which seemingly leads to an electronic phase transition.

**12:15PM S28.00004 Discovery of a Weyl fermion state with Fermi arcs in niobium arsenide<sup>1</sup>** , NASSER ALIDOUST, SU-YANG XU, ILYA BELOPOLSKI, GUANG BIAN, HAO ZHENG, DANIEL S SANCHEZ, TITUS NEUPERT, M ZAHID HASAN, Princeton University, ZHUJUN YUAN, CHENGLONG ZHANG, SHUANG JIA, Peking University, DAIXIANG MOU, YUN WU, LUNAN HUANG, ADAM KAMINSKI, Iowa State University, VLADIMIR N STROCOV, Paul Scherrer Institute, BAOKAI WANG, ARUN BANSIL, Northeastern University, TAY-RONG CHANG, HORNG-TAY JENG, National Tsing Hua University, GUOQING CHANG, CHI-CHENG LEE, SHIN-MING HUANG, HSIN LIN, National University of Singapore — Three types of fermions play a fundamental role in our understanding of nature: Dirac, Majorana and Weyl. A Weyl semimetal is a novel crystal whose low-energy electronic excitations behave as Weyl fermions. Here, we present the experimental discovery of the Weyl semimetal state in an inversion-symmetry-breaking single-crystalline solid, niobium arsenide (NbAs). Utilizing the combination of soft X-ray and ultraviolet photoemission spectroscopy, we systematically study both the surface and bulk electronic structure of NbAs. We experimentally observe both the Weyl cones in the bulk and the Fermi arcs on the surface of this system. Our ARPES data, in agreement with our theoretical calculations, identify the Weyl semimetal state in NbAs, which provides a platform to test the potential of Weyltronics.

<sup>1</sup>The work at Princeton and Princeton-led ARPES measurements were supported by Gordon and Betty Moore Foundations EPiQS Initiative, grant GBMF4547 (Hasan), and by U.S. DOE DE-FG-02-05ER46200.

**12:27PM S28.00005 Discovery of the first Weyl fermion semimetal and topological Fermi arcs in TaAs<sup>1</sup>** , SUYANG XU, ILYA BELOPOLSKI, NASSER ALIDOUST, Princeton University, MADHAB NEUPANE, Los Alamos National Laboratory, GUANG BIAN, Princeton University, CHENGLONG ZHANG, Peking University, RAMAN SANKAR, National Taiwan University, GUOQING CHANG, National University of Singapore, ZHUJUN YUAN, Peking University, CHI-CHENG LEE, SHIN-MING HUANG, National University of Singapore, HAO ZHENG, Princeton University, JIE MA, Oak Ridge National Laboratory, DANIEL SANCHEZ, Princeton University, BAOKAI WANG, ARUN BANSIL, Northeastern University, FANGCHENG CHOU, National Taiwan University, PAVEL SHIBAYEV, Princeton University, HSIN LIN, National University of Singapore, SHUANG JIA, Peking University, M. ZAHID HASAN, Princeton University — Weyl semimetals have opened a new era in condensed matter physics and materials science. They host Weyl fermions as emergent quasiparticles and admit a topological classification that protects Fermi arc surface states on the boundary. This unusual electronic structure has deep analogies with particle physics and leads to unique topological properties. We report the experimental discovery of the first Weyl semimetal, TaAs. We directly observe Fermi arcs on the surface, as well as the Weyl fermion cones and Weyl nodes in the bulk of TaAs single crystals. We find that Fermi arcs terminate on the Weyl fermion nodes, consistent with their topological character. Our work opens the field for the experimental study of Weyl fermions in physics and materials science.

<sup>1</sup>The work at Princeton and Princeton-led ARPES measurements were supported by the Gordon and Betty Moore Foundations EPiQS Initiative through grant GBMF4547 (Hasan) and by U.S. Department of Energy DE-FG-02-05ER46200.

**12:39PM S28.00006 Electronic structures and evolution in a transition metal pnictide Weyl semimetal family** , YULIN CHEN, Oxford University — Topological Weyl semimetals (TWSs) represent a novel state of quantum matter which not only possesses Weyl fermions (massless chiral particles that can be viewed as magnetic monopoles in momentum space) in the bulk and unique Fermi arcs generated by topological surface states, but also exhibits appealing physical properties such as extremely large magnetoresistance and ultra-high carrier mobility. By performing angle-resolved photoemission spectroscopy (ARPES) on compounds from a transition metal pnictide family (NbP, TaP and TaAs), we systematically investigated their electronic structures and discovered the unique surface “Fermi-arcs” and linear bulk band dispersion across the Weyl points. Furthermore, we also illustrated their Fermiology evolution with the spin-orbit coupling (SOC) strength. Our experimental findings not only reveal the mechanism to realize and fine-tune the electronic structures of TWSs, but also provide a rich material base for exploring many exotic physical phenomena (for example, chiral magnetic effects, negative magnetoresistance, and the quantum anomalous Hall effect) and novel future applications.

**12:51PM S28.00007 Experimental discovery of a topological Weyl semimetal state in TaP<sup>1</sup>** , SU-YANG XU, ILYA BELOPOLSKI, DANIEL SANCHEZ, Princeton Univ, CHENG GUO, Peking University, GUOQING CHANG, National University of Singapore, CHENGLONG ZHANG, Peking University, GUANG BIAN, Princeton Univ, ZHUJUN YUAN, HONG LU, YIYANG FENG, Peking University, TAY-RONG CHANG, National Tsing Hua University, PAVEL SHIBAYEV, Princeton Univ, MYKHAILO PROKOPOVYCH, Paul Scherrer Institute, NASSER ALIDOUST, HAO ZHENG, Princeton Univ, CHI-CHENG LEE, SHIN-MING HUANG, National University of Singapore, RAMAN SANKAR, National Taiwan University, HORN-TAY JENNY, National Tsing Hua University, ARUN BANSIL, Northeastern University, TITUS NEUPERT, Princeton Univ, VLADIMIR STROCOV, Paul Scherrer Institute, HSIN LIN, National University of Singapore, SHUANG JIA, Peking University, M. ZAHID HASAN, Princeton Univ — We observed Weyl fermion cones and nodes in the bulk and the Fermi arcs on the surface of Weyl semimetal TaP. Also, we found that the surface states show an unexpectedly rich structure, including both topological Fermi arcs and topologically trivial closed contours in the vicinity of the Weyl points. A rigorous scheme for directly demonstrating the bulk-boundary correspondence and, hence, establishing the Weyl semimetal state in TaP is discussed.

<sup>1</sup>The work at Princeton and Princeton-led ARPES measurements were supported by the Gordon and Betty Moore Foundations EPiQS Initiative through grant GBMF4547 (Hasan) and by U.S. Department of Energy DE-FG-02-05ER46200

**1:03PM S28.00008 Spin polarization of the Fermi arcs in the Weyl semimetal TaAs<sup>1</sup>**, SU-YANG XU, ILYA BELOPOLSKI, DANIEL SANCHEZ, Princeton Univ, MADHAB NEUPANE, Princeton Univ; Los Alamos National Laboratory, GUOQING CHANG, National University of Singapore, KOICHIRO YAJI, University of Tokyo, ZHUJUN YUAN, CHENGLONG ZHANG, Peking University, KENTA KURODA, University of Tokyo, GUANG BIAN, Princeton Univ, TAY-RONG CHANG, National Hua University, NASSER ALIDOUST, HAO ZHENG, Princeton Univ, CHI-CHENG LEE, SHIN-MING HUANG, GUANG-HAN HSU, National University of Singapore, HORNG-TAY JENG, National Tsing Hua University, ARUN BANSIL, Northeastern University, ARIS ALEXANDRADINATA, Yale University, TITUS NEUPERT, Princeton Univ, TAKESHI CONDO, SHIK SHIN, Institute of Solid State Physics (ISSP), HSIN LIN, National University of Singapore, SHUANG JIA, Peking University, M. ZAHID HASAN, Princeton Univ — In a Weyl semimetal, Weyl fermion quasiparticle excitations correspond to points of bulk band degeneracy separated in  $k$ -space and connected on the surface by Fermi arcs. Our spin-resolved ARPES measurements on the experimentally discovered Weyl semimetal TaAs have revealed that the Fermi arcs have spin polarization larger than 80% and that the spin texture is in-plane and does not match with that of the bulk Weyl cones where they meet.

<sup>1</sup>The work at Princeton and Princeton-led ARPES measurements were supported by the Gordon and Betty Moore Foundations EPiQS Initiative through grant GBMF4547 (Hasan) and by U.S. Department of Energy DE-FG-02-05ER46200.

**1:15PM S28.00009 Observation of surface states derived from topological Fermi arcs in the Weyl semimetal NbP<sup>1</sup>**, ILYA BELOPOLSKI, SU-YANG XU, DANIEL SANCHEZ, Princeton University, GUOQING CHANG, National University of Singapore, CHENG GUO, Peking University, MADHAB NEUPANE, Los Alamos National Laboratory, HAO ZHENG, Princeton University, CHI-CHENG LEE, SHIN-MING HUANG, National University of Singapore, GUANG BIAN, NASSER ALIDOUST, Princeton University, TAY-RONG CHANG, National Tsing Hua University, BAOKAI WANG, National University of Singapore, XIAO ZHANG, Peking University, ARUN BANSIL, Northeastern University, HORNG-TAY JENG, National Tsing Hua University, HSIN LIN, National University of Singapore, SHUANG JIA, Peking University, ZAHID HASAN, Princeton University — The recent experimental discovery of the first Weyl semimetal (WSM) provides the first observation of a Weyl fermion in nature and demonstrates a novel type of anomalous surface state band structure, consisting of Fermi arcs. NbP may realize the first WSM in the limit of weak spin-orbit coupling. Here we study the surface states of NbP by ARPES and we find that we cannot show Fermi arcs based on our experimental data alone. However, the excellent agreement between our data and calculations suggests that NbP is a WSM and that we observe trivial surface states which evolve continuously from topological Fermi arcs above the Fermi level.

<sup>1</sup>The work at Princeton and Princeton-led ARPES measurements were supported by the Gordon and Betty Moore Foundation EPiQS Initiative through grant GBMF4547 (Hasan) and by the U.S. Department of Energy, DE-FG-02-05ER46200.

**1:27PM S28.00010 Observation of Fermi Arcs in non-Centrosymmetric Weyl Semi-metal Candidate NbP**, DIFEI XU, State Key Laboratory of Surface Physics, Department of Physics, and Laboratory of Advanced Materials, Fudan University, YONGPING DU, National Laboratory of Solid State Microstructures, Collaborative Innovation Center of Advanced Microstructures, and College of Physics, Nanjing Univ., ZHEN WANG, YUPENG LI, Department of Physics, and State Key Lab of Silicon Materials, Zhejiang University, XIAOHAI NIU, QI YAO, State Key Laboratory of Surface Physics, Department of Physics, and Laboratory of Advanced Materials, Fudan University, PAVEL DUDIN, Diamond Light Source, Harwell Science and Innovation Campus, ZHUAN XU, Department of Physics, Zhejiang University, XIANGANG WAN, National Laboratory of Solid State Microstructures, Collaborative Innovation Center of Advanced Microstructures, and College of Physics, Nanjing Univ., DONGLAI FENG, State Key Laboratory of Surface Physics, Department of Physics, and Laboratory of Advanced Materials, Fudan University — We report the surface electronic structure of niobium phosphide NbP single crystal on (001) surface by vacuum ultraviolet angle-resolved photoemission spectroscopy. Combining with our first principle calculations, we identify the existence of the Fermi arcs originated from topological surface states. Furthermore, the surface states exhibit circular dichroism pattern, which may correlated with spin texture. Our results not only provide critical evidence for the existence of the Weyl Fermions in NbP, but also lay foundations for further investigations.

**1:39PM S28.00011 Observation of Fermi arc spin texture in TaAs**, TIAN QIAN, BAIQING LV, HONGMING WENG, GENFU CHEN, HONG DING, Institute of Physics, Chinese Academy of Sciences — We have investigated the spin texture of surface Fermi arcs in the recently discovered Weyl semimetal TaAs using spin- and angle-resolved photoemission spectroscopy. The experimental results demonstrate that the Fermi arcs are spin-polarized. The measured spin texture fulfills the requirement of mirror and time reversal symmetries and is well reproduced by our first-principles calculations, which gives strong evidence for the topologically nontrivial Weyl semimetal state in TaAs. The consistency between the experimental and calculated results further confirms the distribution of chirality of the Weyl nodes determined by first-principles calculations.

**1:51PM S28.00012 Complete Fermi Surface and Surface State in WTe<sub>2</sub> Revealed by High-Resolution Laser-Based Angle-Resolved Photoemission Spectroscopy**, CHENLU WANG, YAN ZHANG, GUODONG LIU, Institute of Physics, Chinese Academy of Sciences, ZHIQIANG MAO, Department of Physics and Engineering Physics, Tulane University, SHAOLONG HE, LIN ZHAO, Institute of Physics, Chinese Academy of Sciences, CHUANGTIAN CHEN, ZUYAN XU, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, XINGJIANG ZHOU, Institute of Physics, Chinese Academy of Sciences — WTe<sub>2</sub>, an unique transition metal dichalcogenide, attracts considerable attention recently, which shows an extremely large magnetoresistance (MR) with no saturation under very high field. In this talk, we will present our high resolution laser-ARPES study on WTe<sub>2</sub>. Our distinctive ARPES system is equipped with the VUV laser and the time-of-flight (TOF) electron energy analyzer, being featured by super-high energy resolution, simultaneous data acquisition for two-dimensional momentum space and much reduced nonlinearity effect. With this advanced apparatus, the very high quality of electronic structure data are obtained for WTe<sub>2</sub> which gives a full picture of the Fermi surface. Meanwhile, the obtained systematic temperature dependence of its electronic state leads us to a better understanding on the origin of large magnetoresistance in WTe<sub>2</sub>.

**2:03PM S28.00013 First-principles study of temperature effects in topological insulator phase diagrams<sup>1</sup>**, GABRIEL ANTONIUS, STEVEN LOUIE, University of California at Berkeley and Lawrence Berkeley National Lab — Recent studies have identified several tunable three-dimensional topological insulators. Upon varying experimental parameters such as pressure or doping, these materials exhibit a transition between a trivial and a topological insulating phase. We present a first-principles study of temperature effects in the family of alloyed BiTeS<sub>2</sub> / BiTeSe<sub>2</sub> topological phase transition materials. Through the electron-phonon coupling, the electronic bands being renormalized at finite temperature allow for a topological phase transition at some critical temperature. We find a temperature-doping phase diagram having a confined topological phase region, with the topological phase suppressed at high temperature. We also discuss the converse scenario in which phonons might favour the topological phase, as previously anticipated.

<sup>1</sup>This work was supported by the NSF under Grant No. DMR15-1508412 and the DOE under Contract No. DE-AC02-05CH11231.

**Thursday, March 17, 2016 11:15AM - 2:15PM —**  
Session S29 DCMP DMP: Two-dimensional Topological Insulators: Growth, Structure and Electronic Properties 328 - Hua Chen, University of Texas, Austin

**11:15AM S29.00001 Quantum Anomalous Hall Effect in Low-buckled Honeycomb Lattice with In-plane Magnetization**, YAFEI REN<sup>1</sup>, University of Science and Technology of China, HUI PAN, FEI YANG, XIN LI, Beihang University, ZHENHUA QIAO, University of Science and Technology of China, ZHENHUA QIAO'S GROUP TEAM, HUI PAN'S GROUP TEAM — With out-of-plane magnetization, the quantum anomalous Hall effect has been extensively studied in quantum wells and two-dimensional atomic crystal layers [1]. Here, we investigate the possibility of realizing quantum anomalous Hall effect (QAHE) in honeycomb lattices with in-plane magnetization. We show that the QAHE can only occur in low-buckled honeycomb lattice where both intrinsic and intrinsic Rashba spin-orbit coupling appear spontaneously. The extrinsic Rashba spin-orbit coupling is detrimental to this phase. In contrast to the out-of-plane magnetization induced QAHE, the QAHE from in-plane magnetization is achieved in the vicinity of the time reversal symmetric momenta at  $M$  points rather than Dirac points. In monolayer case, the QAHE can be characterized by Chern number  $C = \pm 1$  whereas additional phases with Chern number  $C = \pm 2$  appear in chiral stacked bilayer system. The Chern number strongly depends on the orientation of the magnetization. The bilayer system also provides additional tunability via out-of-plane electric field, which can reduce the critical magnetization strength required to induce QAHE. It can also lead to topological phase transitions from  $C = \pm 2$  to  $\pm 1$  and finally to 0. [1] Review article: arXiv:1509.09016

<sup>1</sup>Equal contribution from Yafei Ren and Hui Pan

**11:27AM S29.00002 The theoretical studies of topology electronic states in HgTe Hall Bar and Quantum Dot**, JIN-XIAN QU, SHU-HUI ZHANG, WEN YANG, Beijing CSRC — In recent years, there is an extensive attention on the new properties of topology materials and their potential applications. Our interest is on the physics in the quantum confined systems based on topology materials. To consider two such systems, i.e., quantum dot and Hall bar constructed on the HgTe quantum well, we study the electronic properties and their dependence on various material parameters with and without an in-plane electric field. For both systems, we find that 1) the exotic edge states appear in bulk energy gap, resulting from the non-trivial topological property of quantum well system. 2) by the magnetic doping, there are tunable phase transitions, e.g., transition from trivial insulating phase to topological insulating phase or anomalous quantum Hall insulating phase. 3) the in-plane electric field can introduce effective control on the electronic states.

**11:39AM S29.00003 A new structure of two-dimensional allotropes of group V elements**, PING LI, WEIDONG LUO, Shanghai Jiao Tong University — The elemental two-dimensional (2D) materials such as graphene, silicene, germanene, and black phosphorus have attracted considerable attention due to their fascinating physical properties. Structurally they possess the honeycomb or distorted honeycomb lattices, which are composed of six-atom rings. Here we find a new structure of 2D allotropes of group V elements composed of eight-atom rings, which we name as the octagonal tiling (OT) structure. First-principles calculations indicate that these allotropes are dynamically stable and are also thermally stable at temperatures up to 600 K. These allotropes are semiconductors with band gaps ranging from 0.3 to 2.0 eV, thus they are potentially useful in near- and mid-infrared optoelectronic devices. OT-Bi is also a 2D topological insulator (TI) with a band gap of 0.33 eV, which is the largest among the reported elemental 2D TIs, and this gap can be increased further by applying compressive strains.

**11:51AM S29.00004 Topological phase transition in layered transition metal dichalcogenides**, DUK-HYUN CHOE, HA-JUN SUNG, KEE JOO CHANG, Department of Physics, KAIST — Despite considerable interests in transition metal dichalcogenides (TMDs), such as  $\text{MX}_2$  with  $M = (\text{Mo}, \text{W})$  and  $X = (\text{S}, \text{Se}, \text{Te})$ , the physical origin of their topological nature is still in its infancy. The conventional view of topological phase transition (TPT) in TMDs is that the band inversion occurs between the metal  $d$  and chalcogen  $p$  orbital bands. More precisely, the former is pulled down below the latter. Here we introduce an explicit scheme for analyzing TPT in topological materials and find that the TPT in TMDs is different from the conventional speculation. When the  $1T$  phase undergoes a structural transformation to the  $1T'$  phase in monolayer  $\text{MX}_2$ , the band topology changes from trivial to non-trivial, leading to the TPT. We discuss the exact role of the metal  $d$  and chalcogen  $p$  orbital bands during the TPT. Our finding would provide clear guidelines for understanding the topological nature not only in TMDs but also in other topological materials yet to be explored.

**12:03PM S29.00005 Effects of edge terminations on monolayer topological crystalline insulators via group theory and DFT<sup>1</sup>**, GERSON J. FERREIRA, AUGUSTO L. ARAUJO, Federal University of Uberlandia, ERNESTO O. WRASSE, Universidade Tecnológica Federal do Parana, TOME M. SCHMIDT, Federal University of Uberlandia — Topological crystalline insulators (TCIs) are a counterpart of usual topological insulators in materials where the topological edge (or surface) states are protected by the underlying crystal symmetries. Here we discuss the band structure of IV-VI monolayer materials, where the edge states are protected by mirror symmetry, considering ribbons cutted in different orientations and distinct edge terminations. We show that although the Chern numbers and the topological classification remain a bulk property, the nature of edge terminations and orientation play a significant role in TCIs. For each ribbon an effective Hamiltonian is derived by group theory and proper boundary conditions are presented. These show good agreement with DFT calculations and illustrate the effects of the distinct reduced symmetry of each ribbon type.

<sup>1</sup>This work was supported by the Brazilian agencies FAPEMIG, CAPES, and CNPq.

**12:15PM S29.00006 Antiperovskite  $\text{Sr}_3\text{PbO}$  thin films grown by molecular beam epitaxy**, DEBAKANTA SAMAL, HIROYUKI NAKAMURA, HIDENORI TAKAGI, Max Planck Institute for Solid State Research — Several antiperovskite compounds have recently been predicted to host bulk three dimensional Dirac dispersion as well as surface states protected by crystal symmetry. Here, we present fabrication of cubic antiperovskite  $\text{Sr}_3\text{PbO}$  films epitaxially grown on  $\text{LaAlO}_3$  by molecular beam epitaxy. Fabricated films were capped with polymer without breaking vacuum to facilitate ex-situ transport characterization. All of the films showed metallic temperature dependence. The Hall effect measurement suggests that the carrier type is hole, whose density is around  $5 \times 10^{19} \text{ cm}^{-3}$ . Details of magnetotransport at low temperature is also described.

**12:27PM S29.00007 Spin-Phonon coupling in a candidate 2D atomic crystal magnetic semiconductor<sup>1</sup>**, YAO TIAN, University of Toronto, HUIWEN JI, ROBERT CAVA, Princeton University, KENNETH BURCH, Boston College —  $\text{Cr}_2\text{Ge}_2\text{Te}_6$  is a particularly interesting material since it is in the very rare class of ferromagnetic semiconductors and possesses a layered, nearly two dimensional structure due to van Der Waals bonds. The van Der Waals bonds make it a candidate two dimensional atomic crystal, which is predicted as a platform to study 2D semiconducting ferromagnets and for single layered spintronics devices. Spin-phonon coupling can be a key factor for the spin relaxation in a spintronics devices. We use polarized temperature dependent Raman scattering to study  $\text{Cr}_2\text{Ge}_2\text{Te}_6$ . The spin-phonon coupling has been confirmed in three ways: below  $T_C$  we observe a split of two phonon modes due to the breaking of time reversal symmetry; an anomalous hardening of an additional three modes; and dramatic decrease of the phonon lifetimes upon warming into the paramagnetic phase. Our results also suggest the possibility of probing the magneto-elastic coupling using Raman spectroscopy, opening a door for the further study of exfoliated 2D  $\text{Cr}_2\text{Ge}_2\text{Te}_6$ . We gratefully acknowledge support from the National Science Foundation (Grant No. DMR-1410846)

<sup>1</sup>ks.burch@bc.edu

**12:39PM S29.00008 Magnetism at grain boundary interfaces in the colossal permittivity dielectric material; In+Nb Co-Doped Rutile**, ADAM BERLIE, ISIS Neutron and Muon Source, STFC Rutherford Appleton Laboratory, Chilton, Oxfordshire, OX11 0QX, United Kingdom., IAN TERRY, Department of Physics, Durham University, South Road, Durham, DH13LE, United Kingdom., STEPHEN COTTRELL, ISIS Neutron and Muon Source, STFC Rutherford Appleton Laboratory, Chilton, Oxfordshire, OX11 0QX, United Kingdom., WANBIAO HU, YUN LIU, Research School of Chemistry, Australian National University, Acton, Canberra, 2601, Australia. — With the emphasis in recent years on understanding novel materials with potential technological applications this work seeks to understand magnetic ordering within the colossal-permittivity material, In+Nb co-doped rutile ( $\text{TiO}_2$ ). Evidence for a spin-freezing transition was reported from a step like feature in the dielectric data below 50 K but this was largely glossed over. Within this work we show that below 300 K there is a slowing down of magnetic fluctuations associated with the electronic magnetism due to the defect-dipoles created by the co-doping, but the muon spectroscopy results are strongly suggestive of the behaviour being localised to the edges/interfaces of particles/grains. The  $T_C$  is strongly dependent on the doping level of the samples that presents novel way to control the magnetism and ultimately magneto-electric coupling within a dielectric material.

**12:51PM S29.00009 Photoconductivity of transparent perovskite oxide semiconductors  $\text{BaSnO}_3$  and  $\text{SrTiO}_3$  epitaxial thin films**, JISUNG PARK, USEONG KIM, KOOKRIN CHAR, Seoul Natl Univ, INSTITUTE OF APPLIED PHYSICS, DEPARTMENT OF PHYSICS AND ASTRONOMY, SEOUL NATIONAL UNIVERSITY, SEOUL TEAM — We have measured the photoconductivity (PC) of epitaxial thin films of transparent semiconductor  $\text{BaSnO}_3$  (BSO) and  $\text{SrTiO}_3$  (STO) at room temperature. The epitaxial thin films of BSO and STO were grown by pulsed laser ablation technique on the MgO substrates to exclude any conductance from the substrate owing to its large bandgap ( $\sim 7.8$  eV). Despite the same crystalline structure and similar band gap sizes ( $\sim 3.2$  eV), the PC of BSO behaved very differently. The slowly varying component in the PC of BSO is much larger than that of STO; the PC of BSO increased slowly, reached higher magnitude after the same duration of illumination, and persisted longer than many hours after the light was turned off, whereas the PC of STO showed little persistent conductivity. The spectral responses of the PC of BSO and STO showed their highest peaks below 400 nm when measured by a UV monochromator system, suggesting that the electron-hole pair generation is the main mechanism of the PC for both materials. The higher mobility of BSO should be partially responsible for the higher PC. The large persistent PC of BSO seems related to the dislocations that trap electrons easily.

**1:03PM S29.00010 Change In The Electronic Structure And Optical Absorption Of Cuprate Delafossites Via B-site Alloying**, RAMON BEESLEY, GIHAN PANAPITIYA, JAMES LEWIS, West Virginia University, LEWIS GROUP TEAM — Delafossite oxides are a family of materials with the form  $\text{ABO}_2$ , where the A-site is a monovalent cation ( $\text{Cu}, \text{Ag}, \text{Au}$ ) and the B-site is a trivalent cation ( $\text{Ga}, \text{Al}, \text{In}$ ). Delafossites typically have a wide optical band gap, this band gap may be tuned by adding a second B-site element forming an  $\text{AB}_{(1-x)}^1\text{B}_{(x)}^2\text{O}_2$  alloy. We investigate changes in the electronic structure of  $\text{CuAlO}_2$ ,  $\text{CuGaO}_2$ , and  $\text{CuInO}_2$  when alloyed with  $\text{CuFeO}_2$ . Using the FIREBALL program to optimize the atomic structure, calculate the total and partial density of states, calculate the valence band edge for each alloy level, and investigate the clustering factor of the second B-site atom, it is found that alloying with  $\text{Fe}$  creates midgap states caused by  $\text{Fe}-\text{O}$  interactions. From the partial density of state, each type of atoms contribution to the change in the valence band edge can be seen. Observed changes to the materials include increased optical absorption in the visible range, and symmetry breaking because of the deformation in the crystal structure. The  $\text{CuFeO}_2$  alloying percentages range from 0-5%. We are synthesizing these alloys to experimentally verify the changes in the optical absorption spectra.

**1:15PM S29.00011 Growth, structural, dielectric and magnetic properties of epitaxial multiferroic  $\text{NaMnF}_3$  thin films<sup>1</sup>**, AMIT KC, PAVEL BORISOV, West Virginia Univ, DAVID LEDERMAN, West Virginia Univ, University of California Santa Cruz — Epitaxial  $\text{NaMnF}_3$  thin films were grown on  $\text{SrTiO}_3$  (100) single crystal substrates via molecular beam epitaxy (MBE). The orthorhombically distorted perovskite fluoride  $\text{NaMnF}_3$  ( $Pnma$  space group) has been predicted to have a polar instability at low temperatures due to  $\text{MnF}_6$  octahedral tilts. Structural, magnetic and dielectric properties were studied. Thin film structural quality as a function of the substrate temperature and film thickness was investigated using X-ray diffraction (XRD), in-situ reflection high-energy electron diffraction (RHEED), and atomic force microscopy (AFM). The best films were smooth and single phase grown with four different twin domains. Magnetic characterization was performed using superconducting quantum interference device (SQUID) magnetometry. In-plane magnetization measurements revealed antiferromagnetic ordering with a Neel temperature  $T_N = 66$  K. For the dielectric studies,  $\text{NaMnF}_3$  films were grown on top of  $\text{SrRuO}_3$  (100) buffer layers grown via pulsed laser deposition that were used as bottom electrodes. Dielectric spectroscopy was performed at different temperatures between 11K and room temperature in a frequency range 100 Hz to 100 kHz. Significant temperature dependent dielectric properties were observed.

<sup>1</sup>This work was supported by the National Science Foundation.

**1:27PM S29.00012 Molecular Beam Epitaxial (MBE) Growth and Characterization of Thin Films of Semiconductor Tin**, P. FOLKES, P. TAYLOR, C. RONG, B. NICHOLS, H. HIER, R. BURKE, US Army Rsch Lab - Adelphi, M. NEUPANE, US Army Rsch Lab - Aberdeen — Recent theoretical predictions that a two-dimensional monolayer of semiconductor tin is a two-dimensional topological insulator and experimental evidence of three-dimensional topological insulator behavior in strained ultrathin films of semiconductor tin grown by MBE on InSb has generated intense research interest. This research is primarily focused on the MBE growth and topological characteristics of ultrathin films of semiconductor tin. In this talk we present results of a study on the MBE growth and the transport, structural and optical characterization of thin films of semiconductor tin on several different substrates.

**1:39PM S29.00013 Phase dependent structural and electronic properties of Lanthanum Orthophosphate ( $\text{LaPO}_4$ )**, MAHESH NEUPANE, US Army Research Laboratory, Aberdeen Proving Ground, MD, GREGORY GARRETT, SERGEY RUDIN, US Army Research Laboratory, Adelphi, MD, JAN ANDZELM, US Army Research Laboratory, Aberdeen Proving Ground, MD — Lanthanum orthophosphate ( $\text{LaPO}_4$ ) belongs to the family of rare-earth (RE) orthophosphates. The La-ion lacks valence 4f-electron, so for it to exhibit f-electron dependent physics, it must be doped with additional RE elements. In the bulk form,  $\text{LaPO}_4$  exist in both a stable monoclinic and a metastable hexagonal phase, which both possess indirect energy transition characteristics. Though the overall optoelectronic properties of the RE-doped  $\text{LaPO}_4$  depend on the accuracy of the observed bulk energy gap, the reported experimental and theoretical energy gaps varies between  $\sim 8^{1,2}$  and  $\sim 5^3$  eV, respectively. Through this theoretical study, we attempt to establish a correlation between electronic properties of bulk  $\text{LaPO}_4$  and various levels of first principle theories. Compared to experimental data, the PBE0 functional over-predicts energy gaps and the energy differences between the indirect-to-direct transition energies by 25%. The HSE06 gives a good description of electronic properties and predicts the energy gaps to be 7.68 (monoclinic) and 7.29 eV (hexagonal). Analysis on the structural stability also reveals that the total energy difference between the two phases is 6meV, consistent with the experimentally observed instantaneous pressure and temperature dependent phase transition. [1] J. Lumin. 72–74, 255, 1997, [2] J. Lumin. 15-18, 255, 1977, [3] App. Surface Science, 268, 458-463, 2013.

**1:51PM S29.00014 Landau Theory of Trifluoride Negative Thermal Expansion Materials<sup>1</sup>**, GIAN GUZMAN-VERRI, U of Costa Rica and Argonne Natl Lab, RICHARD BRIERLEY, Yale University, PETER LITTLEWOOD, Argonne Natl Lab and U of Chicago — Negative thermal expansion (NTE) is a desirable property in designing materials that are dimensionally stable and resistant to thermal shocks. Transition metal trifluorides (MF<sub>3</sub>, M=Al, Cr, Fe, Ga, In, Ti, V) are a class of materials with ReO<sub>3</sub> structure that exhibit large, isotropic, and tunable NTE over a wide temperature range, which makes them attractive material candidates. They exhibit large coefficients of thermal expansion near their cubic-to-rhombohedral structural phase change, which can be thermally or pressure induced. Though they have recently been the subject of intense experimental research, little work has been done on the theory side and it has almost exclusively focused on zero temperature properties. In this talk, we construct a simple Landau theory of trifluorides and use it to calculate the temperature dependence of the elastic constants, soft phonon frequencies, and volume expansion near their structural transition. We compare our results to existing experimental data on trifluorides.

<sup>1</sup>Work at the U of Costa Rica is supported by the Vicerrectoria de Investigacion under project no. B5220. Work at Argonne Natl Lab is supported by the U.S. Department of Energy, Office of Basic Energy Sciences under contract no. DE-AC02-06CH11357

**2:03PM S29.00015 Type-II Dirac cones as unified topological origin of the exotic electronic properties of WTe<sub>2</sub><sup>1</sup>**, LUKAS MUECHLER, Dept. of Chemistry, Princeton University, ARIS ALEXANDRADINATA, Dept. of Physics, Yale University, TITUS NEUPERT, Princeton Center for Theoretical Science, ROBERTO CAR, Dept. of Chemistry, Princeton University — WTe<sub>2</sub> is a recently discovered layered material with remarkable electronic properties. Transport measurements show an extremely large non-saturating magnetoresistance (MR) with mobilities as high as 167 000 cm<sup>2</sup>/Vs at 2 K. Furthermore, recent photoemission experiments discovered circular dichroism in the bulk band structure. We propose a unified explanation for these exotic observations by relating key properties of the bulk electronic structure to that of to that of the mono- and bi-layer material. In particular, we demonstrate that the monolayer is a novel type-II Dirac semimetal in absence of spin-orbit coupling, with Dirac cones that are sufficiently anisotropic to simultaneously harbor electron and hole pockets. The band structure can be characterized by a new  $Z_2 \times Z_2$  topological invariant defined through non-Abelian Wilson loops. We develop a tight-binding model for the mono- and bilayer of WTe<sub>2</sub> based on Wannier functions from *ab-initio* calculations and extend our findings to the iso-structural compounds MoTe<sub>2</sub> and ZrI<sub>2</sub>.

<sup>1</sup>LM and RC are supported by the DOE grant DE-FG02-05ER46201

## Thursday, March 17, 2016 11:15AM - 2:15PM – Session S30 DMP: Theory of Ferroic Systems 329 - Steve Johnson, ETHZ

**11:15AM S30.00001 New design strategy for realizing multiferroic materials**, DANILO PUGGIONI, Department of Materials Science and Engineering, Northwestern University, Evanston, IL60208, USA, GIANLUCA GIOVANNETTI, MASSIMO CAPONE, CNR-IOM-Democritos National Simulation Centre and International School for Advanced Studies (SISSA), Via Bonomea 265, I-34136, Trieste, Italy, JAMES RONDINELLI, Department of Materials Science and Engineering, Northwestern University, Evanston, IL60208, USA — Ferroelectricity is a property that only insulating materials can exhibit. For this reason, nearly all searches for new multiferroic compounds, those simultaneously exhibiting ferroelectric and magnetic order, have focused on *insulating* magnetic oxides. Here, we propose a different approach: Start from a *conducting* oxide with broken inversion symmetry and search for routes to induce long-range magnetic order [1]. Using density-functional and dynamical mean-field theories, we investigate the electronic properties of the polar metallic oxide LiOsO<sub>3</sub>. We show that a multiferroic state can be engineered by enclosing LiOsO<sub>3</sub> between an insulating material, LiNbO<sub>3</sub>. We predict that the 1/1 superlattice of LiOsO<sub>3</sub> and LiNbO<sub>3</sub> exhibits strong coupling between magnetic and ferroelectric degrees of freedom with a ferroelectric polarization of 41.2  $\mu\text{Ccm}^{-2}$ , Curie temperature of 927 K, and Néel temperature of 379 K. Our results show that one can start with polar metallic oxides to make multiferroics.

[1] D. Puggioni *et al*, Phys. Rev. Lett. **115**, 087202 (2015).

**11:27AM S30.00002 Crystal structure and electronic properties of bulk and thin-film brownmillerite oxides**, JOSHUA YOUNG, Drexel University, JAMES RONDINELLI, Northwestern University — The equilibrium structure and functional properties exhibited by brownmillerite oxides (general formula  $A_2B_2O_5$ ), a family of perovskite-derived structures with alternating layers of  $BO_6$  octahedra and  $BO_4$  tetrahedra arising from ordered arrangements of oxygen vacancies, is dependent on a variety of competing crystal-chemistry factors. Using first principles electronic structure calculations, we investigate two antiferromagnetic brownmillerite ferrites, Sr<sub>2</sub>Fe<sub>2</sub>O<sub>5</sub> and Ca<sub>2</sub>Fe<sub>2</sub>O<sub>5</sub>, and find that the stability of the equilibrium ground state is governed by complex interactions among several structural descriptors, including ionic size, distortions of nominally regular oxygen octahedral, and in-plane and out-of-plane separation of tetrahedral chains. Furthermore, we find that these same effects control the preferred oxygen vacancy orientation under epitaxial strain, a tunable parameter which also strongly influences the magnitude of the electronic band gap via an asymmetric-vacancy alignment dependent response. Finally, we show that A-site cation ordering in these materials can lift inversion symmetry, providing a potential new route to room temperature multiferroics.

**11:39AM S30.00003 Unveiling hidden ferrimagnetism and giant magnetoelectricity in polar magnet Fe<sub>2</sub>Mo<sub>3</sub>O<sub>8</sub>**, YAZHONG WANG, GHEORGHE L. PASCUT, BIN GAO, RCEM, Rutgers Univ, TREVOR A. TYSON, New Jersey Institute of Technology, KRISTJAN HAULE, VALERY KIRYUKHIN, SANG-WOOK CHEONG, RCEM, Rutgers Univ, RUTGERS CENTER FOR EMERGENT MATERIALS TEAM, DEPARTMENT OF PHYSICS, NEW JERSEY INSTITUTE OF TECHNOLOGY COLLABORATION — Polar magnets, belonging to the polar crystallographic symmetry groups and containing magnetic ions, can exhibit non-trivial magnetoelectric (ME) effects below magnetic ordering temperatures due to the broken time reversal and space inversion symmetries. Mono-domain polar single crystals can often be grown, and eliminate the need for any poling procedures to reveal the possible ME response. Here, we report a giant ME effect in a polar magnet Fe<sub>2</sub>Mo<sub>3</sub>O<sub>8</sub> at temperature as high as 60 K. Polarization jumps of 0.3  $\mu\text{C}/\text{cm}^2$  and repeated mutual control of ferroelectric and magnetic moments with differential ME coefficients on the order of 10<sup>4</sup> ps/m are achieved. The sign of the ME coefficients can be switched by changing the direction of the applied “bias” magnetic field. Importantly, no electric or magnetic poling is needed, as necessary for applications. Using first principles calculations, we show that exchange striction is the leading mechanism responsible for the observed ME effect.

**11:51AM S30.00004 Theory of colossal magnetoelectric response near spin-flop transition in Ni<sub>3</sub>TeO<sub>6</sub>**<sup>1</sup>, SERGEY ARTYUKHIN, Italian Institute of Technology — The manipulation of magnetic ordering with applied electric fields is of pressing interest for new spintronic and information storage applications. Recently, such magnetoelectric control was realized in multiferroics [1]. However, their magnetoelectric switching is often accompanied by significant hysteresis, resulting from a large barrier, separating different ferroic states. Hysteresis prevents robust switching, unless the applied field overcomes a certain value (coercive field). I will discuss the role of a switching barrier on magnetoelectric control, in particular, in a collinear antiferromagnetic and pyroelectric Ni<sub>3</sub>TeO<sub>6</sub> [2,3]. The barrier between two magnetic states in the vicinity of a spinflop transition is almost flat, and thus small changes in external electric/magnetic fields allow to switch the ferroic state through an intermediate state in a continuous manner, resulting in a colossal magnetoelectric response. This colossal magnetoelectric effect resembles the large piezoelectric effect at the morphotropic phase boundary in ferroelectrics. [1] T. Kimura, T. Goto, H. Shintani et al., Nature 426, 5 (2003) [2] Y.-S. Oh, S. Artyukhin J. J. Yang et al., Nature Communications 5, 3201 (2014) [3] J. W. Kim, S. Artyukhin, E. D. Mun et al., Phys. Rev. Lett. 115, 137201 (2015)

<sup>1</sup>NSF-DMREF-1233349, ONR N00014-12-1-1035

**12:27PM S30.00005 Multiferroic behavior at a spin state transition**, VIVIEN ZAPF, SHALINEE CHIKARA, JOHN SINGLETON, National High Magnetic Field Laboratory, Los Alamos National Lab (LANL), SHIZENG LIN, CRISTIAN BATISTA, Theory Division, LANL, BRIAN SCOTT, MPA-11, LANL, NATHAN SMYTHE, Chemistry Division C-IIAC, LANL — Traditionally, multiferroic behavior is studied in materials with coexisting long-range orders, such as ferromagnetism and ferroelectricity. Here we present multiferroic behavior at a spin-state transition (SST). SSTs, for example, the  $S = 1$  to  $S = 2$  transition in Mn<sup>3+</sup> can become cooperative magneto-structural phase transitions due to structural coupling between ions. SSTs are accompanied by change in the orbital occupation and hence, strongly coupled to the lattice and charge degrees of freedom. They are a dominant functionality in metal-organic materials, persisting up to room temperature in some compounds. We demonstrate that a magnetic SST can induce ferroelectricity. We study a Mn-based metal-organic system in which a three-fold degenerate dynamic Jahn-Teller effect at high temperatures vanishes when the temperature is lowered, and the system drops into a lower spin state. Application of a magnetic field restores the high spin Jahn-Teller-active state and allows the Jahn Teller distortions to order cooperatively, creating a dielectric constant change and a net electric polarization. We use high magnetic fields at the NHMFL to study the magnetic and electric behavior of this system across a significant fraction of its T-H phase space, and compare to theoretical modeling.

**12:39PM S30.00006 Electric polarization induced by the inverse DM interactions in canted antiferromagnets**, NOBUO FURUKAWA, Department of Physics, Aoyama Gakuin Univ, SHIN MIYAHARA, Department of Applied Physics, Fukuoka University — We investigate electric polarizations induced by antisymmetric spin pairs  $S_i \times S_j$  on distorted lattices through the inverse Dzyaloshinsky-Moriya (DM) interaction. From an extended Hubbard model, we microscopically derive a generic form of the electric polarization,  $p = \hat{d}(S_i \times S_j)$ , with a tensor  $\hat{d}$ . This includes components of the electric polarization other than those given by the Katsura-Nagaosa-Balatsky formula  $p \propto e_{ij} \times (S_i \times S_j)$ . Our results indicate that various magnetic structures, such as canted antiferromagnetic as well as proper screw spin structures, show multiferroic properties owing to these non-Katsura-Nagaosa-Balatsky components of the coupling. We also discuss possible novel multiferroic behaviours through these couplings in various compounds.

**12:51PM S30.00007 Spin polarized electronic states and spin textures at the surface of oxygen-deficient SrTiO<sub>3</sub>**<sup>1</sup>, HARALD O. JESCHKE, MICHAELA ALTMAYER, Institut für Theoretische Physik, Goethe-Universität Frankfurt, Germany, MARCELO ROZENBERG, MARC GABAY, Laboratoire de Physique des Solides, Université Paris-Sud, France, ROSER VALENTI, Institut für Theoretische Physik, Goethe-Universität Frankfurt, Germany — We investigate the electronic structure and spin texture at the (001) surface of SrTiO<sub>3</sub> in the presence of oxygen vacancies by means of *ab initio* density functional theory (DFT) calculations of slabs. Relativistic non-magnetic DFT calculations exhibit Rashba-like spin winding with a characteristic energy scale  $\sim 10$  meV. However, when surface magnetism on the Ti ions is included, bands become spin-split with an energy difference  $\sim 100$  meV at the  $\Gamma$  point. This energy scale is comparable to the observations in SARPES experiments performed on the two-dimensional electronic states confined near the (001) surface of SrTiO<sub>3</sub>. We find the spin polarized state to be the ground state of the system, and while magnetism tends to suppress the effects of the relativistic Rashba interaction, signatures of it are still clearly visible in terms of complex spin textures.

<sup>1</sup>We gratefully acknowledge financial support from the Deutsche Forschungsgemeinschaft through grants SFB/TR 49 and FOR 1346.

**1:03PM S30.00008 Electronic structure studies on competing phases of Aurivillius Bi<sub>4</sub>Ti<sub>3</sub>O<sub>12</sub> using first-principles calculations**, FU-CHANG SUN, University of Connecticut, Department of Physics, SANJEEV NAYAK, University of Connecticut, Department of Materials Science & Engineering, DEEPAM MAURYA, SHASHANK PRIYA, Virginia Tech, Bio-inspired Materials and Devices Laboratory (BMDL), Center for Energy Harvesting Materials and Systems (CEHMS), S. PAMIR ALPAY, University of Connecticut, Department of Materials Science & Engineering — The low temperature ferroelectric to high temperature paraelectric phase transition in bismuth titanate (Bi<sub>4</sub>Ti<sub>3</sub>O<sub>12</sub>) has been experimentally observed at Curie temperature ( $T_C$ ) around 675 °C. The first-principles calculations using density functional theory as implemented in the Vienna *ab initio* simulation package (VASP) with generalized gradient approximation (GGA) for the exchange-correlation interaction are performed to investigate this monoclinic (*b1a1*) to tetragonal (*I4/mmm*) crystal structural transition. We further, provide discussion of the band structure and the Ti-O orbital hybridization, in addition to the frequency dependent dielectric and optical properties of Bi<sub>4</sub>Ti<sub>3</sub>O<sub>12</sub> due to the potential applications in the electronic devices.

**1:15PM S30.00009 ABSTRACT WITHDRAWN —**

**1:27PM S30.00010 Microscopic description of oxide perovskites and automated high-throughput analysis of their energy landscape**, GIOVANNI PIZZI, ANDREA CEPELLOTTI, Ecole Polytechnique Federale de Lausanne, Switzerland, BORIS KOZINSKY, Research and Technology Center, Robert Bosch LLC, Cambridge (MA), NICOLA MARZARI, Ecole Polytechnique Federale de Lausanne, Switzerland — Even if ferroelectric materials like BaTiO<sub>3</sub> or KNbO<sub>3</sub> have been used for decades in a broad range of technological applications, there is still significant debate in the literature concerning their microscopic behavior. For instance, many perovskite materials display a high-temperature cubic phase with zero net polarization, but its microscopic nature is though still unclear, with some materials displaying a very complex energy landscape with multiple local minima. In order to investigate and clarify the microscopic nature of oxide perovskites, we perform a study on a set of about 50 representative ABO<sub>3</sub> systems. We use spacegroup techniques to systematically analyze all possible local displacement patterns that are compatible with a net paraelectric phase, but can provide local non-zero ferroelectric moments. The energetics and the stability of these patterns is then assessed by combining the spacegroup analysis with DFT calculations. All calculations are managed and analyzed using our high-throughput platform AiiDA (www.aiida.net) [1]. Using this technique, we are able to describe the different classes of microscopic models underlying the perovskite systems. [1] G. Pizzi et al., Comp. Mat. Sci 111, 218-230 (2016).

**1:39PM S30.00011 Temperature-dependent phase transition of ferroelectric perovskites: A Wang-Landau-DFT approach<sup>1</sup>**, SIMUCK YUK, YING WAI LI, MARKUS EISENBACH, VALENTINO COOPER, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA — Since the discovery of ferroelectricity in perovskite oxides, considerable efforts have been devoted to understanding their phase transition behaviors in terms of temperature, pressure, and composition. Such materials have regularly been used in transducer and actuator applications. As our first step to make accurate predictions of the crystal phases of more complex oxides such as  $\text{Pb}(\text{Zr}_x\text{Ti}_{1-x})\text{O}_3$ , we have used the Wang-Landau (WL) algorithm and density functional theory (DFT) to examine the temperature-dependent phase transition of  $\text{PbTiO}_3$ ,  $\text{BaTiO}_3$ , and  $\text{KNbO}_3$ . DFT was employed to evaluate the energetics of important crystal-structure candidates, which were later used as the input for WL algorithm. In addition, we examine how the choice of exchange-correlation functionals affects our predictions of the relevant phase transition temperatures.

<sup>1</sup>Research supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division and the Office of Science Early Career Research Program (V.R.C.) and used resources at NERSC and OLCF.

**1:51PM S30.00012 First Principle Studies of Electromechanical Properties in Mn-Doped  $\text{BaTiO}_3$ <sup>1</sup>**, HIROYUKI TAKENAKA, Carnegie Institution for Science, Washington, DC, USA, R.E. COHEN, Carnegie Institution of Washington, Washington, DC, US, Department für Geo-und Umweltwissenschaften, Ludwig-Maximilians-Universität, Munich, Germany — We are performing density functional calculations to elucidate the electromechanical properties for Mn-doped  $\text{BaTiO}_3$  with an oxygen vacancy, applying electric field perpendicular to polarization directions. We find that local dipole switching and lattice changes take place at 3MV/m. Spontaneous polarization along x is 0.251 C/m<sup>2</sup> and c/a ratio changes from 1.021 to 1.000. This indicates that coercive field of Mn-doped  $\text{BaTiO}_3$  increases as were experimentally reported since our results for pure  $\text{BaTiO}_3$  exhibit onset of the switching and changes at 0.8 MV/m. We report our computational dielectric constant and strain as a function of electric field for Mn-doped  $\text{BaTiO}_3$ .

<sup>1</sup>This work is supported by ONR and the ERC Advanced Grant ToMCaT.

**2:03PM S30.00013 Towards an understanding of antiferroelectricity in  $\text{PbZrO}_3$  from first principles**, BRIAN M. ABBETT, School of Applied and Engineering Physics, Cornell University, KARIN M. RABE, Department of Physics and Astronomy, Rutgers University, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University — For decades,  $\text{PbZrO}_3$  has been referred to as the prototypical antiferroelectric. According to a recent analysis, an essential requirement for antiferroelectricity is that there is a polar phase almost degenerate with the nonpolar ground state. Indeed, as previously reported, first-principles calculations show that the polar  $R3c$  structure of  $\text{PbZrO}_3$  is only 1 meV per formula unit higher in energy than the nonpolar ground state  $P6mm$  structure. Here, we explore the question of how these two structures, which seem to be only distantly related, can be so close in energy. Using first-principles methods we investigate the energy landscape of  $\text{PbZrO}_3$ . We introduce a simple structural model that both describes the relevant, low-energy, structural motifs and captures the gross energy landscape relating to both structures. We use this model (and test with direct first-principles calculations) to explore a possible switching path between the non-polar ground state and the metastable polar structure. Our results provide insight into why  $\text{PbZrO}_3$  is antiferroelectric, which may prove useful in identifying new antiferroelectric materials.

**Thursday, March 17, 2016 11:15AM - 2:03PM –**

**Session S31 DCP GSOFT: Ice Nucleation, Amorphous Ices and the Role of Interfaces** 331 -

Nicolas Giovambattista

**11:15AM S31.00001 The Many Faces of Ice and Nonlinear Interferometry.**, MARY JANE SHULTZ, Tufts University — Ice is likely the most ubiquitous solid in the Universe, yet even here on Earth its surface contains many mysteries. At atmospheric pressure, the stable form of ice is hexagonal ice; known as  $I_h$ . This contribution will present data about (i) equilibrium growth at the ice-water interface, (ii) procedures to generate any targeted ice face, and (iii) vibrational spectra of the ice-air interface. Contrary to common belief, the stable ice-water interfaces does not consist of the basal face; rather it consists of pyramidal or prism faces. Growth results from a balance between the molecular density and the top half-bilayer configuration. Arguments reminiscent of Pauling's residual entropy of ice generate the configurational contribution. Prism faces are favored due to greater entropy. Ice grows cryptomorphologically: the macroscopic sample does not reveal the crystalline axes. Locating the crystal axes as well as generating authentic faces for fundamental studies use a combination of the birefringence of ice and etch profiles. Surface vibrational spectroscopy supports an ice model consisting of extended, cooperative motion and beyond-bonding-partner determination of hydrogen bond strength. The surface vibrational spectrum is probed with the nonlinear spectroscopy sum frequency generation (SFG). Currently, nonlinearity limits use of SFG to diagnose interactions. This limitation can be circumvented by measuring the full, complex spectrum. We will report initial results from a newly invented nonlinear interferometer that reveals the full complex spectrum.

**11:51AM S31.00002 Direct Calculation of the Rate of Homogeneous Ice Nucleation for a Molecular Model of Water**, AMIR HAJI-AKBARI, PABLO DEBENEDETTI, Department of Chemical and Biological Engineering, Princeton University — Ice formation is ubiquitous in nature, with important consequences in many systems and environments. However, its intrinsic kinetics and mechanism are difficult to discern with experiments. Molecular simulations of ice nucleation are also challenging due to sluggish structural relaxation and the large nucleation barriers, and direct calculations of homogeneous nucleation rates have only been achieved[1-2] for mW, a monoatomic coarse-grained model of water. For the more realistic molecular models, only indirect estimates have been obtained by assuming the validity of classical nucleation theory[3]. Here, we use a coarse-grained variant of a path sampling approach known as forward-flux sampling to perform the first direct calculation of the homogeneous nucleation rate for TIP4P/Ice, which is the most accurate water model for studying ice polymorphs. By using a novel topological order parameter, we are able to identify a freezing mechanism that involves a competition between cubic and hexagonal ice polymorphs[4]. In this competition, cubic ice wins as its growth leads to more compact crystallites[4]. [1] Li, et al., PCCP, 13, 19807 (2011) [2] Haji-Akbari, et al., PCCP, 16, 25916 (2014) [3] Sanz et al., JACS 135, 15008 (2013) [4] Haji-Akbari, Debenedetti, PNAS, 112, 10582 (2015)

**12:03PM S31.00003 Scratching the surface of ice: Interfacial phase transitions and their kinetic implications.**, DAVID LIMMER, Princeton University — The surface structure of ice maintains a high degree of disorder down to surprisingly low temperatures. This is due to a number of underlying interfacial phase transitions that are associated with incremental changes in broken symmetry relative to the bulk crystal. In this talk I summarize recent work attempting to establish the nature and locations of these different phase transitions as well as how they depend on external conditions and nonequilibrium driving. The implications of this surface disorder is discussed in the context of simple kinetic processes that occur at these interfaces. Recent experimental work on the roughening transition is highlighted.

**12:39PM S31.00004 Exploring the coupling between surface crystallinity and surface hydrophilicity in heterogeneous ice nucleation**, YUANFEI BI, RAFFAELA CABRIOLU, TIANSHU LI, the George Washington University — Heterogeneous ice nucleation has significant influence in a variety of fields ranging from global climate change to intracellular freezing. Although its prevalence can be explained quantitatively by the classical nucleation theory [1], there is a lack of molecular level understanding of the key factors governing ice nucleation at the interface between water and ice nucleator. Here, by employing advanced molecular simulation, we show [2] that heterogeneous ice nucleation on graphitic surface is controlled by the coupling of surface crystallinity and surface hydrophilicity. Molecular level analysis shows that the crystalline graphitic surface with an appropriate hydrophilicity templates ice basal plane forming in the contact layer, thus significantly enhances its ice nucleation efficiency. Remarkably, the templating effect is found to transit from within the first contact layer of water to the second as the hydrophilicity increases, yielding an oscillating distinction between the crystalline and amorphous graphitic surfaces in their ice nucleation efficiencies. Our study sheds new light on the long-standing question of what constitutes a good ice nucleator. 1 R. Cabriolu and T. Li, *Physical Review E* 91, 052402 (2015). 2 Y. Bi, R. Cabriolu, and T. Li, arXiv:1510.01371 (2015).

**12:51PM S31.00005 Two Dimensional Ice crystals intercalated between graphene and mica**, PANTELIS BAMPOULIS, MARTIN H. SIEKMAN, E. STEFAN KOOIJ, DETLEF LOHSE, HAROLD J.W. ZANDVLIET, BENÉ POELSEMA, University of Twente, MESA+ INSTITUTE FOR NANOTECHNOLOGY TEAM — The physics and chemistry of the interfacial contact between water and solid surfaces are of the highest fundamental and practical interest in environmental sciences, many biological systems and corrosion effects. Water intercalated between graphene and mica has recently received much interest, even amplified by intriguing intercalation effects and by the evolution of fractals. These confined water layers are argued to be ice-like at room temperature. Due to its good thermal isolation from the environment, as a result of poor perpendicular heat transport through both mica and graphene, this system is uniquely suited for studying the consequences of heat transport, due to latent heat effects, during growth and melting of 2D ice crystals. The enigmatic growth of ice crystals poses a longstanding fundamental problem and its solution is possibly hidden in influences of heat and particle transport. Indeed, we find that heat and particle transport play a crucial role in the growth of ice crystals under high-temperature and high supersaturation conditions.

**1:03PM S31.00006 2D ice from first principles: structures and phase transitions**, JI CHEN, Thomas Young Centre, University College London, London Centre for nanotechnology, GEORG SCHUSTERITSCH, CHRIS J. PICKARD, Thomas Young Centre, University College London, University of Cambridge, CHRISTOPH G. SALZMANN, University College London, ANGELOS MICHAELIDES, Thomas Young Centre, University College London, London Centre for nanotechnology — Despite relevance to disparate areas such as cloud microphysics and tribology, major gaps in the understanding of the structures and phase transitions of low-dimensional water ice remain. Here we report a first principles study of confined 2D ice as a function of pressure. We find that at ambient pressure hexagonal and pentagonal monolayer structures are the two lowest enthalpy phases identified. Upon mild compression the pentagonal structure becomes the most stable and persists up to ca. 2 GPa at which point square and rhombic phases are stable. The square phase agrees with recent experimental observations of square ice confined within graphene sheets. We also find a double layer AA stacked square ice phase, which clarifies the difference between experimental observations and earlier force field simulations. This work provides a fresh perspective on 2D confined ice, highlighting the sensitivity of the structures observed to both the confining pressure and width.

**1:15PM S31.00007 Using nanoscale amorphous solid water films to create and study deeply supercooled liquid water at interfaces**, BRUCE KAY, Pacific Northwest National Laboratory — Molecular beam vapor deposition of water on cryogenic substrates is known to produce amorphous solid films. When heated above their glass transition these films transform into deeply supercooled liquid water. These nanoscale liquid films can be used to study kinetic processes such as diffusion, isotope exchange, crystallization, and solvent mediated reactions in unprecedented detail. This talk will highlight our recent advances in this area. My colleagues Yuntao Xu, Chunqing Yuan, Collin Dibble, R. Scott Smith, Nick Petrik, and Greg Kimmel made important contributions to this work. This work was supported by the U.S. Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences. The research was performed using EMSL, a national scientific user facility sponsored by DOE's Office of Biological and Environmental Research and located at Pacific Northwest National Laboratory, which is operated by Battelle, operated for the U.S. DOE under Contract DE-AC05-76RL01830.

**1:51PM S31.00008 Local Structure in *Ab Initio* Liquid Water: Signatures of Amorphous Phases<sup>1</sup>**, BISWAJIT SANTRA, Princeton University, Princeton, USA, ROBERT A. DISTASIO, JR., Cornell University, Ithaca, USA, FAUSTO MARTELLI, ROBERTO CAR, Princeton University, Princeton, USA — Within the framework of density functional theory, the inclusion of exact exchange and non-local van der Waals/dispersion interactions is crucial for predicting a microscopic structure of ambient liquid water that quantitatively agrees with experiment [1]. In this work, we have used the local structure index (LSI) order parameter to analyze the local structure in such highly accurate *ab initio* liquid water. At ambient conditions, the LSI probability distribution,  $P(I)$ , was unimodal with most water molecules characterized by more disordered high-density-like local environments. With thermal excitations removed, the resultant bimodal  $P(I)$  in the inherent potential energy surface (IPES) exhibited a 3:1 ratio between high- and low-density-like molecules, with the latter forming small connected clusters amid the predominant population. By considering the spatial correlations and hydrogen bond network topologies among water molecules with the same LSI identities, we demonstrate that the signatures of the experimentally observed low- and high-density amorphous phases of ice are present in the IPES of ambient liquid water [2]. [1] DiStasio *et al.*, *J. Chem. Phys.* **141**, 084502 (2014). [2] Santra *et al.*, *Mol. Phys.* **113**, 2829 (2015).

<sup>1</sup>This work was supported by the DOE: DE-SC0008626, DE-SC0005180.

**Thursday, March 17, 2016 11:15AM - 2:15PM —**

**Session S32 DCP: Chemical Physics of Extreme Environments I** 332 - Arthur Suits, University of Missouri

**11:15AM S32.00001 Reaction Product Identification in Extreme Chemical Environments by Broadband Rotational Spectroscopy<sup>1</sup>**, BROOKS PATE, University of Virginia — Molecular rotational spectroscopy has several advantages for detection of reaction intermediates and products under extreme laboratory conditions. Rotational spectroscopy has high sensitivity to the molecular structure and provides high spectral resolution in low pressure environments. Furthermore, quantum chemistry provides accurate estimates of the spectroscopic parameters. As a result, rotational spectroscopy can identify molecular species in complex reaction mixtures without the need for chromatographic separation and without the need for a previously recorded "library spectrum" of the molecule. The application of chirped pulse Fourier transform rotational spectroscopy methods for the identification of molecules of astrochemical interest formed in pulsed discharge sources will be described including recent advances for high-throughput mm-wave spectroscopy. The set of reaction products created in the experiment can provide insight into the reaction mechanism. Reactions involving the CN radical will be discussed. These reactions can be barrierless making them candidates for interstellar gas reactions. The possibility that interstellar cyanomethanimine is produced by gas phase radical-neutral reactions instead of surface chemistry on grain-supported ices will be discussed using recent spatially resolved chemical images in Sagittarius B2 observed with the Jansky Very Large Array.

<sup>1</sup>This work supported by NSF CHE 1213200

**11:51AM S32.00002 Observation of *K*-dependent Reaction Rates in Pulsed Uniform Supersonic Flows by Chirped-Pulse Microwave Spectroscopy**, BERNADETTE BRODERICK, NUWANDI ARIYASINGHA, ARTHUR SUITS, University of Missouri, UNIVERSITY OF MISSOURI TEAM — Chirped-pulse Fourier-transform microwave spectroscopy was used to interrogate the reaction of Cl atoms with propyne in a pulsed uniform supersonic flow. The technique, termed "CPUF", utilizes broad-band microwave spectroscopy to extract structural information with MHz resolution and near universal detection, in conjunction with a Laval flow system, which offers thermalized conditions at low temperatures and high number densities. Previous studies have exploited this approach to obtain multichannel product branching fractions in a number of polyatomic systems, with isomer and often vibrational level specificity. This report highlights an additional capability of the CUF technique: here, the state-specific reactant depletion is directly monitored on a microsecond timescale. In doing so, a clear dependence on the rotational quantum number *K* in the rate of the reaction between Cl atoms and propyne is revealed. Future prospects for the technique will be discussed.

**12:03PM S32.00003 Rotational Spectroscopic Studies and Observational Searches for HO<sub>3</sub>**, SUSANNA WIDICUS WEAVER<sup>1</sup>, Emory University — Interstellar chemistry is largely driven by reactions of unstable molecules that serve as reaction intermediates in terrestrial chemistry. One such class of compounds are weakly-bound clusters. These clusters could form in interstellar environments through radiative association reactions, but their identification and characterization in interstellar environments is limited by a lack of rotational spectral information. One such species is HO<sub>3</sub>, which could be formed in the interstellar medium from O<sub>2</sub> and OH. HO<sub>3</sub> has been studied extensively in the infrared, and there are a few microwave spectral studies that have also been reported. However, no millimeter or submillimeter spectral information is available to guide astronomical observations. In this talk, we will present the laboratory characterization of *trans*-HO<sub>3</sub> and *trans*-DO<sub>3</sub> from 70 to 450 GHz using our newly developed fast sweeping technique. The molecular constants have been significantly refined, and additional higher order centrifugal distortion constants have been determined. We will also present an initial observational search for HO<sub>3</sub> in 32 star forming regions. Although no HO<sub>3</sub> lines have been detected thus far, strict upper limits can be placed on the HO<sub>3</sub> column density in these sources based on this analysis.

<sup>1</sup>Additional Authors: Luyao Zou, Brian M. Hays

**12:39PM S32.00004 The Extreme Chemical Environments Associated with Dying Stars**, LUCY ZIURYS, University of Arizona — Mass loss from dying stars is the main avenue by which material enters the interstellar medium, and eventually forms solar systems and planets. When stars consume all the hydrogen burning in their core, they start to burn helium, first in their centers, and then in a surrounding shell. During these phases, the so-called "giant branches," large instabilities are created, and stars begin to shed their outer atmospheres, producing so-called circumstellar envelopes. Molecules form readily in these envelopes, in part by LTE chemistry at the base of the stellar photosphere, and also by radical reactions in the outer regions. Eventually most stars shed almost all their mass, creating "planetary nebulae," which consist of a hot, ultraviolet-emitting white dwarf surrounded by the remnant stellar material. The environs in such nebulae are not conducive to chemical synthesis; yet molecular gas exists. The ejecta from these nebulae then flows into the interstellar medium, becoming the starting material for diffuse clouds, which subsequently collapse into dense clouds and then stars. This molecular "life cycle" is repeated many times in the course of the evolution of our Galaxy. We have been investigating the interstellar molecular life cycle, in particular the chemical environments of circumstellar shells and planetary nebulae, through both observational and laboratory studies. Using the facilities of the Arizona Radio Observatory (ARO), we have conducted broad-band spectral-line surveys to characterize the contrasting chemical and physical properties of carbon (IRC+10216) vs. oxygen-rich envelopes (VY CMa and NML Cyg). The carbon-rich types are clearly more complex in terms of numbers of chemical compounds, but the O-rich variety appear to have more energetic, shocked material. We have also been conducting surveys of polyatomic molecules towards planetary nebulae. Species such as HCN, HCO<sup>+</sup>, HNC, CCH, and H<sub>2</sub>CO appear to be common constituents of these objects, and their abundances do not appear to vary with age. These results contradict the predictions of all chemical models. We have also been using millimeter-wave and Fourier transform microwave methods to measure rotational spectra of potential new interstellar molecules to complete the chemical inventories. The current results of these studies will be presented.

**1:15PM S32.00005 Complex Mixture Analysis Using Rotational Spectroscopy**, MICHAEL MCCARTHY, Harvard-Smithsonian Center for Astrophysics — Owing to its very high intrinsic resolution, exceeding ppm levels in supersonic jet sources, rotational spectroscopy is a powerful analytical tool to analyze complex mixtures that consist of both familiar and exotic molecules. We present here an experimental method to rapidly sort rotational lines in broadband spectra and assign them to individual chemical compounds in the cm-band. This method combines a chirped-pulse FT microwave (CP-FTMW) spectrometer with follow-up analysis using an automated cavity FTMW spectrometer with double resonance (DR) capabilities. The CP-FTMW spectrum acts as a filter, identifying only those regions of frequency space that contain molecular signal, and discarding the vast majority of frequency space that is devoid of molecular information. With superior sensitivity and resolution per unit time, a cavity spectrometer is then used for follow-up assays on these bright spectral lines, to group transitions which share common characteristics, such as elemental composition, etc. These groups can be further partitioned into smaller sub-groups by exhaustive DR experiments whereby only those rotational lines that share a common energy level from the same molecule are linked together. From these series of measurements and assays, rotational transitions of multiple, individual chemical compounds can be empirically sorted and identified, without the need for any theoretical guidance or input. Significant automation greatly enhances the overall efficiency, enabling rapid, exhaustive testing with little oversight. Examples illustrating the power of this methodology for rapid analysis of broadband spectra will be presented.

**1:51PM S32.00006 Stretching molecules under extreme tensile strain: density functional theory versus multireference methods.**, GARY KEDZIORA, Engility Corp., STEPHEN BARR, RAJIV BERRY, Air Force Research Lab., Materials and Manufacturing Directorate, JAMES MOLLER, Miami University, Department of Mechanical and Manufacturing Engineering, TIMOTHY BREITZMAN, Air Force Research Lab., Materials and Manufacturing Directorate — A more refined understanding of how molecules behave under extreme tensile strain is desirable for modeling fracture initiation in polymers and other mecho-chemical studies. We investigated several quantum mechanical methods for use in multiscale models of highly strained polymers where bond breaking occurs. A small set of molecules and a protocol for stretching them were used as model test systems. The results from these tests using several functionals were compared with complete active space self-consistent field results. These test systems provide unique challenges for quantum mechanical models. Quantum mechanics is required for accurate bond breaking prediction because the results are dependent on the conformation and secondary electronic structure effects such as hyperconjugation. GGA methods with unrestricted solutions to the Kohn-Sham equations provide adequate results for our purposes even though there are some minor flaws based on the spin symmetry breaking.

**2:03PM S32.00007 Mixed quantum/semiclassical studies of condensed-phase dynamics and spectroscopy**<sup>1</sup>, JEFFREY A CINA, PHILIP A KOVAC, Department of Chemistry & Biochemistry, Oregon Center for Optical, Molecular, and Quantum Science — We report on theoretical and computational studies of molecular-level chemical dynamics and their time-resolved spectroscopic signatures for small molecules embedded in low-temperature crystalline-host environments. Our calculations are based on a mixed quantum mechanical/semiclassical theory, referred to as the variational fixed vibrational basis/Gaussian bath theory (v-FVB/GB), in which certain optically addressed coordinates driven to large-amplitude motion by laser pulses are treated fully quantum mechanically and a larger number of others executing small-amplitude motion are treated semiclassically. Model systems under investigation incorporate a dihalogen molecule isolated in a symmetrical cluster of rare-gas atoms, with the outer layer of host atoms bound together in a harmonic net that preserves the initial equilibrium structure, but emulates an extended medium by preventing dynamical reconstruction and host-atom evaporation.

<sup>1</sup>Supported by the US NSF.

## Thursday, March 17, 2016 11:15AM - 2:15PM –

Session S33 DPOLY: Ion Containing Polymer Membranes 336 - Phil Griffin, University of Pennsylvania

**11:15AM S33.00001 Proton conducting, high modulus polymer electrolyte membranes by polymerization-induced microphase separation**, SUJAY CHOPADE, MARC HILLMYER, TIMOTHY LODGE, Univ of Minn - Minneapolis — Robust solid-state polymer electrolyte membranes (PEMs) are vital for designing next-generation lithium-ion batteries and high-temperature fuel cells. However, the performance of diblock polymer electrolytes is generally limited by poor mechanical stability and network defects in the conducting pathways. We present the *in-situ* preparation of robust cross-linked PEMs via polymerization-induced microphase separation, and incorporation of protic ionic liquid (IL) into one of the microphase separated domains. The facile design strategy involves a delicate balance between the controlled growth of polystyrene from a poly(ethylene oxide) macro-chain transfer agent (PEO-CTA) and simultaneous chemical cross-linking by divinylbenzene in the presence of IL. Small angle X-ray scattering and transmission electron microscopy confirmed the formation of a disordered structure with bicontinuous morphology and a characteristic domain size of order 20 nm. The long-range continuity of the PEO/protic IL conducting nanochannels and cross-linked polystyrene domains imparts high thermal and mechanical stability to the PEMs, with elastic modulus approaching 10 MPa and a high ionic conductivity of 15 mS/cm at 180 C.

**11:27AM S33.00002 The role of tortuosity on ion conduction in block copolymer electrolyte thin films<sup>1</sup>**, YU KAMBE, University of Chicago, CHRISTOPHER G. ARGES, PAUL F. NEALEY, University of Chicago / Argonne National Laboratory — This talk discusses the role of grain tortuosity on ion conductivity in block copolymer electrolyte (BCE) thin films. In particular, we studied lamellae forming BCEs with both domains oriented perpendicular to the substrate surface and connected directly from one electrode to another – i.e., tortuosity of one. The BCE is composed of ion-conducting, poly(2-vinyl n-methylpyridinium) blocks and non-ionic polystyrene blocks. Prior to creating the BCE, the pristine block copolymer, poly(styrene-*b*-2-vinyl pyridine), was directly self-assembled (DSA) on topographical or chemical patterns via graphoepitaxy and chemoepitaxy. A chemical vapor infiltration reaction modified the P2VP block into positively charged, fixed quaternary ammonium groups paired with mobile counteranions. The graphoepitaxy process utilized topographical interdigitated gold nanoelectrodes (100s of nanometers spacing between electrodes) created via e-beam lithography. Alternatively, chemical patterns had gold electrodes incorporated into them with 10s to 100s of microns spacing using conventional optical lithography. The interdigitated gold electrodes enabled in-plane ion conductivity measurements of the DSA BCEs to study the role of grain tortuosity on ion conductivity.

<sup>1</sup>U.S. Department of Energy Office of Science: Contract No. DE-AC02-06CH11357

**11:39AM S33.00003 Building non-tortuous ion-conduction pathways using self-assembled block copolymers**, ONNURI KIM, MOON JEONG PARK, Pohang Univ of Sci & Tech — Ion-containing polymers with self-assembled morphologies are becoming important ingredients of a wide range of electrochemical devices such as lithium-ion batteries, fuel cells and electroactive actuators. Although several studies have reported the relationship between morphologies and ion transport properties of such polymers, the most of quantitative analysis have been limited to two-dimensional morphologies as they occupy a large window of the phase diagrams. In present study, we investigated the effects of morphology on the ion transport efficiency with a focus on three-dimensional symmetry. A range of three-dimensional self-assembled morphologies, i.e., ill-defined cubic, orthorhombic network (O<sup>70</sup>), and face-centered cubic phases (fcc) were achieved for a single sulfonated block copolymer upon the addition of non-stoichiometric ionic liquids. The type of three-dimensional lattice was found out to play a crucial role in determining the ion transport properties of composite membranes, where the most efficient ion-conduction was demonstrated for fcc phases with lowest tortuosity of 1 over orthorhombic networks phases (tortuosity:1.5). This intriguing result suggests a new avenue to designing polymer electrolytes with improved transport properties.

**11:51AM S33.00004 Nanostructured anion conducting block copolymer electrolyte thin films<sup>1</sup>**, CHRISTOPHER ARGES, YU KAMBE, PAUL NEALEY, University of Chicago/Argonne National Laboratory — Lamellae forming block copolymer electrolyte (BCE) thin-films with perpendicular aligned orientation were registered with high fidelity over large areas via a self-assembly process followed by a novel chemical vapor infiltration reaction (CVIR) technique. In this scheme, poly(styrene-*b*-2-vinyl pyridine) (PS<sub>6</sub>P2VP) block copolymers were self-assembled with perpendicular orientations on neutral chemical brushes using solvent vapor annealing. The ionic groups were selectively introduced into the P2VP block via a Menshutkin reaction that converted the nitrogen in the pyridine to n-methylpyridinium - anion carrier groups. FTIR-ATR and XPS tools confirmed the formation of the aforementioned ionic moieties post CVIR process and structure imaging tools (e.g., SEM and AFM imaging, GI-SAXS and RSOXs) established that incorporation of the ionic groups did not alter the self-assembled nanostructured films nor did subsequent ion-exchange processes. Electrochemical impedance spectroscopy determined the in-plane ion conductivity of different counteranions in the BCE thin films and alteration to the symmetry of the block copolymer film substantially improved (or hindered) BCE ion conductivity if the P2VP block's volume fraction was slightly greater than (or less than) 0.5.

<sup>1</sup>U.S. Department of Energy, Office of Science under Contract No. DE-AC02-06CH11357

**12:03PM S33.00005 Surface Structure of Thin Films of Multifunctional Ionizable Copolymers<sup>1</sup>**, ANURADHI WICKRAMASINGHE, DVORA PERAHIA, Clemson University — Phase segregation results in a rich variety of structures in co-polymers where interfacial forces often dominate the structure of thin films. Introduction of ionizable segments often drives the formation of compounded structures with multiple blocks residing at the interfaces. Here we probe thin films, 40-50nm, of an A-B-C-B-A co-polymer where C is a randomly sulfonated polystyrene with sulfonation fractions of 0, 26 and 52 mole %, B is poly (ethylene-*r*-propylene), and A is poly (t-butyl styrene) as the sulfonation level and temperature are varied using Neutron Reflectivity AFM, and surface tension measurements. As cast films form layers with both hydrophobic blocks dominating the solid and air interfaces and the ionizable block segregating to the center. Following annealing at 170°C, above T<sub>g</sub> of styrene sulfonate, the films coarsen, with surface aggregation dominating the structure, though interfacial regions remain dominated by the hydrophobic segments. We show that in contrast to non-ionic co-polymers, formation of micelles dominated the structure of these ionic structured films.

<sup>1</sup>Supported in part by DOE Grant No. DE-SC007908

**12:15PM S33.00006 Effects of repeated wet/dry cycling on the structure and performance of sulfonated pentablock copolymer membranes.**, PHUC TRUONG, GILA STEIN, university of houston — Sulfonated block copolymers have shown potential as membranes for water purification. However, the performance of these materials under cyclic wet/dry conditions is not well understood. We measured the membrane structure, mechanical properties, and water vapor transport rates in a sulfonated pentablock copolymer as a function of the number of wet/dry cycles. The polymer is synthesized with an ABCBA block sequence, where A is poly(t-butyl styrene), B is poly(hydrogenated isoprene), and C is poly(styrene sulfonate). The ion exchange capacity is 2 meq, and membranes were prepared by coating from a solution. Using small angle X-ray scattering, we find the structure in as-prepared membranes resembles disordered micelles, and the characteristic length scale swells slightly with each wet/dry cycle. This lattice swelling is likely constrained by the glassy end-blocks. We also detect a lower yield point and less overall tensile strength with repeated cycling. Water vapor transport rates vary with the number of wet/dry cycle, however no specific trend was observed.

**12:27PM S33.00007 Influence of Substrate on PFSA Thin-Film Morphology** , PETER DUDENAS, UC Berkeley, AHMET KUSOGLU, SINGANALLUR VENKATAKRISHNAN, ALEXANDER HEXEMER, ADAM WEBER, Lawrence Berkeley Natl Lab — Perfluorosulfonic-acid (PFSA) ionomers are the most commonly used electrolyte for polymer-electrolyte fuel cells (PEFCs) due to their high conductivity and good electrochemical and thermo-mechanical stability. A PFSA's chemical structure is comprised of a polytetrafluoroethylene (PTFE) backbone that provides mechanical and chemical stability, and randomly placed tethered perfluoroether side chains terminated with sulfonic-acid groups, which impart its remarkable proton-conduction capabilities. Controlled by substrate/film interactions, long-range structural order in PFSAs change when confined to thin films (<200 nm), as does its transport and mechanical properties. The nature of change is substrate dependent, where stronger interactions create a more dramatic change in properties. In this talk, grazing-incidence c-Ray scattering (GIXS) is used to demonstrate induced structural order on metallic substrates, which is not present on other substrates like silicon and carbon. The higher degree of ordering is correlated with measured changes in mechanical properties for the thin films. Scattering data is also modeled using the recently released program high-performance GISAXS (HipGISAXS), to estimate the size and distribution of the ordered domains. -/a

**12:39PM S33.00008 Structure and Properties of a Semi-crystalline Cationic Polymer for Anion Exchange Membranes** , FREDERICK BEYER, SAMUEL PRICE, ALICE SAVAGE, XIAOMING REN, US Army Research Laboratory, INSANE MEMBRANES COLLABORATION — Nafion has long been studied in order to understand its combination of good mechanical properties, chemical resistance, and excellent charge transport characteristics. In the past decade, uncertainty regarding the morphological behavior of Nafion has largely been resolved, allowing researchers to mimic and improve on the structure of this material. In this presentation, work to incorporate key characteristics of Nafion into a model cation-containing polymer will be described. In these new materials, semi-crystalline atactic poly(norbornene) is used to introduce good mechanical properties to anion-exchange membranes, analogous to the PTFE crystallites in Nafion. The ether linkages between the charged species and backbone are also utilized to place the cationic species (trimethylamine) in our materials into a mechanically soft environment. The resulting polymer shows some characteristics that are similar to those of Nafion. In this presentation, the synthesis, alkaline stability, mechanical properties, morphological behavior and charge transport properties will all be described.

**12:51PM S33.00009 Exploring the Parameters Controlling the Crystallinity-Conductivity Correlation of PFSA Ionomers** , AHMET KUSOGLU, SHOUWEN SHI, ADAM WEBER, Lawrence Berkeley Natl Lab — Perfluorosulfonic-acid (PFSA) ionomers are the most commonly used solid-electrolyte in electrochemical energy devices because of their remarkable conductivity and chemical/mechanical stability, with the latter imparted by their semi-crystalline fluorocarbon backbone. PFSAs owe this unique combination of transport/stability functionalities to their phase-separated morphology of conductive hydrophilic ionic domains and the non-conductive hydrophobic backbone, which are connected via pendant chains. Thus, phase-separation is governed by fractions of backbone and ionic groups, which is controlled by the equivalent weight (EW). Therefore, EW, along with the pendant chain chemistry, directly impact the conductive vs non-conductive regions, and consequently the interrelation between transport and stability. Driven by the need to achieve higher conductivities without disrupting the crystallinity, various pendant-chain chemistries have been developed. In this talk, we will report the results of a systematic investigation on hydration, conductivity, mechanical properties and crystallinity of various types and EWs of PFSA ionomers to (i) develop a structure/property map, and (ii) identify the key parameters controlling morphology and properties. It will be discussed how the pendant-chain and backbone lengths affect the conductivity and crystallinity, respectively. Lastly, the data set will be analyzed to explore universal structure/property relationships for PFSAs.

**1:03PM S33.00010 Water's Role in the Relaxation of Polyelectrolyte Complexes and Multilayers** , JODIE LUTKENHAUS, YANPU ZHANG, DARIYA REID, Texas AM University, HANNE ANTILA, EROL YILDIRIM, RAN ZHANG, MARIA SAMMALKORPI, Aalto University — In the last decade, evidence for an intriguing glass-transition-like phase transition has emerged in hydrated polyelectrolyte complex precipitates and polyelectrolyte multilayers. Although the transition is weak, it stimulates large-scale macroscopic phenomena such as multilayer shrinking, swelling, and rearrangement. To date, there is not a clear consensus on what causes this transition, although a growing body of evidence indicates that salt and water are key parameters. Recent simulations of hydrated polyelectrolyte complexes show that water molecules form a stabilizing hydrogen-bonded network and that this network is disrupted by dehydration of the polyanion at the thermal transition, leading to segmental relaxation of polymer chains. If true, this would explain the transition's dependence on water and extrinsic compensation as well as its glass transition-like character. This talk will focus upon water's role in the transition, in which a strong dependence on hydration is observed. Quartz crystal microbalance with dissipation (QCM-D) and modulated differential scanning calorimetry (MDSC) are used to track the transition in polyelectrolyte complexes as a function of hydration.

**1:15PM S33.00011 Probing the mechanism of non-linear growth of polyelectrolyte multilayers** , VICTOR SELIN, Department of Materials Science & Engineering, Texas AM University, College Station, Texas 77843, USA, JOHN ANKNER, Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, SVETLANA A. SUKHISHVILI, Department of Materials Science & Engineering, Texas AM University, College Station, Texas 77843, USA — We report a study of the non-linear growth of electrostatically assembled polyelectrolyte multilayer films (PEM). PEM films were assembled by the layer-by-layer (LbL) technique using poly(methacrylic acid) as a polyanion and quaternized poly-2-(dimethylamino)ethyl methacrylate as a polycation. During film build-up, the thickness evolution as well as water uptake of PEM films were measured by in situ ellipsometry, whereas neutron reflectometry was used to probe the evolution of film internal structure as a function of deposition time. First, we found that during non-linear growth, films remain in a highly swollen hydrogel-like state, but the swelling ratio demonstrated an odd/even effect, with much larger hydration of the PEM when the terminal layer was the polycation. Second, while polycation chains were able to diffuse into the bulk of the film with a diffusion constant several orders of magnitude lower than in their free, unbound state, polyanion invasion was limited to the film surface. The amounts of the polycation and the polyanion adsorbed per deposition cycle were also drastically different. We quantify chemical composition and water content in the film, and correlate these data with the depth polyelectrolyte chains penetrate within the film during PEM construction.

**1:27PM S33.00012 Effect of Aggregation on the Mechanical Properties of Ionomers from MD Simulations<sup>1</sup>** , JANANI SAMPATH, LISA M. HALL, The Ohio State University-Columbus — Ionomers are polymers with a small fraction of charged monomers; these bound ions, along with free counterions, tend to aggregate together strongly in the absence of solvent. Ionic aggregates can act like temporary cross-links, giving rise to interesting mechanical properties. We perform coarse-grained molecular dynamics simulations of ionomers with various spacings of charges along the chain, representing experimental precisely spaced, neutralized poly(ethylene-co-acrylic acid) materials. We calculate aggregate morphology, dynamics, and scattering profiles and study the systems during uniaxial tensile strain to understand how aggregate structure changes under deformation and affects mechanical properties. Anisotropic structure factors (parallel and perpendicular to the direction of pull) and visualization shows that the aggregates align, in qualitative agreement with experimental findings. Stress-strain curves at different strain rates are also obtained. A modification of the model to account for unneutralized acid groups by adjusting their Lennard-Jones interaction strengths with each other and with ionic groups will also be discussed.

<sup>1</sup>This material is based upon work supported by the National Science Foundation under Grant 1463103

**1:39PM S33.00013 Structure and ionic conductivity of block copolymer electrolytes over a wide salt concentration range**, MAHATI CHINTAPALLI, THAO LE, UC Berkeley, NAVEEN VENKATESAN, UC Santa Barbara, JACOB THELEN, ADRIANA ROJAS, NITASH BALSARA, UC Berkeley — Block copolymer electrolytes are promising materials for safe, long-lasting lithium batteries because of their favorable mechanical and ion transport properties. The morphology, phase behavior, and ionic conductivity of a block copolymer electrolyte, SEO mixed with LiTFSI was studied over a wide, previously unexplored salt concentration range using small angle X-ray scattering, differential scanning calorimetry and ac impedance spectroscopy, respectively. SEO exhibits a maximum in ionic conductivity at twice the salt concentration that PEO, the homopolymer analog of the ion-containing block, does. This finding is contrary to prior studies that examined a more limited range of salt concentrations. In SEO, the phase behavior of the PEO block and LiTFSI closely resembles the phase behavior of homopolymer PEO and LiTFSI. The grain size of the block copolymer morphology was found to decrease with increasing salt concentration, and the ionic conductivity of SEO correlates with decreasing grain size. Structural effects impact the ionic conductivity-salt concentration relationship in block copolymer electrolytes. SEO: polystyrene-*block*-poly(ethylene oxide); also PS-PEO LiTFSI: lithium bis(trifluoromethanesulfonyl imide)

**1:51PM S33.00014 Role of Acid Functionality and Placement on Morphological Evolution and Strengthening of Acid Copolymers**, LURI ROBERT MIDDLETON, ERIC SCHWARTZ, KAREN WINEY, University of Pennsylvania — Functional polymers with specific interactions produce hierarchical morphologies that directly impact mechanical properties. We recently reported that the formation of acid-rich layered morphologies in precise poly(ethylene-co-acrylic acid) copolymers improves tensile strength. We now explore the generality of this phenomenon through variations in pendant acid chemistries, acid content and precision in placement of acid groups in polyethylene-based copolymers. In situ X-ray scattering measurements during tensile deformation reveal that the precision in acid group placement is critical to forming well-defined layered morphologies. This phenomenon was observed in both semi-crystalline and amorphous precise acid copolymers with varied acid chemistries (acrylic, geminal acrylic and phosphonic acids). Compositionally identical polymers but with pseudo random acid placement do not form layered morphologies. Acid chemistry and acid content influence morphological evolution predominately through modification of the copolymer Tg and crystallinity. Our results indicate that hierarchical layered structures, commensurate with improved mechanical properties, form in the presence of uniformity in chemical structure and sufficient chain mobility to strongly align during deformation.

**2:03PM S33.00015 States of Salt Water in Polyampholyte Hydrogel Networks at Ice Forming Temperatures**, HYUN-JOONG CHUNG, XINDA LI, JANET A.W. ELLIOTT, Univ of Alberta — The behavior of water in polymers, including ice formation, is of increasing interest. For example, one can achieve improved longevity of water-borne polymeric coatings and aqueous electrolytes that operate at low temperature by understanding the polymer-water interaction. Water molecules that are bound to hydrophilic polymer backbones are known to be non-freezable at extremely low temperatures such as -100C, whereas non-bound water is still freezable at higher temperatures. Polyampholyte, which contains both cationic and anionic groups in its backbone, is an interesting class of anti-fouling coating material with a hygroscopic nature and self-healing ability. In real operational condition, for example in maritime petroleum production in the arctic climate, multiple species of salt ions can complicate the ice formation, but their effect has not been exhaustively studied. Using a random copolymer of sodium p-styrenesulphonate (NaSS) and 3-(methacryloylamino)propyl-trimethylammonium chloride as a model system to study the phase behavior of NaCl salt in the hydrogel, this work presents (i) intriguing mechanical and electrical properties of polyelectrolytes at low temperature (<-20C), (ii) differential scanning calorimetry studies on the effects of salt concentration, polymer chain density, degree of polymerization, and (iii) effect of dialysis on microstructure and phase water behavior in the polyampholyte hydrogel.

**Thursday, March 17, 2016 11:15AM - 2:15PM —**  
**Session S34 GSOF: Small Molecule Glasses** 337 - Kate Jensen, Yale University

**11:15AM S34.00001 Point-to-set correlations and rugged landscapes**, SHO YAJIDA, Duke University, LUDOVIC BERTHIER, Université de Montpellier, PATRICK CHARBONNEAU, Duke University, GILLES TARJUS, Université Pierre et Marie Curie — Upon approaching the glass transition a liquid gets sluggish without obvious structural changes. The glassy slowdown is instead attributed to an increasing roughness in the underlying free-energy landscape. Cavity point-to-set (PTS) correlations are real-space tools for characterizing the evolution of this rugged landscape, but their measurement is a serious computational challenge. Here, we first describe how advanced Monte Carlo techniques can be used to dramatically enhance sampling in cavities, extending the range over which PTS correlations can be obtained. By suitably generalizing the notion of PTS correlations to capture any type of growing order in liquids, be it local or amorphous, we then establish a criterion for distinguishing a dynamical slowdown due to critical ordering from one due to glassiness. These methodological advances shed a new light on the interplay between structure and dynamics in model glass formers, and tie in with recent field-theoretic results about the nature of jumps between metastable minima in rough landscapes.

**11:27AM S34.00002 Evidence for a second-order phase transition to a low-entropy glass**, C. PATRICK ROYALL, FRANCESCO TURCI, University of Bristol, THOMAS SPECK, Johannes Gutenberg-Universität Mainz — The physics underlying the glass transition is a major outstanding. Central to its solution is whether there is some kind of thermodynamic transition to an ideal glass, a disordered state with extremely low entropy, or whether in principle a liquid may be supercooled to arbitrary low temperature. Among the challenges that lie in tackling the glass transition are the immense timescales involved. Computer simulation, which might otherwise be able to pick up hints of a thermodynamic transition is limited by the small time-window over which a liquid can be equilibrated. Here we address this challenge using trajectory sampling in a system undergoing a first order nonequilibrium phase transition to a glassy state rich in low-energy geometric motifs. Extrapolation to equilibrium indicates that the transition would occur at a similar temperature at which the ideal glass transition is expected from extrapolation of dynamic and thermodynamic measurements. We further reweight nonequilibrium data to equilibrium leading to configurations representative of extremely low temperature, which indicate a transition to a low energy state at the ideal glass transition temperature. We thus interpret the ideal glass transition as the lower critical endpoint of this nonequilibrium transition.

**11:39AM S34.00003 Softness Correlations Across Length Scales<sup>1</sup>**, ROBERT IVANCIC, University Of Pennsylvania, AMIT SHAVIT, Thomson Reuters, JENNIFER RIESER, SAMUEL SCHOENHOLZ, University Of Pennsylvania, EKIN CUBUK, Harvard, DOUGLAS DURIAN, ANDREA LIU, ROBERT RIGGLEMAN, University Of Pennsylvania — In disordered systems, it is believed that mechanical failure begins with localized particle rearrangements. Recently, a machine learning method has been introduced to identify how likely a particle is to rearrange given its local structural environment, quantified by *softness*. We calculate the softness of particles in simulations of atomic Lennard-Jones mixtures, molecular Lennard-Jones oligomers, colloidal systems and granular systems. In each case, we find that the length scale characterizing spatial correlations of softness is approximately a particle diameter. These results provide a rationale for why localized rearrangements—whose size is presumably set by the scale of softness correlations—might occur in disordered systems across many length scales.

<sup>1</sup>supported by DOE DE-FG02-05ER46199

**11:51AM S34.00004 Onset of cooperative dynamics in equilibrium glass-forming metallic liquids**<sup>1</sup>, ABHISHEK JAISWAL, YANG ZHANG, Univ of Illinois - Urbana — Onset of cooperative dynamics has been observed in the metastable regime of many molecular liquids, colloids, and granular materials approaching their respective glass or jamming transition points. It is also considered to play a significant role in the emergence of slow dynamics. However, the nature of such dynamical cooperativity remains elusive in multicomponent metallic liquids characterized by complex many-body interactions and high mixing entropy. Herein, we report indications of the onset of cooperative dynamics in an equilibrium glass-forming metallic liquid (ZrCuNiAl). This is revealed by deviation of the experimentally measured mean diffusion coefficient from its high temperature Arrhenius behavior below  $T_o \approx 1300$  K, i.e., a crossover from uncorrelated dynamics above  $T_o$  to landscape-influenced correlated dynamics below  $T_o$ . The onset/crossover in this system is observed at approximately twice of its calorimetric glass transition temperature ( $T_g \approx 697$  K) and in the stable liquid phase, unlike many molecular liquids. Furthermore, we show the presence of such a dynamical onset phenomenon in ten other glass-forming metallic liquids, universally occurring at approximately twice of their  $T_g$  and in their liquid phases.

**12:03PM S34.00005 Differences in dynamic heterogeneity in strong and fragile glass formers**<sup>1</sup>, HANNAH STALEY, ELIJAH FLENNER, GRZEGORZ SZAMEL, Colorado State University — We study dynamic heterogeneity in a model strong glass former. We examine the spatial extent  $\xi_4^a(t)$  and the strength  $\chi_4^a(t)$  of the heterogeneity of the dynamics at two length scales  $a$ . One length scale corresponds to the nearest neighbor separation and the other length scale corresponds to the length scale of the tetrahedral network. We find that the dynamic correlation length  $\xi_4^a$  grows much slower with increasing relaxation time at both length scales than for model fragile glass formers. We also find that the dynamically correlated regions are more ramified for the strong glass former than for model fragile glass formers. However, we do find that Stokes-Einstein violation indicates a change in the character of the dynamic heterogeneities for the strong glass former and the fragile glass formers.

<sup>1</sup>This research used the CSU ISTeC Cray HPC system supported by NSF Grant CNS-0923386. We gratefully acknowledge the support of NSF grant CHE 1213401.

**12:15PM S34.00006 Correlating structural and dynamic fragility in glass-forming liquids**<sup>1</sup>, DMITRY VOYLOV, Univ of Tennessee, Knoxville, PHILIP GRIFFIN, University of Pennsylvania, BRANDON MERCADO, Yale University, JONG KEUM, Oak Ridge National Laboratory, VLADIMIR NOVIKOV, ALEXEI SOKOLOV, Univ of Tennessee, Knoxville — The glass transition was attracting wide interest over the last several decades, but still remains the topic of intensive research and discussions. One of the most intriguing and well-known observations is a drastic change of dynamic properties with only slight variations of structure upon cooling down to the glass transition temperature  $T_g$ . This has led many to believe that the changes of dynamics during approach to  $T_g$  have no structural signatures which would be significant and common to different types of glass-forming liquids. Here we demonstrate analysis of temperature dependence of the main diffraction peak in a static structure factor of various glass-formers. We show that the relative changes of its width with temperature correlates with fragility of these materials. This observation was analyzed using Adam-Gibbs approach establishing a connection between the structural and dynamical properties of glass-forming materials.

<sup>1</sup>We acknowledge partial financial support from the Division of Materials Science and Engineering, U.S. Department of Energy, Office of Basic Energy Sciences

**12:27PM S34.00007 Aging and random-field magnetism in ferromagnet/antiferromagnet bilayers.**<sup>1</sup>, TIANYU MA, RYAN FREEMAN, XIANG CHENG, STEFAN BOETTCHER, SERGEI URAZHDIN, Emory University — Exchange interaction at the interface between a ferromagnet (F) and an antiferromagnet (AF) results in a random effective exchange field acting on both F and AF [1], which can produce complex equilibrium and dynamical states. We utilized anisotropic magnetoresistance to look for signatures of such states in epitaxial Py=Permalloy/Fe50Mn50 and polycrystalline CoO/Py bilayers. For thin AF layers, both systems exhibit slow cooperative aging indicative of a complex glassy state [2]. Aging follows the same small power-law or logarithmic dependence and is observed over a wide range of temperatures and fields, suggesting a universal aging mechanism. Glassy relaxation is not observed at any temperature for AF thickness above 3.5nm. We argue that these observations are inconsistent with the usual “granular” and “domain-state” models of F/AF systems. We discuss the implications of our results for the random field magnetism, and the relationship between the dimensionality and the topological properties of magnetic systems.

1. A.P. Malozemoff, Phys. Rev. B 35, 3679(R) (1987).
2. T.C. Proctor, D.A. Garanin, and E.M. Chudnovsky, Phys. Rev. Lett. 112, 097201 (2014).

<sup>1</sup>Supported by NSF DMR-1504449

**12:39PM S34.00008 Aging in the two-dimensional random-field systems**<sup>1</sup>, XIANG CHENG, TIANYU MA, SERGEI URAZHDIN, STEFAN BOETTCHER, Department of Physics, Emory University — Random fields introduced into the classical Ising and Heisenberg spin models can roughen the energy landscape, leading to complex nonequilibrium dynamics. The effects of random fields on magnetism have been previously studied in the context of dilute antiferromagnets (AF), impure substrates, and magnetic alloys [1]. We utilized random-field spin models to simulate the observed magnetic aging in thin-film ferromagnet/antiferromagnet (F/AF) bilayers. Our experiments show extremely slow cooperative relaxation over a wide range of temperatures and magnetic fields [2]. In our simulations, the experimental system is coarse-grained into a random field Ising model on a 2D square lattice. Monte Carlo simulations indicate that aging processes may be associated with the glassy evolution of the magnetic domain walls, due to the pinning by the random fields. The scaling of the simulated aging agrees well with experiments. Both are consistent with either a small power-law or logarithmic dependence on time. We further discuss the topological effects on aging due to the dimensional crossover from the Ising to the Heisenberg regime.

[1] T. Nattermann, Spin glasses and random fields, 12 (1997):277

[2] S. Urazhdin, arXiv:1503.08380 (2015)(arxiv.org/pdf/1503.08380.pdf)

<sup>1</sup>Supported through NSF grant DMR-1207431

**12:51PM S34.00009 Qualitative change in structural dynamics of some glass-forming systems**<sup>1</sup>, VLADIMIR NOVIKOV, ALEXEI SOKOLOV, Univ of Tennessee, Knoxville — Analysis of temperature dependence of structural relaxation time  $\tau(T)$  in supercooled liquids revealed a qualitatively distinct feature - a sharp, cusp-like maximum in the second derivative of  $\log \tau_\alpha(T)$  at some  $T_{max}$ . It suggests that the super-Arrhenius temperature dependence of  $\tau_\alpha(T)$  in glass-forming liquids eventually crosses over to an Arrhenius behavior at  $T < T_{max}$ , and there is no divergence of  $\tau_\alpha(T)$  at non-zero  $T$ .  $T_{max}$  can be above or below  $T_g$ , depending on sensitivity of  $\tau(T)$  to change in liquid's density quantified by the exponent  $\gamma$  in the scaling  $\tau_\alpha(T) \sim \exp(A/T\rho^{-\gamma})$ . These results might turn the discussion of the glass transition to the new avenue – the origin of the limiting activation energy for structural relaxation at low  $T$ .

<sup>1</sup>The authors acknowledge the support from the NSF Chemistry program (grant CHE-1213444).

**1:03PM S34.00010 Percolation Thresholds in Angular Grain media: Drude Directed Infiltration**, DONALD PRIOUR, Youngstown State University — Pores in many realistic systems are not well delineated channels, but are void spaces among grains impermeable to charge or fluid flow which comprise the medium. Sparse grain concentrations lead to permeable systems, while concentrations in excess of a critical density block bulk fluid flow. We calculate percolation thresholds in porous materials made up of randomly placed (and oriented) disks, tetrahedrons, and cubes. To determine if randomly generated finite system samples are permeable, we deploy virtual tracer particles which are scattered (e.g. specularly) by collisions with impenetrable angular grains. We hasten the rate of exploration (which would otherwise scale as  $n_{\text{coll}}^{1/2}$  where  $n_{\text{coll}}$  is the number of collisions with grains if the tracers followed linear trajectories) by considering the tracer particles to be charged in conjunction with a randomly directed uniform electric field. As in the Drude treatment, where a succession of many scattering events leads to a constant drift velocity, tracer displacements on average grow linearly in  $n_{\text{coll}}$ . By averaging over many disorder realizations for a variety of systems sizes, we calculate the percolation threshold and critical exponent which characterize the phase transition.

**1:15PM S34.00011 Influence of Hydrogen Bonding on the Kinetic Stability of Vapor Deposited Triazine Glasses**, AUDREY LAVENTURE, University of Montreal; University of Wisconsin-Madison, ANKIT GUJRAL, University of Wisconsin-Madison, OLIVIER LEBEL, Royal Military College of Canada, CHRISTIAN PELLERIN, University of Montreal, MARK D. EDIGER, University of Wisconsin-Madison — Physical vapor deposition (PVD) can produce glasses with enhanced kinetic stability, high density and anisotropy. However, the influence of hydrogen bonding on these properties has not been fully explored. We vapor deposit a series of triazine derivatives containing functional groups with different H-bonding capability, i.e. NHMe (H-bond donor), OMe (H-bond acceptor) and Et (none) using a wide range of substrate temperatures, from 0.60 to 1.05T<sub>g</sub>. PVD glasses of the NHMe derivative have inferior kinetic stability compared to its OMe and Et analogues. This behavior can be rationalized by the higher average number of bonded NH per molecule found in PVD glasses of the NHMe derivative, as quantified by infrared spectroscopy (IR). Despite this difference in H-bonding, IR and wide angle X-ray scattering reveal that all three compounds show a tendency to orient parallel to the substrate at low substrate temperatures. Our results support the hypothesis that strong intermolecular interactions, such as H-bonds, can hinder mobility of the molecules at the interface and thus limit their possibility to sample the potential energy landscape to produce stable glasses.

**1:27PM S34.00012 Thermal properties of composite materials: a complex systems approximation**<sup>1</sup>, J. L. CARRILLO, BEATRIZ BONILLA, J. J. REYES, Instituto de Física BUAP, VICTOR DOSSETTI, CIDS- BUAP — We propose an effective media approximation to describe the thermal diffusivity of composite samples made of polyester resin and magnetite inclusions. By means of photoacoustic spectroscopy, the thermal diffusivity of the samples were experimentally measured. The volume fraction of the inclusions was systematically varied in order to study the changes in the effective thermal diffusivity of the composites. For some samples, a static magnetic field was applied during the polymerization process, resulting in anisotropic inclusion distributions. Our results show a significant difference in the thermal properties of the anisotropic samples, compared to the isotropic randomly distributed. We correlate some measures of the complexity of the inclusion structure with the observed thermal response through a multifractal analysis. In this way, we are able to describe, and at some extent predict, the behavior of the thermal diffusivity in terms of the lacunarity and other measures of the complexity of these samples [1]. [1] F. Cervantes-Alvarez, J J Reyes-Salgado, V Dossetti, and J L Carrillo, J. Phys. D: Appl. Phys. 47 (2014) 235303; J. J. Reyes-Salgado, B. Bonilla, V. Dossetti, and J L Carrillo, J. Phys. D: Appl. Phys. 48, (2015)

<sup>1</sup>Partial Financial Support by CONACyT Mexico and VIEP-BUAP.

**1:39PM S34.00013 Preparing anisotropic glasses from structural analogs of liquid crystal formers by physical vapor deposition**, JARITZA GOMEZ, MARK EDIGER, University of Wisconsin - Madison — Physical vapor deposition (PVD) can be used to tune molecular orientation in glasses by depositing at substrate temperatures ( $T_{\text{substrates}}$ ) just below the glass transition temperature ( $T_g$ ). Glasses of a smectic A liquid crystal (LC) former, itraconazole, deposited at a  $T_{\text{substrate}} = T_g$  have been shown to inherit the structure of the equilibrium smectic liquid and orient nearly perpendicular to the substrate. Here we report the deposition of glasses prepared from molecules that are structural analogs to known LC formers: posaconazole and a functionalized perylenemonoimide (PMI), analogs to itraconazole and a previously reported columnar LC, respectively. Spectroscopic ellipsometry and infrared spectroscopy are used to characterize average molecular orientation in the as-deposited glasses. Surprisingly, we find that molecular orientation in glasses of posaconazole deposited at different  $T_{\text{substrates}}$  does not follow the previously observed trends for linear molecules without LC states, but more closely follows itraconazole. In addition, we find that glasses deposited at  $T_g$  are not isotropic, even though liquid-cooled glasses do not show preferential molecular orientation. Similarly, glasses from a functionalized PMI, structural analog to a known columnar LC, show molecular orientation at  $T_{\text{substrate}} = T_g$ . These results may provide insights into the mechanism by which physical vapor deposition can produce glasses with tunable molecular orientation.

**1:51PM S34.00014 Fragility of Ionic Liquids Measured by Flash Differential Scanning Calorimetry**, RAN TAO, NIST - Natl Inst of Stds & Tech, ESHAN GURUNG, EDWARD L. QUITEVIS, SINDEE L. SIMON, Texas Tech University — Ionic liquids are a class of materials that possess attractive properties. They generally have low rates of crystallization due to their bulky and asymmetrical ion structure, and are often considered as good glass-forming materials. In this work, a series of imidazolium-based ionic liquids with varying functionalities from aliphatic to aromatic groups and a fixed anion are characterized using fast scanning differential scanning calorimetry. The limiting fictive temperature  $T_f^*$ , which is equivalent to the glass transition temperature  $T_g$ , is measured on heating as a function of cooling rate using Flash differential scanning calorimetry. Different calculation methods are employed and compared for the determination of  $T_f^*$ . The dynamic fragility is obtained for the series of ionic liquids, and using this data along with a compilation of data from the literature reveals the relationship between molecular structure and fragility for ionic liquids.

**2:03PM S34.00015 Generating tunable structures in glassy materials: Smectic-like layering in glasses of a liquid crystal system prepared by vapor deposition**, ANKIT GUJRAL, JARITZA GOMEZ, JING JIANG, CHENGBIN HUANG, University of Wisconsin-Madison, KATHRYN O'HARA, University of California Santa Barbara, MICHAEL TONEY, Stanford Synchrotron Radiation Lightsource, MICHAEL CHABINYC, University of California Santa Barbara, LIAN YU, MARK EDIGER, University of Wisconsin-Madison — Anisotropic packing, particularly in highly ordered liquid crystalline configurations, has been shown to be useful in organic electronic and optoelectronic applications. In this work, vapor deposited glasses of a model smectic liquid crystal-forming molecule, itraconazole, are investigated. The films are characterized using x-ray scattering, FTIR and spectroscopic ellipsometry, and are found to exhibit unprecedented structural and optical anisotropy for a macroscopically homogeneous solid. A smectic-like layered structure is observed in the glasses that are prepared by depositing the glass at a substrate temperature during deposition ( $T_{\text{sub}}$ ) maintained below the glass transition temperature,  $T_g$ , of the molecule. The layer spacing, and the associated average tilt angle of the molecules, is found to be tunable as a function of  $T_{\text{sub}}$ . The layer spacing reduces by 16% as  $T_{\text{sub}}$  is lowered. These features are retained in the films when heated to at least  $T_g$  of the molecule.

**Thursday, March 17, 2016 11:15AM - 1:51PM —**

**Session S35 DBIO GSOF GSNP: Active Matter: Collective Phenomena in Living Systems IV**

338 - Steve Presse, Indiana University-Purdue University Indianapolis

**11:15AM S35.00001 Fluid flows created by swimming bacteria drive self-organization in confined suspensions**, ENKELEIDA LUSHI, Brown University, HUGO WIOLAND, Institut Jacques Monod, Paris 7 Diderot, RAYMOND GOLDSTEIN, DAMTP, University of Cambridge — Concentrated suspensions of micro-swimmers can display intricate self-organized spatiotemporal patterns on scales larger than those of the individual motile units. The collective dynamics of swimming microorganisms exhibits a complex interplay with the surrounding fluid: the motile cells stir the fluid, which in turn can reorient and advect them. This feedback loop can result in long-range interactions between the cells. We present a computational model that takes into account these cell-fluid interactions and cell-cell forces and that predicts counterintuitive cellular order driven by long-range flows. The predictions are confirmed by new experiments with *Bacillus Subtilis* bacteria. Simulations and experiments show that if the micro-swimmers are confined inside thin cylindrical chambers the suspension self-organizes into a stable swirling vortex. If the micro-swimmers are confined in thin racetracks, a persistent unidirectional stream can emerge. Both these phenomena emerge as a result of the complex interplay between the swimmers, the specific confining boundaries and the fluid flow.

**11:27AM S35.00002 Fluid flow in monolayers: Cells under pressure**, KYLE SCHULZE, STEVEN ZEHNDER, GREG SAWYER, THOMAS ANGELINI, University of Florida — Number density fluctuations are intimately tied to collective behavior in particulate soft matter and active matter systems, including tissue cell monolayers. In cell monolayers, there is no free space between cells, so density fluctuations must involve either out of plane motion, or cell volume fluctuations. Recent work has shown that cells fluctuate in volume to accommodate collective density fluctuations, and that fluid moves between cells in this process. However, measurements of the resistance to this flow with controlled applied pressures have never been performed. Here we apply pressure to local regions in cell monolayers with an indentation instrument mounted on an inverted microscope. While simultaneously measuring contact area, indentation depth, and applied force as a function of time we determine a compression modulus and a permeability of cells. We find that cells are highly permeable, and that cytoskeleton-generated stresses are large enough to drive fluid from cell to cell as they spontaneously fluctuate in volume.

**11:39AM S35.00003 Hydrodynamic interactions and their role on the dynamics of bacterial predators.**<sup>1</sup>, HOSSEIN JASHNSAZ, Physics Department, IUPUI, Indianapolis, IN 46202, MOHAMMED AL JUBOORI, Biomedical Engineering, IUPUI, Indianapolis, IN 46202, COREY WEISTUCH, Department of Applied Mathematics and Statistics, Stony Brook University, Stony Brook, NY 11794, TYLER NGUYEN, Stark Neurosciences Research Institute, IUSM, Indianapolis, IN 46202, NICK MILLER, Biomedical Engineering, IUPUI, Indianapolis, IN 46202, VIKTORIA MEYERHOFF, Mechanical Engineering, IUPUI, Indianapolis, IN 46202, KYLE PROCTOR, BRYAN MCCOY, Biological Chemistry, IUPUI, Indianapolis, IN 46202, STEPHANIE PERKINS, GREGORY ANDERSON, Biology Department, IUPUI, Indianapolis, IN 46202, STEVE PRESSE, Physics Department, IUPUI, Indianapolis, IN 46202 — We consider the effects of hydrodynamics on the behavior of bacterial predators searching for bacterial prey. Experimentally, we find that bacterial predators respond to external flow fields in addition to responding to their own self-generated flow fields neighboring surfaces and finite boundaries. We will discuss the implications of this finding on bacterial hunting strategies.

<sup>1</sup>SP acknowledges the NSF (MCB 1412259) and a Graduate Student Imaging Research Fellowship from the IUPUI Office of the Vice Chancellor for Research.

**11:51AM S35.00004 Non-homogeneous flow profiles in sheared bacterial suspensions**, DEVRANJAN SAMANTA<sup>1</sup>, XIANG CHENG<sup>2</sup>, Univ of Minn - Minneapolis — Bacterial suspensions under shear exhibit interesting rheological behaviors including the remarkable superfluidic state with vanishing viscosity at low shear rates. Theoretical studies have shown that such superfluidic state is linked with non-homogeneous shear flows, which are induced by coupling between nematic order of active fluids and hydrodynamics of shear flows. However, although bulk rheology of bacterial suspensions has been experimentally studied, shear profiles within bacterial suspensions have not been explored so far. Here, we experimentally investigate the flow behaviors of *E. coli* suspensions under planar oscillatory shear. Using confocal microscopy and PIV, we measure velocity profiles across gap between two shear plates. We find that with increasing shear rates, high-concentration bacterial suspensions exhibit an array of non-homogeneous flow behaviors like yield-stress flows and shear banding. We show that these non-homogeneous flows are due to collective motion of bacterial suspensions. The phase diagram of sheared bacterial suspensions is systematically mapped as functions of shear rates and bacterial concentrations. Our experiments provide new insights into rheology of bacterial suspensions and shed light on shear induced dynamics of active fluids.

<sup>1</sup>Chemical Engineering and Material Science department

<sup>2</sup>Chemical Engineering and Material Science department

**12:03PM S35.00005 Discontinuous fluidization transition in dense suspensions of actively deforming particles**, ELSÉN TJHUNG, Univ of Cambridge, LUDOVIC BERTHIER, CNRS, Université Montpellier — Collective dynamics of self-propelled particles at high density have been shown to display a glass-like transition with a critical slowing down of 2 to 4 orders of magnitude. In this talk, we propose a new mechanism of injecting energy or activity via volume fluctuations. We show that the behaviour of actively deforming particles is strikingly different from that of self-propelled particles. In particular, we find a discontinuous non-equilibrium phase transition from a flowing state to an arrested state. Our minimal model might also explain the collective dynamics in epithelial tissues. In particular, without needing self-propulsion or cell-cell adhesion, volume fluctuations of individual cells alone might be sufficient to give rise to an active fluidization and collective dynamics in densely packed tissues.

**12:15PM S35.00006 Superfluid-like dynamics in active vortex fluids**, JONASZ SLOMKA, JORN DUNKEL, Massachusetts Inst of Tech-MIT — Active biological fluids exhibit rich non-equilibrium dynamics and share striking similarities with quantum fluids, from vortex formation and magnetic ordering to superfluid-like behavior. Building on universality ideas, we have recently proposed a generalization of the Navier–Stokes equations that captures qualitatively the active bulk flow structures observed in bacterial suspensions. Here, we present new numerical simulations that explicitly account for boundary and shear effects. The theory successfully reproduces recent experimental observations of bacterial suspensions, including a superfluid-like regime of nearly vanishing shear viscosity. Our simulations further predict a geometry-induced ‘quantization’ of viscosity and the existence of excited states capable of performing mechanical work. It is plausible that these results generalize to a broad class of fluids that are subject to an active scale selection mechanism.

**12:27PM S35.00007 Swarming in viscous fluids: three-dimensional patterns in swimmer- and force-induced flows**<sup>1</sup>, YAO-LI CHUANG, MARIA R. D'ORSOGNA, Dept. of Mathematics, CSUN & Dept. of Biomathematics, UCLA, TOM CHOU, Dept. of Biomathematics UCLA & Dept. of Mathematics, UCLA — Mathematical models of self-propelled interacting particles have reproduced various fascinating “swarming” patterns observed in natural and artificial systems. The formulation of such models usually ignores the influence of the surrounding medium in which the particles swarm. Here we develop from first principles a three-dimensional theory of swarming particles in a viscous fluid environment and investigate how the hydrodynamic coupling among the particles may affect their collective behavior. Specifically, we examine the hydrodynamic coupling among self-propelled particles interacting through “social” or “mechanical” forces. We discover that new patterns arise as a consequence of different interactions and self-propulsion mechanisms. Examples include flocks with prolate or oblate shapes, intermittent mills, recirculating peloton-like structures, and jet-like fluid flows that kinetically destabilize mill-like structures. Our results reveal possible mechanisms for three-dimensional swarms to kinetically control their collective behaviors in fluids.

<sup>1</sup>Supported by NSF DMS 1021818 & 1021850, ARO W1911NF-14-1-0472, ARO MURI W1911NF-11-10332

### 12:39PM S35.00008 Numerical study of the hydrodynamic interactions in an *E. coli* suspension

XINLIANG XU, LIPENG LAI, Beijing Computational Science Research Center, YI PENG, XIANG CHENG, Department of Chemical Engineering and Materials Science, University of Minnesota — The active suspension of *E. coli* displays many interesting non-equilibrium phenomena, e.g. “swarming” at high bacteria concentrations, and viscosity change under simple shear. To understand the microscopic mechanism underlying these phenomena requires detailed knowledge about the hydrodynamics within the suspension. Here we numerically study in detail the hydrodynamic interactions between a bacterium and an ellipsoid tracer at small separations, where the tracer can no longer be treated as a point-like particle that creates no disturbance to local flow field. We observed a significant drop in bacterium swimming velocity, in agreement with previous experimental study.

### 12:51PM S35.00009 Anomalous diffusion of an ellipsoid in quasi-2D active fluids<sup>1</sup>, YI PENG, OU

YANG, CHAO TANG, XIANG CHENG, Department of Chemical Engineering and Materials Science, University of Minnesota — Enhanced diffusion of a tracer particle is a unique feature in active fluids. Here, we studied the diffusion of an ellipsoid in a free-standing film of *E. coli*. Particle diffusion is linearly enhanced at low bacterial concentrations, whereas a non-linear enhancement is observed at high bacterial concentrations due to the giant fluctuation. More importantly, we uncover an anomalous coupling between the translational and rotational degrees of freedom that is strictly prohibited in the classical Brownian diffusion. Combining experiments with theoretical modeling, we show that such an anomaly arises from the stretching flow induced by the force dipole of swimming bacteria. Our work illustrates a novel universal feature of active matter and transforms the understanding of fundamental transport processes in microbiological systems.

<sup>1</sup>ACS Petroleum Research Fund 54168-DNI9, NSF Faculty Early Career Development Program, DMR-1452180

### 1:03PM S35.00010 Non-monotonic size-dependent particle diffusion in active fluids<sup>1</sup>, ALISON

PATTESON, Univ of Pennsylvania, ARVIND GOPINATH, University of California, Merced, PAULO ARRATIA, University of Pennsylvania — We experimentally investigate the effect of particle size on the motion of passive polystyrene spheres in suspensions of *Escherichia coli*. Using particles covering a range of sizes from 0.6 to 39 microns, we probe particle dynamics at both short and long time scales. In all cases, the particles exhibit super-diffusive ballistic behavior at short times before eventually transitioning to diffusive behavior. Surprisingly, the long-time hydrodynamic effective diffusivity exhibits a peak in particle size; an anomalous response that is fundamentally different from classical thermal diffusion. Consistent with recent theory, we find that the active contribution to particle diffusion is controlled by a dimensionless parameter, the Peclet number. We propose a minimal model that allows us to predict the requirements for a peak in the diffusivity as well as the magnitude of the peak as a function of particle size and bacterial concentration. Our results have broad implications on characterizing active fluids using concepts drawn from classical thermodynamics.

<sup>1</sup>NSF-DMR-1104705 and NSF-CBET-1437482

### 1:15PM S35.00011 Hydrodynamics of spinning bacteria at a surface, RACHEL BENNETT, Univ of Pennsylvania,

RAMIN GOLESTANIAN, University of Oxford — Bacteria tethered to a surface by their flagellum show a variety of different spinning behaviors, including different angles made with the surface and rotation velocities. We have developed a hydrodynamic model to show that the different behaviors arise from several factors including the degree of flagellar constraint, the shape of the bacterium, the flexibility of the flagellar hook and the motor torque. Our minimal model produces the wide variety of behaviors observed in experiments and successfully predicts the detachment angle for bacteria with three different body curvatures.

### 1:27PM S35.00012 Mobile wedges in an active turbulent bath, ANDREAS KAISER, ANDREY SOKOLOV, Argonne

Natl Lab, HARTMUT LOWEN, Heinrich-Heine Universität Düsseldorf, IGOR S. ARONSON, Argonne Natl Lab — The motion of micro-wedges in a turbulent bacterial bath is explored using computer simulations with explicit modeling of the bacteria and experiments. We demonstrate that collective turbulentlike motion in a bacterial bath can power and steer the directed transport of mesoscopic carriers through the suspension. We will show that both polar ordering and swirl shielding inside the wedge yield an optimal transport velocity. Finally, we show the behavior of several wedges exposed to a bacterial bath.

### 1:39PM S35.00013 Entrainment dominates the interaction of microalgae with micron-sized objects, RAPHAEL JEANNERET, VASILY KANTSLER, MARCO POLIN, University of Warwick —

Swimming microorganisms usually navigate through fluids containing a variety of microparticles, with which they inevitably interact with important biological and ecological implications. Regarding the prokaryotic realm, it has been shown that the colloidal dynamics within bacterial suspensions is well described by a persistent random walk. As to the other major class of microorganisms, the eukaryotes, much less is known. By directly tracking polystyrene colloids in baths of the model puller-type alga *Chlamydomonas reinhardtii*, a pioneering work [1] has shown that they still behave diffusively asymptotically with diffusivities linearly increasing with the concentration. The values reported as well as the distribution of displacements having exponential tails are well explained theoretically when considering the hydrodynamic far-field contribution of the algae. However nothing has yet been described regarding the short range interactions that inevitably exist. In this work we show, by means of 3 different experiments, that the coarse-grained dynamics of the colloids is in fact dominated by very rare but large jumps due to entrainment by the algae leading to a total effective diffusion an order of magnitude higher than previously reported. [1] Leptos et al, PRL 103, 198103 (2009).

## Thursday, March 17, 2016 11:15AM - 2:15PM –

Session S36 GSOF: Soft Matter at Interfaces: Wetting and Thin Films 339 - Justin Burton, Emory University

### 11:15AM S36.00001 Quantifying stick-slip contact line motion of evaporating sessile droplets,

CLAY WOOD, JUSTIN PYE, JUSTIN BURTON, Department of Physics, Emory University — Sessile droplet evaporation often involves an apparent stick-slip motion of pinning and de-pinning of the drop's edge. The small forces and complex hydrodynamics at the contact line make this phenomena difficult to quantify, although easily observable. We have characterized the stick-slip motion on gold and glass surfaces with the use of a quartz crystal microbalance (QCM). We observe changes in both the resonant frequency and dissipation during droplet evaporation. Depositing a droplet onto this oscillating surface greatly decreases the frequency while the dissipation increases. Evaporation occurs in two stages; when the droplet's contact line is pinned to the surface, its contact angle decreases. Then, at a critical angle, the contact line is pulled over pinning points and continues to evaporate with a receding contact area. These stick-slip events appear in our data as a sharp increase in frequency, followed by a sharp decrease; simultaneously, the dissipation displays a single sharp peak. QCMs pre-cleaned in an oxygen plasma environment exhibited a significantly reduced occurrence and magnitude of these features. We interpret these features and quantify the forces involved in the stick-slip motion using a dynamic model of the QCM with additional surface forces at the contact line.

### **11:27AM S36.00002 High-precision measurements of molecular slip at a solid/liquid interface**

, JUSTIN PYE, CLAY WOOD, JUSTIN BURTON, Department of Physics, Emory University — As fluidic devices get smaller and measurements become more precise and stringent, the need to fully understand the dynamics at interfaces becomes more important. It is now clear that slip near an interface is common at the nanoscale in Newtonian liquids. In simple systems, there is a general trend to larger slip lengths for non-wetting liquid/solid combinations, but many conflicting measurements and interpretations remain. We have developed a novel differential technique using a quartz crystal microbalance (QCM) to measure slip lengths on various substrates. A drop of one liquid is grown on the QCM in the presence of a second, ambient liquid. By choosing the two liquids such that their bulk effects on the QCM frequency and dissipation are identical in the presence of no-slip, we are able to isolate anomalous boundary effects due to interfacial slip. Our data for water on gold (in undecane) are consistent with a slip length of 5nm (for water). A glass surface, wetted by both gold and undecane has also shown strongly anomalous results for the water-undecane pair. In addition to investigating other liquid pairs, future work will include extending this technique to surfaces with independently controllable chemistry and roughness, both of which are known to strongly affect interfacial hydrodynamics.

### **11:39AM S36.00003 Asymmetric and speed-dependent contact angle hysteresis and relaxation of a suddenly stopped moving contact line<sup>1</sup>**

, DONGSHI GUAN, YONG JIAN WANG, Hong Kong University of Science and Technology, ELISABETH CHARLAIX, Université Grenoble Alpes , PENG ER TONG, Hong Kong University of Science and Technology — We report direct atomic-force-microscope measurements of capillary force hysteresis and relaxation of a circular moving contact line (CL) formed on a long micron-sized hydrophobic fiber intersecting a water-air interface. The measured capillary force hysteresis and CL relaxation show a strong asymmetric speed dependence in the advancing and receding directions. A unified model based on force-assisted barrier-crossing is utilized to find the underlying energy barrier  $E_b$  and size  $\lambda$  associated with the defects on the fiber surface. The experiment demonstrates that the pinning (relaxation) and depinning dynamics of the CL can be described by a common microscopic frame-work, and the advancing and receding CLs are influenced by two different sets of relatively wetting and non-wetting defects on the fiber surface.

<sup>1</sup>Work supported in part by the Research Grants Council of Hong Kong SAR.

### **11:51AM S36.00004 Visualizing the shape of soft solid and fluid contacts between two surfaces**

, JONATHAN PHAM, FRANK SCHELLENBERGER, MICHAEL KAPPL, DORIS VOLLMER, HANS-JÜRGEN BUTT, Max Planck Institute for Polymer Research — The soft contact between two surfaces is fundamentally interesting for soft materials and fluid mechanics and relevant for friction and wear. The deformation of soft solid interfaces has received much interest because it interestingly reveals similarities to fluid wetting. We present an experimental route towards visualizing the three-dimensional contact geometry of either liquid-solid (i.e., oil and glass) or solid-solid (i.e., elastomer and glass) interfaces using a home-built combination of confocal microscopy and atomic force microscopy. We monitor the shape of a fluid capillary bridge and the depth of indentation in 3D while simultaneously measuring the force. In agreement with theoretical predictions, the height of the capillary bridge depends on the interfacial tensions. By using a slowly evaporating solvent, we quantify the temporal evolution of the capillary bridge and visualized the influence of pinning points on its shape. The position dependence of the advancing and receding contact angle along the three-phase contact line, particle-liquid-air, is resolved. Extending our system, we explore the contact deformation of soft solids where elasticity, in addition to surface tension, becomes an important factor.

**12:03PM S36.00005 Imbibition kinetics of spherical aggregates** , PASCAL HBRAUD, IPCMS/CNRS, DIDIER LOOTENS, SIKA, ALBAN DEBACKER, IPCMS/CNRS — The imbibition kinetics of a millimeter-sized aggregate of 300 nm diameter colloidal particles by a wetting pure solvent is studied. Three successive regimes are observed : in the first one, the imbibition proceeds by compressing the air inside the aggregate. Then, the solvent stops when the pressure of the compressed air is equal to the Laplace pressure at the meniscus of the wetting solvent in the porous aggregate. The interface is pinned and the aggregate slowly degases, up to a point where the pressure of the entrapped air stops decreasing and is controlled by the Laplace pressure of small bubbles. Depending on the curvature of the bubble, the system may then be in an unstable state. The imbibition then starts again, but with an inner pressure in equilibrium with these bubbles. This last stage leads to the complete infiltration of the aggregate.

**12:15PM S36.00006 Tracking single particles motion in shaken wet powder clusters** , JENNIFER WENZL, National Superconducting Cyclotron Laboratory, MSU, GUENTER K. AUERNHAMMER, LAURENT GILSON, Max-Planck Institute for Polymer Research, Mainz — In many industrial branches wet granulate powders, where the particles are connected via an additional binding liquid, are widely used. Ample investigated were model systems, where the binding liquid is homogeneously distributed, i.e. building a connecting capillary network. In contrast wet granulate model systems with an inhomogeneous liquid distribution have been rarely in focus of research. In this work a model system for wet powders was developed, which is suitable for 3D imaging with confocal microscopy. Fluorescent silica particles were immersed in a mixture of two immiscible liquids, one continuous and one binding liquid. In detail a wet powder cluster, where the binding liquid formed droplets was studied in 3D. During applying a mechanical load the motion of the powder particles and the binding liquid droplets was followed. Deformation of the binding liquid droplets led to an increase of its surface area and energy. When the droplet relaxed to an energetically more favored shape upon further cluster deformation, the sudden release of the stored surface energy led to complex powder particle and droplet motions. The model system illustrated the complex dynamics upon shaking, and showed that the binding liquid dominated the cluster dynamics on a local scale.

**12:27PM S36.00007 Force vs. extension of colloidal membranes<sup>1</sup>** , LEROY JIA, ROBERT PELCOVITS, THOMAS POWERS, Brown University, MARK ZAKHARY, ZVONIMIR DOGIC, Brandeis University — In experiments, disk-shaped colloidal membranes composed of long rod-like viruses will take on a twisted ribbon shape under the application of a diametric stretching force. We use an effective model valid for membranes with small twist penetration to study this phase transition and calculate the force necessary to stretch the membrane to a given extension. The model predicts that for small deformations, the force is linear with spring constant depending on the effective edge bending stiffness of the membrane, while for large extensions, the force is found to saturate to a constant value. Surprisingly, the force is not a monotonic function of the extension. Finally, we use simple numerical calculations to find a power law that accurately describes the critical stretch at which the membrane starts to twist, which may be used to estimate the value of unknown parameters by comparison with experimental data.

<sup>1</sup>We are grateful for support from the Brandeis Center for Bioinspired Soft Materials, NSFMRSEC, DMR-1420382.

### **12:39PM S36.00008 Thermal-mechanical behavior of self-assembled nanoparticle membranes**

, YIFAN WANG, SEAN MCBRIDE, University of Chicago, XIAO-MIN LIN, Argonne National Laboratory, HEINRICH JÄGER, University of Chicago — Monolayers composed of colloidal nanoparticles with a thickness of less than ten nanometers have remarkable mechanical strength and can suspend over micron-sized holes to form free-standing membranes. However, previous measurements on mechanical properties of these monolayers were typically carried out at room temperature. Here, we report the first systematic experimental study of the stiffness of free-standing nanoparticle membranes as a function of temperature. At room temperature and below, these membranes exhibit reversible changes in stiffness, which increases with temperature. At higher temperatures irreversible membrane relaxation was found. This work provides a better understanding of the sub-nanometer scale ligand interactions in self-assembled nanoparticle membranes, and opens up opportunities for using these membranes as thermal-mechanical devices.

**12:51PM S36.00009 Direct observation of critical adsorption on colloidal particles**, HONGYU GUO, ZHIYUAN WANG, C. E. BERTRAND, NIST - Natl Inst of Stds & Tech, PAUL DOUGLAS GODFRIN, University of Delaware, YUN LIU, NIST - Natl Inst of Stds & Tech — We report our direct measurements of critical adsorption on the surface of small spherical silica particles suspended in a binary mixture of lutidine and water, using small-angle neutron scattering (SANS). The surface concentration profile and excess adsorption are studied as functions of temperature, lutidine concentrations, and surface curvature. The profile shape agree with scaling laws. The adsorption associated with the profile shape is found to increase monotonically with increasing lutidine concentration and to decrease with increasing temperature. These observations are important to understand colloidal aggregation behaviors close to the critical point of a binary solvent.

**1:03PM S36.00010 Obtaining self-similar scalings in focusing flows**, JOSHUA DIJKSMAN, Wageningen University, SHOMEK MUKHOPADHYAY, Yale University, CAMERON GAEBLER, Harvey Mudd College, THOMAS WITELSKI, ROBERT BEHRINGER, Duke University — The surface structure of converging thin fluid films displays self-similar behavior, as was shown in the work by Diez et al [Q. Appl. Math 210, 155, 1990]. Extracting the related similarity scaling exponents from either numerical or experimental data is non-trivial. Here we provide two such methods. We apply them to experimental and numerical data on converging fluid films driven by both surface tension and gravitational forcing. In the limit of pure gravitational driving, we recover Diez' semi-analytic result, but our methods also allow us to explore the entire regime of mixed capillary and gravitational driving, up to entirely surface tension driven flows. We find scaling forms of smoothly varying exponents up to surprisingly small Bond numbers. Our experimental results are in reasonable agreement with our numerical simulations, which confirm theoretically obtained relations between the scaling exponents.

**1:15PM S36.00011 Visualizing Nanoscopic Topography and Patterns in Freely Standing Thin Films**, VIVEK SHARMA, YIRAN ZHANG, SUBINUR YILIXIATI, Chemical Engineering, University of Illinois at Chicago — Thin liquid films containing micelles, nanoparticles, polyelectrolyte-surfactant complexes and smectic liquid crystals undergo thinning in a discontinuous, step-wise fashion. The discontinuous jumps in thickness are often characterized by quantifying changes in the intensity of reflected monochromatic light, modulated by thin film interference from a region of interest. Stratifying thin films exhibit a mosaic pattern in reflected white light microscopy, attributed to the coexistence of domains with various thicknesses, separated by steps. Using Interferometry Digital Imaging Optical Microscopy (IDIOM) protocols developed in the course of this study, we spatially resolve for the first time, the landscape of stratifying freely standing thin films. We distinguish nanoscopic rims, mesas and craters, and follow their emergence and growth. In particular, for thin films containing micelles of sodium dodecyl sulfate (SDS), these topological features involve discontinuous, thickness transitions with concentration-dependent steps of 5-25 nm. These non-flat features result from oscillatory, periodic, supramolecular structural forces that arise in confined fluids, and arise due to complex coupling of hydrodynamic and thermodynamic effects at the nanoscale.

**1:27PM S36.00012 Out-of-contact elastohydrodynamic deformation due to lubrication forces.**<sup>1</sup>, YUMO WANG, CHARLES DHONG, JOELLE FRECHETTE, Johns Hopkins University — We characterize the spatiotemporal deformation of an elastic film during the radial drainage of fluid from a narrowing gap. Elastic deformation of the film takes the form of a dimple and prevents full contact to be reached. With thinner elastic film the stress becomes increasingly supported by the underlying rigid substrate, the dimple formation is suppressed, which allows the surfaces to reach full contact. We highlight the lag due to viscoelasticity on the surface profiles, and that for a given fluid film thickness deformation leads to stronger hydrodynamic forces than for rigid surfaces.

<sup>1</sup>This work is partially supported by the Office of Naval Research Young Investigator Award (N000141110629), by the Hopkins Extreme Materials Institute (HEMI), and NSF-CMMI 1538003.

**1:39PM S36.00013 Approaching a flat boundary with a block copolymer coated emulsion drop: late stage drainage dynamics.**, DAMITH ROZAIRO, ANDREW CROLL, North Dakota State Univ — Understanding the dynamics of the formation and drainage of the thin fluid film that becomes trapped by a deformable droplet as it approaches another object is crucial to the advancement of many industrial and biomedical applications. Adding amphiphilic diblock copolymers, which are becoming more commonly used in drug delivery and oil recovery, only add to the complexity. Despite their increased use, little is known about how long polymer chains fill an emulsion drops interface or how the molecules influence hydrodynamic processes. We study the drainage dynamics of a thin water film trapped between mica and a diblock copolymer saturated oil droplet. Specifically, we examine several different polystyrene-b-poly(ethylene oxide) (PS-PEO) molecules self-assembled at a toluene-water interface using laser scanning confocal microscopy. Our experiments reveal that the molecular details of the polymer chains deeply influence the drainage times, indicating that they are not acting as a simple surfactant. The presence of the chains creates a much slower dynamic as fluid is forced to drain through an effective polymer brush, the brush itself determined by chain packing at the interface. We present a simple model which accounts for the basic physics of the interface.

**1:51PM S36.00014 Soft Levelling: Capillary Relaxation of a Thin Liquid Film on an Elastic Substrate**, MARCO RIVETTI, CHRISTINE LINNE, Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany, THOMAS SALEZ, MAXENCE ARUTKIN, ELIE RAPHAEL, UMR 7083 Gulliver, ESPCI and CNRS, PSL Research University, Paris, France, OLIVER BAEUMCHEN, Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany — A thin liquid film with non-zero curvature at its free surface spontaneously relaxes towards a flat configuration. The flow of this liquid film is driven by Laplace pressure gradients and it is resisted by viscosity. In the last few years the dynamics of this system has been studied experimentally, numerically and analytically. Inspired by recent progresses on the wetting behaviour of liquid droplets on soft substrates, we here consider the relaxation of a thin viscous film supported by an elastic foundation. We present experiments involving thin polystyrene films on polydimethylsiloxane substrates, where the dynamics of the liquid-air interface is monitored using an atomic force microscope. In this system, Laplace pressure gradients not only drive the flow but they also induce elastic deformations on the substrate. These deformations affect the flow and the shape of the liquid-air interface itself, giving rise to an original example of elasto-capillary interaction that is not mediated by the presence of a contact line. We show that the width of the profile scales with the time to the power 1/6, rather than 1/4 which has been observed on rigid substrates. A theoretical model that describes the coupled evolution of the elastic-liquid and liquid-air interfaces is also presented.

**2:03PM S36.00015 Slowing of Dynamics of Hydration Water Depends on Length Scale of Measurement**, JONATHAN NICKELS, Oak Ridge National Laboratory, JOHN ATKINSON, University of Guelph, SOULEYMANE DIALLO, STEFANIA PERTICAROLI, JOHN KATSARAS, Oak Ridge National Laboratory, JOHN DUTCHER, University of Guelph — The dynamics of hydration water associated with biomolecules is often slower than in bulk. We have used quasielastic neutron scattering (QENS) to study the dynamics of hydration water associated with soft colloidal, monodisperse phytylglycogen nanoparticles. The large water content of the phytylglycogen nanoparticles makes this an ideal system for investigations of hydration water in hydrophilic environments. We find that the hydration water translation is sub-diffusive, occurring, on average,  $\sim 5.8$  times slower than that of bulk water. Significantly, these data demonstrate a clear  $q$ -dependence in the measured retardation factor, implying a corresponding length scale dependence. This observation may help to reconcile the often-conflicting range of hydration water retardation factors reported in the literature using different experimental techniques.

**Thursday, March 17, 2016 11:15AM - 2:15PM —**

**Session S37 GSOF: Liquid Crystals, Membranes, Micelles and Vesicles** 340 - L J Martinez-Miranda, University of Maryland, College Park

**11:15AM S37.00001 Tetratic, triatic and nematic liquid crystals on a complex plane<sup>1</sup>**, OKSANA MANYUHINA, MARK BOWICK, Syracuse University — Liquid crystals are elastic materials able to resolve geometric and topological frustration by creating disclinations, discontinuities in their continuous orientation field. The strength and the nature of disclinations depend on the symmetry of elements forming liquid crystal phase. Several examples of confined nematic (director field), triatic (Y-field) and tetratic (cross-field) liquid crystals will be considered to show that their ground state contains topological defects. Next, we analyze shape variation of the boundary, enclosing different defect textures. We argue that topological defects can capture essential features of macroscopic shape and relate it to microscopic order, providing a natural way to connect different length scales and to account for large deformations in soft and biological systems.

<sup>1</sup>Soft Matter Program of Syracuse University

**11:27AM S37.00002 Nano-electromechanical Rotation of Graphene and Giant Enhancement in Dielectric Anisotropy in a Liquid Crystal**, RAJRATAN BASU, DANIEL KINNAMON, ALFRED GARVEY, US Naval Academy — A nematic liquid crystal (LC) is doped with dilute concentrations of pristine monolayer graphene flakes (GP), and the LC+GP hybrids are found to exhibit a dramatic increase in the dielectric anisotropy. Electric field-dependent conductance studies reveal that the graphene flakes follow the nematic director that mechanically rotates on increasing an applied electric field. Further studies show that the  $\pi-\pi$  electron stacking, between the graphene's honeycomb structure and the LC's benzene rings, stabilizes *pseudo-nematic domains* that collectively amplify the dielectric anisotropy by improving the orientational order parameter in the nematic phase. These anisotropic domains interact with the external electric field, resulting in a *nonzero* dielectric anisotropy in the isotropic phase as well. The enhancement in dielectric anisotropy, due to the LC – graphene coupling, is found to have subsequent positive impacts on the LC's orientational threshold field and elasticity that allows the nematic director to respond quicker on switching the electric field off.

**11:39AM S37.00003 Smectic Liquid Crystal-Nanoparticle arrangement observed with X-ray Scattering<sup>1</sup>**, LUZ J MARTINEZ-MIRANDA, University of Maryland, College Park, MD, PATRICIO ROMERO-HASLER, ARIEL MENESES-FRANCO, EDUARDO A. SOTO-BUSTAMANTE, Universidad de Chile, Santiago, Chile — We observed the alignment of two different monomeric liquid crystals combined with TiO<sub>2</sub> in a concentration of 0.3 wt of TiO<sub>2</sub>. The liquid crystals are M6R8 and I6R8. These two monomeric compounds have a crystal-SmC-SmA-isotropic phase progression. The two monomeric compounds differ in the final group at the end of one of the carbon chains. The nanoparticle ties itself to the monomers through hydrogen bonding. The difference in the final group determines where the nanoparticle attaches to the liquid crystal molecule. This difference in the way it attaches can be observed using X-ray scattering. The way the nanoparticle attaches has consequences in the current-voltage curve obtained [1]. Under the influence of an electric field, the M6R8 polymerizes. We observe by X-ray scattering that the nanoparticles migrate and the scan is very similar to the scan of the I6R8 monomer with the nanoparticle. In addition the nanoparticle is ordered along one direction and does not seem as ordered in the direction perpendicular to this direction. [1] A. Meneses-Franco, J. Mater. Chem. C, 2015, 3, 8566.

<sup>1</sup>This work supported by grant NSF- OISE-1157589 in the USA and grant Fondecyt 1130187 in Chile

**11:51AM S37.00004 Organized composites of Carbon Nanotubes and Lyotropic Liquid Crystals at very low Surfactant Concentration**, GIUSY SCALIA, University of Luxembourg, Physics & Materials Science Research Unit, HYERAN JO, Seoul National University, Graduate School of Convergence Science & Technology, JI HYUN PARK, JAN LAGERWALL, University of Luxembourg, Physics & Materials Science Research Unit — The difficulties in dispersing and organizing carbon nanotubes (CNTs) can be efficiently tackled using surfactant-based lyotropic liquid crystals, combining high nanotube loading with long-range order. A problem with surfactants is, however, that their residues negatively affect CNT device performance. Here we show aligned CNT-lyotropic composites at reduced surfactant concentration. By combining cat- and anionic surfactants a lyotropic nematic phase forms at just 8% surfactant concentration, and CNTs can be well dispersed and aligned in it [1]. The CNTs themselves were first dispersed below the Krafft temperature of the surfactant used for their stabilization, minimizing also its concentration [2]. The composites exhibit very interesting properties with strong sensitivity to the surfactant ratios. They were investigated by Polarized Optical Microscopy and Polarized Raman spectroscopy, and also the electrical properties were studied. [1] G. Scalia, C. J. von Buehler, C. Haegeler, S. Roth, F. Giesselmann, J. P. F. Lagerwall. Soft Matter, 4, 570, 2008. [2] S. Dölle, B.-D. Lechner, J. H. Park, S. Schymura, J. P. F. Lagerwall and G. Scalia, Angewandte Chemie, 51, 13, 3254, 2012

**12:03PM S37.00005 Effects of graphene on in-plane electro-optic switching for a nematic liquid crystal**, DANIEL KINNAMON, NICOLE SKAGGS, ALFRED GARVEY, RAJRATAN BASU, US Naval Academy — A small quantity of graphene flakes was doped in a nematic liquid crystal (LC), and the in-plane electro-optic switching was found to be significantly faster in the LC+graphene hybrid than that of the pure LC. Additional studies revealed that the presence of graphene reduced the rotational viscosity and the twist elastic constant of the LC, allowing the nematic director to respond faster on switching the electric field on.

**12:15PM S37.00006 Flow of anisotropic and isotropic objects in quasi-twodimensional fluids<sup>1</sup>**, RALF STANNARIUS, ALEXEY EREMIN, SARAH DÖLLE, KIRSTEN HARTH, CHRISTOPH KLOPP, Otto von Guericke University, Magdeburg — We study the motion of microscopic objects in very thin freely suspended smectic liquid-crystal films. The aspect ratios of these films are of the order of  $1:10^6$ . Hydrodynamic motion is restricted to the film plane. Thus such films represent quasi-twodimensional fluids. Not only do they provide the opportunity to test theoretical models on mobilities in thin membranes, they also allow access to viscosity parameters of in-plane isotropic (smectic A) and anisotropic (smectic C) fluids. Combinations of these environments with isotropic and anisotropic geometries of inclusions provide rich information about interactions of rotational and translational particle motions, the anchoring-induced and flow-induced alignments of the embedding fluid, and interactions of particles via flow and director fields. Thermal diffusion in horizontal films as well as controlled effective gravity in tilted films are explored.

<sup>1</sup>Funding by DLR with grant 50WM1430 and by DFG with grant STA 425/28 is acknowledged.

**12:27PM S37.00007 ABSTRACT WITHDRAWN —**

### **12:39PM S37.00008 Field-driven dynamics of microcapillaries filled with nematic liquid crystal<sup>1</sup>**

, FRED FU, POUYA KHAYATZADEH, NASSER M ABUKHDEIR, University of Waterloo — Polymer-dispersed liquid crystal (PDLC) composites have long been a focus of study for their unique electro-optical properties and the feasibility of manufacturing them on a large scale, resulting in applications such as switchable windows. LC domains within PDLCs are typically spheroidal, as opposed to rectangular in LCD technology, and thus exhibit substantially different behaviour in the presence of an external field. In this work, continuum simulations were performed in order to capture the complex formation and electric field-driven switching dynamics of approximations of PDLC domains. A simplified elliptic cylinder (microcapillary) geometry is used and the effects of varying aspect ratio, surface anchoring, and external field strength were studied using the Landau-de Gennes model. The observed nematic formation and reorientation dynamics were found to be governed by the presence and motion of defects within the domain. Aspect ratio was found to strongly influence domain texture by providing regions of high curvature to which defects are attracted. Simulations also predict the presence of a geometry-controlled transition from nematic order enhanced by an external field (low aspect ratio) to nematic order frustrated by an external field (high aspect ratio).

<sup>1</sup>This work was made possible by the Natural Sciences and Engineering Research Council of Canada and Compute Ontario.

### **12:51PM S37.00009 Structural organization of liquid crystals at liquid crystal-air interface: Synchrotron X-ray reflectivity and computational simulations**

, MONIRO SADAT, HADI RAMEZANI-DAKHEL, IME, UChicago, WEI BU, CARS, UChicago, EMRE SEVGEN, IME, UChicago, ZHU LIANG, CEM EROL, Dept. Phys., UIC, NADER TAHERI QAZVINI, MOHAMMAD RAHIMI, IME, UChicago, BINHUA LIN, CARS, UChicago, BENOIT ROUX, Dept. Biochem. Molecular Biol., UChicago, MARK SCHLOSSMAN, Dept. Phys., UIC, JUAN J. DE PABLO, IME, UChicago — Numerous applications of liquid crystals (LC) rely on control of molecular orientation at an interface. However, little is known about the precise molecular structure of such interfaces. In this work, we have performed synchrotron X-ray reflectivity measurements accompanied by an advanced theoretical and computational analysis to study the structural organization of liquid crystals at the air-liquid crystal interface. The X-ray reflectivity was measured from two nematic (5CB) and smectic (8CB) liquid crystals at several temperatures, in the nematic phase and above the nematic-isotropic transition. Our computational simulations and X-ray reflectivity results indicate that in the case of 8CB nematic phase, incipient bulk smectic fluctuations are pinned at the interface to form temperature-dependent multilayers at the interface. Such layers can extend far from the interface. However, the interface of 5CB in the nematic phase exhibits a relatively small number of layers. These measurements will be extended to the study of the LC-aqueous electrolyte interfaces to understand the effects of electrostatic interactions and external stimuli on the interfacial anchoring energy and LC orientational ordering.

### **1:03PM S37.00010 Gold nanoparticle encapsulation into a mixed lipid nanodisk: molecular dynamics simulations**

, HARI SHARMA, ZILU WANG, ELENA DORMIDONTOVA, Department of Physics and Institute of Materials Science, University of Connecticut, Storrs, CT — There is a growing interest in applications of nanoparticles in biomedicine. For practical applications of gold nanoparticles it is often desirable to encapsulate them into lipid nanocarriers. To this end it is important to understand gold-lipid interactions at the molecular level. We have performed coarse grained molecular dynamics simulations using a MARTINI force field of a lipid nanodisk composed of long and short tail lipids, DPPC and DHPC mixed in the ratio of 3:1 and studied its interaction with small gold nanoparticles (AuNP) functionalized with hydrophobic alkane tethers. We found that the inhomogeneous distribution of lipids in the nanodisk affects the outcome the AuNP-nanodisk interaction. The ordered arrangement of long chain lipids forming the interior region of the nanodisk are found to be less accessible for AuNP penetration compared to the rim of the nanodisk, where more mobile short lipids are located. Once encapsulated into a nanodisk, AuNP's have tendency to aggregate, especially if temperature is not too low. The results of computer modeling will be compared to experiment and the implications of our findings for experimental design of lipid nanocarriers for AuNP delivery will be discussed.

### **1:15PM S37.00011 Nanoscale Membrane Curvature detected by Polarized Localization Microscopy**

, CHRISTOPHER KELLY, ABIR MAAROUF, XINXIN WOODWARD, Wayne State University — Nanoscale membrane curvature is a necessary component of countless cellular processes. Here we present Polarized Localization Microscopy (PLM), a super-resolution optical imaging technique that enables the detection of nanoscale membrane curvature with order-of-magnitude improvements over comparable optical techniques. PLM combines the advantages of polarized total internal reflection fluorescence microscopy and fluorescence localization microscopy to reveal single-fluorophore locations and orientations without reducing localization precision by point spread function manipulation. PLM resolved nanoscale membrane curvature of a supported lipid bilayer draped over polystyrene nanoparticles on a glass coverslip, thus creating a model membrane with coexisting flat and curved regions and membrane radii of curvature as small as 20 nm. Further, PLM provides single-molecule trajectories and the aggregation of curvature-inducing proteins with super-resolution to reveal the correlated effects of membrane curvature, dynamics, and molecular sorting. For example, cholera toxin subunit B has been observed to induce nanoscale membrane budding and concentrate at the bud neck. PLM reveals a previously hidden and critical information of membrane topology.

### **1:27PM S37.00012 Membrane Domain Formation on Nanostructured Scaffolds**

, FANGJIE LIU, BERNADETA SRIJANTO, Oak Ridge National Laboratory — The spatial organization of lipids and proteins in biological membranes seems to have a functional role in the life of a cell. Separation of the lipids into distinct domains of greater order and anchoring to the cytoskeleton are two main mechanisms for organizing the membrane in cells. We propose a novel model membrane consisting of a lipid bilayer suspended over a nanostructured scaffold consisting of arrays of fabricated nanopillars. Unlike traditional model membranes, our model will have well-defined lateral structure and distributed substrate attachments that will emulate the connections of cellular membranes to the underlying cytoskeleton. Membranes will be characterized using neutron reflectometry, atomic force microscopy and fluorescence to verify a suspended, planar geometry with restricted diffusion at suspension points, and free diffusion in between. This architecture will allow the controlled study of lipid domain reorganization, viral infection and signal transduction that depend on the lateral structure of the membrane.

### **1:39PM S37.00013 Structure and dynamics of a hydrated phospholipid bilayer in the presence of a silica substrate<sup>1</sup>**

, MATTHEW MCCUNE, IOAN KOSZTIN, University of Missouri — We study the structure and dynamics of a hydrated diiristoyl-phosphatidylcholine (DMPC) lipid bilayer supported on a silica substrate using all-atom molecular dynamics (MD) simulation. A similar MD simulation of a freestanding DMPC bilayer is used as a reference to determine changes to both lipid and hydration water properties due to the introduction of the substrate. Long time (0.1 microsecond) MD trajectories were used to investigate the effect of the substrate on the structure and dynamics of the lipid bilayer by determining (i) the spatial distribution of water molecules and selected lipid atoms; (ii) the out of plane fluctuations of the lipid molecules; (iii) the dipole moment orientation of hydration waters; and (iv) the lateral mean-square-displacement of both lipid and water molecules. The obtained results suggest that (i) at equilibrium the space between the substrate and lipid bilayer is filled by only hydration water; (ii) the presence of the substrate has no major influence on the structure of hydration water layers and on the out-of-plane fluctuations of the lipids; and (iii) the silica substrate alters considerably the lateral diffusion of the lipids in the closest bilayer leaflet and the hydration waters between the substrate and DMPC membrane. The reported results appear to be consistent with previous MD and neutron scattering studies.

<sup>1</sup>Work supported by National Science Foundation Integrative Graduate Education and Research Traineeship (DGE-1069091). The computations were performed on the HPC resources at the University of Missouri Bioinformatics Consortium (UMBC).

**1:51PM S37.00014 Insight into cholesterol transport in different lipid environments: a simulation study**, KLAS KARIS, URSULA PEREZ-SALAS, FATEMEH KHALILI-ARAGHI, Univ of Illinois - Chicago — With molecular dynamics simulations employing the MARTINI coarse grained force field, we investigate the difference in the dynamic behavior of cholesterol, linked to the absorption and desorption of cholesterol in two phospholipid environments consisting of either an uncharged, zwitterionic lipid (POPC) or the charged counterpart (POPS). The work is motivated by results from recent neutron scattering experiments measuring the transfer rate of inter-membrane cholesterol transfer, revealing that cholesterol inter-membrane transport is significantly slower in lipid membranes composed of charged lipids, than in membranes composed of uncharged lipids. By systematically investigating dynamical and equilibrium parameters such as the free energy of desorption, lateral diffusion, tilt angle distribution, structural parameters and estimated absorption rates, we map the key differences in interaction of the two lipid species with cholesterol. Results point towards a shift in cholesterol absorption rates for POPS compared to POPC.

**2:03PM S37.00015 Phase separation in artificial vesicles driven by light and curvature**, MELISSA RINALDIN, WIM POMP, THOMAS SCHMIDT, LUCA GIOMI, DANIELA KRAFT, Leiden University, PHYSICS OF LIFE PROCESSES TEAM, SOFT AND BIO MECHANICS COLLABORATION, SELF-ASSEMBLY IN SOFT MATTER SYSTEMS COLLABORATION — The role of phase-demixing in living cells, leading to the lipid-raft hypothesis, has been extensively studied. Lipid domains of higher lipid chain order are proposed to regulate protein spatial organization. Giant Unilamellar Vesicles provide an artificial model to study phase separation. So far temperature was used to initiate the process. Here we introduce a new methodology based on the induction of phase separation by light. To this aim, the composition of the lipid membrane is varied by photo-oxidation of lipids. The control of the process gained by using light allowed us to observe vesicle shape fluctuations during phase-demixing. The presence of fluctuations near the critical mixing point resembles features of a critical process. We quantitatively analyze these fluctuations using a 2d elastic model, from which we can estimate the material parameters such as bending rigidity and surface tension, demonstrating the non-equilibrium critical behaviour. Finally, I will describe recent attempts toward tuning the membrane composition by controlling the vesicle curvature.

## Thursday, March 17, 2016 11:15AM - 2:15PM —

Session S38 DPOLY DBIO: Mechanics of Biopolymers: Networks and Assemblies 341 - Louis Foucard, UCLA

**11:15AM S38.00001 Rheology and nonlinear mechanics of transiently cross linked semiflexible networks: Bundling, ripping, healing, and mechnomemory**, ALEX LEVINE, UCLA — Transiently cross linked networks of semiflexible filaments make up the principal structural component of the cell the cytoskeleton. This intracellular network, along with molecular motors, forms the basis for cellular control of morphology and force generation. In this talk, I report on investigations of the effect of transiently bound cross linkers on the structure and mechanics of semiflexible networks. Specifically, I address the role of Casimir or fluctuation-induced interactions between cross linkers in the formation of filament bundles. I report on the linear viscoelasticity of transiently cross-linked networks of bundles. Finally, I discuss the nonlinear mechanical response of such networks, where applied stress induces a persistent structural rearrangement of the network that can dramatically alter its nonlinear response to stresses subsequently applied.

**11:51AM S38.00002 A coarse-grained model of microtubule self-assembly**, CHOLA REGMI, SHENGFENG CHENG, Virginia Polytechnic Institute and State University — Microtubules play critical roles in cell structures and functions. They also serve as a model system to stimulate the next-generation smart, dynamic materials. A deep understanding of their self-assembly process and biomechanical properties will not only help elucidate how microtubules perform biological functions, but also lead to exciting insight on how microtubule dynamics can be altered or even controlled for specific purposes such as suppressing the division of cancer cells. Combining all-atom molecular dynamics (MD) simulations and the essential dynamics coarse-graining method, we construct a coarse-grained (CG) model of the tubulin protein, which is the building block of microtubules. In the CG model a tubulin dimer is represented as an elastic network of CG sites, the locations of which are determined by examining the protein dynamics of the tubulin and identifying the essential dynamic domains. Atomistic MD modeling is employed to directly compute the tubulin bond energies in the surface lattice of a microtubule, which are used to parameterize the interactions between CG building blocks. The CG model is then used to study the self-assembly pathways, kinetics, dynamics, and nanomechanics of microtubules.

**12:03PM S38.00003 Molecular Simulations of Actomyosin Network Self-Assembly and Remodeling<sup>1</sup>**, JAMES KOMIANOS, Univ of Maryland-College Park, KONSTANTIN POPOV, Univ of North Carolina-Chapel Hill, GAREGIN PAPOIAN, Univ of Maryland-College Park, PAPOIAN LAB TEAM — Actomyosin networks are an integral part of the cytoskeleton of eukaryotic cells and play an essential role in determining cellular shape and movement. Actomyosin network growth and remodeling in vivo is based on a large number of chemical and mechanical processes, which are mutually coupled and spatially and temporally resolved. To investigate the fundamental principles behind the self-organization of these networks, we have developed a detailed mechanochemical, stochastic model of actin filament growth dynamics, at a single-molecule resolution, where the nonlinear mechanical rigidity of filaments and their corresponding deformations under internally and externally generated forces are taken into account. Our work sheds light on the interplay between the chemical and mechanical processes governing the cytoskeletal dynamics, and also highlights the importance of diffusional and active transport phenomena. Our simulations reveal how different actomyosin micro-architectures emerge in response to varying the network composition.

<sup>1</sup>Support from NSF Grant CHE-1363081.

**12:15PM S38.00004 Active mechanics in living oocytes reveal molecular-scale force kinetics**, WYLIE AHMED, Institut Curie, ETIENNE FODOR, Université Paris Diderot, MARIA ALMONACID, Collège de France, MATTHIAS BUSSONNIER, Institut Curie, MARIE-HELENE VERLHAC, Collège de France, NIR GOV, Weizmann Institute of Science, PAOLO VISCO, FREDERIC VAN WIJLAND, Université Paris Diderot, TIMO BETZ, University of Muenster — Unlike traditional materials, living cells actively generate forces at the molecular scale that change their structure and mechanical properties. This nonequilibrium activity is essential for cellular function, and drives processes such as cell division. Single molecule studies have uncovered the detailed force kinetics of isolated motor proteins in-vitro, however their behavior in-vivo has been elusive due to the complex environment inside the cell. Here, we quantify active forces and intracellular mechanics in living oocytes using in-vivo optical trapping and laser interferometry of endogenous vesicles. We integrate an experimental and theoretical framework to connect mesoscopic measurements of nonequilibrium properties to the underlying molecular-scale force kinetics. Our results show that force generation by myosin-V drives the cytoplasmic-skeleton out-of-equilibrium (at frequencies below 300 Hz) and actively softens the environment. In vivo myosin-V activity generates a force of  $F \sim 0.4$  pN, with a power-stroke of length  $\Delta x \sim 20$  nm and duration  $\tau \sim 300$   $\mu$ s, that drives vesicle motion at  $v_v \sim 320$  nm/s. This framework is widely applicable to characterize living cells and other soft active materials.

**12:27PM S38.00005 Biopolymer mechanics across the force regimes**, OMAR SALEH, Materials Department and BMSE Program, UCSB — The elastic response of a single polymer can explain certain material properties, including the thickness of polymer brushes and the mechanics of gels; in turn, these material properties have a variety of biological applications, such as to the brush-like pericellular matrix surrounding certain cells. More fundamentally, the force-extension relation of a polymer can be predicted theoretically, making it possible to probe the structure of a polymer by measuring its elastic response. This works in a manner similar to scattering: just as scattering at a wave vector  $q$  gives information on structure at a length scale  $1/q$ , the elastic response under applied tension  $f$  gives information on structure at a length scale of  $kT/f$ . Thus, in exact analogy to low-angle scattering, low-force elastic measurements are needed to probe the interesting long-range structure of polymers. I will discuss the basic physics of low-force elasticity, and present our experiments on various polymers, including nucleic acids and polysaccharides, that validate the power of low-force elastic measurements.

**1:03PM S38.00006 Investigating collagen self-assembly with optical tweezers microrheology**, NANCY FORDE, Department of Physics, Simon Fraser University, MARJAN SHAYEGAN<sup>1</sup>, Department of Chemistry, Simon Fraser University, TUBA ALTINDAL, Department of Physics, Simon Fraser University — Collagen is the fundamental structural protein in vertebrates. Assembled from individual triple-helical proteins to make strong fibres, collagen is a beautiful example of a hierarchical self-assembling system. Using optical tweezers to perform microrheology measurements, we explore the dynamics of interactions between collagens responsible for their self-assembly and examine the development of heterogeneous mechanics during assembly into fibrillar gels. Telopeptides, short non-helical regions that flank the triple helix, have long been known to facilitate fibril self-assembly. We find that their removal not only slows down fibril nucleation but also results in a significant frequency-dependent reduction in the elastic modulus of collagens in solution. We interpret these results in terms of a model in which telopeptides facilitate transient intermolecular interactions, which enhance network connectivity in solution and lead to more rapid assembly in fibril-forming conditions.

<sup>1</sup>Current address: Department of Physics, McGill University

**1:15PM S38.00007 Nonlinear microrheology and molecular imaging to map microscale deformations of entangled DNA networks**, TSAI-CHIN WU, RAE ANDERSON, University of San Diego — We use active microrheology coupled to single-molecule fluorescence imaging to elucidate the microscale dynamics of entangled DNA. DNA naturally exists in a wide range of lengths and topologies, and is often confined in cell nuclei, forming highly concentrated and entangled biopolymer networks. Thus, DNA is the model polymer for understanding entangled polymer dynamics as well as the crowded environment of cells. These networks display complex viscoelastic properties that are not well understood, especially at the molecular-level and in response to nonlinear perturbations. Specifically, how microscopic stresses and strains propagate through entangled networks, and what molecular deformations lead to the network stress responses are unknown. To answer these important questions, we optically drive a microsphere through entangled DNA, perturbing the system far from equilibrium, while measuring the resistive force the DNA exerts on the bead during and after bead motion. We simultaneously image single fluorescent-labeled DNA molecules throughout the network to directly link the microscale stress response to molecular deformations. We characterize the deformation of the network from the molecular-level to the mesoscale, and map the stress propagation throughout the network. We further study the impact of DNA length (11 – 115 kbp) and topology (linear vs ring DNA) on deformation and propagation dynamics, exploring key nonlinear features such as tube dilation and power-law relaxation.

**1:27PM S38.00008 Dual-feedback microrheology in cytoskeletal networks**, NATSUKI HONDA, KENJI NISHIZAWA, TAKAYUKI ARIGA, DAISUKE MIZUNO, Kyushu Univ — Cytoskeletons are critical for understanding cell behaviors since they generate forces together with molecular motors and supply mechanical integrity to cells. Since response of cytoskeletons to motor-generated forces is highly nonlinear, cell behaviors intricately depend on activities and mechanics of cytoskeletons. Investigating local response of cytoskeletons to forces generated by molecular motors, which optical trap can imitatively reproduce, is therefore essential. Here, we performed this by developing a novel optical-trap-based microrheology implemented with dual-feedback control. With the slow feedback of piezo-stage, probes under drift, caused by the traction force applied by the optical trap, were stably tracked. By the rapid feedback of trapping laser, artifacts in probes motion, that had been caused by strong optical trap potential, were completely removed. We observed that fluctuations of probes embedded in various cytoskeletons were significantly reduced when subjected to forces. Under the assumption that the fluctuation-dissipation theorem is satisfied, our results indicate the stress stiffening of cytoskeletons, that became now possible to be studied in micro-scales and in a frequency range appropriate for cell behaviors.

**1:39PM S38.00009 Coupled actin-lamin biopolymer networks and protecting DNA**, TAO ZHANG, Chemical Engineering Department, University of Pittsburgh, D. ZEB ROCKLIN, XIAOMING MAO, University of Michigan, Department of Physics, J. M. SCHWARZ, Department of Physics, Syracuse University — The mechanical properties of cells are largely determined by networks of semiflexible biopolymers forming the cytoskeleton. Similarly, the mechanical properties of cell *nuclei* are also largely determined by networks of semiflexible biopolymers forming the *nuclear* cytoskeleton. In particular, a network of filamentous lamin sits just inside the inner nuclear membrane to presumably protect the heart of the cell nucleus—the DNA. It has been demonstrated over the past decade that the actin cytoskeletal biopolymer network and the lamin biopolymer network are coupled via a sequence of proteins bridging the outer and inner nuclear membranes, known as the LINC complex. We, therefore, probe the consequences of such a coupling in a model biopolymer network system via numerical simulations to understand the resulting deformations in the lamin network in response to perturbations in the actin cytoskeletal network. We find, for example, that the force transmission across the coupled system can depend sensitively on the concentration of LINC complexes. Such study could have implications for mechanical mechanisms of the regulation of transcription since DNA couples to lamin via lamin-binding domains so that deformations in the lamin network may result in deformations in the DNA.

**1:51PM S38.00010 The Effect of Crosslinking on the Microscale Stress Response and Molecular Deformations in Actin Networks**, BEKELE GURMESSA, ROBERT FITZPATRICK, JONATHON VALDIVIA, RAE M. R. ANDERSON, Univ of San Diego — Actin, the most abundant protein in eukaryotic cells, is a semi-flexible biopolymer in the cytoskeleton that plays a crucial structural and mechanical role in cell stability, motion and replication, as well as muscle contraction. Most of these mechanically driven structural changes in cells stem from the complex viscoelastic nature of entangled actin networks and the presence of a myriad of proteins that cross-link actin filaments. Despite their importance, the mechanical response of actin networks is not yet well understood, particularly at the molecular level. Here, we use optical trapping - coupled with fluorescence microscopy - to characterize the microscale stress response and induced filament deformations in entangled and cross-linked actin networks subject to localized mechanical perturbations. In particular, we actively drive a microsphere 10 microns through an entangled or cross-linked actin network at a constant speed and measure the resistive force that the deformed actin filaments exert on the bead during and following strain. We simultaneously visualize and track individual sparsely-labeled actin filaments to directly link force response to molecular deformations, and map the propagation of the initially localized perturbation field throughout the rest of the network (~100  $\mu$ m). By varying the concentration of actin and cross-linkers we directly determine the role of crosslinking and entanglements on the length and time scales of stress propagation, molecular deformation and relaxation mechanisms in actin networks.

**2:03PM S38.00011 Mechanically tunable actin networks using programmable DNA based cross-linkers** , JOERG SCHNAUSS, University of Leipzig & Fraunhofer Institute for Cell Therapy and Immunology IZI, JESSICA LORENZ, Fraunhofer Institute for Cell Therapy and Immunology IZI, CARSTEN SCHULDT, University of Leipzig & Fraunhofer Institute for Cell Therapy and Immunology IZI, JOSEF KAES, University of Leipzig, DAVID SMITH, Fraunhofer Institute for Cell Therapy and Immunology IZI — Cells employ multiple cross-linkers with very different properties. Studies of the entire phase space, however, were infeasible since they were restricted to naturally occurring cross-linkers. These components cannot be controllably varied and differ in many parameters. We resolve this limitation by forming artificial actin cross-linkers, which can be controllably varied. The basic building block is DNA enabling a well-defined length variation. DNA can be attached to actin binding peptides with known binding affinities. We used bulk rheology to investigate mechanical properties of these networks. We were able to reproduce mechanical features of actin networks cross-linked by fascin by using a short version of our artificial complex with a high binding affinity. Additionally, we were able to resemble findings for the cross-linker alpha-actinin by employing a long cross-linker with a low binding affinity. Between these natural limits we investigated three different cross-linker lengths each with two different binding affinities. With these controlled variations we are able to precisely screen the phase space of cross-linked actin networks by changing only one specific parameter and not the entire set of properties as in the case of naturally occurring cross-linking complexes.

**Thursday, March 17, 2016 11:15AM - 2:15PM –**

**Session S39 DBIO DPOLY GSNP: Physics of Genome Organization: from DNA to Chromatin**

II 342 - Leonid Mirny, MIT

**11:15AM S39.00001 Inferring the locations of DNA bound proteins from Hi-C data** , PAU FARRE, ELDON EMBERLY, Simon Fraser University — Eukaryotic DNA can be found in either a tightly packed state (heterochromatin) or an open conformation (euchromatin). Certain proteins that bind to the DNA are responsible for setting up these two types of states. They interact with each other, and generate spatially separated compartments in the DNA through the formation of loops. In this talk I will present a combination of analytic and simulation results for the effects of protein-protein interactions on the large-scale 3D structure of chromatin. Using these findings we have developed a maximum-likelihood method for inferring the distribution of DNA bound factors that can help refine and make new predictions for the locations of proteins responsible of structuring the chromosome.

**11:27AM S39.00002 Coalescence Model for Crumpled Globules Formed in Polymer Collapse** , GUY BUNIN, MEHRAN KARDAR, Massachusetts Inst of Tech-MIT — The rapid collapse of a polymer, due to external forces or changes in solvent, yields a long-lived "crumpled globule." The conjectured fractal structure shaped by hierarchical collapse dynamics has proved difficult to establish, even with large simulations. To unravel this puzzle, we study a coarse-grained model of in-falling spherical blobs that coalesce upon contact. Distances between pairs of monomers are assigned upon their initial coalescence, and do not "equilibrate" subsequently. Surprisingly, the model reproduces quantitatively the dependence of distance on segment length, suggesting that the slow approach to scaling is related to the wide distribution of blob sizes.

**11:39AM S39.00003 Probing nuclear dynamics and architecture using single-walled carbon nanotubes** , YOON JUNG, JUNANG LI, NIKTA FAKHRI, Department of Physics, Massachusetts Institute of Technology — Chromatin is a multiscale dynamic architecture that acts as a template for many biochemical processes such as transcription and DNA replication. Recent developments such as Hi-C technology enable an identification of chromatin interactions across an entire genome. However, a single cell dynamic view of chromatin organization is far from understood. We discuss a new live cell imaging technique to probe the dynamics of the nucleus at a single cell level using single-walled carbon nanotubes (SWNTs). SWNTs are non-perturbing rigid rods (diameter of 1 nm and length of roughly 100 nm) that fluoresce in the near infrared region. Due to their high aspect ratio, they can diffuse in tight spaces and report on the architecture and dynamics of the nucleoplasm. We develop 3D imaging and tracking of SWNTs in the volume of the nucleus using double helix point spread function microscopy (DH-PSF) and discuss the capabilities of the DH-PSF for inferring the 3D orientation of nanotubes based on vectorial diffraction theory.

**11:51AM S39.00004 Fractionation of Exosomes and DNA using Size-Based Separation at the Nanoscale** , BENJAMIN WUNSCH, JOSHUA SMITH, IBM Research Labs, CHAO WANG, Arizona State University, STACEY GIFFORD, MARKUS BRINK, ROBERT BRUCE, GUSTAVO SOLOVITZKY, IBM Research Labs, ROBERT AUSTIN, Princeton University, YANN ASTIER, IBM Research Labs — Exosomes, a key target of liquid biopsies, are nano-vesicles found in nearly all biological fluids. Exosomes are secreted by eukaryotic and prokaryotic cells alike, and contain information about their originating cells, including surface proteins, cytoplasmic proteins, and nucleic acids. One challenge in studying exosome morphology is the difficulty of sorting exosomes by size and surface markers. Common separation techniques for exosomes include ultracentrifugation and ultrafiltration, for preparation of large volume samples, but these techniques often show contamination and significant heterogeneity between preparations. To date, deterministic lateral displacement (DLD) pillar arrays in silicon have proven an efficient technology to sort, separate, and enrich micron-scale particles including human parasites, eukaryotic cells, blood cells, and circulating tumor cells in blood; however, the DLD technology has never been translated to the true nanoscale, where it could function on bio-colloids such as exosomes. We have fabricated nanoscale DLD (nanoDLD) arrays capable of rapidly sorting colloids down to 20 nm in continuous flow, and demonstrated size sorting of individual exosome vesicles and dsDNA polymers, opening the potential for on-chip biomolecule separation and diagnosis.

**12:03PM S39.00005 The impact of non-uniform capsid charge density on virus assembly<sup>1</sup>** , SIYU LI, GONCA ERDEMCI-TANDOĞAN, University of California,riverside, JEF WAGNER, Lawrence University, ROYA ZANDI, University of California,riverside — Many spherical viruses efficiently encapsulate their genome into shells (capsids) with icosahedral symmetry. Under many circumstances, this process is spontaneous and is primarily driven by the electrostatic interaction between positively charged capsid proteins and negatively charged genome. Through the free energy minimization of a generic potential, we calculate the optimal encapsulated genome length. In this talk, I will present our results due to a non-uniform charge distribution on the shell and its impact on the optimal size of encapsulated genome.

<sup>1</sup>This work was supported by the National Science Foundation through Grant No. DMR-13-10687.

**12:15PM S39.00006 Single molecule fluorescence studies of transition paths in DNA hairpin folding** , KATHERINE TRUEX, HOI SUNG CHUNG, JOHN LOUIS, WILLIAM EATON, National Institutes of Health — DNA hairpins are the simplest structures for investigating fundamental aspects of nucleic acid folding mechanisms. For two-state hairpins, all of the mechanistic information on how the hairpin folds is contained in the transition path (TP), the rare event in single molecule trajectories when the free energy barrier between folded and unfolded states is actually crossed. The only previous experimental study of TPs in nucleic acids used optical tweezer measurements and Szabo's analytical theory for diffusive barrier crossing to reconstruct the free energy surface for an indirect determination of average TP times (Neupane *et al.* *PRL* 2012). We used confocal single molecule FRET and maximum likelihood analysis of photon trajectories to determine an upper bound of 2.5  $\mu$ s for the average TP time of a DNA hairpin (Truex *et al.*, *PRL* 2015), compared to the value of 4  $\mu$ s predicted by Neupane *et al.*, providing an important test of energy landscape theory. Current experiments are aimed at eventually characterizing structural changes during TPs, which will provide a very demanding test of mechanisms predicted by both theoretical models and simulations.

**12:27PM S39.00007 The Molecular Atlas Project** , JESSE SILVERBERG, PENG YIN, Wyss Institute for Biologically Inspired Engineering, Harvard University — The promise of super-resolution microscopy is a technology to discover new biological mechanisms that occur at smaller length scales than previously observable. However, with higher-resolution, we generally lose the larger spatial context of the image itself. The *Molecular Atlas Project* (MAP) directly asks how these competing interests between super-resolution imaging and broader spatially contextualized information can be reconciled. MAP enables us to acquire, visualize, explore, and annotate proteomic image data representing 7 orders of magnitude in length ranging from molecular (nm) to tissue (cm) scales. This multi-scale understanding is made possible by combining multiplexed DNA-PAINT, a DNA nanotechnology approach to super-resolution imaging, with “big-data” strategies for information management and image visualization. With these innovations combined, MAP enables us to explore cell-specific heterogeneity in ductal carcinoma for every cell in a cm-sized tissue section, analyze organoid growth for advances in high-throughput tissue-on-a-chip technology, and examine individual synapses for connectome mapping over extremely wide areas. Ultimately, MAP is a fundamentally new way to interact with multiscale biophysical data.

**12:39PM S39.00008 simulation of the DNA force-extension curve** , GREGORY SHINABERRY, IVAN MIKHAYLOV, ALEXANDER BALAEFF, University of Central Florida — A molecular dynamics simulation study of the force-extension curve of double-stranded DNA is presented. Extended simulations of the DNA at multiple points along the force-extension curve are conducted with DNA end-to-end length constrained at each point. The calculated force-extension curve qualitatively reproduces the experimental one. The DNA conformational ensemble at each extension shows that the famous plateau of the force-extension curve results from B-DNA melting, whereas the formation of the earlier-predicted novel DNA conformation called ‘zip-DNA’ takes place at extensions past the plateau. An extensive analysis of the DNA conformational ensemble in terms of base configuration, backbone configuration, solvent interaction energy, etc., is conducted in order to elucidate the physical origin of DNA elasticity and the main interactions responsible for the shape of the force-extension curve.

**12:51PM S39.00009 Characterization of the full base pairing probability distribution in RNA secondary structure folding<sup>1</sup>** , WILLIAM BAEZ, Ohio State University, KAY WIESE, CNRS-LPTENS, RALF BUNDSCHUH, Ohio State University — Below the denaturation temperature of RNA, its secondary structures can exist in one of two phases: a strongly disordered, low-temperature glass phase and a weakly disordered, high-temperature molten phase. The probability of two bases pairing in these phases have been shown to scale with the distance between the two bases as  $-3/2$  and  $-4/3$  in the molten and glass phases, respectively. In this study, we characterize the full probability distributions of pair binding both near and far from the critical point rather than just the behavior of their means studied before. We anticipate that this approach allows one to more closely probe the nature of the phase transition and better measure the system's critical exponents close to and at its critical point.

<sup>1</sup>This material is based upon work supported by the National Science Foundation under Grants No. DMR-01105458 and DMR-01410172.

**1:03PM S39.00010 Gene dosage imbalance during DNA replication controls bacterial cell-fate decision<sup>1</sup>** , OLEG IGOSHIN, Rice University — Genes encoding proteins in a common regulatory network are frequently located close to one another on the chromosome to facilitate co-regulation or couple gene expression to growth rate. Contrasting with these observations, here we demonstrate a functional role for the arrangement of *Bacillus subtilis* sporulation network genes on opposite sides of the chromosome. We show that the arrangement of two sporulation network genes, one located close to the origin, the other close to the terminus leads to a transient gene dosage imbalance during chromosome replication. This imbalance is detected by the sporulation network to produce cell-cycle coordinated pulses of the sporulation master regulator Spo0A~P. This pulsed response allows cells to decide between sporulation and continued vegetative growth during each cell-cycle spent in starvation. Furthermore, changes in DNA replication and cell-cycle parameters with decreased growth rate in starvation conditions enable cells to indirectly detect starvation without the need for evaluating specific metabolites. The simplicity of the uncovered coordination mechanism and starvation sensing suggests that it may be widely applicable in a variety of gene regulatory and stress-response settings.

<sup>1</sup>This work is supported by National Science Foundation grants MCB-1244135, EAGER-1450867, MCB-1244423, NIH NIGMS grant R01 GM088428 and HHMI International Student Fellowship.

**1:39PM S39.00011 Torque-induced buckling behavior in stretched intertwined DNAs<sup>1</sup>** , SUMITABHA BRAHMACHARI, JOHN F. MARKO, Northwestern Univ — Two intertwined DNA molecules (a DNA ‘braid’) is a common occurrence in the cell and is a relevant substrate for the study of topoisomerase and recombination enzymes. Single molecule experiments have observed the signature of a buckling transition in braids under tensile and torsional stress. We present a free energy model for braided DNA to investigate the mechanical properties of these structures. Our model is based on the semi-flexible polymer model for double helix DNA and is in quantitative accord with the experiments. We identify coexistence of a force-extended state with a plectonemically buckled state, which is reminiscent of single supercoiled DNA behavior. However, the absence of an intrinsic twist modulus in braided DNA results in unique mechanical properties such as non-linear torque in the extended state. At the buckling transition, we predict a jump in the braid extension due to the plectoneme end loop which acts as a nucleation barrier. We investigate the effect of salt concentration on the mechanical response of braids, e.g. we find that buckling starts at a lower linking number for lower salt concentration, the opposite of what is seen for single supercoiled DNAs. Also, concentrations less than 20 mM monovalent salt favor formation of multiple plectoneme domains.

<sup>1</sup>NSF grant: DMR-9734178

**1:51PM S39.00012 Sequence Heterogeneity Accelerates Protein Search for Targets on DNA<sup>1</sup>** , ALEXEY SHVETS, ANATOLY KOLOMEISKY, Rice Univ — The process of protein search for specific binding sites on DNA is fundamentally important since it marks the beginning of all major biological processes. We present a theoretical investigation that probes the role of DNA sequence symmetry, heterogeneity and chemical composition in the protein search dynamics. Using a discrete-state stochastic approach with a first-passage events analysis, which takes into account the most relevant physical-chemical processes, a full analytical description of the search dynamics is obtained. It is found that, contrary to existing views, the protein search is generally faster on DNA with more heterogeneous sequences. In addition, the search dynamics might be affected by the chemical composition near the target site. The physical origins of these phenomena are discussed. Our results suggest that biological processes might be effectively regulated by modifying chemical composition, symmetry and heterogeneity of a genome.

<sup>1</sup>The work was supported by the Welch Foundation (Grant C-1559), by the NSF (Grant CHE-1360979), and by the Center for Theoretical Biological Physics sponsored by the NSF (Grant PHY-1427654)

**2:03PM S39.00013 SA1 and TRF1 synergistically bind to telomeric DNA and promote DNA-DNA pairing**, HONG WANG, JIANGGUO LIN, PRESTON COUNTRYMAN, HAI PAN, North Carolina State University, PARMINDER KAUR TEAM, ROBERT RIEHN TEAM, PATRICIA OPRESKO TEAM, JANE TAO TEAM, SUSAN SMITH TEAM — Impaired telomere cohesion leads to increased aneuploidy and early onset of tumorigenesis. Cohesion is thought to occur through the entrapment of two DNA strands within tripartite cohesin ring(s), along with a fourth subunit (SA1/SA2). Surprisingly, cohesion rings are not essential for telomere cohesion, which instead requires SA1 and shelterin proteins including TRF1. However, neither this unique cohesion mechanism at telomeres or DNA-binding properties of SA1 is understood. Here, using single-molecule fluorescence imaging of quantum dot-labeled proteins on DNA we discover that while SA1 diffuses across multiple telomeric and non-telomeric regions, the diffusion mediated through its N-terminal domain is slower at telomeric regions. However, addition of TRF1 traps SA1 within telomeric regions, which form longer DNA-DNA pairing tracts than with TRF1 alone, as revealed by atomic force microscopy. Together, these experimental results and coarse-grained molecular dynamics simulations suggest that TRF1 and SA1 synergistically interact with DNA to support telomere cohesion without cohesin rings.

**Thursday, March 17, 2016 11:15AM - 2:15PM –**  
**Session S40 GSNP: Systems with Large Fluctuations and Strong Correlations II** 343 - Uwe Tauber, Virginia Tech

**11:15AM S40.00001 First-Passage Statistics of Extreme Values**, ELI BEN-NAIM, Los Alamos National Laboratory — Theoretical concepts from nonequilibrium statistical physics such as scaling and correlations are used to analyze first-passage processes involving extreme values. The focus of this talk is statistics of the running maxima, defined as the largest variable in a sequence of random variables. In particular, the running maxima of multiple independent sequences of stochastic variables are compared. The probability that these maxima remain perfectly ordered decays algebraically with the number of random variables, and the decay exponent characterizing this decay is nontrivial. Exact solutions for the scaling exponents will be discussed for uncorrelated variables as well as Brownian trajectories which are correlated. Relevance of such statistical measures for analysis of empirical data will be discussed as well.

**11:51AM S40.00002 Emergence of universal statistics from conserved topological features of underlying network dynamics**, SRIVIDYA IYER-BISWAS, Department of Physics, Purdue University — In this talk I will discuss how universal statistics emerge from conserved topological features of underlying network dynamics. I will indicate how dynamical phase transitions between different network structures also encode universal signatures. I will connect these results with our single-cell experiments on *C. crescentus* cells.

**12:03PM S40.00003 Anomalous Dimension in a Two-Species Reaction-Diffusion Model**, JOSHUA HELLERICK, BENJAMIN VOLLMAYR-LEE, Bucknell University — We consider particles ( $A$ ) diffusing in the presence of traps ( $B$ ), which themselves are diffusing and reacting, i.e. the two-species reaction diffusion model  $A + B \rightarrow B$  and  $B + B \rightarrow (0, B)$ . We introduce a simulation technique that provides the full probability distribution of particles for a given realization of the trap dynamics. Previous renormalization group analysis predicted that the density of  $A$  particles decays as  $a t^{-\theta}$  where  $\theta$  is a nontrivial, universal exponent for  $d < 2$ . We compare our results with these predictions, and also demonstrate the scaling of the correlation functions. We discover an anomalous dimension in the particle-particle correlation function, described by  $G_{AA}(0) \sim t^\phi$ , and we report our measurements for this new exponent.

**12:15PM S40.00004 Non-equilibrium steady states of stochastic processes with intermittent resetting**, STEPHAN EULE, Max-Planck-Institute, JAKOB METZGER, Rockefeller University — Stochastic processes that are randomly reset to an initial condition serve as a showcase to analytically investigate non-equilibrium steady states. Here we study such processes for which the time between the resets is random and drawn from a generic waiting time distribution. We obtain the general solution for the stationary state and quantify the temporal relaxation of the process in terms of its moments. Our results are applied to analyze the efficiency of constrained random search processes. For a fixed mean reset time, we show that the search efficiency can be optimized by adapting the shape of the waiting time distribution.

**12:27PM S40.00005 Persistent Probability Currents in Non-equilibrium Steady States<sup>1</sup>**, ROYCE ZIA, Iowa State and Virginia Tech, ANDREW MELLOR, MAURO MÖBILIA, University of Leeds, BAYLOR FOX-KEMPER, Brown University, JEFFREY WEISS, University of Colorado at Boulder — For many interesting phenomena in nature, from all life forms to the global climate, the fundamental hypothesis of equilibrium statistical mechanics does not apply. Instead, they are perhaps better characterized by non-equilibrium steady states, evolving with dynamical rules which violate detailed balance. In particular, such dynamics leads to the existence of non-trivial, persistent probability currents - a principal characteristic of non-equilibrium steady states. In turn, they give rise to the notion of 'probability angular momentum'. Observable manifestations of such abstract concepts will be illustrated in two distinct contexts: a heterogeneous nonlinear voter model and our ocean heat content.

<sup>1</sup>Supported in part by grants from the Bloom Agency (Leeds, UK) and the US National Science Foundation: OCE-1245944. AM acknowledges the support of EPSRC Industrial CASE Studentship, Grant No. EP/L50550X/1

**12:39PM S40.00006 From randomly accelerated particles to Lévy walks: non-ergodic behavior and aging**, GUENTER RADONS, TONY ALBERS, Tech Univ Chemnitz, INSTITUTE OF PHYSICS, COMPLEX SYSTEMS AND NONLINEAR DYNAMICS TEAM — For randomly accelerated particles we detected, and were able to analyze in detail (PRL 113, 184101 (2014)), the phenomenon of weak-ergodicity breaking (WEB), i.e. the inequivalence of ensemble- and time-averaged mean-squared displacements (MSD). These results, including their aging time dependence, are relevant for anomalous chaotic diffusion in Hamiltonian systems, for passive tracer transport in turbulent flows, and many other systems showing momentum diffusion. There are, however, several related models, such as the integrated random excursion model, or, space-time correlated Lévy walks and flights, with similar statistical behavior. We compare the WEB related properties of these models and find surprising differences although, for equivalent parameters, all of them are supposed to lead to the same ensemble-averaged MSD. Our findings are relevant for distinguishing possible models for the anomalous diffusion occurring in experimental situations.

**12:51PM S40.00007 Disordered confinement and anomalous diffusion<sup>1</sup>**, GERALD LAPEYRE, IDAEA-CSIC / ICFO — We discuss the effect of disordered confinement on anomalous diffusion. We treat confinement in conjunction with ordinary diffusion and with anomalous diffusions associated with aging and with correlated displacements. In particular, we compute the altered anomalous exponents. Finally, we relate these results to previous work and show that they shed light on the nature of diffusion on percolation clusters.

<sup>1</sup>Supported by the European Research Council (ERC), project MHetScale (617511), (Grant No. 2009 SGR 597), ERC AdG Osyris, and Spanish Ministry Projects (FOQUS (FIS2013-46768-P) and No. MAT2011-22887)

**1:03PM S40.00008 Non-equilibrium dynamics of the complex Ginzburg-Landau equation<sup>1</sup>**, WEIGANG LIU, UWE TAUBER, Virginia Tech — The complex Ginzburg-Landau equation combines the quantum many-particle nonlinear Schrödinger equation with the time-dependent Ginzburg-Landau equation or model A relaxational dynamics. It arises in quite diverse contexts that include spontaneous pattern formation out of equilibrium, chemical oscillations, multi-mode lasers, thermal convection in binary fluids, cyclic population dynamics, and driven-dissipative Bose-Einstein condensates. Indeed, the complex Ginzburg-Landau equation exhibits a remarkably rich phase diagram with intriguing dynamics. We employ detailed numerical studies as well as analytical tools such as the perturbative renormalization group and the spherical model limit to study the non-equilibrium coarsening and critical aging scaling for the complex Ginzburg-Landau equation following quenches from an initial disordered configuration to either one of the ordered phases or the critical point.

<sup>1</sup>This research is supported by the U. S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering under Award DE-FG02-09ER46613.

**1:15PM S40.00009 Multiscale phenomena and crossover in fluctuations in non-equilibrium systems**, A. SURJALAL SHARMA, VENKAT ANURAG SETTY, University of Maryland — Fluctuations in multiscale phenomena in natural systems, e. g., Earth's magnetosphere, exhibit crossover behavior in the scaling exponents. These exponents represent the nature of correlation in the system and the crossover shows the presence of more than one type of correlation. An accurate characterization of the crossover behavior is thus needed for a better understanding of the inherent correlations in the system. A multi-step process is developed for accurate computation of the crossover behavior. First the detrended fluctuation analysis is used to remove the trends in the data and the scaling exponents are computed. The crossover point is then computed by a Hyperbolic regression technique, with no prior assumptions. The time series data of the magnetic field variations in the Earth's magnetosphere is analyzed with these techniques and yields a crossover behavior with a time scale of ~ 4 hrs. A Langevin model of the magnetospheric dynamics yields an excellent fit to the crossover in the scaling exponents and thus provide a model of the non-equilibrium system.

**1:27PM S40.00010 Ligand binding kinetics in surface plasmon resonance devices: A Monte Carlo simulation analysis**, JACOB CARROLL, UWE TAUBER, Virginia Tech — Surface plasmon resonance (SPR) chips are widely used to measure association and dissociation rates for the binding kinetics between two species of chemicals, e.g., cell receptors and ligands. It is commonly assumed that ligands are spatially well mixed in the SPR region, and hence a mean-field rate equation description is appropriate. This approximation however ignores the spatial fluctuations as well as temporal correlations induced by multiple local rebinding events, which become prominent for slow diffusion rates. We report detailed Monte Carlo simulations of ligand binding kinetics in an SPR cell subject to laminar flow. We extract the binding and dissociation rates by means of the techniques frequently employed in experimental analysis that are motivated by the mean-field approximation. We find major discrepancies in a wide parameter regime between the thus extracted rates and the input simulation values. These results underscore the crucial quantitative importance of spatio-temporal correlations in binary reaction kinetics in SPR cell geometries.

**1:39PM S40.00011 Thermodynamic and Information Entropy in Electroconvection**, JOHN CRESSMAN, George Mason University, MARCUS DAUM, George Institute of Technology, DAVID PATRICK, George Mason University, RORY CERBUS, WALTER GOLDBURG, University of Pittsburgh — Transitions in driven systems often produce wild fluctuations that can be both detrimental and beneficial. Our fundamental understanding of these transients is inadequate to permit optimal interactions with systems ranging from biology, to energy generation, to finance. Here we report on experiments performed in electroconvecting liquid crystals where we abruptly change the electrical forcing across the sample from a state below defect turbulence into a state of defect turbulence. We simultaneously measure the electrical power flow through the liquid crystal as well as image the structure in the sample. These measurements enable us to simultaneously track the evolution of the thermodynamic and information entropies. Our experiments demonstrate that there are strong correlations between the fluctuations in these two entropic measures however they are not exact. We will discuss these discrepancies as well as the relevance of large transient fluctuations in non-equilibrium transitions in general.

**1:51PM S40.00012 Low dissipation in non-equilibrium control: sampling the ensemble of efficient protocols.**, GRANT ROTSKOFF, Univ of California - Berkeley, TODD GINGRICH, Massachusetts Institute of Technology, GAVIN CROOKS, Lawrence Berkeley National Laboratory, PHILLIP GEISSLER, Univ of California - Berkeley — Designing schemes to efficiently control fluctuating, non-equilibrium systems is problem of fundamental importance and tremendous practical interest. A number of optimization techniques have proven fruitful in the pursuit of optimal control, but these approaches focus on the singular goal of finding the exact, optimal protocol. Here, we investigate the diversity of protocols that achieve low dissipation with a Monte Carlo path sampling algorithm. Akin to Boltzmann weighting configurations in Metropolis Monte Carlo, each protocol is exponentially biased by its mean dissipation. We show that the ensemble of low dissipation protocols can be sampled exactly in the Gaussian limit and that the method continues to robustly generate low dissipation protocols, even as the external control drives the system far from equilibrium.

**2:03PM S40.00013 Geometry of dissipative evolution equations**, CELIA REINA, University of Pennsylvania — The modeling of continuum dissipative evolution equations remains a challenge and is primarily based on phenomenological constitutive relations. In this talk we present some connections between the geometry of dissipative gradient flows, the principle of maximum entropy production, large deviation principles for stochastically augmented evolution equations and fluctuation-dissipation relations.

**Thursday, March 17, 2016 11:15AM - 2:03PM –**

**Session S41 DBIO DPOLY DCOMP: Physics of Proteins: Protein Structure and Interactions**

344 - Aihua Xie, Oklahoma State University

**11:15AM S41.00001 Dynamics and mechanism of ultrafast water-protein interactions**, DONGPING ZHONG<sup>1</sup>, Ohio State Univ - Columbus — Protein hydration is essential to protein stability, flexibility, dynamics and function. We have used a tryptophan scan with femtosecond spectroscopy to probe global surface water dynamics and characterize the coupled interactions of water and proteins. With extensive temperature-dependent studies, we found that water plays the dominant role to drive relaxation on the picosecond time scales. By measuring both water and protein relaxations, it shows that hydration water drives local protein fluctuations, a clear beta-relaxation, and such results are significant for the understanding of protein dynamics and functions.

<sup>1</sup>This is an invited speaker.

**11:51AM S41.00002 Effect of protein crystal hydration on side chain conformational heterogeneity**, HAKAN ATAKISI, DAVID MOREAU, JESSE HOPKINS, ROBERT THORNE, Cornell University, ROBERT THORNE'S GROUP TEAM — The structure of protein crystals is determined in part by water-mediated interactions involving both protein surface-ordered (hydration) and bulk water, and so is sensitive to the relative humidity of the environment. Monoclinic lysozyme provides a remarkable model for studying structural changes induced by dehydration, as it maintains excellent order for relative humidities (r.h.) down to 5%, corresponding to solvent content of 9% by volume, much smaller than the 88% (22% by volume) at which lysozyme loses its enzymatic activity. Although the main chain conformation does not change significantly, the effect of dehydration on side chain conformations has not been systematically studied. High resolution (1.1 to 1.7 Å) structural data sets for monoclinic lysozyme at r.h. between 99% and 11% have been analyzed to identify major and minor side chain conformers at each humidity, and to map out how the side chain conformational ensemble evolves with hydration. Modest dehydration produces comparable overall effects to cooling to  $T=100$  K, but with conformational changes largely confined to solvent-exposed residues. The largest side chain conformation changes occur at humidities that deplete water within the first two hydration shells.

**12:03PM S41.00003 Determination of Protein Surface Hydration by Systematic Charge Mutations.**, JIN YANG, Department of Physics, The Ohio State University, MENGHUI JIA, State Key Laboratory of Precision Spectroscopy, East China Normal University, YANGZHONG QIN, Department of Physics, The Ohio State University, DIHAO WANG, Program of Biochemistry, The Ohio State University, HAIFENG PAN, State Key Laboratory of Precision Spectroscopy, East China Normal University, LIJUAN WANG, Department of Physics, The Ohio State University, JIANHUA XU, State Key Laboratory of Precision Spectroscopy, East China Normal University, DONGPING ZHONG, Department of Physics, Department of Chemistry and Biochemistry, and Programs of Biophysics, Chemical Physics and Biochemistry, The Ohio State University, DONGPING ZHONG COLLABORATION, JIANHUA XU COLLABORATION — Protein surface hydration is critical to its structural stability, flexibility, dynamics and function. Recent observations of surface solvation on picosecond time scales have evoked debate on the origin of such relatively slow motions, from hydration water or protein charged sidechains, especially with molecular dynamics simulations. Here, we used a unique nuclease with a single tryptophan as a local probe and systematically mutated neighboring three charged residues to differentiate the contributions from hydration water and charged sidechains. By mutations of alternative one and two and all three charged residues, we observed slight increases in the total tryptophan Stokes shifts with less neighboring charged residue(s) and found insensitivity of charged sidechains to the relaxation patterns. The dynamics is correlated with hydration water relaxation with the slowest time in a dense charged environment and the fastest time at a hydrophobic site. On such picosecond time scales, the protein surface motion is restricted. The total Stokes shifts are dominantly from hydration water relaxation and the slow dynamics is from water-driven relaxation, coupled with local protein fluctuations.

**12:15PM S41.00004 Biomolecular solvation study of proteins in liquid water by a wide range gigahertz-to-terahertz spectroscopy**, ALI CHARKHESHT, DEEPU GEORGE, VINH NGUYEN, Virginia Tech — Solvent dynamics within biomolecular solvation layers play a major role in enzyme activity, but obtaining an accurate and quantitative picture of solvent activity around proteins is challenging. Due to the strong absorption of water in the gigahertz-to-terahertz frequencies, it is challenging to study properties of the solvent dynamics as well as conformational changes protein in water. We have developed a highly sensitive dielectric gigahertz-to-terahertz frequency-domain spectroscopy system for probing the collective dynamics of proteins and solvent. Using this technique, we investigate the complex dielectric response of bovine serum albumin and lysozyme proteins in aqueous environment on a wide frequency range from 0.1 GHz up to 2 THz. We explore the conformation flexibility of proteins and compare the hydration dynamics around proteins to understand the effects of surface-mediated solvent dynamics, relationships among different measures of interfacial solvent dynamics, and protein-mediated solvent dynamics.

**12:27PM S41.00005 Structure and conformation of peptides at air/aqueous interface and their impact on interfacial water structure.**, KAILASH CHANDRA JENA<sup>1</sup>, Assistant Professor, DEEPAK TOMAR<sup>2</sup>, Research Scholar — Process of protein folding is very essential for the proper functioning of the protein molecules at membrane surface and other organelles. Understanding the process of protein folding at various biological relevant aqueous interfaces are very important to understand various complicated chemical and physical processes relevant to chemistry, physics, and medicine. The building blocks of proteins molecules are amino acids and the chemistry of each amino acid is very different; as a consequence their sequence plays an important role for various conformations upon adsorption for the protein molecules. In the present study, we have investigated the interfacial structure and conformation of two amino acids (L-Proline and L-Tyrosine) and peptide molecules formed from these two amino acids (L-Tyr-Pro). We have used sum frequency generation (SFG) vibrational spectroscopy to probe the air/aqueous interface. We have studied the impact of adsorption of the amino acids and the peptide molecules on the interfacial water structure by slowly varying concentration and ionic strength of the solutions. Our preliminary result shows a huge impact of the adsorption process of peptide molecules on the hydrogen bonding environment of interfacial structure of water.

<sup>1</sup>Indian Institute of Technology Ropar, Nangal Road, Rupnagar, Punjab-140001

<sup>2</sup>Indian Institute of Technology Ropar, Nangal Road, Rupnagar, Punjab-140001

**12:39PM S41.00006 Roles of urea and TMAO on the interaction between extended non-polar peptides**, ZHAOQIAN SU<sup>1</sup>, CRISTIANO DIAS<sup>2</sup>, New Jersey Inst of Tech — Urea and trimethylamine n-oxide (TMAO) are small molecules known to destabilize and stabilize, respectively, the structure of proteins when added to aqueous solution. To unravel the molecular mechanisms of these cosolvents on protein structure we perform explicit all-atom molecular dynamics simulations of extended poly-alanine and polyleucine dimers. We use an umbrella sampling protocol to compute the potential of mean force (PMF) of dimers at different concentrations of urea and TMAO. We find that the large non-polar side chain of leucine is affected by urea whereas backbone atoms and alanine's side chain are not. Urea is found to occupy positions between leucine's side chains that are not accessible to water. This accounts for extra Lennard-Jones bonds between urea and side chains that favors the unfolded state. These bonds compete with urea-solvent interactions that favor the folded state. The sum of these two energetic terms provide the enthalpic driving force for unfolding. We show here that this enthalpy correlate with the potential of mean force of poly-leucine dimers. Moreover, the framework developed here is general and may be used to provide insights into effects of other small molecules on protein interactions. The effect of the TMAO will be in the presentation.

<sup>1</sup>Department of Physics, University Heights, Newark, New Jersey, 07102-1982

<sup>2</sup>Department of Physics, University Heights, Newark, New Jersey, 07102-1982

**12:51PM S41.00007 Theory Of Salt Effects On Protein Solubility**<sup>1</sup>, YUBA DAHAL, JEREMY SCHMIT, Kansas State Univ — Salt is one of the major factors that effects protein solubility. Often, at low salt concentration regime, protein solubility increases with the salt concentration (salting in) whereas at high salt concentration regime, solubility decreases with the increase in salt concentration (salting out). There are no quantitative theories to explain salting in and salting out. We have developed a model to describe the salting in and salting out. Our model accounts for the electrostatic Coulomb energy, salt entropy and non-electrostatic interaction between proteins. We analytically solve the linearized Poisson Boltzmann equation modelling the protein charge by a first order multipole expansion. In our model, protein charges are modulated by the anion binding. Consideration of only the zeroth order term in protein charge doesn't help to describe salting in phenomenon because of the repulsive interaction. To capture the salting in behaviour, it requires an attractive electrostatic interaction in low salt regime. Our work shows that at low salt concentration, dipole interaction is the cause for salting in and at high salt concentration a salt-dependent depletion interaction dominates and gives the salting out. Our theoretical result is consistent with the experimental result for Chymosin protein

<sup>1</sup>NIH Grant No R01GM107487

### 1:03PM S41.00008 Computational and Experimental Study of Neuroglobin and Mutants<sup>1</sup>

LAUREN NELSON, Wake Forest University Department of Physics, SAMUEL CHO, Wake Forest University Departments of Physics and Computer Science, DANIEL KIM-SHAPRIO, Wake Forest University Department of Physics —

Neuroglobin (Ngb) is a hexacoordinated heme protein that is closely related to hemoglobin and myoglobin and normally found in the brain and nervous systems. It is involved in cellular oxygen homeostasis and reversibly binds to oxygen with a higher binding affinity than hemoglobin. To protect the brain tissue from hypoxic or ischemic conditions, Ngb increases oxygen availability. We have previously shown that a mutant form of Ngb reduces nitrite to nitric oxide 50x faster than myoglobin and 500x faster than hemoglobin. It also tightly binds to carbon monoxide (CO) with an association rate that is 500x faster than hemoglobin. To analyze the structure of neuroglobin and the characteristics causing these phenomena, we performed 3 sets of 1 microsecond molecular dynamic (MD) simulations of wild-type oxidized and reduced human Ngb and their C46A, C55A, H64L, and H64Q mutants. We also directly compare our MD simulations with time-resolved absorption spectroscopy. These studies will help identify treatments for diseases involving low nitric oxide availability and carbon monoxide poisoning.

<sup>1</sup>This research was supported by an NIH NSRA predoctoral fellowship in the Structural and Computational Biophysics Program training grant (T32GM095440-05).

### 1:15PM S41.00009 Analysis of Cavity Volumes in Proteins Using Percolation Theory , SHERIDAN GREEN, The University of North Carolina at Chapel Hill, DONALD JACOBS, JENNY FARMER, The University of North Carolina at Charlotte —

Molecular packing is studied in a diverse set of globular proteins in their native state ranging in size from 34 to 839 residues. An new algorithm has been developed that builds upon the classic Hoshen-Kopelman algorithm for site percolation combined with a local connection criterion that classifies empty space within a protein as a cavity when large enough to hold a spherical shaped probe of radius, R, otherwise a microvoid. Although microvoid cannot fit an object (e.g. molecule or ion) that is the size of the probe or larger, total microvoid volume is a major contribution to protein volume. Importantly, the cavity and microvoid classification depends on probe radius. As probe size decreases, less microvoid forms in favor of more cavities. As probe size is varied from large to small, many disconnected cavities merge to form a percolating path. For fixed probe size, microvoid, cavity and solvent accessible boundary volume properties reflect conformational fluctuations. These results are visualized on three-dimensional structures. Analysis of the cluster statistics within the framework of percolation theory suggests interconversion between microvoid and cavity pathways regulate the dynamics of solvent penetration during partial unfolding events important to protein function.

### 1:27PM S41.00010 Characterization of DNA-protein interactions using high-throughput sequencing data from pulldown experiments<sup>1</sup> , BLYTHE MORELAND, Ohio State Univ - Columbus, KENJI OMAN, Fred Hutchinson Cancer Research Center, JOHN CURFMAN, PEARLLY YAN, RALF BUNDSCHUH, Ohio State Univ - Columbus —

Methyl-binding domain (MBD) protein pulldown experiments have been a valuable tool in measuring the levels of methylated CpG dinucleotides. Due to the frequent use of this technique, high-throughput sequencing data sets are available that allow a detailed quantitative characterization of the underlying interaction between methylated DNA and MBD proteins. Analyzing such data sets, we first found that two such proteins cannot bind closer to each other than 2 bp, consistent with structural models of the DNA-protein interaction. Second, the large amount of sequencing data allowed us to find rather weak but nevertheless clearly statistically significant sequence preferences for several bases around the required CpG. These results demonstrate that pulldown sequencing is a high-precision tool in characterizing DNA-protein interactions.

<sup>1</sup>This material is based upon work supported by the National Science Foundation under Grant No. DMR-1410172.

### 1:39PM S41.00011 Molecular stripping in the $NF\kappa B/I\kappa B/DNA$ genetic regulatory network ,

DAVIT POTOYAN, PETER WOLYNES, Rice University — Genetic switches based on the  $NF\kappa B/I\kappa B/DNA$  system are master regulators of an array of cellular responses. Recent kinetic experiments have shown that  $I\kappa B$  can actively remove  $NF\kappa B$  bound to its genetic sites via a process called "molecular stripping". This allows the  $NF\kappa B/I\kappa B/DNA$  switch to function under kinetic control rather than the thermodynamic control contemplated in the traditional models of gene switches. Using molecular dynamics simulations of coarse grained predictive energy landscape models for the constituent proteins by themselves and interacting with the DNA we explore the functional motions of the transcription factor  $NF\kappa B$  and its various binary and ternary complexes with DNA and the inhibitor  $I\kappa B$ . These studies show that the function of the  $NF\kappa B/I\kappa B/DNA$  genetic switch is realized via an allosteric mechanism. Molecular stripping occurs through the activation of a domain twist mode by the binding of  $I\kappa B$  which occurs through conformational selection. Free energy calculations for DNA binding show that the binding of  $I\kappa B$  not only results in a significant decrease of the affinity of the transcription factor for the DNA but also kinetically speeds DNA release. Projections of the

### 1:51PM S41.00012 Modeling Adsorption Kinetics (Bio-remediation of Heavy Metal Contaminated Water).<sup>1</sup> , CHRIS MCCARTHY, BMCC CUNY —

My talk will focus on modeling the kinetics of the adsorption and filtering process using differential equations, stochastic methods, and recursive functions. The models have been developed in support of our interdisciplinary lab group which is conducting research into bio-remediation of heavy metal contaminated water via filtration through biomass such as spent tea leaves. The spent tea leaves are available in large quantities as a result of the industrial production of tea beverages. The heavy metals bond with the surfaces of the tea leaves (adsorption).

<sup>1</sup>Funding: CUNY Collaborative Incentive Research Grant

## Thursday, March 17, 2016 11:15AM - 2:15PM —

Session S42 DPOLY GSOFT: Assembly of Nanoparticles 345 - Chang Ryu, Rensselaer Polytechnic Institute

### 11:15AM S42.00001 Polydots, Soft Nanoparticles, at Membrane Interfaces , SIDATH WIJESINGHE,

DVORA PERAHIA, Clemson University, CHRISTOPH JUNGHANS, Los Alamos National Laboratory, GARY GREEST, Sandia National Laboratories — Luminescent polymers confined into long lived nano-configurations form dynamic nanoparticles (NPs) or polydots with a potential for new bio imaging markers and targeted drug delivery vehicles. A key step in the use of any NP for therapeutic applications is their translocation across membranes. Here we report the results of all-atom molecular dynamics simulation of a polydot that consists of carboxylate decorated dinonyl poly para phenylene ethynylene, at the interface with a 1,2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC) bilayer. The polydot size and surface charge are controlled by varying the polymer molecular weight and degree of carboxylation. The polydot structure and its effect on the membrane structure are probed. We find that the polydot remains stable as it transcends the membrane where the initial curvature of the membrane is strongly affected as polydot inserted, but it relaxes with time. The larger the polydots are the less dynamic the DPPC molecules become. Further we find that neutral-surface polydots reside in the center of the bilayer, while increasing the polydot surface charge, the polydot migrates towards the hydrophilic leaflet of the bilayer.

**11:27AM S42.00002 Surface-Engineered Graphene Quantum Dots for Shape Control of Block Copolymer Particles**, HYUNSEUNG YANG, KANG HEE KU, JAE MAN SHIN, JUNHYUK LEE, CHAN HO PARK, HAN-HEE CHO, KAIST, SE GYU JANG, KIST, BUMJOON KIM, KAIST, KIST COLLABORATION — Surface-engineered, 10 nm-sized graphene quantum dots (GQDs) are shown to be efficient surfactants for producing poly(styrene-*b*-4-vinylpyridine) (PS-*b*-P4VP) particles that feature tunable shapes and internal morphologies. The surface properties of GQDs were modified by grafting different alkyl ligands, such as hexylamine and oleylamine, to generate the surfactant behavior of the GQDs. In stark contrast to the behavior of the unmodified GQDs, hexylamine-grafted GQDs and oleylamine-grafted GQD surfactants were selectively positioned on the PS and P4VP domains, respectively, at the surface of the particles. This positioning effectively tuned the interfacial interaction between two different PS/P4VP domains of the particles and the surrounding water during emulsification and induced a dramatic morphological transition to an unconventional convex lens-shaped particles. Precise and systematic control of interfacial activity of GQD surfactants was also demonstrated by varying the density of the alkyl ligands on the GQDs. The excellent surface tunability of 10 nm-sized GQDs combined with their significant optical and electrical properties highlight their importance as surfactants for producing colloidal particles with novel functions.

**11:39AM S42.00003 Self-Assembled Soft Porous Particles with Tailored Nano-Porosity.**, KANG HEE KU, JAEMAN SHIN, KAIST, DANIEL KLINGER, U.C. Santa Barbara, RYAN C. HAYWARD, University of Massachusetts, SE GYU JANG, KIST, CRAIG J. HAWKER, U.C. Santa Barbara, BUMJOON J. KIM, KAIST — A series of porous block copolymer (BCP) particles with controlled porosity and nanostructure was fabricated by tuning interfacial hydrodynamics of toluene-in-water emulsion droplets. A synergistic adsorption of polystyrene-*b*-poly(4-vinylpyridine) (PS-*b*-P4VP) BCPs and sodium dodecyl sulfate (SDS) to the surface of emulsion particle induced a dramatic decrease in the interfacial tension and generated the interfacial instability at the particle surface, thus producing different types of particles including closed pore particles, open pore particles, capsules and micelles. In particular, the SDS concentration and the P4VP volume fraction of PS-*b*-P4VP were key parameters in determining the degree of interfacial instability of the emulsion, producing porous particles with tunable pore sizes ranging from 10 to 500 nm. These porous particles could be used as pH responsive carriers, which were demonstrated by combining and releasing of different colored dyes to particles at desired pH conditions.

**11:51AM S42.00004 Particle-Directed Assembly of Semiflexible Polymer Chains**, MICHAEL MCGOVERN, KEVIN DORFMAN, DAVID MORSE, University of Minnesota — We use molecular dynamics simulations to investigate several models of semiflexible polymers that exhibit an attractive interaction with spherical particles. The organization of semiflexible polymer chains through attractive interactions with spherical particles occurs in several important processes in nature, such as the winding of DNA around histones and counter-ion condensation of charged polymers. The process is also of technological interest in the packaging of DNA for delivery to cells. In this presentation, we will present data on both the phase behavior and the kinetics of self-assembly as a function of the stiffness of the polymers, the attractive potential between the monomers and the particles, and the relative size of the monomers and particles. Our simulations suggest a transition between globular and rod-like aggregates that changes from a gradual to a sudden transition depending on particle size, and that rod formation is a slow, nucleation dependent process.

**12:03PM S42.00005 Structure and Entanglement Factors on Dynamics of Polymer Grafted Magnetic Nanoparticles**, SIQI LIU, Stevens Institute of Technology, ERKAN SENSES, NCNR NIST, YANG JIAO, Air Force Research Laboratory, SURESH NARAYANAN, Argonne National Laboratory, PINAR AKCORA, Stevens Institute of Technology — Magnetic nanoparticles functionalized with long polymer chains at low graft density are interesting systems to study structure-dynamic relationships in polymer nanocomposites since they are shown to aggregate into strings in both solution and melts, and also into spheres and branched aggregates in the presence of free polymer chains. This work investigates the structure, free volume and entanglement effects in composites of polystyrene grafted iron oxide nanoparticles by measuring particle dynamics with x-ray photon correlation spectroscopy technique. Particles of highly ordered strings and aggregated systems follow heterogeneous dynamics commonly observed in jammed soft glassy systems and other nanocomposites. On the other hand, particle dynamics becomes diffusive in branched structures which could be caused by the less penetration of long matrix chains into the brushes. These results show that particle dynamics is dictated through the strong interactions of low graft density chains with the host polymer.

**12:15PM S42.00006 Selective Permeability of Uranyl Peroxide Nanocages to Different Alkali Ions: Influences from Surface Pores and Hydration Shells<sup>1</sup>**, YUNYI GAO, Univ of Akron, JENNIFER SZYMANOWSKI, PETER BURNS, University of Notre Dame, TIANBO LIU, Univ of Akron — The precise guidance to different ions across the biological channels is essential for many biological processes. An artificial nanopore system will facilitate the study of ion transport mechanism through nanosized channels and offer new views for designing nanodevices. Here we reveal that a 2.5-nm-size, fullerene-shaped molecular cluster  $\text{Li}_{48+m}\text{K}_{12}(\text{OH})_m[\text{UO}_2(\text{O}_2)(\text{OH})]_{60-(\text{H}_2\text{O})_n}$  ( $m \approx 20$  and  $n \approx 310$ ) ( $\text{U}_{60}$ ) shows selective permeability to different alkali ions. The sub-nanometer pores on the water-ligand-rich surface of  $\text{U}_{60}$  are able to block  $\text{Rb}^+$  and  $\text{Cs}^+$  ions from passing through, while allow  $\text{Na}^+$  and  $\text{K}^+$  ions, which possess larger hydrated sizes, to enter the interior space of  $\text{U}_{60}$ . An interestingly high entropy gain during the binding process between  $\text{U}_{60}$  and alkali ions suggest that the hydration shells of  $\text{Na}^+/\text{K}^+$  and  $\text{U}_{60}$  are damaged during the interaction. The ion selectivity of  $\text{U}_{60}$  is greatly influenced by both the morphologies of surface nanopores and the dynamics of the hydration shells.

<sup>1</sup>This material is based upon work supported as part of the Materials Science of Actinides Center, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001089

**12:27PM S42.00007 Understanding of DNA directed nanoparticle superlattices in bulk and thin film**, BYEONGDU LEE, Argonne National Laboratory — Over the years, there have been significant advances in assembling nanoparticles with DNA into superlattices. Since the first reports on DNA directed FCC and BCC superlattices consisting of single type of spherical nanoparticles,[1,2] building blocks for the DNA-nanoparticle superlattices have been extended from a spherical gold nanoparticle to various types of other particles including quantum dots, magnetic, hollow, or polyhedral particles.[3,4] Not only single component, but superlattices of binary[5] and ternary components[6] have also been synthesized. Although still many details are unclear, now there is a general consensus about thermodynamics of this type of assembly, which led us to fabricate thin films of DNA directed nanoparticle superlattices on substrate for applications such as optical materials.[7] Since the structures are formed in aqueous condition, small angle x-ray scattering (SAXS) that does not disturb the system has been a critical tool to determine structural and thermodynamic characteristics of the assemblies. Thus, we have also been improving SAXS instrumentations and computational methods to calculate scattering profiles for the nanoparticle superlattices.[8] In this talk, we will summarize our works with a focus on some structural details of these superlattices and DNA and understanding about the role of DNA in the crystallization processes in bulk and thin film. 1. Park, S. Y. et al, C. A. Nature 2008, 451, 553. 2. Nykypanchuk, D. et al, Nature 2008, 451, 549. 3. Jones, M. R. et al, Nat Mater 2010, 9, 913. 4. O'Brien, M. N. et al, Nat Mater 2015, 14, 833. 5. Macfarlane, R. J. et al, Science 2011, 334, 204. 6. Macfarlane, R. J. et al, Science 2013, 341, 1222. 7. Senesi, A. J. et al, Angew. Chem. Intern. Ed. 2013, 52, 6624. 8. Senesi, A. J. and Lee, B. J. of Appl. Crystallog. 2015, 48, 1172.

**1:03PM S42.00008 Modeling of water-borne coating: stress relaxation of suspensions of colloids linked by telechelic HEUR polymers.**<sup>1</sup> , SHIHU WANG, RONALD G. LARSON, Univ of Michigan - Ann Arbor — In water-borne coatings, the rheology of colloidal suspensions is modified by the presence of rheological modifiers, such as Hydrophobic Ethoxylated Urethane (HEUR) polymers. HEUR is a telechelic polymer with two hydrophobic tails (hydrophobes) and a long hydrophilic interblock consisting of poly(ethylene oxide), and its thickening effect is largely determined by the self-association of hydrophobes as well as their adsorption onto latex particles. Here we describe a model that simulates the complex interactions among latex particles due to the formation of bridges or superbridges via model HEURs. We calculate the stress relaxation of the system and identify different relaxation modes. We explore the relaxation time at different latex volume fractions, HEUR concentrations and energies of association between hydrophobes and latex particles, and discuss its relationship with the bridge or latex cluster formation. These results provide important insights for HEUR adsorption and water-borne coating rheology.

<sup>1</sup>We acknowledge the financial support from The Dow Chemical Company.

**1:15PM S42.00009 Anisotropic Packing of DNA-Mediated Colloidal Self-Assembly** , THI VO, Chemical Engineering, Columbia University, FANG LU, YUGANG ZHANG, OLEG GANG, Center for Functional Nanomaterials, Brookhaven National Lab, SANAT KUMAR, Chemical Engineering, Columbia University — The self-assembly of DNA-grafted nanoparticles has garnered considerable interest in recent years. However, many efforts focused on the usage of spherical nanoparticles, which limits us to the formation of only a handful of crystal lattices. Recent advances in the synthesis of non-spherical particles have directed attention towards the usage of these anisotropic particles for self-assembly. Here we combine experiments and theory on a series of DNA-grafted nanocubes. Our studies indicate that anisotropy not only directs where DNA linkers graft onto the particle but also affects how they pack and orient within a lattice, giving rise to both a preferential attachment effect and orientation-directed self-assembly. These results emphasize anisotropic self-assembly as a powerful new tool that allows for precise and directed control of nanoparticle self-assembly.

**1:27PM S42.00010 Giant soft-memory in liquid crystal-nanocomposites** , RAVINDRA KEMPAIAH, YIJING LIU, ZHIHONG NIE, University of Maryland, College Park, RAJRATAN BASU, US Naval Academy — Here, we report a novel way of introducing giant, non-volatile soft-memory in a nanocomposite comprising of amphiphilic polymer functionalized barium titanate ( $\text{BaTiO}_3$ ) nanoparticles and *isotropic* phase of 5CB liquid crystal. Doping of pure ferroelectric NPs in isotropic phase of 5CB creates nanoscopic domains of highly ordered regions as 5CB molecules arrange themselves around the NPs and we call these regions, *pseudonematic domains*. Here, mesogens can *electromechanically* rotate the  $\text{BaTiO}_3$  NPs within the domain, along the direction of applied electric field. These domains are spatially and thermodynamically locked-in and retain their directional orientation and net polarization even after the applied electric field is switched off. We call this net remnant polarization or hysteresis, '*soft memory*'. When NPs are functionalized with amphiphilic block copolymers, self-assembly of mesogens occurs at the interface of polymer tethers and nanoparticles via combination of non-covalent coupling and  $\pi$ - $\pi$  stacking interaction and this results in multi-fold enhancement in the volume of pseudonematic domains and subsequent increase in the soft memory. This work provides new insight into understanding the interaction of nanoparticles, polymers and liquid crystal and potentially lead to the creation of nanoelectromechanical (NEMS) storage device using functionalized nanoparticles.

**1:39PM S42.00011 Temperature Effects on Soft Polymeric Nanoparticles: Molecular Dynamics Study**<sup>1</sup> , SABINA MASKEY, Clemson University, GARY S. GRETT, Sandia National Laboratory, DVORA PERAHIA, Clemson University — Luminescent polymers collapsed into soft nanoparticles or polydots have emerged as the potential candidates for biomedical applications such as drug delivery and biosensing. Here, using fully atomistic molecular dynamics simulation, the temperatures effects on the stability, internal structure and dynamics of polydots formed by substituted and bare dialkyl *para* phenylene ethynylenes (PPEs) will be discussed. We find that with increasing temperature from 300 K to 600K both substituted and bare PPE polydots expand but do not fully unfold and remain in their confined state. As observed visually and by measurement of structure factor  $S(q)$ , the overall shape of the both type of polydots changes from spherical to elongated with the increase in temperature. These effects are more pronounced for bare PPE polydots which show that interdigitation of side chains in substituted PPE polydots enhances stability. In addition, the side chains are more dynamic than the backbone..

<sup>1</sup>NSF CHE 1308298 2013-2016

**1:51PM S42.00012 Spectroscopic Investigations on PVDF-MWCNTs Nanocomposites.** , OSCAR GUERRERO, SAMANTHA RAMIREZ, ROBERT JONES, BRIAN YUST, JAMES HINTHORNE, MIRCEA CHIPARA, Univ of Texas Rio Grande Valley — Nanocomposites have been obtained by dispersing Multi Walled Carbon Nanotubes (MWCNTs) within polyvinylidene fluoride. Various samples loaded by 0 to 20 % wt. MWCNTs have been obtained by melt mixing using a Haake RheoMixer, with two counter rotating screws. The effect of the nanofiller concentration on the glass, melting, and crystallization temperatures, as determined from Differential Scanning Calorimetry measurements, is reported. Small shifts towards higher temperatures as the loading with MWCNTs was increased have been noticed. A detailed analysis on the effect of MWCNTs on the degree of crystallinity of PVDF is reported. Raman data obtained by using a Renishaw InVia spectrometer have been used to estimate the stress transfer. Additional information was obtained by FTIR and Wide Angle X-Ray Scattering. The nature of the crystalline phases was determined for each sample. Thermogravimetric data showed a small increase of the thermal stability of the polymeric matrix upon the loading with MWCNTs.

**2:03PM S42.00013 Investigation of Molecular Interactions between AFM-Tip and Thiol Films**<sup>1</sup> , AHMED TOUHAMI, JUSTIN MOORE, University of Texas Rio Grande Valley, T. RANDALL LEE, University of Houston — Among various self-assembly processes, the formation of a self-assembled monolayer (SAM) is one of the most elegant ways for making an organic film with specific surface properties. Recently, much effort has been devoted in using AFM-based single-molecule force spectroscopy (SMFS) to understanding the formation of alkanethiol SAMs on gold surfaces. Investigating the factors that affect the AFM tip-SAMs interactions is necessary to clarify the controversial results of these studies. Here, we investigated the interactions between bare AFM-tips and several SAMs thiols-gold surfaces under controlled humidity conditions. Our results demonstrate that the Tip-SAM interactions can be used to precisely determine the length of the thiol chains, the adhesion force between thiols head groups and the AFM tip, and the strength of the thiol-gold contact. Our findings on the dynamics and the structure of the SAMs of alkanethiols on gold are useful for detail understanding of the thermodynamics, kinetics and mechanisms of SAM technology assembly.

<sup>1</sup>NSF

**Thursday, March 17, 2016 11:15AM - 1:51PM –**  
**Session S43 GSNP: Nonlinear Dynamics in Networks II** 346 - Adilson Motter, Northwestern University

## 11:15AM S43.00001 Quantifying Stability in Complex Networks: From Linear to Basin Stability

JÜRGEN KURTHS, Humboldt University — The human brain, power grids, arrays of coupled lasers and the Amazon rainforest are all characterized by multistability. The likelihood that these systems will remain in the most desirable of their many stable states depends on their stability against significant perturbations, particularly in a state space populated by undesirable states. Here we claim that the traditional linearization-based approach to stability is in several cases too local to adequately assess how stable a state is. Instead, we quantify it in terms of basin stability, a new measure related to the volume of the basin of attraction. Basin stability is non-local, nonlinear and easily applicable, even to high-dimensional systems. It provides a long-sought-after explanation for the surprisingly regular topologies of neural networks and power grids, which have eluded theoretical description based solely on linear stability. Specifically, we employ a component-wise version of basin stability, a nonlinear inspection scheme, to investigate how a grid's degree of stability is influenced by certain patterns in the wiring topology. Various statistics from our ensemble simulations all support one main finding: The widespread and cheapest of all connection schemes, namely dead ends and dead trees, strongly diminish stability. For the Northern European power system we demonstrate that the inverse is also true: 'Healing' dead ends by addition of transmission lines substantially enhances stability. This indicates a crucial smart-design principle for tomorrow's sustainable power grids: add just a few more lines to avoid dead ends. Further, we analyse the particular function of certain network motifs to promote the stability of the system. Here we uncover the impact of so-called detour motifs on the appearance of nodes with a poor stability score and discuss the implications for power grid design. Moreover, it will be shown that basin stability enables uncovering the mechanism for explosive synchronization and understanding of evolving networks.

Reference: P. Menck, J. Heitzig, N. Marwan, and J. Kurths, *Nature Physics* 9, 89 (2013) P. Menck, J. Heitzig, J. Kurths, and H. Schellnhuber, *Nature Communication* 5, 3969 (2014) P. Schultz, J. Heitzig, and J. Kurths, *New Journal Physics* 16, 125001 (2014) V. Kohar, P. Ji, A. Choudhary, S. Sinha, and J. Kurths, *Phys. Rev. E* 90, 022812 (2014) Y. Zou, T. Pereira, M. Small, Z. Liu, and J. Kurths, *Phys. Rev. Lett.* 112, 114102 (2014)

## 11:51AM S43.00002 Control of State Transitions in Complex and Biophysical Networks<sup>1</sup>

ADILSON MOTTER, DANIEL WELLS, WILLIAM KATH, Northwestern University — Noise is a fundamental part of intracellular processes. While the response of biological systems to noise has been studied extensively, there has been limited understanding of how to exploit it to induce a desired cell state. Here I will present a scalable, quantitative method based on the Freidlin-Wentzell action to predict and control noise-induced switching between different states in genetic networks that, conveniently, can also control transitions between stable states in the absence of noise. I will discuss applications of this methodology to predict control interventions that can induce lineage changes and to identify new candidate strategies for cancer therapy. This framework offers a systems approach to identifying the key factors for rationally manipulating network dynamics, and should also find use in controlling other classes of complex networks exhibiting multi-stability. Reference: D. K. Wells, W. L. Kath, and A. E. Motter, *Phys. Rev. X* 5, 031036 (2015).

<sup>1</sup>Work funded by CBC, NCI, NIGMS, and NSF.

## 12:03PM S43.00003 Landscape Construction in Dynamical Systems

YING TANG, RUOSHI YUAN, GAOWEI WANG, PING AO, Shanghai Jiao Tong Univ — The idea of landscape has been recently applied to study various of biological problems. We demonstrate that a dynamical structure built into nonlinear dynamical systems allows us to construct such a global optimization landscape, which serves as the Lyapunov function for the ordinary differential equation. We find exact constructions on the landscape for a class of dynamical systems, including a van der Pol type oscillator, competitive Lotka-Volterra systems, and a chaotic system. The landscape constructed provides a new angle for understanding and modelling biological network dynamics.

## 12:15PM S43.00004 Cell fate reprogramming by control of intracellular network dynamics<sup>1</sup>

JORGE G. T. ZANUDO, REKA ALBERT, The Pennsylvania State University — Identifying control strategies for biological networks is paramount for practical applications that involve reprogramming a cell's fate, such as disease therapeutics and stem cell reprogramming. Although the topic of controlling the dynamics of a system has a long history in control theory, most of this work is not directly applicable to intracellular networks. Here we present a network control method that integrates the structural and functional information available for intracellular networks to predict control targets. Formulated in a logical dynamic scheme, our control method takes advantage of certain function-dependent network components and their relation to steady states in order to identify control targets, which are guaranteed to drive any initial state to the target state with 100% effectiveness and need to be applied only transiently for the system to reach and stay in the desired state. We illustrate our method's potential to find intervention targets for cancer treatment and cell differentiation by applying it to a leukemia signaling network and to the network controlling the differentiation of T cells. We find that the predicted control targets are effective in a broad dynamic framework. Moreover, several of the predicted interventions are supported by experiments.

<sup>1</sup>This work was supported by NSF grant PHY 1205840.

## 12:27PM S43.00005 Predictive Control of Large Complex Networks

ALEKSANDAR HABER, ADILSON E. MOTTER, Northwestern University — Networks of coupled dynamical subsystems are increasingly used to represent complex natural and engineered systems. While recent technological developments give us improved means to actively control the dynamics of individual subsystems in various domains, network control remains a challenging problem due to difficulties imposed by intrinsic nonlinearities, control constraints, and the large-scale nature of the systems. In this talk, we will present a model predictive control approach that is effective while accounting for these realistic properties of complex networks. Our method can systematically identify control interventions that steer the trajectory to a desired state, even in the presence of strong nonlinearities and constraints. Numerical tests show that the method is applicable to a variety of networks, ranging from power grids to chemical reaction systems.

## 12:39PM S43.00006 Reconstructing Directed Networks From Noisy Dynamics<sup>1</sup>

HIU CHING TAM, EMILY SC CHING, Department of Physics, The Chinese University of Hong Kong — Complex systems can be fruitfully studied as networks of many elementary units, known as nodes, interacting with one another with the interactions being the links between the nodes. The overall behavior of the systems depends crucially on the network structure depicting how the nodes are linked with each other. It is usually possible to measure the dynamics of the individual nodes but difficult, if not impossible, to directly measure the interactions or links between the nodes. For most systems of interest, the links are directional in that one node affects the dynamics of the other but not vice versa. Moreover, the strength of interaction can vary for different links. Reconstructing directed and weighted networks from dynamics is one of the biggest challenges in network research. We have studied directed and weighted networks modelled by noisy dynamical systems with nonlinear dynamics and developed a method that reconstructs the links and their directions using only the dynamics of the nodes as input. Our method is motivated by a mathematical result derived for dynamical systems that approach a fixed point in the noise-free limit. We show that our method gives good reconstruction results for several directed and weighted networks with different nonlinear dynamics.

<sup>1</sup>Supported by Hong Kong Research Grants Council under Grant No. CUHK 14300914

**12:51PM S43.00007 Hamiltonian-Based Model to Describe the Nonlinear Physics of Cascading Failures in Power-Grid Networks**, YANG YANG, ADILSON MOTTER, Department of Physics and Astronomy, Northwestern University — A local disturbance to the state of a power-grid system can trigger a protective response that disables some grid components, which leads to further responses, and may finally result in large-scale failures. In this talk, I will introduce a Hamiltonian-like model of cascading failures in power grids. This model includes the state variables of generators, which are determined by the nonlinear swing equations and power-flow equations, as well as the on/off status of the network components. This framework allows us to view a cascading failure in the power grid as a phase-space transition from a fixed point with high energy to a fixed point with lower energy. Using real power-grid networks, I will demonstrate that possible cascade outcomes can be predicted by analyzing the stability of the system's equilibria. This work adds an important new dimension to the current understanding of cascading failures.

**1:03PM S43.00008 Cascading Failures in Flow-Driven Networks Induced by Multiple Initiators**<sup>1</sup>, ALAA MOUSSAWI, NOEMI DERZSY, XIN LIN, BOLESŁAW SZYMANSKI, GYORGY KORNISS, Rensselaer Polytechnic Institute — Flow-driven networks are particularly prone to cascading failures. These failures are non self-averaging and this makes them very difficult to predict or subdue [1, 2]. Previous work has suggested that uniformly increasing edge or node capacities may lead to larger failures [1]. This suggests that some nodes/edges may act as fuses and mitigate cascading failures. We investigate this idea, and analyze how properties of the initiators of the cascade influence its outcome. We also discuss how stochastic node capacity allocation can be utilized to mitigate cascades induced by multiple initiators. We demonstrate the efficacy of these strategies on random geometric graphs (RGG) and the UCTE European electrical power transmission network, with capacities allocated in a fashion similar to the industry standard. [1] A. Asztalos, S. Sreenivasan, B.K. Szymanski, and G. Korniss, "Cascading Failures in Spatially-Embedded Random Networks", PLOS ONE 9(1): e84563 (2014). [2] Bernstein et al., ACM SIGMETRICS Performance Eval. Rev. 40, 33-37 (2012).

<sup>1</sup>Supported in part by DTRA and NSF

**1:15PM S43.00009 Cascading processes on multiplex networks: Impact of weak layers**, KYU-MIN LEE, KWANG-IL GOH, Korea University — Many real-world complex systems such as biological and socio-technological systems consist of manifold layers in multiplex networks. The multiple network layers give rise to the nonlinear effect for the emergent dynamics of systems. Especially, the weak layers plays the significant role in nonlinearity of multiplex networks, which can be neglected in single-layer network framework overlaying all layers. Here we present a simple model of cascades on multiplex networks of heterogeneous layers. The model is simulated on the multiplex network of international trades. We found that the multiplex model produces more catastrophic cascading failures which were the result of collective behaviors from coupling layers rather than the simple summation effect. Therefore risks can be systematically underestimated in simply overlaid network system because the impact of weak layers is overlooked. Our simple theoretical model would have some implications to investigate and design optimal real-world complex systems.

**1:27PM S43.00010 Long-term Failure Prediction based on an ARP Model of Global Risk Network**<sup>1</sup>, XIN LIN, ALAA MOUSSAWI, BOLESŁAW SZYMANSKI, GYORGY KORNISS, Rensselaer Polytechnic Institute — Risks that threaten modern societies form an intricately interconnected network. Hence, it is important to understand how risk materializations in distinct domains influence each other. In the paper <sup>2</sup>, we study the global risks network defined by World Economic Forum experts in the form of Stochastic Block Model. We model risks as Alternating Renewal Processes with variable intensities driven by hidden values of exogenous and endogenous failure probabilities. Based on the expert assessments and historical status of each risk, we use Maximum Likelihood Evaluation to find the optimal model parameters and demonstrate that the model considering network effects significantly outperforms the others. In the talk, we discuss how the model can be used to provide quantitative means for measuring interdependencies and materialization of risks in the network. We also present recent results of long-term predictions in the form of predicated distributions of materializations over various time periods. Finally we show how the simulation of ARPs enables us to probe limits of the predictability of the system parameters from historical data and ability to recover hidden variable.

<sup>1</sup>Supported in part by DTRA, ARL NS-CTA.

<sup>2</sup>Szymanski et al., Sci. Rep. 5:10998 (2015)

**1:39PM S43.00011 Hybrid dynamics in delay-coupled swarms with “mothership” networks**<sup>1</sup>, JASON HINDES, IRA SCHWARTZ, U.S. Naval Research Laboratory — Swarming behavior continues to be a subject of immense interest because of its centrality in many naturally occurring systems in biology and physics. Moreover, the development of autonomous mobile agents that can mimic the behavior of swarms and can be engineered to perform complex tasks without constant intervention is a very active field of practical research. Here we examine the effects on delay-coupled swarm pattern formation from the inclusion of a small fraction of highly connected nodes, “motherships”, in the swarm interaction network. We find a variety of new behaviors and bifurcations, including new hybrid motions of previously analyzed patterns. Both numerical and analytic techniques are used to classify the dynamics and construct the phase diagram. The implications for swarm control and robustness from topological heterogeneity are also discussed.

<sup>1</sup>This research was funded by the office of Naval Research (ONR), and was performed while JH held a National Research Council Research Associateship Award

**Thursday, March 17, 2016 11:15AM - 2:03PM –**  
**Session S44 GQI: Quantum Architectures and Control 347 - Ryan Babbush, Google**

**11:15AM S44.00001 A universal scheme for indirect quantum control**<sup>1</sup>, DAVID LAYDEN, University of Waterloo (Department of Applied Mathematics), Institute for Quantum Computing, EDUARDO MARTIN-MARTINEZ, ACHIM KEMPF, University of Waterloo (Department of Applied Mathematics), Institute for Quantum Computing, Perimeter Institute for Theoretical Physics — The goal of indirect quantum control is to coherently steer a quantum system solely by acting on a quantum actuator to which it is coupled. This approach to quantum control is convenient in many physical settings, as it allows one to avoid direct addressing of the system—and any associated difficulties—altogether. While it is known in principle that control of the actuator typically yields universal control of the system, the practical details of how such indirect control can be achieved are less clear. This deficiency has led to a number of implementation- and model-specific indirect control schemes, in lieu of a general recipe applicable to any physical setting. Here, we present such a recipe, in the form of an open-loop control scheme which implements arbitrary unitary operations on the system by exploiting open dynamics in the actuator.

<sup>1</sup>arXiv:1506.06749

## 11:27AM S44.00002 Symmetry-protected topologically ordered states for universal quantum computation<sup>1</sup>

HENDRIK POULSEN NAUTRUP, Department of Physics and Astronomy, Stony Brook University, TZU-CHIEH WEI, C. N. Yang Institute for Theoretical Physics, Stony Brook University — Measurement-based quantum computation (MBQC) is a model for quantum information processing utilizing only local measurements on suitably entangled resource states for the implementation of quantum gates. A complete characterization for universal resource states is still missing. It has been shown that symmetry-protected topological order (SPTO) in one dimension can be exploited for the protection of certain quantum gates in MBQC. Here we investigate whether any 2D nontrivial SPTO states can serve as resource for MBQC. In particular, we show that the nontrivial SPTO ground state of the CZX model on the square lattice by Chen et al. [Phys. Rev. B **84**, 235141 (2011)] can be reduced to a 2D cluster state by local measurement, hence a universal resource state. Such ground states have been generalized to qudits with symmetry action described by three cocycles of a finite group  $G$  of order  $d$  and shown to exhibit nontrivial SPTO. We also extend these to arbitrary lattices and show that the generalized two-dimensional plaquette states on arbitrary lattices exhibit nontrivial SPTO in terms of symmetry fractionalization and that they are universal resource states for quantum computation. SPTO states therefore can provide a new playground for measurement-based quantum computation.

<sup>1</sup>This work was supported in part by the National Science Foundation.

## 11:39AM S44.00003 Two-dimensional quantum walk under artificial magnetic field

ISKENDER YALCINKAYA, ZAFER GEDIK, Sabanci University — We introduce the Peierls substitution to a two-dimensional discrete-time quantum walk on a square lattice to examine the spreading dynamics and the coin-position entanglement in the presence of an artificial gauge field [1]. We use the ratio of the magnetic flux through the unit cell to the flux quantum as a control parameter. For a given flux ratio, we obtain faster spreading for a small number of steps and the walker tends to be highly localized around the origin. Moreover, the spreading of the walk can be suppressed and decreased within a limited time interval for specific rational values of flux ratio. When the flux ratio is an irrational number, even for a large number of steps, the spreading exhibit diffusive behavior rather than the well-known ballistic one as in the classical random walk and there is a significant probability of finding the walker at the origin. We also analyze the coin-position entanglement and show that the asymptotic behavior vanishes when the flux ratio is different from zero and the coin-position entanglement become nearly maximal in a periodic manner in a long time range.

[1] I. Yalcinkaya, Z. Gedik, Phys. Rev. A **92**, 042324 (2015).

## 11:51AM S44.00004 Quantum Ultra-Walks: Walks on a Line with Spatial Disorder<sup>1</sup>

STEFAN BOETTCHER<sup>2</sup>, STEFAN FALKNER<sup>3</sup>, Physics Department, Emory University — We discuss the model of a heterogeneous discrete-time walk on a line with spatial disorder in the form of a set of ultrametric barriers. Simulations show that such a quantum ultra-walk spreads with a walk exponent  $d_w$  that ranges from ballistic ( $d_w = 1$ ) to complete confinement ( $d_w = \infty$ ) for increasing separation  $1 \leq 1/\epsilon < \infty$  in barrier heights. We develop a formalism by which the classical random walk as well as the quantum walk can be treated in parallel using a coined walk with internal degrees of freedom. For the random walk, this amounts to a 2<sup>nd</sup>-order Markov process with a stochastic coin, better known as an (anti-)persistent walk. The exact analysis, based on the real-space renormalization group (RG), reproduces the results of the well-known model<sup>4</sup> of “ultradiffusion,”  $d_w = 1 - \log_2 \epsilon$  for  $0 < \epsilon \leq 1/2$ . However, while the evaluation of the RG fixed-points proceeds virtually identical, for the corresponding quantum walk with a unitary coin<sup>5</sup> it fails to reproduce the numerical results. A new way to analyze the RG is indicated.

<sup>1</sup>supported by NSF-DMR 1207431

<sup>2</sup><http://www.physics.emory.edu/faculty/boettcher/>

<sup>3</sup>now U. of Freiburg,

<http://aad.informatik.uni-freiburg.de/people/falkner/>

<sup>4</sup>J. Phys. A **19**(1986)L269

<sup>5</sup>Phys. Rev. A **90**(2014)032324,

<http://arxiv.org/abs/1311.3369>

## 12:03PM S44.00005 Quantum walks outside of boolean domain as a gate for one, two, or three qubits.

THOMAS CAVIN, DMITRY SOLENOV, Department of Physics, Saint Louis University, St. Louis, MO 63103 — Quantum computing needs entangling quantum gates to perform computation and error correction. We will discuss a novel way to implement quantum gates, such as CNOT, using quantum walks that are directed through a network of states outside of the boolean domain. In such implementations it is important to investigate walks on networks of different connectivities. Specifically, we will discuss solutions to non-symmetric linear chain networks and demonstrate how solutions to more complex networks that have branching, such as cubes, can be expressed in terms of linear chain solutions. We then show examples of implementing single qubit and two-qubit entangling gates.

## 12:15PM S44.00006 Duality quantum computer and the efficient quantum simulations

SHIJIE WEI, GUILU LONG, Tsinghua Univ, TSINGHUA NATIONAL LABORATORY FOR INFORMATION SCIENCE AND TECHNOLOGY COLLABORATION, COLLABORATIVE INNOVATION CENTER OF QUANTUM MATTER COLLABORATION — Duality quantum computer is a new kind of quantum computer which is able to perform an arbitrary sum of unitaries, and therefore a general quantum operator. This gives more computational power than a normal quantum computer. All linear bounded operators can be realized in a duality quantum computer, and unitary operators are just the extreme points of the set of generalized quantum gates. Duality quantum computer can provide flexibility and clear physical picture in designing quantum algorithms, serving as a useful bridge between quantum and classical algorithms. In this report, we will firstly briefly review the theory of duality quantum computer. Then we will introduce the application of duality quantum computer in Hamiltonian simulation. We will show that duality quantum computer can simulate quantum systems more efficiently than ordinary quantum computer by providing descriptions of the recent efficient quantum simulation algorithms.

## 12:27PM S44.00007 Optimized probabilistic quantum processors: A unified geometric approach

JANOS BERGOU, CUNY Hunter College, EMILIO BAGAN, Fisica Teorica: Informacio i Fenomens Quanticos, Universitat Autonoma de Barcelona, EDGAR FELDMAN, Department of Mathematics, Graduate Center of the City University of New York — Using probabilistic [1] and deterministic quantum cloning [2], and quantum state separation [3] as illustrative examples we develop a complete geometric solution for finding their optimal success probabilities. The method is related to the approach that we introduced earlier for the unambiguous discrimination of more than two states [4]. In some cases the method delivers analytical results, in others it leads to intuitive and straightforward numerical solutions. We also present implementations of the schemes based on linear optics employing few-photon interferometry. [1] V. Yerkhin, A. Shehu, E. Feldman, E. Bagan, and J. Bergou, Probabilistically perfect cloning, submitted to PRL (2015). [2] V. Yerkhin, A. Shehu, E. Bagan, E. Feldman, and J. Bergou, Approximate probabilistic cloning, in preparation. [3] V. Yerkhin, A. Shehu, E. Feldman, E. Bagan, and J. Bergou, A geometric approach to state separation, submitted to NJP (2015). [4] J. Bergou, U. Futschik, and E. Feldman, Optimal unambiguous discrimination of pure quantum states, Phys. Rev. Lett. **108**, 250502 (2012).

**12:39PM S44.00008 Three step implementation of any unitary matrix with complete graph of  $n$  qubits**, AMARA KATABARWA, MICHAEL GELLER, Univ of Georgia — The use of programmable array of superconducting qubits for general purpose quantum computation has been recently proposed, and applications to amplitude amplification, phase estimation and simulation of realistic molecular collisions. This Single Excitation Subspace (SES) approach does not require error correction and is practical now. We show that any element in the unitary group  $U(n)$  can be generated in three steps, for any  $n$ . This allows for implementation of highly complex operations in constant time.

**12:51PM S44.00009 Recursive linear optical networks for realizing quantum algorithms<sup>1</sup>**, GELO NOEL TABIA, Univ of Tartu — Linear optics has played a leading role in the development of practical quantum technologies. In recent years, advances in integrated quantum photonics have significantly improved the functionality and scalability of linear optical devices [1]. In this talk, I present recursive schemes for implementing quantum Fourier transforms and inversion about the mean in Grover's algorithm with photonic integrated circuits [2]. By recursive, I mean that two copies of a  $d$ -dimensional unitary operation is used to build the corresponding unitary operation on  $2d$  modes. The linear optical networks operate on path-encoded qudits and realize  $d$ -dimensional unitary operations using  $O(d^2)$  elements. To demonstrate that the recursive circuits are viable in practice, I conducted simulations of proof-of-principle experiments using a fabrication model of realistic errors in silicon-based photonic integrated devices. The results indicate high-fidelity performance in the circuits for 2-qubit and 3-qubit quantum Fourier transforms, and for quantum search on 4-item and 8-item databases. Ref: [1] G. D. Marshall, et al., Opt. Express 17, 12546 (2009); [2] G. N. M. Tabia, arXiv:1509.04246 (2015).

<sup>1</sup>This work was funded by institutional research grant IUT2-1 from the Estonian Research Council and by the European Union through the European Regional Development Fund.

**1:03PM S44.00010 Controlling Quantum Transport with a Programmable Nanophotonic Processor**, NICHOLAS HARRIS, GREGORY STEINBRECHER, JACOB MOWER, YOAV LIHINI, MIHIKA PRABHU, Massachusetts Institute of Technology, TOM BAEHR-JONES, MICHAEL HOCHBERG, Coriant Advanced Technology, SETH LLOYD, DIRK ENGLUND, Massachusetts Institute of Technology — Recent experimental and theoretical work has revealed emergent, counter-intuitive quantum transport effects in a range of physical media including solid-state and biological systems. Photonic integrated circuits are promising platforms for studying such effects. A central goal in for photonic quantum transport simulators has been the ability to rapidly control all parameters of the transport problem. Here, we present a large-scale programmable nanophotonic processor composed of 56 Mach-Zehnder interferometers that enables control over modal couplings and differential phases between modes—enabling observations of Anderson localization, environment-assisted quantum transport, ballistic transport, and a number of intermediate quantum transport regimes. Rapid programmability enables tens of thousands of realizations of disordered and noisy systems. In addition, low loss makes this nanophotonic processor a promising platform for many-boson quantum simulation experiments.

If possible schedule directly before Universal Linear Optics: A Testbed for Optical Quantum Logic, author Chris Sparrow.

**1:15PM S44.00011 Universal Linear Optics: An implementation of Boson Sampling on a Fully Reconfigurable Circuit**, CHRISTOPHER HARROLD, JACQUES CAROLAN, CHRIS SPARROW<sup>1</sup>, NICHOLAS J. RUSSELL, JOSHUA W. SILVERSTONE, GRAHAM D. MARSHALL, MARK G. THOMPSON, JONATHAN C.F. MATTHEWS, JEREMY L. O'BRIEN, ANTHONY LAING, University of Bristol, ENRIQUE MARTIN-LOPEZ, Nokia Technologies, Cambridge, PETER J. SHADBOLT, Imperial College London, NOBUYUKI MATSUDA, NTT Basic Research Laboratories, NTT Corporation, MANABU OGUMA, MIKITAKA ITOH, TOSHIKAZU HASHIMOTO, NTT Device Technology Laboratories, NTT Corporation — Linear optics has paved the way for fundamental tests in quantum mechanics and has gone on to enable a broad range of quantum information processing applications for quantum technologies. We demonstrate an integrated photonics processor that is universal for linear optics. The device is a silica-on-silicon planar waveguide circuit (PLC) comprising a cascade of 15 Mach Zehnder interferometers, with 30 directional couplers and 30 tunable thermo-optic phase shifters which are electrically interfaced for the arbitrary setting of a phase. We input ensembles of up to six photons, and monitor the output with a 12-single-photon detector system. The calibrated device is capable of implementing any linear optical protocol. This enables the implementation of new quantum information processing tasks in seconds, which would have previously taken months to realise. We demonstrate 100 instances of the boson sampling problem with verification tests, and six-dimensional complex Hadamards.

<sup>1</sup>Also Imperial College London

**1:27PM S44.00012 Universal Linear Optics: A Testbed for Optical Quantum Logic**, CHRIS SPARROW, Centre for Quantum Photonics, University of Bristol, UK and Department of Physics, Imperial College London, UK, JACQUES CAROLAN, CHRISTOPHER HARROLD, NICHOLAS RUSSELL, GRAHAM MARSHALL, JOSHUA SILVERSTONE, MARK THOMPSON, JONATHAN MATTHEWS, JEREMY O'BRIEN, ANTHONY LAING, Centre for Quantum Photonics, University of Bristol, UK, ENRIQUE MARTIN-LOPEZ, Nokia Technologies, Cambridge, UK, PETER SHADBOLT, Department of Physics, Imperial College London, UK, NOBUYUKI MATSUDA, NTT Basic Research Laboratories, NTT Corporation, Japan, MANABU OGUMA, MIKITAKA ITOH, TOSHIKAZU HASHIMOTO, NTT Device Technology Laboratories, NTT Corporation, Japan — Linear optics is a promising platform for scalable quantum information processing. We demonstrate a single reprogrammable optical circuit that is sufficient to implement all possible linear optical protocols up to the size of the circuit [Carolan et al., Science, 349, (2015)]. The system is an ideal testbed for rapidly prototyping new linear optical quantum gates, and testing known protocols in experimentally realistic scenarios. We use the device to perform a series of postselected and heralded quantum logic gates including a new scheme for heralded bell state generation, a key primitive in measurement-based linear optical quantum computation. We propose and demonstrate techniques for efficiently and accurately characterising and verifying these gates operation. The ability to rapidly reprogram linear optical devices promises to replace a multitude of existing and future prototype systems, pointing the way to applications across quantum technologies.

**1:39PM S44.00013 Entanglement Dynamics in Heisenberg spin systems coupled to a dissipative environment**, GEHAD SADIEK, Department of Applied Physics, University of Sharjah, Sharjah 27272, UAE, SAMAHER ALMALKI, Department of Physics, King Saud University, Riyadh 11451, Saudi Arabia — Heisenberg Spin chains and lattices have been intensively used to represent many of the physical systems that are considered as promising candidates for quantum computing and quantum information processing. The main obstacle toward realizing the ultimate goals in these fields is decoherence caused by the surrounding dissipative and thermal environments. We are studying spin relaxation and entanglement dynamics in one and two-dimensional XYZ Heisenberg spin systems under coupling with a dissipative Lindblad environment at finite temperature. We investigate the effect of the anisotropy of the coupling between the spins on the asymptotic steady state of the system and the spin relaxation rates at different temperatures of the environment. We demonstrate the role played by the initial system setup on the entanglement and spin dynamics and steady state properties. Also we examine the effect of the long range interaction between the spins on the asymptotic behavior of the system.

**1:51PM S44.00014 Geometrical, response, and gap properties of Lindbladians**, VICTOR V. ALBERT, Yale University, BARRY BRADLYN, Princeton University, MARTIN FRAAS, University of Munich, LIANG JIANG, Yale University — We study Lindbladians admitting multi-dimensional steady-state subspaces (SSS) which can be used to store, protect, and process quantum information. We derive an analytical formula for the left eigenmatrices of such Lindbladians corresponding to purely imaginary eigenvalues. This formula resolves how Lindbladian evolution affects perturbative response and geometrical features of the SSS and allows us to generalize recent work to all types of SSS. We show that Hamiltonian and certain jump operator perturbations induce, to first order, exclusively unitary evolution on the SSS. Similarly, the holonomy (generalization of geometric phase) induced on the SSS after adiabatic traversal of a closed path in parameter space is unitary. We derive a new Riemannian metric tensor in parameter space induced by one type of SSS, generalizing the Fubini-Study metric to Lindbladians possessing one or more mixed steady states. We derive a Kubo formula governing linear response of the SSS to Hamiltonian perturbations. Finally, we show that the energy scale governing leakage out of the SSS is different from the conventional Lindbladian dissipative gap.

**Thursday, March 17, 2016 11:15AM - 2:03PM —**

**Session S45 GQI DAMOP: Atomic, Molecular and Optical Quantum Information and Metrology**  
348 - Jonathan Home, ETH

**11:15AM S45.00001 Quantum Rabi Model in Quantum Technologies**, JULEN PEDERNALES, URTZI LAS HERAS, LUCAS LAMATA, University of the Basque Country, Spain, ENRIQUE SOLANO, University of the Basque Country and IKERBASQUE, Spain — We will discuss how to simulate a wide range of regimes of the Quantum Rabi Model (QRM) in quantum platforms as trapped ions and circuit QED. Directly accessible regimes of the QRM correspond to a very narrow set of values of the ratio between the coupling strength and the characteristic frequencies of the system, typically in the strong coupling regime or in the perturbative zone of the ultrastrong coupling regime. However, with analog and digital quantum simulation techniques we can access the most elusive regimes of the QRM. Recent theoretical developments have disclosed a plethora of physical phenomena appearing at these previously unexplored regimes of the QRM, making its experimental implementation timely and of high interest.

**11:27AM S45.00002 What can we learn from the dynamics of entanglement and quantum discord in the Tavis-Cummings model?**<sup>1</sup>, JULIANA RESTREPO, Universidad Antonio Nario, BORIS A. RODRIGUEZ, Universidad de Antioquia — We revisit the problem of the dynamics of quantum correlations in the exact Tavis-Cummings model. We show that many of the dynamical features of quantum discord attributed to dissipation are already present in the exact framework and are due to the well known non-linearities in the model and to the choice of initial conditions. Through a comprehensive analysis, supported by explicit analytical calculations, we find that the dynamics of entanglement and quantum discord are far from being trivial or intuitive. In this context, we find states that are indistinguishable from the point of view of entanglement and distinguishable from the point of view of quantum discord, states where the two quantifiers give opposite information and states where they give roughly the same information about correlations at a certain time. Depending on the initial conditions, this model exhibits a fascinating range of phenomena that can be used for experimental purposes such as: Robust states against change of manifold or dissipation, tunable entanglement states and states with a counterintuitive sudden birth as the number of photons increase. We furthermore propose an experiment called quantum discord gates where discord is zero or non-zero depending on the number of photons.

<sup>1</sup>This work was supported by the Vicerrectoria de Investigacion of the Universidad Antonio Nario, Colombia under project number 20141031 and by the Departamento Administrativo de Ciencia, Tecnologia e Innovacion (COLCIENCIAS) of Colombia under grant number

**11:39AM S45.00003 ABSTRACT WITHDRAWN —**

**11:51AM S45.00004 Robust quantum state transfer with suppressed parametric noise**, MENGZHEN ZHANG, CHANGLING ZOU, LIANG JIANG, Yale University — For opto-electro-mechanical transducers, there are undesirable parametric processes that introduce parametric noise, which will limit the fidelity of the transferred quantum state<sup>1</sup>. To overcome this imperfection, we propose a quantum state transfer scheme with squeezed input states and measurement dependent compensation to eliminate the parametric noise from the quantum state transfer. Besides parametric noise, we also investigate the sensitivity of our scheme to thermal noise, signal frequency detuning and imperfect impedance matching, and show a good quantum state fidelity and applicability to quantum state transfer.

<sup>1</sup>R. W. Andrews, R. W. Peterson, T. P. Purdy, K. Cicak, R. W. Simmonds, C. A. Regal & K. W. Lehnert, Nature Physics **10**, 321-326 (2014)

**12:03PM S45.00005 High efficiency in Mode Selective Frequency Conversion for Optical Quantum Information Processing**, NICOLAS QUESADA, Universite de Sherbrooke, J.E. SIPE, University of Toronto — Mode selective Frequency conversion (FC) is an enabling process in many quantum information protocols<sup>1</sup>. Recently, it has been observed that upconversion efficiencies in single-photon, mode-selective FC are limited to around 80%<sup>2</sup>. In this contribution we show that these limits can be understood as time ordering corrections (TOCs) that modify the joint conversion amplitude of the process<sup>3</sup>. Furthermore we show, using a simple scaling argument, that recently proposed cascaded FC protocols<sup>4</sup> that overcome the aforementioned limitations act as “attenuators” of the TOCs. This observation allows us to argue that very similar cascaded architectures can be used to attenuate TOCs in photon generation via spontaneous parametric down-conversion<sup>5</sup>. Finally, by using the Magnus expansion, we argue that the TOCs, which are usually considered detrimental for FC efficiency, can also be used to increase the efficiency of conversion in partially mode selective FC.

<sup>1</sup>B. Brecht et al. Phys. Rev. X **5**, 041017 (2015)

<sup>2</sup>B. Brecht et al. Phys. Rev. A **90**, 030302 (2014)

<sup>3</sup>N. Quesada et al. Phys. Rev. A **90**, 063840 (2014).

<sup>4</sup>D.V. Reddy et al. Opt. Lett. **39**, 2924-2927 (2014).

<sup>5</sup>N. Quesada et al., Phys. Rev. Lett. **114**, 093903 (2015).

**12:15PM S45.00006 Maximal adaptive-decision speedups in quantum-state readout<sup>1</sup>**, BENJAMIN D'ANJOU, LOUTFI KURET, LILIAN CHILDRESS, WILLIAM A. COISH, McGill University — The average time  $T$  required for high-fidelity readout of quantum states can be significantly reduced via a real-time adaptive decision rule. An adaptive decision rule stops the readout as soon as a desired level of confidence has been achieved, as opposed to setting a fixed readout time  $t_f$ . The performance of the adaptive decision is characterized by the “adaptive-decision speedup”,  $t_f/T$ . In this work, we reformulate this readout problem in terms of the first-passage time of a particle undergoing stochastic motion. This formalism allows us to theoretically establish the maximum achievable adaptive-decision speedups for several physical two-state readout implementations. We show that for two common readout schemes (the Gaussian latching readout and a readout relying on state-dependent decay), the speedup is bounded by 4 and 2, respectively, in the limit of high single-shot readout fidelity. We experimentally study the achievable speedup in a real-world scenario by applying the adaptive decision rule to a readout of the nitrogen-vacancy-center (NV-center) charge state. We find a speedup of  $\approx 2$  with our experimental parameters. Our results should lead to immediate improvements in nano-scale magnetometry based on spin-to-charge conversion of the NV-center spin.

<sup>1</sup>We acknowledge support from NSERC, INTRIQ, CIFAR and the Walter C. Sumner Foundation.

**12:27PM S45.00007 Negatively-charged NV-center in SiC: Electronic structure properties**, PRATIBHA DEV, Dept. of Physics and Astronomy, Howard University, Washington, D.C., SOPHIA ECONOMOU, Dept. of Physics, Virginia Tech, Blacksburg, Virginia — Deep defects with high-spin states in semiconductors are promising candidates as solid-state systems for quantum computing applications. The charged NV-center in diamond is the best-known and most-studied defect center, and has proven to be a good proof-of-principle structure for demonstrating the use of such defects in quantum technologies. Increasingly, however, there is an interest in exploring deep defects in alternative semiconductors such as SiC. This is due to the challenges posed by diamond as host material for defects, as well as the attractive properties of SiC. In this density functional theory work, we study the spin-1 structure of the negatively charged NV-center in two polytypes: 3C-SiC and 4H-SiC. The calculated zero phonon line for the excited state of the defect is in telecom range (0.90eV), making it a very good candidate for quantum technologies. This work provides basic ingredients required to understand the physics of this color center at a quantitative and qualitative level. We also design quantum information applications, such as a spin-photon interface and multi-photon entanglement.

**12:39PM S45.00008 Optical patterning of trapped charge in nitrogen-doped diamond<sup>1</sup>**, SIDDHARTH DHOMKAR, HARISHANKAR JAYAKUMAR, DANIELA PAGLIERO, ABDELGHANI LARAOU, REMUS ALBU, City College of New York-CUNY, NEIL MANSON, MARCUS DOHERTY, Australian National University, JACOB HENSHAW, CARLOS MERILES, City College of New York-CUNY, Graduate Center-CUNY — The nitrogen-vacancy (NV) center in diamond is emerging as a promising platform for solid-state quantum information processing and nanoscale metrology. Of interest in these applications is the manipulation of the NV charge state, which can be attained by optical illumination. Here we use two-color optical microscopy to investigate the dynamics of NV photo-ionization, charge diffusion, and trapping in type-1b diamond. We combine fixed-point laser excitation and scanning fluorescence imaging to locally alter the concentration of negatively charged NVs and to subsequently probe the corresponding redistribution of charge. We uncover the formation of various spatial patterns of trapped charge, which we semi-quantitatively reproduce via a model of the interplay between photo-excited carriers and atomic defects in the diamond lattice. Further, by using the NV as a local probe, we map the relative fraction of positively charged nitrogen upon localized optical excitation. These observations may prove important to various technologies, including the transport of quantum information between remote NVs and the development of three-dimensional, charge-based memories.

<sup>1</sup>We acknowledge support from the National Science Foundation through grant NSF-1314205

**12:51PM S45.00009 Towards High Density 3-D Memory in Diamond<sup>1</sup>**, JACOB HENSHAW, City College of New York- CUNY, Graduate Center-CUNY, SIDDHARTH DHOMKAR, City College of New York- CUNY, CARLOS MERILES, City College of New York- CUNY, Graduate Center-CUNY, HARISHANKAR JAYAKUMAR, City College of New York- CUNY — The nitrogen-vacancy (NV) center in diamond is presently the focus of widespread attention for applications ranging from quantum information processing to nanoscale metrology. Of great utility is the ability to optically initialize the NV charge state, which has an immediate impact on the center's light emission properties. Here, we use two-color microscopy in NV-rich, type-1b diamond to demonstrate fluorescence-encoded long-term storage of classical information. As a proof of principle, we write, reset, and rewrite various patterns with 2-D binary bit density comparable to present DVD-ROM technology. The strong fluorescence signal originating from the diffraction-limited bit volume allows us to transition from binary to multi-valued encoding, which translates into a significant storage capacity boost. Finally, we show that our technique preserves information written on different planes of the diamond crystal and thus serves as a platform for three-dimensional storage. Substantial enhancement in the bit density could be achieved with the aid of super resolution microscopy techniques already employed to discriminate between NVs with sub-diffraction, nanometer accuracy, a regime where the storage capacity could exceed  $10^{17}$  bytes/cm<sup>3</sup>

<sup>1</sup>We acknowledge support from the National Science Foundation through grant NSF-1314205

**1:03PM S45.00010 Quantum memory enhanced nuclear magnetic resonance of nanometer-scale samples with a single spin in diamond**, NABEEL ASLAM, MATTHIAS PFENDER, SEBASTIAN ZAISER, FELIPE FAVARO DE OLIVEIRA, S. ALI MOMENZADEH, ANDREJ DENISENKO, 3rd Physics Institute, University of Stuttgart, JUNICHI ISOYA, Research Center for Knowledge Communities, University of Tsukuba, PHILIPP NEUMANN, JOERG WRACHTRUP, 3rd Physics Institute, University of Stuttgart — Recently nuclear magnetic resonance (NMR) of nanoscale samples at ambient conditions has been achieved with nitrogen-vacancy (NV) centers in diamond. So far the spectral resolution in the NV NMR experiments was limited by the sensor's coherence time, which in turn prohibited revealing the chemical composition and dynamics of the system under investigation. By entangling the NV electron spin sensor with a long-lived memory spin qubit we increase the spectral resolution of NMR measurement sequences for the detection of external nuclear spins. Applying the latter sensor-memory-couple it is particularly easy to track diffusion processes, to identify the molecules under study and to deduce the actual NV center depth inside the diamond. We performed nanoscale NMR on several liquid and solid samples exhibiting unique NMR response. Our method paves the way for nanoscale identification of molecule and protein structures and dynamics of conformational changes.

**1:15PM S45.00011 Single molecule spin resonance spectroscopy and imaging by diamond-sensor**, JIANGFENG DU, University of Science and Technology of China — Single-molecule magnetic resonance spectroscopy and imaging is one of the ultimate goals in magnetic resonance and will have great applications in a broad range of scientific areas, from life science to physics and chemistry. The spin of a single nitrogen vacancy (NV) center in diamond is a highly sensitive magnetic-field sensor, which has been proposed for detection of single molecules or nanoscale targets. We and co-workers have successfully obtained the first single-protein spin resonance spectroscopy under ambient conditions [1], high-resolution vector microwave imaging [2], and realized atomic-scale structure analysis of single nuclear-spin clusters in diamond [3]. Moreover, we have tried to improve the quantum control technique and succeed to achieve fault-tolerant universal quantum gates [4]. As the last part, I will briefly introduce our most recently work on single protein imaging in situ in cell. References: [1] Fazhan Shi, et al., Science, 347, 1135 (2015) [2] Pengfei Wang, et al., Nature Commu., 6, 6631 (2015) [3] Fazhan Shi, et al., Nature Physics, 10, 21 (2014) [4] Xing Rong, et al., Nature Commu., In press (2015)

**1:27PM S45.00012 Beating the Shot-Noise Limit with Partially-Distinguishable Photons**, PATRICK M. BIRCHALL, JAVIER SABINES-CHESTERKING, JEREMY L. OBRIEN, HUGO CABLE, JONATHAN C. F. MATTHEWS C. F. MATTHEWS, Centre for Quantum Photonics, University of Bristol — Quantum metrology promises high-precision measurements beyond the capability of any classical techniques. This has the potential to be an integral part of investigative techniques, utilised across all areas of science and technology. However, all sensors must be able to operate despite imperfections to be of practical use. Proposals for photonic quantum sensors typically exploit quantum interference between photons which are perfectly indistinguishable, but achieving this indistinguishability can be a major technical challenge in practice, in particular with immature but promising approaches to photon sources. Here we show that highly indistinguishable photons are not required for quantum-enhanced measurements, nor do partially distinguishable photons have to be engineered to mitigate the effects of distinguishability. We conduct an experiment to verify the utility of two- and four-photon states containing partially distinguishable particles by performing quantum-enhanced measurements with low-visibility quantum interference. This demonstrates that sources producing spectrally-mixed single photons can be readily applied in quantum metrology systems.

**1:39PM S45.00013 How zero light intensity can exert a nonzero force on a charged particle**, JUSTIN DRESSEL, JEFF TOLLAKESEN, Chapman University, YAKIR AHARONOV, Chapman University, Tel Aviv University — A classical electromagnetic field is deterministic and fully specified by a single temporal boundary condition. In contrast, a quantum electromagnetic field is irreducibly stochastic, such that only its average corresponds to a classical field for large ensembles of measurements. Such a field-average may be further refined by a second temporal boundary condition, which can expose fundamentally different classical fields in the same classical averaging limit. To demonstrate this, we consider an ensemble of coherent laser pulses that interact with identically prepared test charges before being collected at an intensity meter. Isolating only the pulses with zero collected intensity reveals a nonzero average classical force on the charge from those pulses. The charge is affected with no light collected.

**1:51PM S45.00014 Sub-Cycle Quantum Optics: Direct Access to Electric Field Vacuum Fluctuations.**, DENIS SELETSKIY, CLAUDIUS RIEK, ANDREY MOSKALENKO, JAN SCHMIDT, PHILIPP KRAUSPE, SEBASTIAN ECKART, STEFAN EGGERT, GUIDO BURKARD, ALFRED LEITENSTORFER, University of Konstanz — Vacuum fluctuations are fundamental to a variety of physical aspects ranging from spontaneous photon emission via the Casimir force all the way to cosmology. Study and manipulation of the ground state of the radiation field is a central subject in quantum optics. In common approaches, such as for example homodyne detection, the information is averaged over multiple cycles of light and amplification to finite intensity is mandatory. Usually, ultrashort pulses are applied for quantum measurements within a slowly-varying envelope approximation. We demonstrate direct detection of the vacuum fluctuations of the local electric field amplitude in free space. Broadband electro-optic sampling with sub-6 femtosecond gate pulses enables quantum-statistic readout [1]. Distinction from the detector shot noise is achieved by modification of the sampled space-time volume. Measuring with a bandwidth matching the 70 THz center frequency maximizes the vacuum amplitude since the ground-state energy approaches half a photon per optical cycle. Our findings open up a new avenue to quantum analysis and manipulation of light working in the time domain and with sub-cycle access to the electric field quadrature.  
[1] C. Riek et al, Science **350**, 420 (2015).

## Thursday, March 17, 2016 11:15AM - 2:15PM –

Session S47 DCP GSOF: Chemical Physics of Surfaces, Interfaces and Colloids 312 - Jeff Owrutsky, Naval Research Laboratory

**11:15AM S47.00001 Effects of Oxide Surface on the Detonation Initiation of Energetic Materials from First Principles**, FENG GONG WANG, ROMAN TSYSHEVSKY, MAIJA KUKLJA, Department of Materials Science and Engineering, University of Maryland, College Park, MD 20742, USA, UMD TEAM — Organic-inorganic interface provides both intrigues and opportunities for designing systems possessing properties and functionalities inaccessible by individual component. The electronic, catalytic, and defect properties of inorganic surfaces can affect the adsorption, chemical reaction, and photo-responsive properties of organic molecules. In particular, the presence of a particular oxide additive prompts the energy absorption for detonation initiation. Here, we choose the highly catalytic oxide  $\text{TiO}_2$  and explosive trinitrotoluene (TNT) as prototypical examples to explore the role of oxide surface on the detonation initiation of explosives from first principles. We show that the TNT- $\text{TiO}_2$  (110) interface induces optical transitions between  $\text{TiO}_2$  and TNT, shifting the light absorption edge to lower energy. This helps to control the detonation initiation by laser light with a modest optical energy. In addition, the presence of surface oxygen vacancies leads to electron transfer from surface to molecule, facilitating the decomposition of TNT. Our results not only provide guidelines for designing a controllable oxide-explosive formulation that can be initiated by available lasers, but also help to understand interfaces with target properties and functionalities.

**11:27AM S47.00002 Effect of surface morphology on kinetic compensation effect**, NAYELI ZUNIGA-HANSEN, Louisiana State University, LEONARDO E. SILBERT, Southern Illinois University Carbondale — The existence of the kinetic compensation effect, observed in many fields of science, continues to be debated and believed to be a mathematical artifact. Recently, we performed a computational study of the thermal desorption of interacting adsorbates from an energetically homogeneous surface and we observed that the kinetic compensation effect indeed occurs to varying degrees depending on interaction strength. However, other factors which may lead to a kinetic compensation effect have yet to be explored. In the present work, using kinetic Monte Carlo simulations, we study the effects of substrate topology on thermal desorption. We focus on differences between ordered and disordered surfaces at a fixed site coordination number. The rates of desorption depend on surface configuration due to the inherent differences in the local environments of adsorbing sites. While the compensation effect persists for the disordered substrate, it is more strongly influenced by variations in the preexponential factor rather than the activation energy which dominates in the ordered lattice. We expect our results to provide a deeper insight into the microscopic events that originate compensation effects in our system of study but also in other fields where these effects have been reported.

**11:39AM S47.00003 Thermodynamics of catalytic nanoparticle morphology**, MICHAEL ZWOLAK, RENU SHARMA, PIN ANN LIN, Center for Nanoscale Science and Technology, National Institute of Standards and Technology — Metallic nanoparticles are an important class of industrial catalysts. The variability of their properties and the environment in which they act, from their chemical nature & surface modification to their dispersion and support, allows their performance to be optimized for many chemical processes useful in, e.g., energy applications and other areas. Their large surface area to volume ratio, as well as varying sizes and faceting, in particular, makes them an efficient source for catalytically active sites. These characteristics of nanoparticles – i.e., their morphology – can often display intriguing behavior as a catalytic process progresses. We develop a thermodynamic model of nanoparticle morphology, one that captures the competition of surface energy with other interactions, to predict structural changes during catalytic processes. Comparing the model to environmental transmission electron microscope images of nickel nanoparticles during carbon nanotube (and other product) growth demonstrates that nickel deformation in response to the nanotube growth is due to a favorable interaction with carbon. Moreover, this deformation is halted due to insufficient volume of the particles. We will discuss the factors that influence morphology and also how the model can be used to extract interaction strengths from experimental observations.

**11:51AM S47.00004 Support- dependent evolution of oxidation state and nanoassembly formation of subnanometer copper clusters under carbon dioxide conversion conditions**, AVIK HALDER, BING YANG, KARTHIKA L. KOLIPAKA, MICHAEL PELLIN, SOENKE SEIFERT, STEFAN VAJDA, Argonne National Laboratory, MATERIALS SCIENCE DIVISION TEAM — Size- and support- dependence of the properties of copper clusters have been investigated during carbon dioxide conversion with hydrogen at high reactant concentrations and atmospheric pressure. The model catalyst systems were prepared by depositing size-selected  $\text{Cu}_n$  clusters ( $n = 3, 4, 12$  and  $20$ ) on various amorphous metal oxide ( $\text{Al}_2\text{O}_3$ ,  $\text{ZnO}$ , and  $\text{ZrO}_2$ ), and carbon-based (UNCD = ultrananocrystalline diamond) supports. During the temperature ramp, the evolution of the chemical state and size of the particles were characterized by *in situ* grazing incidence X-ray absorption near edge structure (GIXANES), and grazing incidence small angle X-ray scattering (GISAXS) respectively. Under reaction conditions the initially oxidized Cu clusters reduced at various temperatures depending on cluster size and support. Clusters supported on  $\text{ZnO}$  and UNCD were found to be sinter-resistant under reactive gases at elevated temperatures and atmospheric pressures, whereas on  $\text{ZrO}_2$  support the clusters formed stable aggregates. Clusters on  $\text{Al}_2\text{O}_3$  support demonstrated unique properties, where a formation of a nanostructure was observed during heating, which then disintegrated during the cool down. Under applied conditions,  $\text{Cu}_4$  clusters on  $\text{Al}_2\text{O}_3$  were found to be the most efficient in methanol formation.

**12:03PM S47.00005 Molecular Imprinting of Silica Nanoparticle Surfaces via Reversible Addition-Fragmentation Polymerization for Optical Biosensing Applications<sup>1</sup>**, ZEHRA OLUZ, TOBB UET Materials Science and Nanotechnology Engineering, SANA NAYAB, Lahore College for Women University Department of Chemistry, TALYA TUGANA KURSUN, TUNCER CAYKARA, Gazi University Department of Chemistry, BASIT YAMEEN, Harvard Medical School Laboratory of Nanomedicine and Biomaterials, HATICE DURAN, TOBB UET Materials Science and Nanotechnology Engineering — Azo initiator modified surface of silica nanoparticles were coated via reversible addition-fragmentation polymerization (RAFT) of methacrylic acid and ethylene glycol dimethacrylate using 2-phenylprop 2-yl dithobenzoate as chain transfer agent. Using L-phenylalanine anilide as template during polymerization led molecularly imprinted nanoparticles. RAFT polymerization offers an efficient control of grafting process, while molecularly imprinted polymers shows enhanced capacity as sensor. L-phenylalanine anilide imprinted silica particles were characterized by X-Ray photoelectron spectroscopy (XPS), atomic force microscopy (AFM). Performances of the particles were followed by surface plasmon resonance spectroscopy (SPR) after coating the final product on gold deposited glass substrate against four different analogous of analyte molecules: D-phenylalanine anilide, L-tyrosine, L-tryptophan and L-phenylalanine. Characterizations indicated that silica particles coated with polymer layer do contain binding sites for L-phenylalanine anilide, and are highly selective for the molecule of interest.

<sup>1</sup>This project was supported by TUBITAK (Project No:112M804)

**12:15PM S47.00006 Sum Frequency Generation at the  $\text{Al}_2\text{O}_3$ - $\text{H}_2\text{O}$  Interface: An Effective Bond Polarizability Model<sup>1</sup>**, MARK DELLOSTRITTO, Physics Dept., Pennsylvania State University, JAMES KUBICKI, Dept. of Geological Sciences, University of Texas at El Paso, JORGE SOFO, Physics Dept., Pennsylvania State University — Sum Frequency Generation (SFG) is a powerful tool for extracting the vibrational spectrum of an interface as it is a second-order optical process and therefore prohibited in centrosymmetric bulk media. When calculating the spectrum, it is often desirable to write the response as a sum over components of the system, such as atoms or molecules. This can pose a number of challenges however, as the response depends upon the total polarizability, which is in general not an additive quantity. We employ a Thole-type model to assign polarizabilities to the bonds of a system, which allows us to treat the contribution of molecules and surface groups to the spectrum. Local field effects are then taken into account using modified Ewald sums. Following the time-dependent approach of Morita, we are able to produce the SFG spectrum at an interface from molecular dynamics simulations ranging in size and detail from small ab-initio to large classical simulations. We tested our method on ab-initio simulations of the  $\text{Al}_2\text{O}_3$ (0001)- $\text{H}_2\text{O}$  interface as  $\text{Al}_2\text{O}_3$  has a low dissolution rate, a well-known surface structure, and thoroughly studied surface-water interactions. We were able to successfully reproduce the experimental spectrum and decompose it in terms of molecular motions and local correlations.

<sup>1</sup>Research Supported by U.S. Dept. of Energy

**12:27PM S47.00007 Electrokinetic Stabilization of Thin Surfactant Films**, SOUMYADIP SETT, RAKESH SAHU, ALEXANDER YARIN, University of Illinois at Chicago — Ionic surfactant solutions were used to study gravitational drainage from thin vertical planar films supported on a frame with the upper and lower parts being electrodes. The imposed electric field resulted in the following physical phenomena: (i) surface charge redistribution, (ii) electroosmotic flow in the diffuse layer, and (iii) pressure build-up near the electrode to which the electroosmotic flow is directed. The interplay of these phenomena stabilized the film drainage irrespectively of polarity. Similar effects were observed with foams.

**12:39PM S47.00008 Tuning surface reactivity by finite size effects: role of orbital symmetry in the *d*-band model<sup>1</sup>**, PAUL SNIJDERS, XIANGSHI YIN, VALENTINO COOPER, Oak Ridge National Laboratory, HANNO WEITERING, University of Tennessee, Knoxville — Catalytic activity depends sensitively on the strength of the interactions between reactant molecules and catalyst surface: too weak and the catalyst cannot capture enough molecules to react; too strong and the reaction products do not desorb, blocking further reactions. The ability to control the binding strength of molecules to metal surfaces is thus fundamental to the design of efficient and selective catalysts. Catalyst design often relies on increasing the interaction strength on relatively non-reactive materials by introducing active sites. Here, we present a complementary approach: we exploit finite size effects in the electronic structure of ultrathin Pd(111) films grown on Ru(0001) to tune their reactivity by changing the film thickness one atom layer at a time. While bulk Pd(111) is reactive toward oxygen, we find that Pd films thinner than 6 atom layers are surprisingly inert to oxidation. This observation can be explained with the *d*-band model only when it is applied to the orbitals directly involved in the bonding. The insight into orbital specific contributions to surface reactivity could be useful in the design of catalysts.

<sup>1</sup>This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

**12:51PM S47.00009 Nonequilibrium thermodynamics of an interface**, THIERRY SAVIN, University of Cambridge, MARCO SCHWEIZER, HANS CHRISTIAN ÖTTINGER, ETH Zurich — Interfacial thermodynamics has deep ramifications in understanding the boundary conditions of transport theories. We present a formulation of local equilibrium for interfaces that extends the thermodynamics of the “dividing surface,” as introduced by Gibbs, to nonequilibrium settings such as evaporation or condensation. By identifying the precise position of the dividing surface in the interfacial region with a gauge degree of freedom, we exploit gauge-invariance requirements to consistently define the intensive variables for the interface. The model is verified under stringent conditions by employing high-precision nonequilibrium molecular dynamics simulations of a coexisting vapor-liquid Lennard-Jones fluid. We conclude that the interfacial temperature is determined using the surface tension as a “thermometer,” and can be significantly different from the temperatures of the adjacent phases.

**1:03PM S47.00010 CO<sub>2</sub> Adsorption on ZIF-8**, ALDO MIGONE, BRICE RUSSELL, Southern Illinois University Carbondale — We present the results of an adsorption isotherm study of CO<sub>2</sub> on the metal-organic framework ZIF-8. This material undergoes a structural transition (“gate-opening”) as a function of increasing pressure and sorbent loading for sorbates. Gate-opening manifests itself in the isotherm data as a quasi-vertical substep, corresponding to an increase in the amount that can adsorb in the ZIF-8. We measured ten CO<sub>2</sub> isotherms from 133 K to 227 K. In this range, we did not find in any of the isotherms the characteristic substep indicative of the gate-opening. It is possible that the temperature range over which this transition would manifest in the data simply has not been explored in our measurements. The adsorption isotherm data was used to determine the isosteric heat of adsorption of CO<sub>2</sub> on this sorbent as a function of sorbent loading. We have studied the adsorption kinetics for this system, i.e., how the equilibration times for adsorption change as a function of sorbent loading. Trends in the isosteric heat, and kinetics of adsorption data will be discussed.

**1:15PM S47.00011 Low frequency ionic conduction across liquid interfaces.**, FRANCISCO J SOLIS, Arizona State University, GUILLERMO IVAN GUERRERO, Universidad Autnoma de San Luis Potos, MONICA OLVERA DE LA CRUZ, Northwestern University — Ionic conduction in liquid media is a central component of many recently proposed technologies. As in the case of solid state systems, the presence of heterogeneous media gives rise to interesting nonlinear phenomena. We present simulations and theoretical analysis of the low frequency ionic conduction in a two-liquid system. In the case analyzed, the conduction is driven by an electric field perpendicular to the liquid-liquid interface. We show that the dielectric contrast between the liquids produces non-linear effects in the effective conductivity of the system and discuss the effects of the ion solubility in the media.

**1:27PM S47.00012 Protonation of octadecylamine Langmuir monolayer by adsorption of halide counterions**, WOONGMO SUNG, ZAURE AVAZBAEVA, JONGGWAN LEE, DOSEOK KIM, Sogang University — Langmuir monolayer consisting of octadecylamine (C<sub>18</sub>H<sub>37</sub>NH<sub>2</sub>, ODA) was investigated by heterodyne vibrational sum-frequency generation (HD-VSFG) spectroscopy in conjunction with surface pressure-area ( $\pi$ -A) isotherm, and the result was compared with that from cationic-lipid (DPTAP) Langmuir monolayer. In case of ODA monolayer on pure water, both SF intensity of water OH band and the surface pressure were significantly smaller than those of the DPTAP monolayer implying that only small portion of the amine groups (-NH<sub>3</sub><sup>+</sup>) is protonated in the monolayer. In the presence of sodium halides (NaCl and NaI) in the subphase water, it was found that the sign of Im $\chi^{(2)}$  of water OH band remained the same as that of the ODA monolayer on pure water, but there was a substantial increase in the SF amplitude. From this, we propose that surface excess of the halide counterions (Cl<sup>-</sup> and I<sup>-</sup>) makes the solution condition near the ODA monolayer/water interface more acidic so that ODA molecules in the monolayer are more positively charged, which works to align the water dipoles at the interface.

**1:39PM S47.00013 Single Molecule Mechanochemistry<sup>1</sup>**, SHAOWEI LI, Dept. of Chemistry, University of California, YANXING ZHANG, Dept. of Physics and Astronomy, University of California, WILSON HO, Dept. of Chemistry, University of California, RUQIAN WU, Dept. of Physics and Astronomy, University of California, RUQIAN WU, YANXING ZHANG TEAM, WILSON HO, SHAOWEI LI TEAM — Mechanical forces can be used to trigger chemical reactions through bending and stretching of chemical bonds. Using the reciprocating movement of the tip of a scanning tunneling microscope (STM), mechanical energy can be provided to a single molecule sandwiched between the tip and substrate. When the mechanical pulse center was moved to the outer ring feature of a CO molecule, the reaction rate was significantly increased compared with bare Cu surface and over Au atoms. First, DFT calculations show that the presence of CO makes the Cu cavity more attractive toward H<sub>2</sub>. Second, H<sub>2</sub> prefers the horizontal adsorption geometry in the Cu-Cu and Au-Cu cavities and no hybridization occurs between the antibonding states of H<sub>2</sub> and states of Cu atoms. While H<sub>2</sub> loses electrons from its bonding state in all three cavities, the filling of its anti-bonding state only occurs in the CO-Cu cavity. Both make the CO-Cu cavity much more effectively to chop the H<sub>2</sub> molecule.

<sup>1</sup>Work was supported by the National Science Foundation Center for Chemical Innovation on Chemistry at the Space-Time Limit (CaSTL) under Grant No. CHE-1414466

**1:51PM S47.00014 Charge-patterning phase transition on a surface lattice of titratable sites adjacent to an electrolyte solution<sup>1</sup>**, JOEL SHORE, GEORGE THURSTON, Rochester Institute of Technology — We discuss a model for a charge-patterning phase transition on a two-dimensional square lattice of titratable sites, here regarded as protonation sites, placed on a square lattice in a dielectric medium just below the planar interface between this medium and an aqueous salt solution. Within Debye-Huckel theory, the analytical form of the electrostatic repulsion between protonated sites exhibits an approximate inverse cubic power-law decrease beyond short distances. The problem can thus be mapped onto the two-dimensional antiferromagnetic Ising model with this longer-range interaction, which we study with Monte Carlo simulations. As we increase pH, the occupation probability of a site decreases from 1 at low pH to 0 at high pH. For sufficiently-strong interaction strengths, a phase transition occurs as the occupation probability of 1/2 is approached: the charges arrange themselves into a checkerboard pattern. This ordered phase persists over a range of pH until a transition occurs back to a disordered state. This state is the analogue of the Neel state in the antiferromagnetic Ising spin model. More complicated ordered phases are expected for sufficiently strong interactions (with occupation probabilities of 1/4 and 3/4) and if the lattice is triangular rather than square.

<sup>1</sup>This work was supported by NIH EY018249 (GMT).

**2:03PM S47.00015 Understanding the electronic band structure of Pt-alloys for surface reactivity**, JONGKEUN JUNG, Seoul Natl Univ, BEOMYOUNG KIM, Lawrence Berkeley National Laboratory, JI SOOK HONG, TAE WON JIN, JI HOON SHIM, Postech, SLAVOMIR NEMSAK, BESSY II, JONATHAN D. DENLINGER, Lawrence Berkeley National Laboratory, ARITA MASASHI, SHIMADA KENYA, Hiroshima Synchrotron Radiation Center, CHANGYOUNG KIM, Seoul Natl Univ, BONGJIN SIMON MUN, GIST — In polymer exchange membrane fuel cell (PEMFC), the oxygen reduction reaction (ORR) at cathode side has been continuously investigated due to its critical importance in performance of fuel cell. So far, even with best industrial catalyst made with Pt, the performance of ORR is too far below from the commercial purpose. In 2007, Stamenkovic et al. showed that Pt alloys with 3-*d*-transition metal exhibited significantly improved ORR performance and pointed out the altered electronic structure of surface as the major contributing factor for enhanced ORR. Since 1990, with the advance of DFT calculation, the trend of surface chemical reactivity is explained with the analysis of *d*-band structures, known as *d*-band model. While *d*-band provides valid insight on surface chemical reactivity based on the valence band DOS, the relation between surface work function and DOS has not been well understood. The element-specific local electronic band structure of Pt alloys are identified by ARPES measurement, and the correlation between surface work function and local charge density is investigated.

**Thursday, March 17, 2016 11:15AM - 2:15PM –**

**Session S48 GQI: Superconducting Circuits: Amplifiers** 349 - Michel Devoret, Yale Univesity

**11:15AM S48.00001 Hybrid-free Josephson Parametric Converter<sup>1</sup>**, N.E. FRATTINI, A. NARLA, K.M. SLIWA, S. SHANKAR, M. HATRIDGE, M.H. DEVORET, Department of Applied Physics, Yale University — A necessary component for any quantum computation architecture is the ability to perform efficient quantum operations. In the microwave regime of superconducting qubits, these quantum-limited operations can be realized with a non-degenerate Josephson junction based three-wave mixer, the Josephson Parametric Converter (JPC). Currently, the quantum signal of interest must pass through a lossy 180 degree hybrid to be presented as a differential drive to the JPC. This hybrid therefore places a limit on the quantum efficiency of the system and also increases the device footprint. We present a new design for the JPC eliminating the need for any external hybrid. We also show that this design has nominally identical performance to the conventional JPC.

<sup>1</sup>Work supported by ARO, AFOSR and YINQE

**11:27AM S48.00002 Simplifying the circuit of Josephson parametric converters**, BALEEGH ABDO, MARKUS BRINK, JOSE CHAVEZ-GARCIA, GEORGE KEEFE, IBM- Research Center — Josephson parametric converters (JPCs) are quantum-limited three-wave mixing devices that can play various important roles in quantum information processing in the microwave domain, including amplification of quantum signals, transduction of quantum information, remote entanglement of qubits, nonreciprocal amplification, and circulation of signals [1-4]. However, the input-output and biasing circuit of a state-of-the-art JPC consists of bulky components, i.e. two commercial off-chip broadband 180-degree hybrids, four phase-matched short coax cables, and one superconducting magnetic coil. Such bulky hardware significantly hinders the integration of JPCs in scalable quantum computing architectures. In my talk, I will present ideas on how to simplify the JPC circuit and show preliminary experimental results. [1] B. Abdo et al., PRB 87, 014508. [2] M. Silveri et al., arxiv:1507.00732. [3] B. Abdo et al., PRL 112, 167701. [4] K. Sliwa et al., arxiv:1503.00209.

**11:39AM S48.00003 Phase-sensitive, through-amplification with a double-pumped JPC.<sup>1</sup>**, K.M. SLIWA, M. HATRIDGE, N.E. FRATTINI, A. NARLA, S. SHANKAR, M.H. DEVORET, Department of Applied Physics, Yale University — The Josephson Parametric Converter (JPC) is now routinely used as a quantum-limited signal processing device for superconducting qubit experiments. The JPC consists of two modes, the signal and the idler, that are coupled by a ring of Josephson junctions that implements a non-degenerate, three-wave mixing process. This device is conventionally operated as either a phase-preserving parametric amplifier, or a coherent frequency converter, by pumping it at the sum or difference of the signal and idler frequencies, respectively. Here we present a novel double-pumping scheme based on theory by Metelmann and Clerk where a coherent conversion process and a gain process are simultaneously imposed between the signal and idler modes. The interference of these two processes results in a phase-sensitive amplifier with only forward gain, and which breaks the traditional gain-bandwidth limit of parametric amplification. We present results on phase-sensitive amplification with increased bandwidth, and on noise performance and dynamic range that are comparable to the traditional mode of operation.

<sup>1</sup>Work supported by ARO, AFOSR, NSF and YINQE

**11:51AM S48.00004 Traveling-Wave Parametric Amplifier Based on a Chain of Coupled Asymmetric SQUIDs<sup>1</sup>**, MATTHEW BELL, ANA SAMOLOV, University of Massachusetts Boston — A traveling-wave parametric amplifier (TWPA) composed of a transmission line made up of a chain of coupled asymmetric superconducting quantum interference devices (SQUIDs) is proposed. The unique nature of this transmission line is that its nonlinearity can be tuned with an external magnetic flux and can even change sign. This feature of the transmission line can be used to perform phase matching in a degenerate four-wave mixing process which can be utilized for the parametric amplification of a weak signal in the presence of a strong pump. Numerical simulations of the TWPA design show that, with tuning, phase matching can be achieved and an exponential gain as a function of the transmission-line length can be realized. The flexibility of the proposed design can realize: compact TWPAs with fewer than 211 unit cells, signal gains greater than 20 dB, 3-dB bandwidth greater than 5.4 GHz, and saturation powers up to -98 dBm. This amplifier design is well suited for the multiplexed readout of quantum circuits or astronomical detectors in a compact configuration which can foster on-chip implementations. Phys. Rev. Applied 4, 024014 (2015).

<sup>1</sup>This work was supported in part by the Joseph P. Healey Research Grant (No. P2016), and University of Massachusetts Boston startup funds.

**12:03PM S48.00005 Strong field dynamics and quantum noise in Josephson traveling wave parametric amplifiers (JTWPAs)**, KEVIN O'BRIEN, NSF Nano-scale Science and Engineering Center, UC Berkeley, CHRIS MACKLIN, Quantum Nanoelectronics Laboratory, UC Berkeley, YUAN WANG, NSF Nano-scale Science and Engineering Center, UC Berkeley, IRFAN SIDDIQI, Quantum Nanoelectronics Laboratory, UC Berkeley, XIANG ZHANG, NSF Nano-scale Science and Engineering Center, UC Berkeley — Josephson traveling wave parametric amplifiers (JTWPAs) with resonant phase matching have demonstrated high gain over a broad bandwidth with near quantum-limited noise performance. Several amplifier non-idealities were observed in experiments, including a rapid drop in gain at a certain pump power and a near, but non-unity intrinsic quantum efficiency. To understand these non-idealities, we solve the full nonlinear wave equation for the JTWPA for a sinusoidal drive, finding higher harmonic generation and observing a blow-up at an input pump current below the junction critical current. We find analytic traveling wave solutions in the form of snoidal waves which propagate without distortion. A snoidal drive scheme may increase the drive power at which the blow-up occurs. The quantum noise properties of JTWPAs are critically important for their role as low noise amplifiers. We calculate the noise figure and find that coupling to higher order sidebands imposes an upper limit for the quantum efficiency, in good agreement with empirical results. We further show that this limit can be increased by modest changes to the phase matching of the pump and the dispersion relation.

**12:15PM S48.00006 Broadband Josephson parametric amplifiers: Beyond the standard gain-bandwidth product**, TANAY ROY, SUMAN KUNDU, MADHAVI CHAND, A. M. VADIRAJ, A. RANADIVE, N. NEHRA, MEGHAN P. PATANKAR, Tata Institute of Fundamental Research, Mumbai 400005, J. AUMENTADO, National Institute of Standards and Technology, Boulder, Colorado 80305, A. A. CLERK, McGill University, 3600 rue University, Montreal, Quebec H3A 2T8, Canada, R. VIJAY, Tata Institute of Fundamental Research, Mumbai 400005 — Recent development of multiplexed qubit measurement schemes demand broadband quantum-limited amplifiers to enable high fidelity readout with minimal resources. We present a simple technique to enhance the bandwidth of a resonator based Josephson Parametric Amplifier (JPA) beyond the standard gain-bandwidth product. This is achieved by introducing a positive linear slope in the imaginary component of the input impedance seen by the JPA using a  $\lambda/2$  transformer. Our theoretical model predicts an extremely flat gain profile with a bandwidth enhancement proportional to the square root of the amplitude gain. Experimentally, we achieved a nearly flat 20 dB gain profile over a 640 MHz band, with a mean 1-dB compression point of -110 dBm along with nearly quantum-limited noise performance. The results are in excellent agreement with our theoretical model. We will then discuss strategies to further enhance the performance in terms of bandwidth and dynamic range of the JPA. Finally, we will consider the applicability of our technique to different parametric pumping methods and other parametric amplifier designs as well.

**12:27PM S48.00007 Microwave design optimization for broadband Josephson parametric amplifiers** , MATTHEW REAGOR, EYOB SETE, DANE THOMPSON, Rigetti Quantum Computing, ARPIT RANADIVE, R. VIJAY, Tata Institute of Fundamental Research, Mumbai, CHAD RIGETTI, Rigetti Quantum Computing — Broadband Josephson parametric amplifiers are crucial components of a scalable superconducting quantum computing architecture. Recently, the bandwidth of a resonator-based Josephson parametric amplifier was significantly enhanced by introducing a controlled reactance in the signal chain. The design was based on a  $\lambda/2$  section fabricated on an RF circuit board. We present the design of an on-chip version that will improve robustness and minimize performance variability from one device to another. Further, we will discuss microwave design optimization for flux pumping mechanism to minimize cross-talk between different input-output ports of the device. Finally, we will discuss design goals for further improvement of amplifier performance.

**12:39PM S48.00008 High dynamic range Josephson parametric amplifiers** , NICOLAS ROCH, CNRS and Universite Grenoble Alpes, Institut Neel, 38042 Grenoble, France, KATER W. MURCH, Department of Physics, Washington University, St. Louis, Missouri 63130, USA, RAJAMANI VIJAY, Tata Institute of Fundamental Research, Mumbai 400005, India — Josephson parametric amplifiers (JPAs) have become the technology of choice to amplify small amplitude microwave signals since they show noise performances close to the quantum limit of amplification. An important challenge that faces this technology is the low dynamic range of current devices, which limits the number of measurements that can be performed concurrently and the rate of information acquisition for single measurements. We have fabricated and tested novel parametric amplifiers based on arrays of up to 100 SQUIDS. The amplifiers produce gain in excess of 20 dB over a large bandwidth and match the dynamic range achieved with traveling wave devices. Compared to the latter devices they are fabricated in a single lithography step and we will show that their bandwidth performance can be further extended using a recently developed impedance matching technique.

**12:51PM S48.00009 Microwave response and photon emission of a voltage biased Josephson junction** , SALHA JEBARI, ALEXANDER GRIMM, DIBYENDU HAZRA, MAX HOFHEINZ, CEA Grenoble — The readout of superconducting qubits requires amplifiers combining noise close to the quantum limit, high gain, large bandwidth, and sufficient dynamic range. Josephson parametric amplifiers using Josephson junctions in the 0-voltage state, driven by a large microwave signals, begin to perform sufficiently well in all 4 of these aspects to be of practical use, but remain difficult to optimize and use. Recent experiments with superconducting circuits consisting of a DC voltage-biased Josephson junction in series with a resonator, showed that a tunneling Cooper pair can emit one or several photons with a total energy of 2e times the applied voltage. We present microwave reflection measurements on this device indicating that amplification is possible with a simple DC voltage-biased Josephson junction. We compare these measurements with the noise power emitted by the junction and show that, for low Josephson energy, transmission and noise emission can be explained within the framework of P(E) theory of inelastic Cooper pair tunneling. Combined with a theoretical model, our results indicate that voltage-biased Josephson junctions might be useful for amplification near the quantum limit, offering simpler design and a different trade-off between gain, bandwidth and dynamic range.

**1:03PM S48.00010 Estimation of the projection error of a qubit readout by quantum Zeno effect** , KOSUKE KAKUYANAGI, YUICHIRO MATSUZAKI, HAYATO NAKANO, NTT Basic Research Laboratories, KOUICHI SEMBA, National Institute of Information and Communications Technology, SHIRO SAITO, NTT Basic Research Laboratories — In a quantum system, frequent projection operations can suppress a specific kind of time evolutions that show quadratic behavior in a time domain. This phenomenon is known as quantum Zeno effect (QZE). Normally, projection operations freeze the qubit state so that the qubit remains in the initially prepared state such as a ground state or an excited state. However, if a projection error occurs, qubit state is flipped. In this case, frequent projection operations do not keep qubit state. This means that, by investigating the efficiency of the QZE, we can in principle estimate the projection error rate of the qubit readout system. A Josephson bifurcation amplifier (JBA) readout method provides us a way to perform fast and low back-action superconducting qubit readout. We fabricate a sample that has a JBA resonator coupled to the superconducting flux qubit. By using this sample, we demonstrated QZE by applying multiple readout pulses during Rabi oscillations. Because of the multiple readout pulses, Rabi oscillation was suppressed and the qubit was kept in its initial state. From the holding time of the state via the QZE, we concluded that the projection error of the JBA readout is less than 2%.

**1:15PM S48.00011 Single-shot Readout of a Superconducting Qubit using a Josephson Parametric Oscillator<sup>1</sup>** , PHILIP KRANTZ, ANDREAS BENGTTSSON, MICHAEL SIMOEN, Chalmers, SIMON GUSTAVSSON, MIT, VITALY SHUMEIKO, Chalmers, W. D. OLIVER, MIT, MIT Lincoln Laboratory, C. M. WILSON, Waterloo, PER DELSING, JONAS BYLANDER, Chalmers — We propose and demonstrate a new read-out technique for a superconducting qubit by dispersively coupling it to a Josephson parametric oscillator. We employ a tunable quarter-wavelength superconducting resonator and modulate its resonant frequency at twice its value with an amplitude surpassing the threshold for parametric instability. We map the qubit states onto two distinct states of classical parametric oscillation: one oscillating state, with  $185 \pm \sum 15$  photons in the resonator, and one with zero oscillation amplitude. This high contrast obviates a following quantum-limited amplifier. We demonstrate proof-of-principle, single-shot readout performance, and present an error budget indicating that this method can surpass the fidelity threshold required for quantum computing.

<sup>1</sup>Support came from the Wallenberg foundation, the European Research Council (ERC), the Royal Swedish Academy of Science (KVA), the European project ScaleQIT, STINT, and Marie Curie CIG.

**1:27PM S48.00012 SLUG Microwave Amplifier as a Nonreciprocal Gain Element for Scalable Qubit Readout** , TED THORBECK, EDWARD LEONARD, SHAOJIANG ZHU, ROBERT MCDERMOTT, University of Wisconsin - Madison — Josephson parametric amplifiers for superconducting qubits require several stages of cryogenic isolation to protect the qubit from strong microwave pump tones and downstream noise. But isolators and circulators are large, expensive and magnetic, so they are an obstacle to scaling up a superconducting quantum computer. In contrast, the SLUG (Superconducting Low-inductance Undulatory Galvanometer) is a high gain, broadband, low noise microwave amplifier that provides built-in reverse isolation. Here, we describe the dependence of the SLUG reverse isolation on signal frequency and device operating point. We show that the reverse isolation of the SLUG can be as large as or larger than that of a bulk commercial isolator. Finally, we discuss the use of the SLUG to read out a transmon qubit without isolators or circulators.

**1:39PM S48.00013 Noise Characteristics of the Josephson Amplifiers by Stochastic Calculus<sup>1</sup>** , WENSHUO LIU, ROBERT MCDERMOTT, MAXIM VAVILOV, University of Wisconsin, Madison — We present theoretical studies of the noise performance of non-reciprocal gain elements based on Josephson junctions including the SQUID and the SLUG. We develop a perturbative approach by means of stochastic calculus which combines both analytical and numerical methods, and calculate the noise characteristics of the amplifiers in the thermal regime. We show that noise in the amplifiers originates mainly from the diffusive behavior of phase slips. This new method could help with the optimization of Josephson amplifiers for high-fidelity multiplexed qubit readout.

<sup>1</sup>Supported by the Army Research Office under contract W911NF-14-1-0080.

**1:51PM S48.00014 Qubit Readout with the Josephson Photomultiplier** , IVAN PECHENEZHSKIY, GUILHEM RIBEILL, University of Wisconsin, Madison, M. HUTCHINGS, CALEB HOWINGTON, Syracuse University, MAXIM VAVILOV, University of Wisconsin, Madison, FRANK WILHELM, Saarland University, B.L.T. PLOURDE, Syracuse University, ROBERT MCDERMOTT, University of Wisconsin, Madison — The realization of a large-scale fault-tolerant quantum processor will require scalable high-fidelity readout of multiqubit parity operators. Here we describe development of a scalable qubit measurement approach based on microwave photon counting. The measurement protocol involves mapping the qubit state to photon occupation of bright and dark cavity pointer states, followed by photodetection using the Josephson photomultiplier (JPM). We discuss use of the qubit as a calibrated source of photons to measure JPM quantum efficiency, and we describe global optimization of the measurement protocol. Finally, we discuss prospects for interfacing the JPM output to single flux quantum circuits to allow low-latency classical postprocessing of the qubit measurement result.

**2:03PM S48.00015 Multi-qubit measurements with a Josephson Photomultiplier<sup>1</sup>** , CALEB HOWINGTON, M HUTCHINGS, Syracuse University, GUILHEM RIBEILL, IVAN PECHENEZHSKIY, MAXIM G. VAVILOV, University of Wisconsin, FRANK K. WILHELM, Saarland University, R. MCDERMOTT, University of Wisconsin, BLT PLOURDE, Syracuse University — The ability to measure multi-qubit parity is critical for the realization of a fault-tolerant quantum information processor. For a system of transmon qubits coupled to a superconducting cavity, a threshold photon detector can provide an efficient path towards the digital readout of qubit parity after the parity information is mapped onto the cavity photon occupation. We will describe progress towards the implementation of such a scheme for measuring the parity of two transmon qubits. On-chip flux bias lines allow us to tune the dispersive cavity shifts related to the state of the two qubits and an appropriately shaped pulse driven to the cavity results in a bright state for one parity but not the other. A Josephson Photomultiplier then serves as a phase-insensitive digital detector of the microwave photons that leak out of the cavity. Future improvements and various technical difficulties will be discussed.

<sup>1</sup>We acknowledge support from ARO under Contract W911NF-14-1-0080.

**Thursday, March 17, 2016 11:15AM - 2:15PM —**  
**Session S50 DAMOP: Strongly Interacting Bose and Fermi Gases** Hilton Baltimore Holiday Ballroom 1 -  
Johannes Hofmann, Cavendish Laboratory

**11:15AM S50.00001 P-wave contacts for two dimensional quantum gas** , YICAI ZHANG, The University of Hong Kong, ZHENHUA YU, Institute for Advanced Study, Tsinghua University, SHIZHONG ZHANG, The University of Hong Kong — The s-wave contact has played an important role in our understanding of the strongly interacting Fermi gases. Recently, theoretical and experimental work has shown that two similar contacts exist for a p-wave interacting Fermi gas in three-dimensions. In this work, we extend the considerations to two dimensional spineless Fermi gas and derive exact results regarding the energy, momentum distributions and in particular, shifts of monopole frequency in a harmonic trap. Asymptotic formula for the frequency shift is given at high temperature via virial expansion and this can be checked by future experiments.

**11:27AM S50.00002 Multi-Branch Spin Chain Models for Strongly interacting Spinor Fermi and Bose gases in One-Dimension** , LI YANG, HAN PU, Rice Univ — By mapping a 1D spinor Fermi or Bose gases wavefunction to a direct product of a spinless fermion wavefunction and a spin chain wavefunction, we obtain a spin-charge coupling Hamiltonian which is a multi-branch spin chain model. The charge part of this model are p-wave  $\vec{\sigma}\delta(x)\vec{\sigma}$  interactions. The spin part of this model are spin parity projection operators. Previously obtained spin chain models (Nature Commun. 5, 5300. Phys. Rev. A 90, 013611. Phys. Rev. A 91, 043634.) are first order perturbation of this multi-branch spin chain model. With this model, for particles in a harmonic trap in strongly interacting regime, we study breathing mode frequencies and the system's response to a spin dependent magnetic gradient and quench dynamics. We also studied the properties of the system with large particle numbers under local density approximation. The resulted spin chain models are studied by exact numerical methods such as Matrix Product States. Other than harmonic trap we also considered traps with  $\delta(x)$  impurity, which can not be approximated by local density approximation.

**11:39AM S50.00003 ABSTRACT WITHDRAWN —**

**11:51AM S50.00004 Efimov correlations in strongly interacting Bose gases** , JOHANNES HOFMANN, University of Cambridge, MARCUS BARTH, Technische Universitaet Muenchen — A series of recent hallmark experiments have demonstrated that Bose gases can be created in the strongly interacting unitary limit in the non-degenerate high-temperature regime. These systems display the three-body Efimov effect, which poses a theoretical challenge to compute observables including these relevant three-body correlations. In this talk, I shall present our results for the virial coefficients, the contact parameters, and the momentum distribution of a strongly interacting three-dimensional Bose gas obtained by means of a virial expansion up to third order in the fugacity, which takes into account three-body correlations exactly. Our results characterize the non-degenerate regime of the interacting Bose gas, where the thermal wavelength is smaller than the interparticle spacing but the scattering length may be arbitrarily large. In addition, we provide a calculation of the momentum distribution at unitarity, which displays a universal high-momentum tail with a log-periodic momentum dependence - a direct signature of Efimov physics. In particular, we provide a quantitative description of the momentum distribution at high momentum as measured by the JILA group [Makotyn et al., Nat. Phys. 10, 116 (2014)]. Our results allow the spectroscopy of Efimov states at unitarity.

**12:03PM S50.00005 Competing order parameters in Fermi systems with engineered band dispersion** , CHIEN-TE WU, RUFUS BOYACK, BRANDON ANDERSON, K LEVIN, James Franck Institute — We explore a variety of competing phases in 2D and 3D Fermi gases in the presence of novel dispersion relations resulting from a shaken optical lattice. We incorporate spin imbalance along with attractive interactions. In 3D, at the mean field level we present phase diagrams reflecting the stability of alternative order parameters in the pairing (including LOFF) and charge density wave channels. We perform analogous studies in 2D, where we focus on the competition between different paired phases. Important in this regard is that our 2D studies [1] are consistent with the Mermin-Wagner theorem, so that, while there is competition, conventional superfluidity cannot occur. [1] C.-T. Wu, B. M. Anderson, R. Boyack, and K. Levin, arXiv:1509.00857 (to be published in Phys. Rev. Lett.)

**12:15PM S50.00006 Spectral function and dark continuum of the resonant Fermi Polaron<sup>1</sup>** , OLGA GOULKO, UMass Amherst, ANDREY MISHCHENKO, RIKEN Center for Emergent Matter Science (CEMS), NIKOLAY PROKOFEV, BORIS SVISTUNOV, UMass Amherst — The Fermi polaron is an impurity interacting with a sea of fermions. It is an exemplary system to study impurity problems, strongly imbalanced Fermi gases and quasiparticles. Experiments probe its spectral function, which is directly linked to many physical properties. We present the first numerical results for the polaron spectral function with controlled error bars, obtained from first principles with diagrammatic Monte Carlo and analytic continuation. The spectral function exhibits a narrow ground state peak and another broad peak at positive energy, which are separated by a region of extremely low spectral weight. This "dark continuum" surprisingly starts to emerge in the absence of a small parameter, around  $k_F a \sim 1$ , and quickly broadens into a gap-like structure deeper on the BEC side. We confirm that the dark continuum is indeed physical and not an artefact of approximate calculations and establish a controlled upper bound on its integrated weight.

<sup>1</sup>This work is supported by the NSF under the Grant No. PHY-1314735.

**12:27PM S50.00007 Finite Temperature Response of a 2D Dipolar Bose Gas at Different Dipolar Tilt Angles<sup>1</sup>**, PENGTAO SHEN, KHANDKER QUADER, Kent State University — We calculate finite temperature (T) response of a 2D Bose gas, subject to dipolar interaction, within the random phase approximation (RPA). We evaluate the appropriate 2D finite-T pair bubble diagram needed in RPA, and explore ranges of density and temperature for various dipolar tilt angles. We find the system to exhibit a collapse transition and a finite momentum instability, signaling a density wave or striped phase. We construct phase diagrams depicting these instabilities and resulting phases, including a normal Bose gas phase. We also consider the finite-T response of a quasi-2D dipolar Bose gas. We discuss how our results may apply to ultracold dense Bose gas of polar molecules, such as <sup>41</sup>K<sup>87</sup>Rb, that has been realized experimentally.

<sup>1</sup>Acknowledge partial support from Institute for Complex Adaptive Matter (ICAM)

**12:39PM S50.00008 Strengthening Supersolids with Disorder in the Extended Bose-Hubbard Model**, FEI LIN, Washington and Lee University, THOMAS MAIER, Oak Ridge National Lab, VITO SCAROLA, Virginia Tech — The extended Bose-Hubbard model captures the essential properties of a wide variety of physical systems including ultracold atoms and molecules in optical lattices, Josephson junction arrays, and narrow band superconductors. It exhibits a rich phase diagram including a supersolid phase where a lattice solid coexists with a superfluid. We use quantum Monte Carlo to map out the phase diagram of the extended Bose-Hubbard model on the simple cubic lattice where the supersolid is expected. We find that the supersolid is very delicate because unexpected phase separated states compete with the supersolid. We add disorder to the extended Bose-Hubbard model and find that the supersolid phase is enhanced by disorder as phase separation is suppressed. Our results establish optimal regimes for observing supersolids and therefore have important implications for their observation.

**12:51PM S50.00009 *p*-wave superfluid shells for trapped fermions with population imbalance<sup>1</sup>**, AMMAR KIRMANI, KHANDKER QUADER, MAXIM DZERO, Kent State University — We present the phase diagram for a *p*-wave fermionic superfluid with imbalanced populations in a potential trap. We find shells of various superfluid phases, whose realization is determined by the parameters of a trap. In order to compute the resulting phase diagram, we use weak-coupling BCS theory together with the local density approximation in which the effect of the trapping potential is accounted for by a spatially inhomogeneous chemical potential. We compare our phase diagram with the one found for the trapped population imbalanced *s*-wave fermionic superfluid [Lin, Yi & Duan, Phys. Rev. A 74, 031604R (2006)], and also point out key differences with results for the population imbalanced *p*-wave case in the absence of a trap [Liao, Popescu & Quader, Phys. Rev. B 88, 134507 (2013)].

<sup>1</sup>NSF-DMR-1506547

**1:03PM S50.00010 Quantum Criticality of the Two-dimensional Bose Gas with the Lifshitz dispersion**, CONGJUN WU, JIANDA WU, UC San Diego — Bosonic systems with the synthetic spin-orbit coupling and Zeeman field can be tuned into a quantum Lifshitz point exhibiting the  $q^4$ -dispersion. They are fundamentally different from the conventional ones with the  $q^2$ -dispersion, and are also connected to quantum frustrated magnets. We set up a generic quantum  $\phi^4$ -theory at the Lifshitz point and investigate quantum critical behaviors at both zero and finite temperatures following the perturbative renormalization group method. Controlled by different fixed points, various physical quantities exhibit significantly different scalings from those of the conventional bosonic systems, exhibiting rich quantum critical physics in different interaction and temperature ranges.

**1:15PM S50.00011 Equation of state of ultracold fermions in the 2D BEC-BCS crossover**, IGOR BOETTCHER, Department of Physics, Simon Fraser University, Burnaby, British Columbia V5A 1S6, Canada, LUCA BAYHA, DHRUV KEDAR, PUNEET MURTHY, MATHIAS NEIDIG, MARTIN RIES, ANDRE WENZ, GERHARD ZUERN, SELIM JOCHIM, Physikalisches Institut, Heidelberg University, D-69120 Heidelberg, Germany, TILMAN ENSS, Institute for Theoretical Physics, Heidelberg University, D-69120 Heidelberg, Germany — We report the experimental measurement of the equation of state of a two-dimensional Fermi gas with attractive *s*-wave interactions throughout the crossover from a weakly coupled Fermi gas to a Bose gas of tightly bound dimers as the interaction strength is varied. We demonstrate that interactions lead to a renormalization of the density of the Fermi gas by several orders of magnitude. We compare our data near the ground state and at finite temperature to predictions for both fermions and bosons from Quantum Monte Carlo simulations and Luttinger-Ward theory. Our results serve as input for investigations of close-to-equilibrium dynamics and transport in the two-dimensional system.

**1:27PM S50.00012 Fluctuation theory of Rashba Fermi gases: Gaussian and beyond<sup>1</sup>**, VIJAY B. SHENOY, Indian Institute of Science Bangalore, JAYANTHA P. VYASANAKERE, Tumkur University — Fermi gases with generalized Rashba spin orbit coupling induced by a synthetic gauge field have the potential of realizing many interesting states such as rashbon condensates and topological phases. Here we address the key open problem of the fluctuation theory of such systems and demonstrate that beyond-Gaussian effects are *essential* to capture finite temperature physics of such systems. We obtain their phase diagram by constructing an approximate non-Gaussian theory. We conclusively establish that spin-orbit coupling can enhance the exponentially small transition temperature ( $T_c$ ) of a weakly attracting superfluid to the order of Fermi temperature, paving a pathway towards high  $T_c$  superfluids.

<sup>1</sup>Work supported by CSIR, DST, DAE and IUSSTF

**1:39PM S50.00013 Superfluidity and BCS-BEC crossover of ultracold atomic Fermi gases in mixed dimensions<sup>1</sup>**, LEIFENG ZHANG, QIJIN CHEN, Zhejiang University — Atomic Fermi gases have been under active investigation in the past decade. Here we study the superfluid and pairing phenomena of a two-component ultracold atomic Fermi gas in the presence of mixed dimensionality, in which one component is confined on a 1D optical lattice whereas the other is free in the 3D continuum. We assume a short-range pairing interaction and determine the superfluid transition temperature  $T_c$  and the phase diagram for the entire BCS-BEC crossover, using a pairing fluctuation theory which includes self-consistently the contributions of finite momentum pairs. We find that, as the lattice depth increases and the lattice spacing decreases, the behavior of  $T_c$  becomes very similar to that of a population imbalance Fermi gas in a simple 3D continuum. There is no superfluidity even at  $T = 0$  below certain threshold of pairing strength in the BCS regime. Nonmonotonic  $T_c$  behavior and intermediate temperature superfluidity emerge, and for deep enough lattice, the  $T_c$  curve will split into two parts. Implications for experiment will be discussed. References: 1. Q.J. Chen, Ioan Kosztin, B. Janko, and K. Levin, Phys. Rev. B 59, 7083 (1999). 2. Chih-Chun Chien, Qijin Chen, Yan He, and K. Levin, Phys. Rev. Lett. 97, 090402(2006).

<sup>1</sup>Work supported by NSF of China and the National Basic Research Program of China

**1:51PM S50.00014 Bose polarons in the strongly interacting regime.**<sup>1</sup>, MING-GUANG HU, MICHAEL VAN DE GRAAFF, DHRUV KEDAR, ERIC CORNELL, DEBORAH JIN, JILA, NIST and CU-Boulder — Impurities immersed in and interacting with a Bose-Einstein condensate (BEC) are predicted to form quasiparticle excitations called Bose polarons. I will present experimental evidence of Bose polarons in cold atoms obtained using radio-frequency spectroscopy to measure the excitation spectrum of fermionic <sup>40</sup>K impurities interacting with a BEC of <sup>87</sup>Rb atoms. We use an interspecies Feshbach resonance to tune the interactions between the impurities and the bosons, and we take data in the strongly interacting regime.

<sup>1</sup>This work is supported by NSF, NASA and NIST

**2:03PM S50.00015 Self consistent theories of superfluid density and collective modes in BCS-BEC**, RUFUS BOYACK, BRANDON ANDERSON, CHIEN-TE WU, KATHRYN LEVIN, James Franck Inst — Establishing fully self consistent and sum rule compatible response functions in strongly correlated Fermi superfluids has been a historically challenging subject. In this talk, we present recent progress pertaining to response functions in many-body Fermi systems. We note that even in strict BCS theory, the textbook derivation of density and current response functions in the gradient expansion breaks certain conservation laws such as the compressibility sum rule. To include additional contributions that preserve all expected conservation laws, we show how to exploit Ward identities within two different t-matrix schemes. In this way we address the density-density response (including collective modes) and the superfluid density. Finally, we characterize approximations made in the literature where some consistency requirements have been dropped.

**Thursday, March 17, 2016 11:15AM - 2:15PM –**  
**Session S51 FIAP: Thermodynamic & Transport Properties of Semiconductors** Hilton Baltimore  
 Holiday Ballroom 2 - Neil Zimmerman, NIST

**11:15AM S51.00001 Magneto-Inter-Subband Oscillations in GaAs quantum wells with three populated subbands placed in tilted magnetic fields.**<sup>1</sup>, WILLIAM MAYER, JESSE KANTER, SERGEY VITKALOV, City College of New York, CUNY Graduate Center, ALEXEY BYKOV, Institute of Semiconductor Physics, Novosibirsk, Russia — The effect of tilted magnetic fields on magnetotransport is studied in GaAs quantum wells with three populated subbands. In perpendicular fields magneto-intersubband oscillations (MISO) are observed. These oscillations obey the relation  $\Delta_{ij} = (E_i - E_j) = k\omega_c$ , where  $E_i$  is the energy of the bottom of  $i$ -th subband and  $k$  is an integer. MISO are periodic in the inverse magnetic field and show three frequencies  $f_{ij} \sim \Delta_{ij}$ . Due to  $E_{1,2} \ll E_3$  two MISO oscillate at high frequencies (HF) demonstrating a beat pattern with the beat frequency  $f_b = (f_{13} - f_{23})/2 \sim \Delta_{12}$ . With increasing tilt angle at small magnetic fields,  $\omega_c < \Delta_{12}$ , the periodicity of HF-MISO changes indicating a change in the subband gap  $\Delta_{12}$ . The dependence of  $\Delta_{12}$  on the parallel magnetic field is found to be in a good agreement with existing theory. At larger parallel magnetic fields and  $\omega_c > \Delta_{12}$ , the high frequency beating disappears leaving only HF-MISO with single frequency  $f = (f_{13} + f_{23})/2$ . It indicates a magnetic breakdown between the lower two subbands. Investigations of the 2D electron system in the regime of the magnetic breakdown are presented.

<sup>1</sup>This work was supported by the National Science Foundation (DMR 1104503), the Russian Foundation for Basic Research (project no.14-02-01158) and the Ministry of Education and Science of the Russian Federation.

**11:27AM S51.00002 Blockade in a silicon double quantum dot via the valley degree of freedom**, JUSTIN PERRON<sup>1</sup>, Cal State Univ - San Marcos, MICHAEL J. GULLANS<sup>2</sup>, JACOB M. TAYLOR<sup>3</sup>, Joint Quantum Institute, National Institute of Standards and Technology, Gaithersburg, Maryland, 20899, M. D. STEWART, JR., NEIL M. ZIMMERMAN, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA — Measuring electrical transport through double quantum dots (DQDs) is a useful way of illuminating several aspects of the states of the carriers. We show transport measurements through a silicon DQD formed in a mesa etched nanowire. Comparing the data at positive and negative bias voltage we observe a size asymmetry in the region of allowed current typically associated with Pauli spin blockade (PSB). However, the qualitative features of the asymmetry in our data, including i) lack of odd/even filling, ii) same polarity of asymmetry across many bias triangles, iii) lack of systematic dependence on magnetic field, and iv) a dependence on gate voltages, are all in disagreement with the predictions of PSB. In contrast, we have developed a model based on the selective filling of valley states in the DQD and the conservation of the valley degree of freedom during tunneling that predicts all of the qualitative features in our data.

<sup>1</sup>Joint Quantum Institute, National Institute of Standards and Technology, Gaithersburg, Maryland 20899

<sup>2</sup>Joint Center for Quantum Information and Computer Science, University of Maryland, College Park, Maryland 20742, USA

<sup>3</sup>Joint Center for Quantum Information and Computer Science, University of Maryland, College Park, Maryland 20742, USA

**11:39AM S51.00003 Negative Differential Conductance from Space Charge Limited Currents in Semiconductors**, ANDREW BROOKS, XIAO GUANG ZHANG, University of Florida — Applying the theory of space charge limited currents (SCLC), we show that negative differential conductance can arise from doubly occupied traps that are nearly degenerate with the bottom of the conduction band. Using degenerate state perturbation theory, the Coulomb energy of the doubly occupied traps is shown to depend on the hybridization with the conduction band states. Initially, when carriers are injected into the solid, traps begin to fill while the conduction band states stay relatively empty and thus accessible to trapped electrons via hopping. Trap and conduction states continue to be filled as current is increased, and the energy of trapped electrons begins to rise. A critical current is reached whereupon a further increase in current leads to a reduction of filled traps (i.e. a reduction of space charge in the solid), and thus a corresponding decrease in voltage. This trend in the current-voltage characteristic curves persists until the bottom of the conduction band has been filled, then voltage rises with current.

**11:51AM S51.00004 Vertical electronic transport in van de waals heterostructures**, ZHENHUA QIAO, University of Science and Technology of China, ZHENHUA QIAO'S GROUP TEAM — In this work, we will introduce the theoretical investigation of the vertical electronic transport in various heterostructures by using both tight-binding method and first-principles calculations. Counterintuitively, we find that the maximum electronic transport is achieved at very limited scattering regions but not at large overlapped catering regions. Based on this finding, we design a special setup to measure the tunneling effect in rotated bilayer systems.

**12:03PM S51.00005 First principles lattice thermal conductivity of  $\text{Li}_2\text{Se}$ ,  $\text{Li}_2\text{Te}$  and alloys: phase space guidelines for thermal transport**<sup>1</sup>, LUCAS LINDSAY, SAIKAT MUKHOPADHYAY, DAVID PARKER, Oak Ridge National Laboratory — The lattice thermal conductivities ( $k$ ) of  $\text{Li}_2\text{Se}$ ,  $\text{Li}_2\text{Te}$  and alloys are examined using a first-principles Peierls-Boltzmann transport methodology. The dominant resistance to heat-carrying acoustic phonons in  $\text{Li}_2\text{Se}$  and  $\text{Li}_2\text{Te}$  comes from the interactions of these modes with two optic phonons, a.o scattering. In typical cubic and hexagonal materials (*e.g.*, Si, GaAs, AlN) a.o scattering does not play a considerable role in determining  $k$ , as it requires significant bandwidth and dispersion of the optic phonon branches, both present in  $\text{Li}_2\text{Se}$  and  $\text{Li}_2\text{Te}$ . We discuss how these properties and other features of the phonon dispersion (*e.g.*, bunching of the acoustic branches and an acoustic-optic frequency gap) combine to determine the overall conductivity of a material. Thus, microscopic scattering phase space arguments are generalized to give a more comprehensive view of intrinsic thermal transport in crystalline solids. We note that these general considerations are important for the discovery and design of new ‘high $k$ ’ and ‘low  $k$ ’ materials for thermal management applications.

<sup>1</sup>L. L., S. M. and D. S. P. acknowledge support from the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division

**12:15PM S51.00006 Thermal Conductivity Accumulation Function of Silicon-Germanium Alloy from Thermorefectance and First-Principles**, KEVIN PARRISH, JUSTIN FREEDMAN, KEITH REGNER, ANKIT JAIN, JONATHAN MALEN, ALAN MCGAUGHEY, Carnegie Mellon Univ — Phonons are the dominant heat carriers in semiconductors. Alloying changes their properties by introducing mass disorder and altering the bonding environment. In this study, we determine the thermal conductivity accumulation functions of silicon-germanium alloys using broadband frequency-domain thermorefectance experiments. The accumulation function describes the cumulative mean free path-dependent contributions to thermal conductivity and provides a measure for determining how alloying alters thermal conductivity compared to pure semiconductors. The experimental results are compared to calculations based in density functional theory, lattice dynamics, the virtual crystal approximation, and the Boltzmann transport equation. In both thermorefectance and lattice dynamics we find alloying increases the proportional accumulation of long MFP phonons.

**12:27PM S51.00007 Study of Thermal properties of  $\text{VO}_2$  and multilayer  $\text{VO}_2$  thin films for application in Thermal Switches.**, GAOHUA ZHU, Toyota Research Institute of North America — Ultrafast nature of the phase transition near room temperature in  $\text{VO}_2$  makes it attractive material for applications in electronics and optical devices however utilization of corresponding drastic change in thermo-physical properties are rarely reported. In this study we investigate thermal and electronic properties of  $\text{VO}_2$  thin films on various substrates across the transition temperature to seek possibility of utilizing  $\text{VO}_2$  based thermal switches for applications in thermal devices. In addition, the interfacial heat transfer in  $\text{VO}_2$ /metal multilayer thin film is mediated by phonons at low temperature, and when temperature is elevated beyond phase transition temperature, the interface thermal conductance is mediated mainly by both phonons and electrons.  $\text{VO}_2$ -multilayers approach is studied to utilize the switching interface thermal conductance in order to obtain higher thermal conductivity switch ratio than what can be achieved in intrinsic  $\text{VO}_2$ . Thermal conductivities and interface thermal conductance of  $\text{VO}_2$  and  $\text{VO}_2$  multilayer thin films are measured using the time-domain thermorefectance (TDTR) method. We will discuss interplay of phononic and electronic component to thermal conductivity in the light of Wiedemann–Franz law across the metal to insulator state of  $\text{VO}_2$  films.

**12:39PM S51.00008 Efros-Shklovskii variable range hopping conductivity without Coulomb gap**, TIANRAN CHEN, Department of Physics, West Chester University of Pennsylvania, BRIAN SKINNER, Center for Excitonics, Massachusetts Institute of Technology — In doped semiconductors and Coulomb glasses, in the limit of weak coupling, the electron conductivity primarily proceeds by phonon-assisted tunneling or hopping between different sites through the insulating gaps that separate them. Electron conduction can occur both through nearest-neighbor hopping and through cotunneling of electrons between distant sites via a chain of intermediate virtual states. In the presence of some disorder, the latter mechanism dominates at low temperatures, where the length of the hops grows to optimize the conductivity. This transport mechanism was introduced by Mott, and is called variable range hopping. When the Coulomb interaction between localized electrons is taken into account, it can be shown that at a sufficiently low temperature, variable range hopping conductivity obeys the Efros-Shklovskii (ES) law, which has been observed in a number of amorphous semiconductors and granular metal systems at low temperatures. ES conductivity has been long understood as the result of a soft, Coulomb gap at the Fermi level. However, such a theory overlooks the presence of spatial correlations between site energies and their possible effects on electrical conductivity. In this talk, we show both analytically and numerically that in systems where spatial correlations must be taken into account, ES conductivity may persist far outside the Coulomb gap, in contrast to conventional transport theory for doped semiconductors and Coulomb glasses where ES conductivity only occurs within the Coulomb gap.

**12:51PM S51.00009 Maximum non-saturating magnetoresistance in  $\text{MoTe}_2$** , MAHMOUD ABDEL-HAFIEZ, ZHEHAO GU, XIAO-JIA CHEN, Center for High Pressure Science and Technology Advanced Research, Shanghai, 201203, China, CENTER FOR HIGH PRESSURE SCIENCE AND TECHNOLOGY ADVANCED RESEARCH, SHANGHAI, 201203, CHINA TEAM — The search for exotic materials with a linear magnetoresistance (MR) is one of the most challenging tasks of the condensed matter community and materials science. Here, we investigated the magnetoresistance behavior of high-quality single crystals  $\text{MoTe}_2$ . A large linear non-saturating MR in a magnetic field of 60 T, was observed with a maximum at a temperature of  $T = 45$  K. The detailed field and temperature dependencies will be presented. Our results not only provide a general scaling approach for the anisotropic MR but also are crucial for correctly understanding the mechanism of the linear MR, including the origin of the remarkable “turn-on” behavior in the resistance versus temperature curve.

**1:03PM S51.00010 Negative thermal expansion above a quantum phase transition**, SAHAN HAN-DUNKANDA, ERIN CURRY, JASON HANCOCK, Univ of Connecticut - Storrs — Strong, thermally persistent, isotropic negative thermal expansion (NTE) is unusual and has been observed in only a handful of materials. Scandium trifluoride ( $\text{ScF}_3$ ) features large isotropic thermal expansion persistent over a 1000K range of temperature. More interestingly, no structural phase transition has been reported above 0.4K and it retains the simple cubic structure up to its high melting point of 1800K, which is unusual compared with other transition metal trifluorides. Here, we present a combined inelastic x-ray scattering (IXS) and x-ray diffraction study of  $\text{ScF}_3$ , which reveals some exciting features of this material. The low-energy ( $\sim 1$  meV) vibrational modes corresponding to M and R points of simple cubic Brillouin zone could explain NTE in  $\text{ScF}_3$ , and we find that the low temperature IXS data show a central peak which is especially strong at these points. In addition, the whole M-R branch undergoes unusual softening at low temperature. We determine that this mode softens nearly to zero energy as the temperature approaches to 0K. These signature portend an approach to a quantum phase transition of this insulating, nonmagnetic simple cubic perovskite material  $\text{ScF}_3$ . The central peak, soft mode and thermal expansion could all be consequences of this incipient transition. The connections we have established in the phenomenology of  $\text{ScF}_3$  may be present in other perovskites as well as other materials that display strong NTE

**1:15PM S51.00011 First Principles Study of structural characteristics and phase change mechanism of Ge-Sb-Te based materials**, HANJIN PARK, CHEOL-WOON KIM, HYUNG-JUNE LEE, HOSIN SONG, YOUNG-KYUN KWON, Department of Physics and Research Institute for Basic Sciences, Kyung Hee University, Seoul, 130-701, Korea — Using *ab initio* density functional theory, we investigate the structural properties and their phase transition mechanism of the crystalline and amorphous phases of Ge-Sb-Te (GST) based phase change materials, which would be utilized for phase change random access memory. Among various stoichiometries of GST, we focus on compositions along the  $(\text{GeTe})_n(\text{Sb}_2\text{Te}_3)_m$  pseudo-binary line, denoted simply by  $(n, m)$  with integer  $n$  and  $m$ . We explore various GST materials corresponding  $(n, m)$  sets including (1,0), (0,1), (1,1), (2,1) and (1,2) by modeling their both phases. Especially, their amorphous phases can be constructed based on experimental data available or molecular dynamics (MD) simulations performing melt-quench processes. To understand the phase transition mechanism, we evaluate their coordination numbers, radial distribution functions, and angle distribution functions, which enables us to identify the characteristic local geometry representing each phase. We further investigate the thermal properties of various phases by evaluating their phonon densities of states obtained by Fourier-transforming the velocity autocorrelation functions calculated directly from our MD simulation.

**1:27PM S51.00012 Nonlinear THz absorption and cyclotron resonance in InSb.**<sup>1</sup>, KATE HEFFERNAN, SHUKAI YU, DIYAR TALBAYEV, Tulane University — The emergence of coherent high-field terahertz (THz) sources in the past decade has allowed the exploration of nonlinear light-matter interaction at THz frequencies. Nonlinear THz response of free electrons in semiconductors has received a great deal of attention. Such nonlinear phenomena as saturable absorption and self-phase modulation have been reported. InSb is a narrow-gap (bandgap 0.17 eV) semiconductor with a very low electron effective mass and high electron mobility. Previous high-field THz work on InSb reported the observation of ultrafast electron cascades via impact ionization. We study the transmission of an intense THz electric field pulse by an InSb wafer at different incident THz amplitudes and 10 K temperature. Contrary to previous reports, we observe an increased transmission at higher THz field. Our observation appears similar to the saturable THz absorption reported in other semiconductors. Along with the increased absorption, we observe a strong modulation of the THz phase at high incident fields, most likely due to the self-phase modulation of the THz pulse. We also study the dependence of the cyclotron resonance on the incident THz field amplitude. The cyclotron resonance exhibits a lower strength and frequency at the higher incident THz field.

<sup>1</sup>The work at Tulane was supported by the Louisiana Board of Regents through the Board of Regents Support Fund Contract No. LEQSF(2012-15)-RD-A-23 and through the Pilot Funding for New Research (PFund) Contract No. LEQSF-EPS(2014)-PFUND-378.

**1:39PM S51.00013 Bound excitons at nitrogen and bismuth isoelectronic impurities**, THERESA CHRISTIAN, Univ of Colorado - Boulder, KIRSTIN ALBERI, DANIEL BEATON, BRIAN FLUEGEL, ANGELO MASCARENHAS, National Renewable Energy Lab — When nitrogen and bismuth dopants are simultaneously incorporated into a host lattice such as gallium arsenide (GaAs) or gallium phosphide (GaP), each dopant species contributes to the evolution of the electronic structure. Bound excitons in these systems luminescence from localized states whose distinctive radiative signatures provide invaluable clues into the nature of impurity clustering and inter-impurity interactions within the host lattice. Spectroscopic studies of these states will be presented for a series of samples grown by molecular beam epitaxy. Research was supported by the U. S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division under contract DE-AC36-08GO28308 and by the Department of Energy Office of Science Graduate Fellowship Program (DOE SCGF), made possible in part by the American Recovery and Reinvestment Act of 2009, administered by ORISE-ORAU under contract no. DE-AC05-06OR23100.

**1:51PM S51.00014 Electron-Phonon Renormalization of Electronic Band Structures of C Allotropes and BN Polymorphs**<sup>1</sup>, ROXANNE M. TUTCHTON, CHRISTOPHER MARCHBANKS, ZHIGANG WU, The Colorado School of Mines — The effect of lattice vibration on electronic band structures has been mostly neglected in first-principles calculations because the electron-phonon (e-ph) renormalization of quasi-particle energies is often small ( $< 100$  meV). However, in certain materials, such as diamond, the electron-phonon coupling reduces the band gap by nearly 0.5 eV, which is comparable to the many-body corrections of the electronic band structures calculated using the density functional theory (DFT). In this work, we compared two implementations of the Allen-Heine-Cardona theory in the EPW code and the ABINIT package respectively. Our computations of Si and diamond demonstrate that the ABINIT implementation converges much faster. Using this method, the e-ph renormalizations of electronic structures of three C allotropes (diamond, graphite, graphene) and four BN polymorphs (zincblende, wurtzite, mono-layer, and layered-hexagonal) were calculated. Our results suggest that (1) all of the zero-point renormalizations of band gaps in these materials, except for graphene, are larger than 100 meV, and (2) there are large variations in e-ph renormalization of band gaps due to differences in crystal structure.

<sup>1</sup>This work was supported by a U.S. DOE Early Career Award (Grant No. DE-SC0006433). Computations were carried out at the Golden Energy Computing Organization at CSM and the National Energy Research Scientific Computing Center (NERSC).

**2:03PM S51.00015 Non-adiabatic effects on the optical response of driven systems**, BENJAMIN M. FREGOSO, MICHAEL KOLODRUBETZ, JOEL MOORE, Univ of California - Berkeley — Periodically driven systems have received renewed interest due to their capacity to engineer non-trivial effective Hamiltonians. A characteristic of such systems is how they respond to weak periodicity-breaking drive, as for example when a laser is pulsed instead of continuous wave. We develop semi-classical equations of motion of a wave packet in the presence of electric and magnetic fields which are turned on non-adiabatically. We then show the emergence of significant corrections to electronic collective excitations and optical responses of topological insulator surface states, Weyl metals and semiconductor mono-chalcogenides.

**Thursday, March 17, 2016 11:15AM - 2:15PM —**  
**Session S52 DAMOP: Photonic Topological Materials** Hilton Baltimore Holiday Ballroom 3 - Xiaopeng Li, Joint Quantum Institute, University of Maryland

**11:15AM S52.00001 The Science and Applications of Photonic Topological Insulators: From Robust Delay Lines to Non-Reciprocal Metawaveguides<sup>1</sup>** , GENNADY SHVETS, The University of Texas at Austin — Electromagnetic (EM) waves propagating through an inhomogeneous medium inevitably scatter whenever the medium's electromagnetic properties change on the scale of a single wavelength. This fundamental phenomenon constrains how optical structures are designed and interfaced with each other. Our theoretical work indicates [1] that electromagnetic structures collectively known as photonic topological insulators (PTIs) can be employed to overcome this fundamental limitation, thereby paving the way to ultra-compact photonic structures that no longer have to be wavelength-scale smooth. Here I present the first experimental demonstration of a photonic structure that supports topologically protected surface electromagnetic waves (TPSWs) that are counterparts to the edge states between two quantum spin-Hall topological insulators in condensed matter. Unlike conventional guided EM waves that do not benefit from topological protection, TPSWs are shown to experience reflections-free time delays when detoured around sharply-curved paths, thus offering a unique paradigm for wave buffers and delay lines. I will also discuss how the photonic analogs of the quantum Hall and valley-Hall topological insulators can be realized and interfaced with each other. [1] T. Ma et. al., "Guiding Electromagnetic Waves around Sharp Corners: Topologically Protected Photonic Transport in Metawaveguides", Phys. Rev. Lett. 114, 127401 (2015).

<sup>1</sup>This work was supported by the National Science Foundation (NSF) Award PHY-1415547 and the Air Force Office of Scientific Research grant number FA9550-15-1-0075

**11:51AM S52.00002 Disordered Interactions and Fractional Quantum Hall States** , WADE DEGOT-TARDI, MOHAMMAD HAFEZI, Joint Quantum Institute, University of Maryland — The possibility that topological ordered states may be realized in photonic systems has recently attracted a great deal of attention. Given the rich phenomenology of the fractional quantum Hall effect, the bosonic Laughlin states have been of particular focus in this context. These states are known to arise in strongly nonlinear photonic lattices with artificial gauge fields, where nonlinearities associated with the resonators mimic on-site interactions. These effective interaction strengths are not universal and are subject to spatial disorder. We present a detailed study of the stability of these states and what implications they have for experiments.

**12:03PM S52.00003 Topological photonic crystal with ideal Weyl points** , LUYANG WANG, SHAO-KAI JIAN, HONG YAO, Institute for Advanced Study, Tsinghua University — Weyl points in three-dimensional photonic crystals behave as monopoles of Berry flux in momentum space. Here, based on symmetry analysis, we show that a minimal number of symmetry-related Weyl points can be realized in time-reversal invariant photonic crystals. We propose to realize these "ideal" Weyl points in modified double-gyroid photonic crystals, which is confirmed by our first-principle photonic band-structure calculations. Photonic crystals with ideal Weyl points are qualitatively advantageous in applications such as angular and frequency selectivity, broadband invisibility cloaking, and broadband 3D-imaging.

**12:15PM S52.00004 Topological photonics: an observation of Landau levels for optical photons<sup>1</sup>** , NATHAN SCHINE, Univ of Chicago, ALBERT RYOU, ARIEL SOMMER, JONATHAN SIMON, University of Chicago — Creating photonic materials with nontrivial topological characteristics has seen burgeoning interest in recent years; however, a major route to topology, a magnetic field for continuum photons, has remained elusive. We present the first experimental realization of a bulk magnetic field for optical photons. By using a non-planar ring resonator, we induce an image rotation on each round trip through the resonator. This results in a Coriolis/Lorentz force and a centrifugal anticonfining force, the latter of which is cancelled by mirror curvature. Spatial- and energy- resolved spectroscopy tracks photonic eigenstates as residual trapping is reduced, and we observe photonic Landau levels as the eigenstates become degenerate. We will discuss the conical geometry of the resulting manifold for photon dynamics and present a measurement of the local density of states that is consistent with Landau levels on a cone. While our work already demonstrates an integer quantum Hall material composed of photons, we have ensured compatibility with strong photon-photon interactions, which will allow quantum optical studies of entanglement and correlation in manybody systems including fractional quantum Hall fluids.

<sup>1</sup>This work was supported by DOE, DARPA, and AFOSR.

**12:27PM S52.00005 Topological crystalline insulators in photonic systems<sup>1</sup>** , JIANXIAO ZHANG, MIKAEL RECHTSMAN, CHAO-XING LIU, Pennsylvania State Univ — Topological crystalline insulators are a class of materials with a bulk energy gap and edge or surface modes, which are protected by crystalline symmetry, at their boundaries. They have been realized in electronic systems: in particular, in SnTe. In this work, we propose a mechanism to realize photonic boundary states topologically protected by crystalline symmetry. We map this one-dimensional system to a two-dimensional lattice model with opposite magnetic fields, as well as opposite Chern numbers, in its even and odd mirror parity subspaces, thus corresponding to a topological mirror insulator. Furthermore, we test how sensitive and robust edge modes depend on their mirror parity by performing time dependent evolution simulation of edge modes in a photonic setting with realistic experimental parameters.

<sup>1</sup>C.-X.L. acknowledge the support from Office of Naval Research (Grant No. N00014-15-1-2675).

**12:39PM S52.00006 Braiding light quanta<sup>1</sup>** , THOMAS IADECOLA, THOMAS SCHUSTER, CLAUDIO CHAMON, Boston University — The possibility that anyons — quantum particles other than fermions or bosons — can emerge in condensed matter systems has motivated generations of physicists. In addition to being of fundamental scientific importance, so-called non-Abelian anyons are particularly sought-after for potential applications to quantum computing. However, experimental evidence of anyons in electronic systems remains inconclusive. We propose to demonstrate non-Abelian braiding by injecting coherent states of light into topological guided modes in specially-fabricated photonic waveguide arrays. These modes are photonic analogues of topological zero modes in electronic systems. Light traveling inside spatially well-separated topological guided modes can be braided, leading to the accumulation of non-Abelian phases. We propose an optical interference experiment to probe this non-Abelian braiding directly.

<sup>1</sup>T.I. is supported by a National Science Foundation Graduate Research Fellowship under grant no. DGE-1247312.

**12:51PM S52.00007 Topological Photonics for Continuous Media<sup>1</sup>** , MARIO SILVEIRINHA, University of Coimbra — Photonic crystals have revolutionized light-based technologies during the last three decades. Notably, it was recently discovered that the light propagation in photonic crystals may depend on some topological characteristics determined by the manner how the light states are mutually entangled. The usual topological classification of photonic crystals explores the fact that these structures are periodic. The periodicity is essential to ensure that the underlying wave vector space is a closed surface with no boundary. In this talk, we prove that it is possible to calculate Chern invariants for a wide class of continuous bianisotropic electromagnetic media with no intrinsic periodicity. The nontrivial topology of the relevant continuous materials is linked with the emergence of edge states. Moreover, we will demonstrate that continuous photonic media with the time-reversal symmetry can be topologically characterized by a  $\mathbb{Z}_2$  integer. This novel classification extends for the first time the theory of electronic topological insulators to a wide range of photonic platforms, and is expected to have an impact in the design of novel photonic systems that enable a topologically protected transport of optical energy.

<sup>1</sup>This work is supported in part by Fundacao para a Ciencia e a Tecnologia grant number PTDC/EEL-TEL/4543/2014.

**1:03PM S52.00008 From Casimir-Polder Force to Dicke Physics: Interaction between Atoms and a Topological Insulator**, SEBASTIAN FUCHS, STEFAN BUHMANN, University of Freiburg — We apply the theory of macroscopic quantum electrodynamics in dispersing and absorbing media to study the Casimir-Polder force between an atom and a topological insulator [1]. The electromagnetic response of a topological insulator surface leads to a mixing of electric and magnetic fields, breaking the time-reversal symmetry [2, 3]. The coupling of these fields to an atom causes shifts of the atom's eigenenergies and modified decay rates near the surface of the topological insulator. Energy shifts and modified decay rates cannot only be triggered by the presence of a material, but can be caused by other atoms in close proximity as well. The collective dynamics of atoms (Dicke Physics) leads to a superradiant burst [4]. Combining macroscopic QED and Dicke physics opens the door to the investigation of cooperative atom-surface interactions. [1] S. Y. Buhmann, Dispersion Forces II, Springer-Verlag Berlin Heidelberg (2012). [2] S. Y. Buhmann, D. T. Butcher, and S. Scheel, New Journal of Physics 14, 083034 (2012). [3] J. A. Crosse, S. Fuchs, and S. Y. Buhmann, arXiv: 1509.03012 (2015). [4] S. Fuchs, J. Ankerhold, M. Blencowe, and B. Kubala, arXiv: 1501.07841 (2015).

**1:15PM S52.00009 Robust topological states in Parity-time (PT) symmetric photonic lattices<sup>1</sup>**, ANDREW HARTER, YOGESH JOGLEKAR, Indiana University Purdue University Indianapolis (IUPUI) — We consider generalized Aubry-Andre models, which support topological states and are experimentally realizable in integrated waveguide lattices, in the presence of balanced gain and loss. When the gain-loss strength exceeds a threshold set by the nearest neighbor tunneling, the non-Hermitian, PT-symmetric Hamiltonian of this system undergoes PT breaking transition. We investigate the interplay between the PT-breaking transition, tuned by the gain-loss strength, and topological transitions between different states with Chern numbers. We show, due to sub-lattice-localization property of the topological edge states in these models, these edge states remain robust across the PT-breaking transition. We present the consequences of this result for light-propagation in such materials, obtained via both tight-binding model and beam-propagation method.

<sup>1</sup>This work is supported by DMR-1054020.

**1:27PM S52.00010 Exciting Reflectionless, Unidirectional Edge Mode in Bianisotropic Meta-waveguide Using Rotating Dipole Antenna.<sup>1</sup>**, BO XIAO, THOMAS ANTONSEN, EDWARD OTT, STEVEN ANLAGE, Univ of Maryland-College Park, TZUHSUAN MA, GENNADY SHVETS, University of Texas Austin — Electronic chiral edge states in Quantum Hall Effect systems has attracted a lot of attention in recent years because of its unique directionality and robustness against scattering from disorder. Its electromagnetic counterpart can be found in photonic crystals, which is a material with periodic dielectric constant. Here we present the experimental results demonstrating the unidirectional edge mode inside a bi-anisotropic meta-waveguide [1] (BMW) structure. It is a parallel plate waveguide with metal rods placed in a hexagonal lattice. Half of the rods are attached to the top plate while the other half are attached to the bottom plate creating a domain wall. The edge mode is excited by two loop antennas placed perpendicular to each other within one wavelength, generating a rotating magnetic dipole that couples to the left or right-going mode. The transmission measurement are taken along the BMW boundary and shows high transmission only around the edge, thus confirming the presence of an edge mode. We also demonstrated that very high directivity can be achieved when the input amplitude and phase of the two loop antennas are tuned properly. [1] T. Ma, A. B. Khanikaev, S. H. Mousavi, And G. Shvets, Phys. Rev. Lett. 114, 127401 (2015).

<sup>1</sup>This work is funded by the ONR under Grants No. N00014130474 and N000141512134, and the Center for Nanophysics and Advanced Materials (CNAM).

**1:39PM S52.00011 Angle-Resolved Mid-Infrared Spectroscopy of Gyroid Photonic Crystals**, EMIL T. KHABIBOULLINE, SIYING PENG, Applied Physics, California Institute of Technology, PHILIP HON, Nanophotonics and Metamaterials Laboratory, Northrop Grumman Aerospace Systems, RUNYU ZHANG, Department of Materials Science and Engineering, UIUC, HONGJIE CHEN, Applied Physics, California Institute of Technology, LUKE A. SWEATLOCK, Nanophotonics and Metamaterials Laboratory, Northrop Grumman Aerospace Systems, PAUL BRAUN, Department of Materials Science and Engineering, UIUC, HARRY A. ATWATER, Applied Physics, California Institute of Technology — Photonic topological insulators form a new class of materials with exciting properties. Theory has indicated that gyroid photonic crystals are photonic topological insulators. In this paper, we experimentally characterize the photonic properties of gyroid photonic crystals at mid-infrared wavelengths, using angle-resolved spectroscopy with coherent light from a quantum cascade laser tuned from  $7.7\ \mu\text{m}$  to  $11.1\ \mu\text{m}$  and focused onto a  $100\ \mu\text{m} \times 100\ \mu\text{m}$  spot. From measurements of reflection and transmission spectra over incidence angles, we construct the band structure of the photonic crystals. In this study, the photonic crystals are single and double gyroid made of amorphous silicon, with unit cell size of  $5\ \mu\text{m}$ , sitting on an intrinsic silicon substrate. Simulations predict band gaps for the single gyroid and Weyl points for the double gyroid. We compare results of angle-resolved spectroscopy experiments with simulations for nanofabricated gyroid structures and discuss the topological features observable in angle-resolved scattering.

**1:51PM S52.00012 Squeezing as a route to photonic analogues of topological superconductors**, MARTIN HOUE, McGill Univ, VITTORIO PEANO, CHRISTIAN BRENDL, FLORIAN MARQUARDT, University of Erlangen-Nrnberg, AASHISH CLERK, McGill Univ — There has been considerable recent interest in studying topological phases of photonic systems. In many cases the resulting system is described by a quadratic particle-conserving Hamiltonian which is directly equivalent to its fermionic counterpart. Here, we consider a class of photonic topological phases where this correspondence fails: photonic systems where particle-number non-conserving terms break time-reversal symmetry [1]. We show that these phases support protected edge modes which facilitate chiral inelastic and elastic transport channels. We also discuss the possibility of quantum amplification using these edge states. Our system could be realized in a variety of systems, including nonlinear photonic crystals, superconducting circuits and optomechanical systems. [1] Vittorio Peano, Martin Houde, Christian Brendel, Florian Marquardt, and Aashish Clerk, arXiv:1508.01383 (2015).

**2:03PM S52.00013 Gyroid photonic crystal with Weyl points: synthesis and mid-infrared photonic characterization**, SIYING PENG, EMIL KHABIBOULLINE, Applied Physics, California Institute of Technology, RUNYU ZHANG, Department of Materials Science and Engineering, UIUC, HONGJIE CHEN, Applied Physics, California Institute of Technology, PHILIP HON, LUKE SWEATLOCK, Nanophotonics and Metamaterials Laboratory, Northrop Grumman Aerospace Systems, PAUL BRAUN, Department of Materials Science and Engineering, UIUC, HARRY ATWATER, Applied Physics, California Institute of Technology — Weyl points are degenerate energy states resulting from crossings of linear bands in 3D momentum space. Unlike their 2D counterparts, Weyl points are bulk degenerate states that are stable to weak perturbation. The topological surface states associated with Weyl points exhibit unidirectional backscattering-immune transport. Double gyroid photonic crystals with a parity-breaking perturbation are predicted to possess Weyl points. We designed and synthesized single and double gyroid mid-IR photonic crystals composed of a-Si. We characterized them by mid-IR spectroscopy. We observed 100% reflection at  $8\ \mu\text{m}$  for single gyroids with unit cell size of  $5\ \mu\text{m}$ , in agreement with the predicted photonic bandgap seen in full-wave EM simulations. As the unit cell size of single gyroids changes to  $6\ \mu\text{m}$ , the observed reflection peak shifted to  $9\ \mu\text{m}$ , also agreeing with simulation. For double gyroids with unit cell size of  $5\ \mu\text{m}$ , we observed a 20% decrease in reflection at  $8\ \mu\text{m}$ , which could be explained by a new pair of states appearing within the bandgap from our simulation of double gyroids. We use angle-resolved mid-IR spectroscopy with a QCL to characterize Weyl points.

**Thursday, March 17, 2016 11:15AM - 2:15PM –**

**Session S53 GIMS: Keithley Award Session** Hilton Baltimore Holiday Ballroom 4 - Francis Hellman, University of California, Berkeley

**11:15AM S53.00001 Joseph F. Keithley Award For Advances in Measurement Science: Resonant Ultrasound Spectroscopy: An Odyssey in Measurement Science<sup>1</sup>**, ALBERT MIGLIORI, Los Alamos Natl Lab

— Perhaps the speeds of sound, or, equivalently, the elastic moduli are some of the most fundamental attributes of a solid, connecting to fundamental physics, metallurgy, non-destructive testing, and more. Unlike most of the quantities used to characterize condensed matter, the elastic moduli are fourth-rank tensors containing a wealth of detail, directional information, and consistency constraints that provide some of the most revealing probes of solids. We describe here the current state of the art in one method, Resonant Ultrasound Spectroscopy, where the mechanical resonances of a specimen of regular shape (easy to measure) are analyzed (difficult computational problem) to obtain the full elastic tensor. With modern advances in electronics and analysis, fractions of a part per million changes in elastic moduli are detectable providing new and important insight into grand challenges in condensed matter physics.

<sup>1</sup>This work was supported as part of the Materials Science of Actinides, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award DE-SC0001089.

**11:51AM S53.00002 Strain coupling and dynamic relaxation dynamics associated with ferroic and multiferroic phase transition**, MICHAEL CARPENTER, Dept. of Earth Sciences, University of Cambridge

— Almost any change that occurs in a crystal structure results in some lattice strain and it is inevitable that this will appear also as a change in elastic properties. It follows that one of the most characteristic features of phase transitions, whether driven by structural, magnetic or electronic effects, will be variations of elastic constants. In addition, transformation microstructures such as ferroelastic twins may be mobile under some conditions of temperature and stress and will give characteristic patterns of acoustic loss when measured by dynamical methods. Thanks substantially to the pioneering work of Dr Albert Migliori in developing the technique of Resonant Ultrasound Spectroscopy (RUS), it has been possible to follow the elastic and anelastic behaviour associated with phase transitions quantitatively as a function of temperature through the interval 2-1600 K. It is also possible to add magnetic and electric fields. The frequency window 0.1-2 MHz and inherently small strains of RUS appear to be particularly sensitive for observing the consequences of strain coupling and microstructure relaxation dynamics. Recent collaborative work carried out using the RUS facilities in Cambridge will be presented, relating to phase transitions in multiferroic perovskites, such as  $\text{PbZr}_{0.53}\text{Ti}_{0.47}\text{O}_3$ - $\text{PbFe}_{0.5}\text{Nb}_{0.5}\text{O}_3$  and  $\text{Sr}_2\text{FeMoO}_6$ , the ferroelectric/improper ferroelastic transition in GeTe, and magnetoelastic behaviour of  $\text{EuTiO}_3$ . A common feature of these is softening of the shear modulus ahead of the transition that is not expected on the basis of linear/quadratic coupling between strain and the driving order parameter (improper ferroelastic). This appears to be due to coupling of acoustic modes with unseen central modes which are related to collective motions of domains with short range order. In some cases the ferroelastic twin walls have a well defined freezing interval (GeTe) whereas anelastic loss and stiffening over a wide temperature interval appears to be diagnostic of a microstructure with heterogeneous strain variations. Elastic softening by 10's of percent is typical of the effect of shear strains in the range 0.005-0.03.

**12:27PM S53.00003 Ultrasonic techniques for measuring physical properties of fluids in harsh environments**, CRISTIAN PANTEA, Los Alamos National Laboratory

— Ultrasonic-based measurement techniques, either in the time domain or in the frequency domain, include a wide range of experimental methods for investigating physical properties of materials. This discussion is specifically focused on ultrasonic methods and instrumentation development for the determination of liquid properties at conditions typically found in subsurface environments (in the U.S., more than 80% of total energy needs are provided by subsurface energy sources). Such sensors require materials that can withstand harsh conditions of high pressure, high temperature and corrosiveness. These include the piezoelectric material, electrically conductive adhesives, sensor housings/enclosures, and the signal carrying cables, to name a few. A complete sensor package was developed for operation at high temperatures and pressures characteristic to geothermal/oil-industry reservoirs. This package is designed to provide real-time, simultaneous measurements of multiple physical parameters, such as temperature, pressure, salinity and sound speed. The basic principle for this sensor's operation is an ultrasonic frequency domain technique, combined with transducer resonance tracking. This multipurpose acoustic sensor can be used at depths of several thousand meters, temperatures up to 250 C, and in a very corrosive environment. In the context of high precision measurement of sound speed, the determination of acoustic nonlinearity of liquids will also be discussed, using two different approaches: (i) the thermodynamic method, in which precise and accurate frequency domain sound speed measurements are performed at high pressure and high temperature, and (ii) a modified finite amplitude method, requiring time domain measurements of the second harmonic at room temperature. Efforts toward the development of an acoustic source of collimated low-frequency (10-150 kHz) beam, with applications in imaging, will also be presented.

**1:03PM S53.00004 Real time studies of Elastic Moduli Pu Aging using Resonant Ultrasound Spectroscopy**, BORIS MAIOROV, Los Alamos National Laboratory

— Elastic moduli are fundamental thermodynamic susceptibilities that connect directly to thermodynamics, electronic structure and give important information about mechanical properties. To determine the time evolution of the elastic properties in  $^{239}\text{Pu}$  and its Ga alloys, is imperative to study its phase stability and self-irradiation damage process. The most-likely sources of these changes include a) ingrowth of radioactive decay products like He and U, b) the introduction of radiation damage, c)  $\delta$ -phase instabilities towards  $\alpha$ -Pu or to  $\text{Pu}_3\text{Ga}$ . The measurement of mechanical resonance frequencies can be made with extreme precision and used to compute the elastic moduli without corrections giving important insight in this problem. Using Resonant Ultrasound Spectroscopy, we measured the time dependence of the mechanical resonance frequencies of fine-grained polycrystalline  $\delta$ -phase  $^{239}\text{Pu}$ , from 300K up to 480K. At room temperature, the shear modulus shows an increase in time (stiffening), but the bulk modulus decreases (softening). These are the first real-time measurements of room temperature aging of the elastic moduli, and the changes are consistent with elastic moduli measurements performed on 44 year old  $\delta$ -Pu. As the temperature is increased, the rate of change increases exponentially, with both moduli becoming stiffer with time. For  $T > 420\text{K}$  an abrupt change in the time dependence is observed indicating that the bulk and shear moduli have opposite rates of change. Our measurements provide a basis for ruling out the decomposition of  $\delta$ -Pu towards  $\alpha$ -Pu or  $\text{Pu}_3\text{Ga}$ , and indicate a complex defect-related scenario from which we are gathering important clues.

**1:39PM S53.00005 TBD talk 5**, TBD TBD, TBD — No abstract available.

**Thursday, March 17, 2016 11:15AM - 2:15PM –**

**Session S55 DBIO GSNP: Inference in Biophysics** Hilton Baltimore Holiday Ballroom 6 - Steve Presse, Indiana University of Pennsylvania

**11:15AM S55.00001 Genetic networks and the flow of positional information in embryonic development** , WILLIAM BIALEK, Princeton University — When we study a biological system, we make inferences about the underlying mechanisms and dynamics. But biological systems themselves must also solve inference problems, as when our brains draw conclusions about the world given (often quite limited) data from our eyes and ears. My colleagues and I have been exploring both of these inference problems as they play out in the first hours of development in the fruit fly embryo. In this system, the concentrations of particular molecules encode the position of each cell in the embryo, and these concentrations are the outputs of a genetic network. Putting ourselves in the place of the cells, we have been able to read the code, building a dictionary that maps gene expression levels back into estimates of position. If our dictionary really is the one used by the embryo, then mutants should build predictably distorted body plans, and preliminary results show quantitative agreement with these predictions. Independent of their role as carriers of information, we can also analyze the patterns of gene expression to draw inferences about the underlying network. Finally, it is possible that the network architecture and parameters have been chosen to optimize the flow of information, and we see signatures of this optimization. Joint work with CG Callan, JO Dubuis, T Gregor, D Krotov, M Petkova, TR Sokolowski, G Tkacik, AM Walczak, and EF Wieschaus.

**11:51AM S55.00002 Deep Learning, Group representations, and the Information-Bottleneck phase transitions.** , NAFTALI TISHBY, Hebrew University — Deep Neural Networks (DNNs) are analyzed via the theoretical framework of the information bottleneck (IB). We first show that any DNN can be quantified by the mutual information between the layers and the input and output variables. Using this representation we can calculate the optimal information theoretic limits of the DNN and obtain finite sample generalization bounds. The advantage of getting closer to the theoretical limit is quantifiable both by the generalization bound and by the network's simplicity. We argue that both the optimal architecture, number of layers and features/connections at each layer, are related to critical points on the information bottleneck tradeoff line, namely, relevant compression of the input layer with respect to the output layer. The hierarchical representations at the layered network naturally correspond to the structural phase transitions along the information curve. An interesting class of solvable DNN's arise by applying this framework to the case of symmetries in the supervised learning task. The case of translation invariance leads to the familiar convolution neural networks. Other symmetry groups yield different types of bifurcation diagrams and network architectures, which correspond to information contained by irreducible representations of the group. These new insights also suggest new sample complexity bounds, architecture design principles (number and widths of layers), and eventually entirely different deep learning algorithms. Based partly on works with Noga Zaslavsky and Ravid Ziv.

**12:27PM S55.00003 Fock spaces for modeling macromolecular complexes** , JUSTIN KINNEY, Cold Spring Harbor Laboratory — Large macromolecular complexes play a fundamental role in how cells function. Here I describe a Fock space formalism for mathematically modeling these complexes. Specifically, this formalism allows ensembles of complexes to be defined in terms of elementary molecular "building blocks and "assembly rules. Such definitions avoid the massive redundancy inherent in standard representations, in which all possible complexes are manually enumerated. Methods for systematically computing ensembles of complexes from a list of components and interaction rules are described. I also show how this formalism readily accommodates coarse-graining. Finally, I introduce diagrammatic techniques that greatly facilitate the application of this formalism to both equilibrium and non-equilibrium biochemical systems.

**1:03PM S55.00004 Causal inference of signaling networks using single cell data** , KAREN SACHS, Stanford University — No abstract available.

**1:39PM S55.00005 Maximum Entropy and the Inference of Pattern and Dynamics in Ecology** , JOHN HARTE, University of California, Berkeley — Constrained maximization of information entropy yields least biased probability distributions. From physics to economics, from forensics to medicine, this powerful inference method has enriched science. Here I apply this method to ecology, using constraints derived from ratios of ecological state variables, and infer functional forms for the ecological metrics describing patterns in the abundance, distribution, and energetics of species. I show that a static version of the theory describes remarkably well observed patterns in quasi-steady-state ecosystems across a wide range of habitats, spatial scales, and taxonomic groups. A systematic pattern of failure is observed, however, for ecosystems either losing species following disturbance or diversifying in evolutionary time; I show that this problem may be remedied with a stochastic-dynamic extension of the theory.

**1:00PM - 1:00PM –**

**Session T1 Poster Session III (Thursday, 1:00 pm - 4:00 pm) Exhibit Hall EF -**

**T1.00001 GENERAL THEORY/COMPUTATIONAL PHYSICS –**

**T1.00002 Formation of graphene flakes from oxidation of SiC nanoparticle** , PANKAJ RAJAK, KENICHI NAMURA, RAJIV KALIA, AIICHIRO NAKANO, PRIYA VASHISHTA, Univ of Southern California — We have performed the largest (112 million atoms) reactive molecular dynamics simulation using reactive force fields to study the oxidation of a SiC nanoparticle on the full Blue Gene/P machine. The SiC nanoparticle of diameter 100 nm is surrounded by O<sub>2</sub> gas and heated to 2,800 K. Subsequently, we let the SiC nanoparticle oxidize at 2,800K. We observe formation of graphene-like flakes despite the harsh oxidation condition. We find the fractal dimension of the flakes is 1.85. We will discuss the implication of reaction kinetics on the structure and distribution of graphene flakes.

**T1.00003 Bayesian Inference of Effective Classical Spin Hamiltonians from Hartree-Fock Calculation** , HIKARU TAKENAKA, KENJI NAGATA, Graduate School of Frontier Sciences, The University of Tokyo, TAKASHI MIZOKAWA, School of Advanced Science and Engineering, Waseda University, MASATO OKADA, Graduate School of Frontier Sciences, The University of Tokyo — A novel method is described for extracting effective classical spin Hamiltonians from mean-field type electronic structural calculations by means of Bayesian inference[1]. The method is applied to a NiS<sub>2</sub> triangular lattice in NiGa<sub>2</sub>S<sub>4</sub> with a spin disordered ground state. Unrestricted Hartree-Fock calculations for the spin configurations of 16 Ni sites led to the estimation that not only the strongest superexchange interaction between the third nearest neighbor sites but also those between the nearest and the second nearest neighbor sites should be taken into account to extract effective classical spin Hamiltonians for NiGa<sub>2</sub>S<sub>4</sub>. Results obtained from the above calculations with the Boltzmann factor are also shown. It was estimated that the superexchange interaction between the nearest neighbor sites is ferromagnetic, which is consistent with magnetic experiment results. This supports the theory that the competition between the antiferromagnetic third neighbor interaction and the ferromagnetic nearest neighbor interaction may lead to the quantum spin liquid in NiGa<sub>2</sub>S<sub>4</sub>. [1]H. Takenaka, K. Nagata, T. Mizokawa, and M. Okada, J. Phys. Soc. Jpn. 83, 124706, (2014).

**T1.00004 Enhancing AFLOW Visualization using Jmol**, JACOB LANASA, ELIZABETH NEW, PATRIK STEFEK, BRIGETTE HONAKER, ROBERT HANSON, St. Olaf College, AFLOW COLLABORATION — The AFLOW library[1,2] is a database of theoretical solid-state structures and calculated properties created using high-throughput *ab initio* calculations. Jmol[3] is a Java-based program capable of visualizing and analyzing complex molecular structures and energy landscapes. In collaboration with the AFLOW consortium, our goal is the enhancement of the AFLOWLIB database through the extension of Jmol's capabilities in the area of materials science. Modifications made to Jmol include the ability to read and visualize AFLOW binary alloy data files, the ability to extract from these files information using Jmol scripting macros that can be utilized in the creation of interactive web-based convex hull graphs, the capability to identify and classify local atomic environments by symmetry, and the ability to search one or more related crystal structures for atomic environments using a novel extension of inorganic polyhedron-based SMILES strings. [1] S. Curtarolo, *et al.*, *AFLOW: an automatic framework for high-throughput materials discovery*, *Comp. Mat. Sci.* **58**, 218-226 (2012). [[doi=10.1016/j.commatsci.2012.02.005](https://doi.org/10.1016/j.commatsci.2012.02.005)]; [2] S. Curtarolo, *et al.*, *AFLOWLIB.ORG: a distributed materials properties repository from high-throughput ab initio calculations*, *Comp. Mat. Sci.* **58**, 227-235 (2012). [[doi=10.1016/j.commatsci.2012.02.002](https://doi.org/10.1016/j.commatsci.2012.02.002)]; [3] R. Hanson, *Jmol – A Paradigm Shift in Crystallographic Visualization*, *J. Appl. Cryst.* **2010** 43, 1250-1260.

**T1.00005 Composition-Dependent Phase Concentrations from First Principles: Simulating Combinatorial Libraries of Transition Metal Oxides<sup>1</sup>**, GUO LI, QIMIN YAN, Lawrence Berkeley Natl Lab, LAN ZHOU, PAUL NEWHOUSE, JOHN GREGOIRE, California Institute of Technology, JEFFREY NEATON, Lawrence Berkeley Natl Lab; UC-Berkeley; Kavli Energy NanoSciences Institute at Berkeley — To identify material phases in experimental combinatorial libraries, we develop a theoretical model as a complementary approach to accelerate phase identification. In this approach, samples in a combinatorial library are simulated as mixtures in chemical equilibria. Each of these mixtures contains all the solid-state phases, which can possibly exist in the library. Using the total energies of these phases obtained in first-principle calculations, we calculate the Gibbs free energy changes in the corresponding chemical reactions, and subsequently evaluate the equilibrium concentrations of the phases in every sample according to the law of mass action. Furthermore, to test this approach, we simulate pseudobinary libraries  $M_nV_{1-x}O_y$  and  $Cu_xV_{1-x}O_y$ . Interestingly, we find that the composition-dependent phase concentrations calculated within our approach agree well with the experimental results measured with XRD spectroscopy.

<sup>1</sup>This work supported by DOE (the JCAP under Award number DE-SC0004993 and the Molecular Foundry of LBNL), and computational resources provided by NERSC.

**T1.00006 Bosonics: Phononics, Magnonics, Plasmonics in Nano-Scale Disorder(Nanonics), Metamaterials, Astro-Seismology (Meganonics): Brillouin-Siegel GENERIC: Generalized-Disorder Collective-Boson Mode-Softening Universality-Principle (G...P) With PIPUB Many-Body Localization**, EDWARD SIEGEL, FUZZYICS=CATEGORYICS=ANALOGYICS=PRAGMATYICS/CATEGORY-SEMANTICS ONTOLOGY COGNITION ANALYTICS — Siegel and Matsubara[Statphys-13('77); Intl.Conf.Lattice-Dyn.('77); Scripta Met.13,913('80)]; JMMM:5, 1, 84 ('77);22,1:41,58('80);Mag.Lett.('80);Phys./Chem.Liquids:4,(4) ('75);5,(1)('76)] generalization to GENERIC Siegel[J.Non-Xline-Sol.40,453('80)] G...P GENERIC Brillouin[Wave-Propagation in Periodic-Structures('22)]-Landau['41]-Feynman['51]-de Boer[in Phonons/Phonon-Interactions('64)]-Egelstaff[Intro.Liquid-State('65)]-Hubbard-Beebe[J.Phys.C('67)]-“Anderson”[1958]- Siegel [J.Non-Xl.-Sol. 40, 453('80)] GENERIC many-body localization. GENERIC Hubbard-Beebe[J.Phys.C('67)] static structure-factor  $S(k)$  modulated kinetic-energy  $\omega(k)=\hbar^2k^2/2mS(k)$  expressing G...P(“bass-ackwardly”) aka homogeneity and isotropy creates GENERIC G...P with GENERIC pseudo-isotropic pseudo-Umklapp backscattering (PIPB) for GENERIC many-body localization of and/or by mutually interacting collective-bosons: phonons(phononics) with magnons(magnonics) with plasmons(plasmonics) with fermions (electrons, holes)...etc. in nano-scale “disorder”, metamaterials and on very-macro-scales (surprisingly) Bildsten et.al. astro-seismology(meganonics) of red-giant main-sequence stars(Mira, Betelgeuse)!

**T1.00007 Introduction to Electromagnetic Fields and Geodesics in a Tokamak**, STEPHEN SHARMA, Univ. of Calif. Berkeley, Univ. of Southern California — Photons mediate electromagnetic radiation such that electric and magnetic particles obey the principle of least action from the applied fields. Elastic and inelastic collisions arise after summation of Lagrangian geodesics. In the case of reacting tritium and deuterium, energy is released in the form of electromagnetic radiation, neutrons, and alpha particles. Within fusion tokamaks, alpha particle energies determine if a self sustaining reaction—or ignition—will proceed. If particle mean free path is confined by electric and magnetic fields, then fusion occurs at higher frequencies. If temperature is increased and particle velocity is increased, then collision frequency increases. Modeling the nucleons as polarizable quark dielectric liquid drops increases differentiation between scattering events and fusion. When the cross section of two reactant liquid drops is coincident, fusion occurs. If cross sections do not overlap sufficiently, Coulomb scattering occurs. One strives for understanding of geometric approaches to solving for reactants' cross sections and fusion collision frequency in order to determine power output per particle and critical density of reactants.

**T1.00008 Global and short-range entanglement properties in excited, many-body localized spin chains**, COLIN WEST, TZU-CHIEH WEI, State Univ of NY- Stony Brook — Many-body localization is a manifestation of the violation of the eigenstate thermalization hypothesis. As one of many characteristic features, eigenstates in a many-body localized regime have been observed to obey an area law in the scaling of the entanglement entropy. Consequently, such states can be efficiently represented by matrix product states (MPS). Here, we use the SIMPS algorithm proposed by Yu, Pekker, and Clark to numerically access these excited states in spin chains with disorder, and study them from the perspective of their global and short range entanglement properties, as well as through other local observables. We compare the behavior across excited states as the strength of disorder varies.

**T1.00009 Atomistic Simulations of High-intensity XFEL Pulses on Diffractive Imaging of Nano-sized Systems<sup>1</sup>**, PHAY HO, CHRISTOPHER KNIGHT, LINDA YOUNG, Argonne National Laboratory, MIKLOS TEGZE, GYULA FAIGEL, Institute for Solid State Physics and Optics of the Wigner Research Centre for Physics — We have developed a large-scale atomistic computational method based on a combined Monte Carlo and Molecular Dynamics (MC/MD) method to simulate XFEL-induced radiation damage dynamics of complex materials. The MD algorithm is used to propagate the trajectories of electrons, ions and atoms forward in time and the quantum nature of interactions with an XFEL pulse is accounted for by a MC method to calculate probabilities of electronic transitions. Our code has good scalability with MPI/OpenMP parallelization, and it has been run on Mira, a petascale system at the Argonne Leadership Computing Facility, with particle number >50 million. Using this code, we have examined the impact of high-intensity 8-keV XFEL pulses on the x-ray diffraction patterns of argon clusters. The obtained patterns show strong pulse parameter dependence, providing evidence of significant lattice rearrangement and diffuse scattering. Real-space electronic reconstruction was performed using phase retrieval methods. We found that the structure of the argon cluster can be recovered with atomic resolution even in the presence of considerable radiation damage.

<sup>1</sup>This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Chemical Sciences, Geosciences, and Biosciences Division under Contract No. DE-AC02-06CH11357.

**T1.00010 Canonical Quantization of Crystal Dislocation and Electron-Dislocation Scattering in an Isotropic Media**, MINGDA LI, MIT, WENPING CUI, Boston College, M. S. DRESSELHAUS, GANG CHEN, MIT, MIT TEAM, BOSTON COLLEGE TEAM — Crystal dislocations govern the plastic mechanical properties of materials but also affect the electrical and optical properties. However, a fundamental and decent quantum-mechanical theory of dislocation remains undiscovered for decades. Here we present an exact and manageable Hamiltonian theory for both edge and screw dislocation line in an isotropic media, where the effective Hamiltonian of a single dislocation line can be written in a harmonic-oscillator-like form, with closed-form quantized 1D phonon-like excitation. Moreover a closed-form, position dependent electron-dislocation coupling strength is obtained, from which we obtained good agreement of relaxation time when comparing with classical results. This Hamiltonian provides a platform to study the effect of dislocation to materials' non-mechanical properties from a fundamental Hamiltonian level.

**T1.00011 Electron binding energies using perturbative delta-SCF method**, SHUSIL BHUSAL, TUNNA BARUAH, RAJENDRA ZOPE, University of Texas at El Paso — The knowledge of fundamental and optical gaps is of significant importance for organic photovoltaics. The electron binding energies estimated from the Kohn-Sham eigenvalues are significantly underestimated. Here, we use our recently outlined perturbative delta-SCF approach to compute the electron binding energies of a number of aromatic organic molecules commonly used in organic photovoltaics. Further, the electron affinities are also computed for the C60, C70 and PCBM. The results show that the perturbative delta-SCF provide adequate description of valence electron binding energies. We also applied the method to compute the core binding energies and the core-valence excited states. While the method can successfully predict the core-valence excited states the results on the core-binding energies are mixed. The strategies for improvement of the core binding energies will be discussed.

**T1.00012 Berry phase oscillations in a one-dimensional Dirac comb**, WILLIAM HODGE, NICHOLAS CASSERA, Stevenson University, MATTHEW RAVE, Western Carolina University — In quantum mechanics, the Berry phase is a geometric phase acquired by a wave function over the course of a cycle, when subjected to adiabatic processes. In general, this phase is due to the geometry of the underlying parameter space and thus depends only on the path taken. In any system described by a periodic potential, the torus topology of the Brillouin zone itself can lead to such a phase. In this work, we numerically calculate the Berry phase for a one-dimensional Dirac comb described by  $N$  distinct wells per unit cell. As expected, the resulting Berry phase exhibits a rich band-dependence. In the case where  $N = 2$ , we find that the Berry phase corresponding to the  $n^{\text{th}}$  energy band oscillates such that  $\gamma_n(x) = A_n \sin(\pi x) \cos[(2n - 1)\pi x]$ , where  $A_n$  is a band-dependent constant and  $0 < x < 1$  is the relative position of the two wells. This expression, obtained using perturbation theory, gives excellent agreement with exact numerical results, even at low energy levels. The Berry phase exhibits a similar behavior for cases where  $N > 2$ .

**T1.00013 Single Electron in Systems of Two and Three Quantum Dots<sup>1</sup>**, IGOR FILIKHIN, BRANISLAV VLAHOVIC, North Carolina Central University — We consider the single electron confinement states in the system of two and three quantum dots (QDs). The InAs/GaAs QDs are modeled as laterally distributed dots, using single sub-band effective mass approach with effective potential simulating the strain effect. Electron localization in double quantum dots (DQDs) and in triple quantum dots (TQDs) is studied over the entire electron energy spectrum by varying the geometry parameters of these QDs arrays. It is shown that a small violation of the DQD shape symmetry drastically affects tunneling. This effect also appears as a numerical instability in calculations of spectral distribution of localized/delocalized electron states for small variations of the input parameters of numerical procedure. The effect of adding a third dot to a DQD is investigated. We show that the presence of a third dot increases the tunneling in the initial DQD. The spectral distribution of localized/delocalized states appears sensitive to the violation of the mirror symmetry of TQDs.

<sup>1</sup>This work was supported by the NSF (HRD-1345219)

**T1.00014 State of the art for ab initio vs empirical potentials for HeH<sup>+</sup> (2e<sup>-</sup>), BeH<sup>+</sup> (4e<sup>-</sup>), BeH (5e<sup>-</sup>), Li<sub>2</sub> (6e<sup>-</sup>) and BH (6e<sup>-</sup>)**, NIKE DATTANI, Kyoto University — For large internuclear distances, the potential energy between two atoms is known analytically, based on constants that are calculated from atomic *ab initio* rather than molecular *ab initio*. This analytic form can be built into models for molecular potentials that are fitted to spectroscopic data. Such empirical potentials constitute the most accurate molecular potentials known. For HeH<sup>+</sup>, and BeH<sup>+</sup>, the long-range form of the potential is based only on the polarizabilities for He and H respectively, for which we have included up to 4th order QED corrections. For BeH, the best ab initio potential matches all but one observed vibrational spacing to  $\pm 1 \text{ cm}^{-1}$  accuracy, and for Li<sub>2</sub> the discrepancy in the spacings is  $\pm 0.08 \text{ cm}^{-1}$  for all vibrational levels. But experimental methods such as photoassociation require the absolute energies, not spacings, and these are still several in several  $\text{cm}^{-1}$  disagreement. So empirical potentials are still the only reliable way to predict energies for few-electron systems. We also give predictions for various unobserved "halo nucleonic molecules" containing the "halo" isotopes: <sup>6,8</sup>He, <sup>11</sup>Li, <sup>11,14</sup>Be and <sup>8,17,19</sup>B.

**T1.00015 Efficient method of finite-size correction in quantum Monte Carlo calculations**, SAM AZADI, Department of Physics and Tomas Young Centre, University College London, MATTHEW FOULKES, Department of Physics, Imperial College London — We present a simple but efficient method of finite size correction for metallic crystals [1]. Our method is based on an accurate combination of twist averaging boundary condition and density functional theory. We compare our method with several previously introduced schemes. Our quantum Monte Carlo results for lithium and aluminium show the accuracy and practicality of our method. :1] Sam Azadi, and W. M. C. Foulkes, J. Chem. Phys. **143**, 102807 (2015).

**T1.00016 Microscopic Picture of Atomic Dynamics in the Double Perovskite, PrBaCo<sub>2</sub>O<sub>6</sub>**, ELVIS SHOKO, UDO SCHWINGENSCHLOGL, PSE Division, KAUST, Saudi Arabia — We have used a combination of lattice dynamics and *ab initio* molecular dynamics to study atomic dynamics in PrBaCo<sub>2</sub>O<sub>6</sub>, a prototype material for a large class of layered compounds of both fundamental and technological interest. We find clear signatures of the layered structure of this compound on the overall atomic dynamics. In particular, we find that O atom dynamics in the PrO layer is predominantly in-plane (*ab*-plane) in contrast to the predominantly out-of-plane dynamics in the CoO<sub>2</sub> layer. This suggests that the oxide ionic conductivity is dominated by the O atoms in the PrO layer, a finding of interest in solid-oxide fuel cells. Additionally, our results reveal sharp low-energy vibrational modes below 20 meV for both Ba and Pr atoms leading to the intriguing possibility that this material may be engineered for thermoelectric applications.

**T1.00017 Obtaining model parameters for real materials from ab-initio calculations: Heisenberg exchange<sup>1</sup>**, DMITRY KOROTIN, Institute of Metal Physics, Yekaterinburg, VLADIMIR MAZURENKO, Ural Federal University, Yekaterinburg, VLADIMIR ANISIMOV, SERGEY STRELTISOV, Institute of Metal Physics, Yekaterinburg — An approach to compute exchange parameters of the Heisenberg model in plane-wave based methods is presented. This calculation scheme is based on the Green's function method and Wannier function projection technique. It was implemented in the framework of the pseudopotential method and tested on such materials as NiO, FeO, Li<sub>2</sub>MnO<sub>3</sub>, and KCuF<sub>3</sub>. The obtained exchange constants are in a good agreement with both the total energy calculations and experimental estimations for NiO and KCuF<sub>3</sub>. In the case of FeO our calculations explain the pressure dependence of the Néel temperature. Li<sub>2</sub>MnO<sub>3</sub> turns out to be a Slater insulator with antiferromagnetic nearest neighbor exchange defined by the spin splitting. The proposed approach provides a unique way to analyze magnetic interactions, since it allows one to calculate orbital contributions to the total exchange coupling and study the mechanism of the exchange coupling.

<sup>1</sup>The work was supported by a grant from the Russian Scientific Foundation (Project No. 14-22-00004)

## **T1.00018 Devil's staircase in a quantum dimer model on the hexagonal lattice**, THOMAS BARTHEL,

Duke University, Department of Physics, GRÉGOIRE MISGUICH, CEA Saclay, Institut de Physique Théorique, THIAGO M. SCHLITTLER, JULIEN VIDAL, RÉMY MOSSERI, Université Paris 6, LPTMC — Quantum dimer models appear in different contexts when describing dynamics in constrained low-energy manifolds, such as for frustrated Ising models in weak transverse fields. In this talk, I address a particularly interesting case, where a quantum dimer model on the hexagonal lattice, in addition to the standard Rokhsar-Kivelson Hamiltonian, includes a competing potential term, counting dimer-free hexagons. It has a rich zero-temperature phase diagram that comprises a cascade of rapidly changing flux quantum numbers (tilt in the height language). This cascade is partially of fractal nature and the model provides, in particular, a microscopic realization of the “devil's staircase” scenario [E. Fradkin *et al.* Phys. Rev. B **69**, 224415 (2004)]. We have studied the system by means of quantum Monte-Carlo simulations and the results can be explained using perturbation theory, RG, and variational arguments.

References: arXiv:1507.04643, arXiv:1501.02242.

## **T1.00019 Fermionic Quantum Monte Carlo simulations without fixed nodes**, TOBIAS DORNHEIM, TIM

SCHOOF, SIMON GROTH, MICHAEL BONITZ, Kiel university — Recent restricted PIMC (RPIMC) simulations [PRL **110**, 146405 (2013)] of the uniform electron gas (UEG) at finite temperature have turned out to be surprisingly inaccurate [PRL **115**, 130402 (2015)]. Therefore, there exists a high need for alternative approaches which circumvent the fermion sign problem (FSP). In this work, we present two independent approaches which exhibit a complementary behavior. The configuration PIMC (CPIMC) method [Contrib. Plasma Phys. **51**, 687-697 (2011)], which operates in Fock space, excels at high density and allows for cutting edge results at strong degeneracy. In contrast, the permutation blocking PIMC (PB-PIMC) approach [New J. Phys. **17**, 073017 (2015)] is formulated in coordinate space and combines antisymmetric imaginary time propagators (determinants) with a higher order factorization of the density matrix. This leads to a significant reduction of the sign problem and extends the range of applicability of standard PIMC towards higher density and lower temperature [arXiv:1508.03221 (2015)]. Joining these two complementary methods allows us to present accurate thermodynamic results for the uniform electron gas over a broad parameter range and, therefore, to partly avoid the FSP.

## **T1.00020 Modeling of Electromagnetic Phenomenon in Fractional Dimensional Space**, MUHAM-

MAD ZUBAIR, L.K. ANG, Engineering Product Development, Singapore University of Technology and Design, East Coast Campus, 8 Somapah Road, Singapore 487372, Singapore — Fractional dimensional space has emerged as an extremely useful concept in many areas of physics, including electromagnetic (EM) theory. The development made in the area of fractional calculus has made it possible to study the most important physical phenomenon in a generalized  $D$ -dimensional fractional space. It is worthwhile to mention that many natural objects, such as clouds, snowflakes, rough surfaces, cracks, turbulence in fluids, are aptly described by dimensions of fractional order. Therefore, EM wave propagation in such fractal media is best characterized by considering an effective space of non-integer (fractional) dimensions. Here we present the recent developments in the study of differential Maxwell equations in a  $D$ -dimensional fractional space, where  $D$  is a non-integer value. Same examples will be used in order to show the transition to the traditional non-fractional conditions or settings.

## **T1.00021 Optimized simulations of Olami-Feder-Christensen systems using parallel algorithms**<sup>1</sup>, RACHELE DOMINGUEZ, RANCE NECAISE, ERIC MONTAG, Randolph-Macon College — The sequential nature of the Olami-Feder-

Christensen (OFC) model for earthquake simulations limits the benefits of parallel computing approaches because of the frequent communication required between processors. We developed a parallel version of the OFC algorithm for multi-core processors. Our data, even for relatively small system sizes and low numbers of processors, indicates that increasing the number of processors provides significantly faster simulations; producing more efficient results than previous attempts that used network-based Beowulf clusters. Our algorithm optimizes performance by exploiting the multi-core processor architecture, minimizing communication time in contrast to the networked Beowulf-cluster approaches. Our multi-core algorithm is the basis for a new algorithm using GPUs that will drastically increase the number of processors available. Previous studies incorporating realistic structural features of faults into OFC models have revealed spatial and temporal patterns observed in real earthquake systems. The computational advances presented here will allow for studying interacting networks of faults, rather than individual faults, further enhancing our understanding of the relationship between the earth's structure and the triggering process.

<sup>1</sup>Support for this project comes from the Chenery Research Fund, the Rashkind Family Endowment, the Walter Williams Craigie Teaching Endowment, and the Schapiro Undergraduate Research Fellowship.

## **T1.00022 CHEMICAL PHYSICS —**

### **T1.00023 Ab initio molecular electrostatic potential of hexanuclear Cu, Ag, and Au clusters**<sup>1</sup>

, ALVARO POSADA-AMARILLAS, Dept de Investigacion en Fisica, Universidad de Sonora — DFT calculations of electrostatic potential (ESP) are carried out under the PBE/SDD theory level. Planar initial structures are given as input to perform DFT optimization with the aim of obtaining ground state structures. ESP is thus calculated and results show the existence of both, nucleophilic and electrophilic sites. In each case, the latter are located over the cluster planes while the former are observed in cluster vertices. Binding energy is provided, as well as structural parameters of ground state structures.

<sup>1</sup>CONACyT-Mxico is acknowledged for funding project No. 180424.

## **T1.00024 Hyperpolarized <sup>13</sup>C NMR lifetimes in the liquid-state: relating structures and T1 relaxation times**<sup>1</sup>, CHRISTOPHER PARISH, PETER NIEDBALSKI, University of Texas at Dallas, ZOHREH HASHAMI, LEILA FIDELINO, ZOLTAN KOVACS, Advanced Imaging Research Center, University of Texas Southwestern Medical Center, LLOYD LUMATA, University of Texas at Dallas — Among the various attempts to solve the insensitivity problem in nuclear magnetic resonance (NMR), the physics-based technique dissolution dynamic nuclear polarization (DNP) is probably the most successful method of hyperpolarization or amplifying NMR signals. Using this technique, liquid-state NMR signal enhancements of several thousand-fold are expected for low-gamma nuclei such as carbon-13. The lifetimes of these hyperpolarized <sup>13</sup>C NMR signals are directly related to their <sup>13</sup>C spin-lattice relaxation times T1. Depending upon the <sup>13</sup>C isotopic location, the lifetimes of hyperpolarized <sup>13</sup>C compounds can range from a few seconds to minutes. In this study, we have investigated the hyperpolarized <sup>13</sup>C NMR lifetimes of several <sup>13</sup>C compounds with various chemical structures from glucose, acetate, citric acid, naphthalene to tetramethylallene and their deuterated analogs at 9.4 T and 25 deg C. Our results show that the <sup>13</sup>C T1s of these compounds can range from a few seconds to more than 60 s at this field. Correlations between the chemical structures and T1 relaxation times will be discussed and corresponding implications of these results on <sup>13</sup>C DNP experiments will be revealed.

<sup>1</sup>US Dept of Defense award no. W81XWH-14-1-0048 and Robert A. Welch Foundation grant no. AT-1877

**T1.00025 Hyperpolarized  $^{89}\text{Y}$  NMR spectroscopic detection of yttrium ion and DOTA macrocyclic ligand complexation: pH dependence and Y-DOTA intermediates<sup>1</sup>**, SARAH FERGUSON, ANDHIKA KISWANDHI, PETER NIEDBALSKI, CHRISTOPHER PARISH, University of Texas at Dallas, ZOLTAN KOVACS, University of Texas Southwestern Medical Center, LLOYD LUMATA, University of Texas at Dallas — Dissolution dynamic nuclear polarization (DNP) is a rapidly emerging physics technique used to enhance the signal strength in nuclear magnetic resonance (NMR) and imaging (MRI) experiments for nuclear spins such as yttrium-89 by >10,000-fold. One of the most common and stable MRI contrast agents used in the clinic is Gd-DOTA. In this work, we have investigated the binding of the yttrium and DOTA ligand as a model for complexation of Gd ion and DOTA ligand. The macrocyclic ligand DOTA is special because its complexation with lanthanide ions such as  $\text{Gd}^{3+}$  or  $\text{Y}^{3+}$  is highly pH dependent. Using this physics technology, we have tracked the complexation kinetics of hyperpolarized Y-triflate and DOTA ligand in real-time and detected the Y-DOTA intermediates. Different kinds of buffers were used (lactate, acetate, citrate, oxalate) and the pseudo-first order complexation kinetic calculations will be discussed.

<sup>1</sup>The authors would like to acknowledge the support by US Dept of Defense award no. W81XWH-14-1-0048 and Robert A. Welch Foundation grant no. AT-1877.

**T1.00026 Temperature dependence of proton NMR relaxation times at earth's magnetic field<sup>1</sup>**, PETER NIEDBALSKI, ANDHIKA KISWANDHI, CHRISTOPHER PARISH, SARAH FERGUSON, EDUARDO CERVANTES, ANISHA OOMEN, ANAGHA KRISHNAN, AAYUSH GOYAL, LLOYD LUMATA, University of Texas at Dallas — The theoretical description of relaxation processes for protons, well established and experimentally verified at conventional nuclear magnetic resonance (NMR) fields, has remained untested at low fields despite significant advances in low field NMR technology. In this study, proton spin-lattice relaxation ( $T_1$ ) times in pure water and water doped with varying concentrations of the paramagnetic agent copper chloride have been measured from 6 to 92°C at earth's magnetic field (1700 Hz). Results show a linear increase of  $T_1$  with temperature for each of the samples studied. Increasing the concentration of the copper chloride greatly reduced  $T_1$  and reduced dependence on temperature. The consistency of the results with theory is an important confirmation of past results, while the ability of an ultra-low field NMR system to do contrast-enhanced magnetic resonance imaging (MRI) is promising for future applicability to low-cost medical imaging and chemical identification.

<sup>1</sup>This work is supported by US Dept of Defense award no. W81XWH-14-1-0048 and the Robert A. Welch Foundation grant no. AT-1877.

**T1.00027 Impact of  $\text{Gd}^{3+}$  doping and glassing solvent deuteration on  $^{13}\text{C}$  DNP at 5 Tesla<sup>1</sup>**, ANDHIKA KISWANDHI, Univ of Texas, Dallas, BIMALA LAMA, AMRIS/NHMFL, Univ of Florida, PETER NIEDBALSKI, MUDREKH GODERYA, Univ of Texas, Dallas, JOANNA LONG, AMRIS/NHMFL, Univ of Florida, LLOYD LUMATA, Univ of Texas, Dallas — Dynamic nuclear polarization (DNP) is a technique which can be used to amplify signals in nuclear magnetic resonance (NMR) and magnetic resonance imaging (MRI) by several thousand-fold. The most commonly available DNP system typically operates at the W-band field or 3.35 T, at which it has been shown that  $^{13}\text{C}$  NMR signal can be enhanced by deuteration and  $\text{Gd}^{3+}$  doping. In this work, we have investigated the applicability of these procedures at 5 T. Our results indicate that the deuteration of the glassing matrix still yields an enhancement of  $^{13}\text{C}$  DNP when 4-oxo-TEMPO free radical is used. The effect is attributed to the lower heat load of the deuterons compared to protons. An addition of a trace amount of  $\text{Gd}^{3+}$  gives a modest enhancement of the signal when trityl OX063 is used, albeit with a less pronounced relative enhancement compared to the results obtained at 3.35 T. The results suggest that the enhancement obtained via  $\text{Gd}^{3+}$  doping may become saturated at higher field. These results will be discussed using a thermodynamic model of DNP.

<sup>1</sup>This work is supported by US Dept of Defense award no. W81XWH-14-1-0048 and Robert A. Welch Foundation grant no. AT-1877.

**T1.00028 STRUCTURAL AND ELEMENTAL ANALYSIS OF DEGRADED SINGLE JUNCTION AMORPHOUS SILICON SOLAR MODULE<sup>1</sup>**, GILBERT OSAYEMWENRE, EDSON MEYER, Fort Hare — Photovoltaic solar modules have different defects and degradation characteristic modes. These degradation modes normally heats up some regions in the PV module. Depending on the degree and size of the localised heat, the localized heat can raise above the temperature limit of the module and cause damage to the structural orientation. The presence of severe defect and degradation correlates with high temperature gradients that usually results in morphological damage especially under outdoor conditions. The present study investigates the effect of defect/degradation on the surface morphology of single junction amorphous silicon modules (a-Si:H) during outdoor deployment. The observed structural damage was analysed using scanning electron microscope (SEM) and energy dispersion X-ray (EDX) to ascertain the elemental composition. Results show huge discrepancies in the chemical composition constitute alone different regions. The presence of high concentration of carbon and oxygen was found in the affected region.

<sup>1</sup>The authors wish to acknowledge GMRDC and the International affairs for the support

**T1.00029 Enhanced confinement in compositionally heterogeneous alloy quantum dots**, ZUBAER HOSSAIN, University of Delaware — While there is a growing need to increase solar cell efficiencies and reduce the cost per watt, reported efficiencies are still well below the thermodynamic limit of photovoltaic energy conversion. The major factor that affects the efficiency (by more than 40%) is the lack of absorption or thermalization of electrons. To improve absorption, existing approaches, till date, are focused on combining multiple materials in the form of heterostructures. This talk will show the application of a physics-based mechanistic approach to engineer absorption by using alloy quantum dots and exploiting its heterogeneous compositional and deformation fields. Using a multiscale computational framework that combines density functional theory, k.p method and the finite element calculations, the work shows that heterogeneous distribution of composition and strain fields can lead to substantial confinement in alloy quantum dots. Subsequently alloy quantum dots that are much larger (on the order of 50 nm) in size – compared to their single crystalline counterparts (which are on the order of 5 nm) – can still provide significant confinement. The findings uncover new fundamental insights for engineering confinement that are unattainable under conventional homogenization approximations.

**T1.00030 Electric Transport Phenomena of Nanocomposite Organic Polymer Thin Films<sup>1</sup>**, NICHOLAS C. JIRA, ILДАР SABIRIANOV, CAROLINA C. ILIE, SUNY Oswego — We discuss herein the nanocomposite organic thin film diodes for the use of plasmonic solar cells. This experimental work follows the theoretical calculations done for plasmonic solar cells using the MNPBEM toolbox for MatLab. These calculations include dispersion curves and amount of light scattering cross sections for different metallic nanoparticles. This study gives us clear ideas on what to expect from different metals, allowing us to make the best choice on what to use to obtain the best results. One specific technique for light trapping in thin films solar cells utilizes metal nanoparticles on the surface of the semiconductor. The characteristics of the metal, semiconductor interface allows for light to be guided in between them causing it to be scattered, allowing for more chances of absorption. The samples were fabricated using organic thin films made from polymers and metallic nanoparticles, more specifically Poly(1-vinylpyrrolidone-co-2-dimethylaminoethyl methacrylate) copolymer and silver or gold nanoparticles. The two fabrication methods applied include spin coating and Langmuir-Blodgett technique. The transport properties are obtained by analyzing the I-V curves. We will also discuss the resistance, resistivity, conductance, density of charge carriers.

<sup>1</sup>SUNY Oswego SCAC Grant

**T1.00031 Optimized growth of gold nanobars for energy responsive applications.** , ERIK HOBBS, ANTHONY JOHNSON, CACIE HART, DAVID SCHAEFER, RAJESWARI KOLAGANI, Department of Physics, Towson University, MARY SAJINI DEVADAS, Department of Chemistry, Towson University — The aim of this research is to create a reliable protocol for the synthesis of plasmonic gold nano bars for energy responsive applications such as light harvesting. The mechanism of growth in these metallic structures is not fully understood. Symmetry breaking by twinning introduces anisotropy in the shape of the nanostructures. This also results in the formation of highly faceted tip geometries that support the propagation of surface plasmon polaritons. Gold nanobars have been synthesized through chemical reduction in the presence of surfactants: cetyltrimethylammonium bromide (CTAB) and polyvinylpyrrolidone (PVP). Synthesis is executed by varying the concentrations of CTAB and PVP, as well as adjusting the growth temperature. The influence of additives such as metal ions will be presented. Resulting plasmonic gold nanobars are viewed using darkfield microscopy and scanning electron microscopy to visualize the nanoparticle product mixture. Atomic force microscopy is employed to measure the length and width of the nanobelts. X-ray diffraction determines the degree of crystallinity in the synthesized gold nanobars.

**T1.00032 Nanostructured SnO<sub>2</sub> current collectors for solar energy conversion devices: relating morphology and conductivity** , BENJAMIN DRINGOLI, Department of Physics, Worcester Polytechnic Institute, L. ZHOU, B. GIRI, H. JOSHI, Department of Mechanical Engineering, Worcester Polytechnic Institute, W. BELLEMAN, Department of Physics, Worcester Polytechnic Institute, P.M. RAO, Department of Mechanical Engineering, Worcester Polytechnic Institute, L.V. TITOVA, Department of Physics, Worcester Polytechnic Institute — Large bandgap (3.8 eV), high bulk conductivity, and a low-lying valence band make nanostructured SnO<sub>2</sub> a promising candidate material for extracting photoexcited electrons from absorbers in solar energy conversion devices. Efficient charge collection requires high surface to volume ratio of a nanostructured SnO<sub>2</sub> network, which comes at a cost of reduced conductivity due to incorporation of defects and grain boundaries, and reduction of electrical connectivity. We use terahertz time-domain spectroscopy (THz-TDS) to measure conductivity in nanoporous SnO<sub>2</sub> films and nanowire arrays with different average lengths and packing densities. THz-TDS allows a non-contact measurement of frequency-resolved conductivity over nanoscale distances. Modeling the THz-TDS data using the the Drude–Smith model, we extract intrinsic properties of SnO<sub>2</sub> as well as the effects of morphology on nanoscale conductivity. We find that the intrinsic carrier mobility of SnO<sub>2</sub> making up a nano-porous film is 100 cm<sup>2</sup>/Vs, while the nanoscale mobility is 25 cm<sup>2</sup>/Vs. Correlating THz conductivity of nanostructured SnO<sub>2</sub> with morphology allows us to establish optimal morphology and growth conditions for achieving highest conductivity while maintaining high surface to volume ratio.

**T1.00033 ABSTRACT WITHDRAWN —**

**T1.00034 Environmental Effects on the Terahertz Surface Plasmons in Epitaxial Graphene** , PAULA FEKETE, Department of Physics and Nuclear Engineering, US Military Academy at West Point, NY, GODFREY GUMBS, Hunter College of the City University of New York, NY, ANDRII IUROV, Center for High Technology Materials, University of New Mexico, Albuquerque, New Mexico, JHAO-YING WU, MING-FA LIN, Department of Physics, National Cheng Kung University, Tainan, Taiwan 701 — We predict the existence of low-frequency nonlocal plasmons at the vacuum-surface interface of a superlattice of  $N$  graphene layers interacting with conducting substrate. We derive a dispersion function that incorporates the polarization function of both the graphene monolayers and the semi-infinite electron liquid at whose surface the electrons scatter specularly. We find a surface plasmon-polariton that is not damped by particle-hole excitations or the bulk modes and which separates below the continuum mini-band of bulk plasmon modes. The surface plasmon frequency of the hybrid structure always lies below a limiting value of the surface plasmon frequency of the conducting substrate. The intensity of this mode depends on the distance of the graphene layers from the conductor's surface, the energy band gap between valence and conduction bands of graphene monolayer and, most importantly, on the number of two-dimensional layers. For a sufficiently large number of layers ( $N > 7$ ) the hybrid structure has no surface plasmon. The existence of two plasmons with different dispersion relations indicates that quasiparticles with different group velocity may coexist for various ranges of wavelengths determined by the number of layers in the superlattice.

**T1.00035 Modeling Wettability and Friction of Water on MoS<sub>2</sub> Surface** , BINQUAN LUAN, RUHONG ZHOU, IBM T J Watson Res Ctr — The molybdenum disulfide (MoS<sub>2</sub>) nanosheet is a promising new two-dimensional (2D) material and has recently been used in biological sensing. While the electronic structure of 2D MoS<sub>2</sub> sheet has been extensively studied, the role of its atomic structure and thus the interfacial interactions with bio-fluids are still elusive. Using Molecular dynamics simulations, we modeled the contact angle of water on the MoS<sub>2</sub> nanosheet and predicted the slip-length of water (that is not measurable in experiment yet). Simulation results suggest that the MoS<sub>2</sub> nanosheet is a hydrophobic and low-friction surface. We expect that our newly developed force fields for depicting surface atoms of MoS<sub>2</sub> will facilitate future research in understanding biomolecule-MoS<sub>2</sub> interactions in MoS<sub>2</sub>-based biosensors.

**T1.00036 Unraveling the microscopic pathway of homogeneous water crystallization at supercooled conditions from direct simulations** , FAUSTO MARTELLI, Department of Chemistry, Princeton University, JEREMY PALMER, Department of Chemical and Biomolecular Engineering, University of Houston, RAKESH SINGH, PABLO DEBENEDETTI, Department of Chemical and Biological Engineering, Princeton University, ROBERTO CAR, Department of Chemistry, Princeton University — By means of unbiased classical molecular dynamics simulations, we identify the microscopic pathways of spontaneous homogeneous crystallization in supercooled ST2 water. By introducing a new order parameter, we are able to monitor formation/disruption of locally ordered regions characterized by small ice clusters with intermediate range order. When two of these regions are close each other, they percolate and form a larger ordered region. The process is slow enough to allow for polymorphic selection in favor of cubic ice (Ic). The formation of an ice nucleus requires percolation of many small clusters so that the transformations at the interface of the nucleus do not involve its core, thus guaranteeing the stability of the nucleus. The growth of the crystalline nucleus is fast and involves direct transformation of interfacial liquid molecules as well as percolation of small Ic/Ih clusters. The growth is too fast to allow conversion of Ih into Ic sites, originating the formation of a stacking fault in the final crystal. We recognize Euclidean structures in the oxygen configuration of the second shell in Ic and Ih clusters. This new point of view allows us to explain the source of the ordered stacking fault geometry.

**T1.00037 Boson peak, Ioffe-Regel Crossover, and Liquid-Liquid phase transition in Supercooled Water** , PRADEEP KUMAR, Univ of Arkansas-Fayetteville — We have investigated the onset of Boson peak in a model of liquid water which exhibits a clear first-order phase transition between a low-density liquid phase and a high-density liquid phase of water at low temperature and high pressure. We find that the at low pressures, the onset of Boson peak coincides with the Widom-line of the system. At high pressures, the onset occurs at the transition temperature between the two liquids. Furthermore, we show that at both low and high pressure, the frequency of the Boson peak coincides with the Ioffe-Regel crossover of the transverse phonons, suggesting that the breakdown of Debye behavior is a general feature of Ioffe-Regel limit crossover in supercooled water. The frequency of the Boson peak is weakly pressure dependent and decreases with increasing pressure. Our work bridges gap between the experimental results on the Boson peak nanoconfined water and the behavior that one would expect from a bulk system.

**T1.00038 Testing and using the Lewin-Lieb bounds in density functional theory<sup>1</sup>**, DAVID FEINBLUM, Department of Chemistry, University of California, Irvine, JOHN KENISON, Department of Physics and Astronomy, University of California, Irvine, KIERON BURKE, Department of Chemistry, University of California, Irvine — Lewin and Lieb have recently proven several new bounds on the exchange-correlation energy that complement the Lieb-Oxford bound. We test these bounds for atoms, for slowly-varying gases, and for Hooke's atom, finding them usually less strict than the Lieb-Oxford bound. However, we also show that, if a generalized gradient approximation (GGA) is to guarantee satisfaction of the new bounds for all densities, new restrictions on the exchange-correlation enhancement factor are implied.

<sup>1</sup>We thank Mathieu Lewin and Elliott Lieb for bringing their new bounds to our attention, and Eberhard Engel for developing the OPMKS atom code. This work was supported by NSF under grant CHE-1112442.

**T1.00039 Ab-Initio Modeling of Embedded Subsystems that Exchange Energy and Charge with the Environment**, MICHELE PAVANELLO, Rutgers University-Newark — We claim that a subsystem formulation of Density-Functional Theory simplifies both the theoretical framework and the computational effort for calculating the electronic structure of condensed phase systems. In addition, the naturally subsystem-like form of molecular aggregates makes subsystem DFT a better descriptor of the underlying physics than regular DFT of the supersystem. Our claims are substantiated by simulations of embedded ground and excited states (including charge transfer) of liquids, crystals, and layered systems. By suppressing the inter-subsystem self-interaction error inherent in the exchange-correlation functional, subsystem DFT yields substantially improved simulations compared to Kohn-Sham DFT at a fraction of the computational cost - achieving a dual saving: time to the researcher, and energy to our planet.

**T1.00040 Correcting for the Self-Interaction Error in Ab-Initio Molecular Dynamics Simulations**, ALESSANDRO GENOVA, Rutgers University - Newark, DAVIDE CERESOLI, CNR, ISTM, ALISA KRISHTAL, MICHELE PAVANELLO, Rutgers University - Newark — The Self-Interaction Error (SIE) in semilocal Kohn-Sham (KS) DFT is omnipresent and it can strongly affect the quality of the properties predicted by ab-initio molecular dynamics (AIMD). Liquid water offers two good examples of this behavior: (1) semilocal KS-DFT overestimates the hydrogen bond strength resulting in an overly structured liquid, similar to ice; (2) in the case of solvated radical species, such as OH, KS-DFT exhibits unphysical spin density leakage to neighboring water molecules. We identify the cause of such behavior to be the SIE in the interaction between different molecules (rather than within). Unfortunately, it is a challenge to only rid of the SIE in the intermolecular interactions without introducing spurious corrections for the intramolecular interactions. Semilocal formulations of subsystem DFT offer an elegant solution to this problem: they remove the intermolecular self interaction, and result in an optimal description of liquid water and solvated OH radical, as compared against the experiment. In addition, the subsystem DFT simulations involve a much reduced computational effort compared to KS-DFT. [1] A. Genova et al., JCP 2014, 141, 174101 [2] A. Genova et al., JPCM 2015, Accepted

**T1.00041 Time-dependent Liouville density functional theory for laser-induced ultrafast demagnetization in ferromagnets<sup>1</sup>**, GUOPING ZHANG, Department of Physics, Indiana State University, Terre Haute, IN 47809, USA, YIHUA BAI, Office of Information Technology, THOMAS F GEORGE, University of Missouri-St. Louis — Abstract: The traditional time-dependent density functional theory is very powerful to simulate the dynamic process, but is very time consuming. When it was first used to understand laser-induced ultrafast demagnetization in ferromagnets, the results were disappointing, with the laser amplitude at least three orders of magnitude larger than the experimental one to achieve the similar spin reduction. We develop a new theory within the density functional theory (DFT) for laser-induced ultrafast demagnetization in ferromagnets. We first solve the Liouville equation in the time domain and then feed the excited state density into the DFT code, so the dynamics proceeds on the excited and constraint potential surface. We test this for several magnetic systems and find a significantly larger demagnetization than the static approach, but is still smaller than the experimental finding. Both the local density approximation and the generalized gradient approximation fail. Our finding strongly suggests that a new functional must be developed. As a first test, we introduce a spin power scaling method. Some primitive results will be presented.

<sup>1</sup>This work was solely supported by the U.S. Department of Energy under Contract No. DE-FG02-06ER46304. The research used resources of the National Energy Research Scientific Computing Center.

**T1.00042 Magnetic Exchange Couplings in Heterodinuclear Transition Metal Complexes based on Differential Local Spin Rotations<sup>1</sup>**, RAJENDRA JOSHI, Department of Physics and Science of Advanced Materials, Central Michigan University, Mount Pleasant, MI, 48859, USA, JORDAN PHILLIPS, Science of Advanced Materials, Central Michigan University, Mount Pleasant, MI, 48859, USA, JUAN PERALTA, Department of Physics and Science of Advanced Materials, Central Michigan University, Mount Pleasant, MI, 48859, USA — We assess the performance of a new method based on a generalized perturbative approach, which uses differential local spin rotations for the calculation of magnetic exchange couplings for the case of heterodinuclear transition metal complexes of Cu, Ni, and V. These types of complexes pose a challenge for estimating exchange couplings, mainly due to the asymmetrical spin on the metal centers and the different mapping schemes that can be applied to such systems. The reliability of calculated couplings has been examined by comparing with couplings obtained from the broken symmetry (BS) energy differences method with different exchange correlational functionals, and experimental values. Results show that our method to calculate magnetic exchange couplings can be reliably employed with heterodinuclear complexes, and gives results similar to BS energy differences, when a proper mapping is used.

<sup>1</sup>NSF DMR-1206920

**T1.00043 Large-Scale Hybrid Density Functional Theory Calculations in the Condensed-Phase: *Ab Initio* Molecular Dynamics in the Isobaric-Isothermal Ensemble<sup>1</sup>**, HSIN-YU KO, BISWAJIT SANTRA, Princeton University, ROBERT A. DISTASIO JR, Cornell University, XIFAN WU, Temple University, ROBERTO CAR, Princeton University — Hybrid functionals are known to alleviate the self-interaction error in density functional theory (DFT) and provide a more accurate description of the electronic structure of molecules and materials. However, hybrid DFT in the condensed-phase has a prohibitively high associated computational cost which limits their applicability to large systems of interest. In this work, we present a general-purpose order(N) implementation of hybrid DFT in the condensed-phase using Maximally localized Wannier function; this implementation is optimized for massively parallel computing architectures. This algorithm is used to perform large-scale *ab initio* molecular dynamics simulations of liquid water, ice, and aqueous ionic solutions. We have performed simulations in the isothermal-isobaric ensemble to quantify the effects of exact exchange on the equilibrium density properties of water at different thermodynamic conditions. We find that the anomalous density difference between ice Ih and liquid water at ambient conditions as well as the enthalpy differences between ice Ih, II, and III phases at the experimental triple point (238 K and 20 Kbar) are significantly improved using hybrid DFT over previous estimates using the lower rungs of DFT. [1] X Wu, A Selloni, and R Car, PRB 79, 08510

<sup>1</sup>This work has been supported by the Department of Energy under Grants No. DE-FG02-05ER46201 and DE-SC0008626

**T1.00044 Calibration of a cavity ring down spectrometer and nephelometer using polystyrene spheres and Mie theory**<sup>1</sup>, KHALIL MCMILLAN, SUJEETA SINGH, MARC FIDDLER, SOLOMON BILILIGN, North Carolina AT State Univ — The extinction and scattering cross section of 700 nm polystyrene spherical particles are measured in the 500-660 nm light wavelength range using CRD (Cavity Ring Down) Spectroscopy and an integrating nephelometer. The measurement using spherical particles can be compared with Mie theory predictions to evaluate sources of errors in the system in order to use the system for studying real aerosols. Measurement of optical properties of aerosols such as absorption and scattering cross sections and single scattering albedo are important to quantify the radiative properties of aerosols for climate models.

<sup>1</sup>We acknowledge the support of NSF through grant number AGS1262876

**T1.00045 Investigation of Growth Patterns due to Environmental Factors on the Surface of Bivalve shells with LIBS and Raman Spectroscopy**<sup>1</sup>, ANDRIA PALMER, JOSEPH MAYS, JAMES AMOS, TOM DYNKA, LASZLO UJJ, University of West Florida — Environmental disturbances (such as temperature or chemical disturbances) can cause bivalve mollusk shells to grow faster or slower and cause changes in color and surface ring pattern. We have selected a few shells from our local habitat in Pensacola Beach, FL to analyze without sample treatment to determine what factors may have come into play during growth and use this as a way to analyze our marine environment. Laser Induced Breakdown Spectroscopy (LIBS) uses high energy laser pulses (355 and 532nm) to ablate the sample and create a micro-plasma from which emission spectra can be recorded. Based upon the analysis of intensities, wavelengths, and band patterns of spectral emission bands, the spatial qualitative elemental composition of the shell samples can be determined. Raman spectra were also recorded and correlated to molecules in the sample. By analyzing these measurements using LIBS-Raman spectroscopic techniques, we will be able to see how the local environment is effecting growth, with the largest chemical disturbance in the area being the BP Oil Spill in the Gulf in 2010. Therefore if samples are selected from this period of time it may be possible to identify the effects on shell growth.

<sup>1</sup>UWF NIH MARC U-STAR 1T34GM110517-01, UWF Office of Undergraduate Research

**T1.00046 Encaged molecules in external electric fields: a molecular ‘tug-of-war’**<sup>1</sup>, RAJEEV PATHAK, NALINI GURAV, SHRIDHAR GEJJI, University of Pune, LIBERO BARTOLOTTI, East Carolina University — We investigate applying ab initio theoretical methods, the molecules Hydrogen peroxide, H<sub>2</sub>O<sub>2</sub>, and Methanol, CH<sub>3</sub>OH, encaged in hydrogen-bonded water “buckyballs” (H<sub>2</sub>O)<sub>20</sub>, subjected to an externally applied electric field. While the water-cage (host) tends to confine the guest-molecule, the external electric field tends to stretch it along with its labile hydrogen-bonded host, resulting into a molecular ‘tug-of-war’. We appraise these two competing effects in terms of the extent of ‘screening’ of the host by the cage and compare the response of the composite system in the form of the consequent structural mutations, redistributions in the electron density and the electrostatic potential leading to emergence and suppression of the covalent O-H characteristic frequency shifts in the infra-red vibrational spectrum. This study brings forth the cooperative effect of hydrogen-bonding up to a maximally sustainable threshold electric field, beyond which fragmentation of the water cage occurs.

<sup>1</sup>Partial support from The Center for Development in Advanced Computing (C-DAC) in terms of Computer time on the PARAM Supercomputing facility at Pune, MH, India, is gratefully acknowledged

**T1.00047 Insights into reactivity properties of the ground state structures of (CuS)<sub>x</sub> (x=1-7) using DFT**, JONATHAN LUQUE CEBALLOS, ALVARO POSADA AMARILLAS, Dpto. de Investigacin en Fsica, Univesidad de Sonora, Hermosillo, Sonora — The extraordinary properties of nanoscale materials have generated an enormous interest in the study of nanomaterials, because of the difference of their properties as compared to the corresponding bulk materials. Polyatomic nanomaterials have become important in recent years, due to the possibility of synthesize new materials with similar or better physical and chemical properties, than those of the monoatomic materials, or with a lower cost, to be used in technological applications in medicine, biology, electronics, or catalysis. Among these materials, copper sulfide is one of the transition metal chalcogenides that exhibits different stoichiometric forms with crystal structure varying from orthogonal to hexagonal. In this work we obtained the ground state structures of copper sulfide nanoparticles (CuS)<sub>x</sub>, x=1-7. The corresponding frontier orbitals (HOMO and LUMO) are analyzed, and different reactivity parameters are obtained. We also present the molecular electrostatic potential, which is used to determine the higher and lower electron density regions on the clusters’ structure. All calculations were performed using the TZVP basis set for S and the Christianssen-Ermeler pseudopotential for Cu, employing two different exchange-correlation functionals, PBE and PBE0.

**T1.00048 Theoretical Study of Carborane:Pyridine and Carborane:Pyrimidine Aggregates and Polymers.**, YI GAO, ZHONG-KANG HAN, Shanghai Institute of Applied Physics, Chinese Academy of Sciences, NAN SHAO, WAI-NING MEI, University of Nebraska-Omaha — The carboranes are cross-linked by the pyridines and pyrimidines to form aggregates and polymers. Their geometries and electronic structures are studied by the first-principle calculations. Our results show different connections influence the orientations of the aromatic rings of pyridines and pyrimidines, which would highly affect the electronic structures of carborane:pyridine and carborane:pyrimidine aggregates and polymers. This study might be helpful for the future design of new class of semiconducting boron carbides.

**T1.00049 INTERACTION OF BORON CLUSTERS WITH OXYGEN: A DFT STUDY**<sup>1</sup>, KAMRON SALAVITABAR, West Chester Univeristy of Pennsylvania, KIRAN BOGGAVARAPU, McNeese State University, ANIL KANDALAM, West Chester Univeristy of Pennsylvania — A controlled combustion involving aluminum nanoparticles has often been the focus of studies in the field of solid fuel propellants. However very little focus has been given to the study of boron nanoparticles in controlled combustion. In contrast to aluminum nanoclusters, boron nanoclusters (B<sub>n</sub>) are known to exhibit a planar geometries even at the size of  $n = 19 - 20$ , and thus offer a greater surface area for interaction with oxygen. Earlier experimental studies have shown that boron nanoclusters exhibit different reactivity with oxygen depending on their size and charge. In this poster, we present our recent density functional theory based results, focusing on the reactivity patterns of neutral and negatively charged B<sub>5</sub> cluster with O<sub>n</sub>, where  $n = 1 - 5$ ; and B<sub>6</sub> cluster with O<sub>n</sub> ( $n = 1 - 2$ ). The effect of charge on the reactivity of boron cluster, variation in the stability of product clusters, i.e., neutral and negatively charged B<sub>5</sub>O<sub>n</sub> ( $n = 1 - 5$ ) and B<sub>6</sub>O<sub>n</sub> ( $n = 1 - 2$ ) are also examined.

<sup>1</sup>Financial Support from West Chester University Foundation under FaStR grant is acknowledged.

**T1.00050 High Temperature Raman Spectroscopy Study of the Conversion of Formate into Oxalate: Search for the Elusive  $\text{CO}_2^{2-}$  Intermediate**, CHARLES RYAN, ANNA MEAD, PRASAD LAKKARAJU, Georgian Court University, Dept. of Chemistry, JERRY KACZUR, Liquid Light Chemical Corp., CHRISTOPHER BENNETT<sup>1</sup>, TABBETHA DOBBINS, Rowan University, Dept. of Physics & Astronomy — Research on conversion of carbon dioxide into chemicals and fuels has the potential to address three problems of global relevance. (a) By removing carbon dioxide from the atmosphere, we are able to reduce the amount of greenhouse gases in the atmosphere, (b) by converting carbon dioxide into fuels, we are providing pathways for renewable energy sources, (c) by converting carbon dioxide into C2 and higher order compounds, and we are able to generate valuable precursors for organic synthesis. Formate salts are formed by the electrochemical reduction of carbon dioxide in aqueous media. However, in order to increase the utilization of carbon dioxide, methods need to be developed for the conversion of formate into compounds containing two carbon atoms such as oxalate or oxalic acid. Recently, we examined the thermal conversion of sodium formate into sodium oxalate utilizing a hydride ion catalyst. The proposed mechanism for this reaction involves the carbon dioxide dianion.

<sup>1</sup>currently at NASA Goddard Space Flight Center

## **T1.00051 ABSTRACT WITHDRAWN —**

**T1.00052 Energy of the quasi-free electron in hydrogen, deuterium and oxygen: Probing intermolecular potentials within the local Wigner-Seitz model**<sup>1</sup>, KAMIL KRYNSKI, Department of Chemistry and Biochemistry and Department of Physics, Queens College – CUNY, ZACHARY STREETER<sup>2</sup>, School of Sciences, University of Louisiana at Monroe, CHERICE EVANS, Department of Chemistry and Biochemistry, Queens College – CUNY and Department of Chemistry, Graduate Center – CUNY, GARY L. FINDLEY, School of Sciences, University of Louisiana at Monroe — We present for the first time the quasi-free electron energy  $V_0(\rho)$  for  $\text{H}_2$ ,  $\text{D}_2$  and  $\text{O}_2$  from gas to liquid densities, on noncritical isotherms and on a near critical isotherm in each fluid. These data illustrate the ability of field enhanced photoemission (FEP) to determine  $V_0(\rho)$  accurately in strongly optically absorbing fluids (e.g.,  $\text{O}_2$ ) and fluids with extremely low critical temperatures (e.g.,  $\text{H}_2$  and  $\text{D}_2$ ). We also show that the isotropic local Wigner-Seitz model for  $V_0(\rho)$  – when coupled with thermodynamic data for the fluid – can yield optimized parameters for intermolecular potentials, as well as zero kinetic energy electron scattering lengths.

<sup>1</sup>All measurements were performed at the University of Wisconsin Synchrotron Radiation Center. This work was supported by a grant from the National Science Foundation (NSF CHE-0956719).

<sup>2</sup>currently at Department of Chemistry, University of California – Davis

**T1.00053 Effect of dissolved ions on dipolar correlations in liquid water**, UPAYAN BAUL, The Institute of Mathematical Sciences, C.I.T. Campus, Taramani, Chennai 600113, India, J. MARUTHI PRADEEP KANTH, Vectra LLC, 191, Hamid Building, Mount Road, Chennai 600006, India, RAMESH ANISHETTY, SATYAVANI VEMPARALA, The Institute of Mathematical Sciences, C.I.T. Campus, Taramani, Chennai 600113, India — Structural correlations in liquid water and the effect of dissolved ions on them have generally been characterized through short range density fluctuations. Recent simulation and experimental results have shown that there exists considerably longer ranged ( $> 24$  Angstroms) orientational order in water that can be studied using dipolar correlations. Using extensive molecular dynamics simulations, we show that the spatially long-range nature of such structural correlations are suppressed by the presence of ions, through reduction in co-operativity in orientational fluctuations. At high ( $\geq 2\text{M}$ ) concentrations, strongly solvated ions induce strong perturbations in the hydrogen bond network of water, leading to the formation of bulk like domains with defect sites on boundaries of such domains. Reorientational autocorrelation functions of dipole vectors of water molecules at such defect sites, which are beyond the first hydration shells of ions, also experience significant slowing of reorientation times. Our results show that the effect of ions on the properties of water can propagate well beyond the first solvation shells. Results are discussed in the context of hydrophobic effect and Hofmeister series.

**T1.00054 External dc bias field effects in the nonlinear ac stationary response of permanent dipoles in a uniaxial potential**, NIJUN WEI, WILLIAM T. COFFEY, Department of Electronic and Electrical Engineering, Trinity College, Dublin 2, Ireland, PIRRE-MICHEL DJARDIN, YURI P. KALMYKOV, LAMPS (EA 4217), Universit de Perpignan Via Domitia, France — External dc bias field effects on the nonlinear dielectric relaxation and dynamic Kerr effect of a system of permanent dipoles in a uniaxial mean field potential are studied via the rotational Brownian motion model. Postulated in terms of the infinite hierarchy of differential-recurrence equations for the statistical moments (the expectation value of the Legendre polynomials), the dielectric and Kerr effect ac stationary responses may be evaluated for arbitrary dc bias field strength via perturbation theory in the ac field. We have given two complementary approaches for treating the nonlinear effects. The first is based on perturbation theory allowing one to calculate the nonlinear ac stationary responses using powerful matrix methods. The second approach based on the accurate two-mode approximation [D.A. Garanin, Phys. Rev. E. **54**, 3250 (1996)] effectively generalizes the existing results for dipolar systems in superimposed ac and dc fields to a mean field potential. The results apply both to nonlinear dielectric relaxation and dynamic Kerr effect of nematics and to magnetic birefringence relaxation of ferrofluids. Furthermore, the given methods of the solution of infinite hierarchies of *multi-term* recurrence relations are quite general and can be applied to analogous nonlinear response problems.

**T1.00055 The hydrogen bond network of water supports propagating optical phonon-like modes**<sup>1</sup>, DANIEL ELTON, MARIVI FERNANDEZ-SERRA, Stony Brook University — The local structure of liquid water as a function of temperature is a source of intense research. This structure is intimately linked to the dynamics of water molecules, which can be measured using Raman and infrared spectroscopies. Vibrational modes in liquids are usually considered to be associated to the motions of single molecules or small clusters. Previously, the librational Raman peaks of water were assigned to the librational motions of single molecules. By comparing experimental Raman and IR spectra we show these assignments are problematic. Using molecular dynamics simulations we study the k-dependent dielectric susceptibility of water. We find dispersive optical phonon-like modes in water's librational and OH stretching bands. We argue that on subpicosecond time scales these modes propagate through water's hydrogen bond network over distances of up to two nanometers. In the long wavelength limit these optical modes exhibit longitudinal-transverse splitting, indicating the presence of coherent long range dipole-dipole interactions. Studying how LO-TO splitting evolves with temperature may yield insight into how local structure changes. Our results indicate the dynamics of liquid water have more similarities to ice than previously thought. Reference: arXiv:1507.06363

<sup>1</sup>This work was partially supported by DOE Award No. DE-FG02-09ER16052 (D.C.E.) and by DOE Early Career Award No. DE-SC0003871 (M.V.F.S.).

**T1.00056 Possible Existence of Two Amorphous Phases of D-Mannitol Related by a First-Order Transition**, MEN ZHU, JUN-QIANG WANG, JOHN PEREPEZKO, LIAN YU, University of Wisconsin-Madison — We report that the common polyalcohol D-mannitol may have two amorphous phases related by a first-order transition. Slightly above  $T_g$  (284 K), the supercooled liquid (SCL) of D-mannitol transforms to a low-energy, apparently amorphous phase (Phase X). The enthalpy of Phase X is roughly halfway between those of the known amorphous and crystalline phases. The amorphous nature of Phase X is suggested by its absence of birefringence, transparency, broad X-ray diffraction, and broad Raman and NIR spectra. Phase X has greater molecular spacing, higher molecular order, fewer intra- and more inter-molecular hydrogen bonds than the normal liquid. On fast heating, Phase X transforms back to SCL near 330 K. Upon temperature cycling, it shows a glass-transition-like change of heat capacity. The presence of D-sorbitol enables a first-order liquid-liquid transition (LLT) from SCL to Phase X. This is the first report of polyamorphism at 1 atm for a pharmaceutical relevant substance. As amorphous solids are explored for many applications, polyamorphism could offer a tool to engineer the properties of materials. (Ref: M. Zhu et al, J. Chem. Phys. 2015, 142, 244504)

**T1.00057 Microfaceting of  $\text{Cu}_2\text{O}$  and its implications in photochemistry**, YUNJAE LEE, TAEHUN LEE, YONGHYUK LEE, ALOYSIUS SOON, Department of Materials Science and Engineering, Yonsei University — The high Miller-index microfacets e.g.  $\{211\}$ ,  $\{311\}$ , and  $\{522\}$  have been proposed to play a key role in shape-controlled crystal engineering of  $\text{Cu}_2\text{O}$  polyhedrons for various clean energy applications. These  $\text{Cu}_2\text{O}$  microcrystals with high Miller-index microfacets are found to have a higher photocatalytic activity than those with octahedra and cube morphologies, and thus suggesting that the catalytically active sites are more abundant on the high Miller-index surfaces. Although much effort has been devoted to the actual synthesis and characterizations of these shaped  $\text{Cu}_2\text{O}$  nanocrystals with various morphologies, a firm theoretical understanding of these system are currently limited to low Miller-index facets of  $\text{Cu}_2\text{O}$ . Here, we perform first-principles density-functional theory (DFT) calculations to study the surface energetics and electronic structure of these high Miller-index  $\text{Cu}_2\text{O}$  surfaces, and evaluate their overpotential for water redox reactions on  $\text{Cu}_2\text{O}$ , in comparison with that for the low Miller-index surfaces.

**T1.00058 Water Adsorption and Dissociation on  $\text{CeO}_2(111)$ .**, YI GAO, ZHONG-KANG HAN, Shanghai Institute of Applied Physics, Chinese Academy of Sciences, NAN SHAO, WAI-NING MEI, University of Nebraska-Omaha — The complexity and flexibility of ceria surface hinders the fully understanding of its reactivity and real applications. Here, we use  $\text{H}_2\text{O}/\text{CeO}_2(111)$  as the model system to investigate the water effect on the electron localization and vacancy diffusion on  $\text{CeO}_2(111)$  surface by the first-principle calculations. Our results indicate the water adsorption would high affect the electronic structures of  $\text{CeO}_2(111)$  surface, which further induce the dissociation of  $\text{H}_2\text{O}$  molecule. This molecular mechanism might provide more guidance to the future applications including the watergas shift reactions.

**T1.00059 Investigating Non-Equilibrium Fluctuations of Nanocolloids in a Magnetic Field Using Direct Imaging Methods<sup>1</sup>**, ASHLEY RICE, ANA OPRISAN, SORINEL OPRISAN, College of Charleston, RICE-OPRISAN COLLEGE OF CHARLESTON TEAM — Nanoparticles of iron oxide have a high surface area and can be controlled by an external magnetic field. Since they have a fast response to the applied magnetic field, these systems have been used for numerous in vivo applications, such as MRI contrast enhancement, tissue repair, immunoassay, detoxification of biological fluids, hyperthermia, drug delivery, and cell separation. We performed three direct imaging experiments in order to investigate the concentration-driven fluctuations using magnetic nanoparticles in the absence and in the presence of magnetic field. Our direct imaging experimental setup involved a glass cell filled with magnetic nanocolloidal suspension and water with the concentration gradient oriented against the gravitational field and a superluminescent diode (SLD) as the light source. Nonequilibrium concentration-driven fluctuations were recorded using a direct imaging technique. We used a dynamic structure factor algorithm for image processing in order to compute the structure factor and to find the power law exponents. We saw evidence of large concentration fluctuations and permanent magnetism. Further research will use the correlation time to approximate the diffusion coefficient for the free diffusion experiment.

<sup>1</sup>Funded by College of Charleston Department of Undergraduate Research and Creative Activities SURF grant

**T1.00060 Capillary Condensation in Polymer Blends: an Analysis of Phase Transitions<sup>1</sup>**, CAROLINA C. ILIE, State University of New York at Oswego, Department of Physics, NICHOLAS C. JIRA, IAN R. EVANS, MATTHEW COHEN, JULIA R. D'ROZARIO, MARIE T. ROMANO, ILDAR SABIRIANOV, SUNY Oswego — We explore herein the capillary condensation for various geometries. Capillary condensation is studied in the presence of van der Waals forces. We derive the grand free energy, and we analyze the phase transitions, the absorption isotherms and the triple point. Phase transitions between full, empty and two films are investigated and the shape of the liquid is calculated. We also analyze an important application of wetting phenomena and capillary condensation in binary polymer blends and investigate the type of wetting transitions presented and the phase diagram.

<sup>1</sup>SUNY Oswego SCAC Grant, NSF Noyce Grant

## **T1.00061 ABSTRACT WITHDRAWN —**

**T1.00062 Frustrated Total Internal Reflection applied to Quantum Tunneling<sup>1</sup>**, NATHANIEL HULL, JIA-AN YAN, Towson Univ — The objective of this project is to demonstrate an optical phenomenon, frustrated total internal reflection (FTIR), by numerically solving the time-dependent Schrodinger equation (TDSE) in quantum mechanics, and to illustrate the correlations between FTIR and the quantum tunneling in one-dimensional quantum structures. We will use a MATLAB program to numerically propagate a Gaussian wave packet to penetrate finite square barriers. The transmission coefficient is then calculated as a function of the distance between two rectangular barriers/wells. The results will be useful to elucidate the correlations between optical FTIR and quantum tunneling.

<sup>1</sup>This work was supported by the FCSM Undergraduate Research Committee, the FCSM Fisher General Endowment and the FDRC grant (OSPR No. 140269) at Towson University

**T1.00063 Photodissociation Spectroscopy of Ruthenium Polypyridyl Complexes in Vacuo**, SHUANG XU, JAMES SMITH, J. MATHIAS WEBER, JILA/University of Colorado at Boulder — Photoelectrochemical water oxidation is a direct way to produce solar fuels from renewable sources. Since this reaction has a high reaction barrier, a cost-effective catalyst is necessary. Ruthenium polypyridyl complexes are promising catalysts for water oxidation. However, the mechanism of catalytic action is not well understood. One major difficulty of a mechanistic understanding is the complexity of reactive solutions under turnover conditions. To circumvent this problem, we applied electronic photodissociation spectroscopy in the UV and visible spectral range to a series of mass selected ruthenium polypyridyl complex ions in vacuo. The ions in this work are of the form  $[\text{Ru}^{II}\text{-L}]^{2+}$ , where  $\text{Ru}^{II}$  represents ruthenium(II)-bipyridine-terpyridine, a prototype catalyst belonging to the ruthenium-polypyridyl family. By varying the ligand L, we were able to study the ligand influence on the photophysical properties of the complex. The cases where  $\text{L} = (\text{H}_2\text{O})_{1,2,3}$  are of particular interest because they are directly related to an intermediate in the catalytic cycle for water oxidation. Our experiment in vacuo is an essential complement to experiments in solution and provides unique information for understanding the photophysics and photochemistry of these complexes on a molecular level.

**T1.00064 Quantum and Classical Electrostatics Among Atoms<sup>1</sup>**, T. P. DOERR, O.I. BOLENSKY, A. Y. OGURTSOV, YI-KUO YU, National Center for Biotechnology Information — Quantum theory has been unquestionably successful at describing physics at the atomic scale. However, it becomes more difficult to apply as the system size grows. On the other hand, classical physics breaks down at sufficiently short length scales but is clearly correct at larger distances. The purpose of methods such as QM/MM is to gain the advantages of both quantum and classical regimes: quantum theory should provide accuracy at the shortest scales, and classical theory, with its somewhat more tractable computational demands, allows results to be computed for systems that would be inaccessible with a purely quantum approach. This strategy will be most effective when one knows with good accuracy the length scale at which quantum calculations are no longer necessary and classical calculations are sufficient. To this end, we have performed both classical and quantum calculations for systems comprising a small number of atoms for which experimental data is also available. The classical calculations are fully exact; the quantum calculations are at the MP4(SDTQ)/aug-cc-pV5Z and CCSD(T)/aug-cc-pV5Z levels. The precision of both sets of calculations along with the existence of experimental results allows us to draw conclusions about the range of utility of the respective calculations.

<sup>1</sup>This research was supported by the Intramural Research Program of the NIH, NLM and utilized the computational resources of the NIH HPC Biowulf cluster.

**T1.00065 Single micelle force microscopy reveals the coordination interaction between catechol and Fe3+.**, YIRAN LI, YI CAO, WEI WANG, Nanjing Univ — Metal coordination bonds are widely found in natural adhesive, load-bearing, and protective materials, which are thought to be responsible for their high strength and toughness. However, it remains unknown how the metal-ligand complexes could give rise to such superb mechanical properties. Here, combining single molecule force spectroscopy and quantum calculation, we study the mechanical properties of individual catechol-Fe3+ complexes, the key elements accounting for the high toughness and extensibility of byssal threads of marine mussels. We find that catechol-Fe3+ complexes possess a unique combination of mechanical features, including high mechanical stability, fast reformation kinetics, and stoichiometry-dependent mechanics. Therefore, they can serve as sacrificial bonds to efficiently dissipate energy in the material, quickly recover the mechanical properties when load is released, and be responsive to environmental conditions. Our study provides the mechanistic understanding of the coordination bond-mediated mechanical properties of biogenetic materials, and could guide future rational design and regulation of the mechanical properties of synthetic materials.

**T1.00066 Band-gap opening properties of graphene binding with low-concentration fluorine**, YUHUA DUAN, DOE-National Energy Technology Laboratory, Pittsburgh, PA 15236, CHARTER STINESPRING, Chemical Engineering Department, West Virginia University, Morgantown, WV 25506, USA, BENJAMIN CHORPENING, DOE-National Energy Technology Laboratory, Pittsburgh, PA 15236 — To better understand the effects of low-level fluorine (F) in graphene-based sensors, the structure and impact of low-concentration of fluorine defects on the electrical properties of single- and multi-layer graphene films were investigated by density functional theory with van der Waals dispersion interactions. When F bonds to a carbon atom of graphene, the carbon atom is pulled slightly above the graphene plane creating what is referred to as a C<sub>F</sub> defect, and a valence band (B<sub>F</sub>) near the Fermi level is formed mainly from the *p* orbitals of the F atoms with some small contribution from the *p* orbitals of the bonded carbon atoms. Depending on the F binding sites, the B<sub>F</sub> can serve as a valence band or a conduction band and only few configurations of the F-binding graphene can open a band gap. Such results indicate that the band gap opening for graphene with low F-adsorption level strongly depends on the F-binding configurations, which is different from the fully or highly partial fluorinated graphene. At low F-adsorption level, the interaction between neighboring pairs of F adatoms is negligible and the most important interaction is between the F and carbon atoms in the C<sub>F</sub> defect. Such results are useful for sensor and nano-electronics developments.

**T1.00067 A simple model for electronic properties of surface adsorbed molecules.**, RAJESH DHAKAL, WILLIAM SCHWALM, Univ of North Dakota — We adapt a minimal approximation to one electron quantum theory of molecules referred as Fast Accurate Kinetic Energy method. This in principle handles large complex molecular structures with less computational effort to compute electronic properties of adsorbed molecules. Kinetic energy integrals are calculated accurately but multi-electron potential energy integrals are approximated. The neighboring atom interactions are included also. For layers of isophthalic acids formed on pyrolytic graphite the configuration changes as a function of length of hydrocarbon tails. We study properties of this system as a function of tail length.

**T1.00068 Spectroscopic Studies on Graphenes Dispersed Within Polymeric Matrices<sup>1</sup>**, FILIPE FERREIRA, FELIPE BRITO, Instituto Tecnológico de Aeronáutica, So Jos dos Campos-SP, Brazil, DORINA CHIPARA, The University of Texas Rio Grande Valley, PULLICKEL AJAYAN, Rice University, WESLEY FRANCISCO, Instituto Tecnológico de Aeronáutica, So Jos dos Campos-SP, Brazil, CRISTIAN CHIPARA, Rice University, EVELYN SIMONETTI, Instituto Tecnológico de Aeronáutica, So Jos dos Campos-SP, Brazil, CHARLES CARTWRIGHT, The University of Texas Rio Grande Valley, LUCIANA CIVIDANES, Instituto Tecnológico de Aeronáutica, So Jos dos Campos-SP, Brazil, JAMES HINTHORNE, The University of Texas Rio Grande Valley, GILMAR THIM, Instituto Tecnológico de Aeronáutica, So Jos dos Campos-SP, Brazil, ROBERT VAJTAI, Rice University, MIRCEA CHIPARA, The University of Texas Rio Grande Valley, INSTITUTO TECNOLÓGICO DE AERONÁUTICA COLLABORATION, THE UNIVERSITY OF TEXAS PAN AMERICAN COLLABORATION, RICE UNIVERSITY COLLABORATION — Graphenes have been dispersed within various polymeric matrices (polyethylene, polyethylene oxide, polystyrene, and epoxy resins). Some have been used as purchased (pristine and functionalized graphene platelets from Cheap Tubes). Pristine and functionalized graphene oxides have been obtained in laboratory according to W. Hummers, R. Offeman, ("Preparation of Graphitic Oxide". J Am Chem Soc **80**, 6, 1339, 1958) and by original functionalization processes. All these samples were investigated by Raman spectroscopy using a Renishaw InVia spectrometer operating at 532 and 785 nm. Additional information has been obtained by Wide Angle X-Ray Scattering using a Bruker Discover 8 spectrometer. Raman spectra have been fitted by a convolution of modified Breit-Wigner-Fano line shapes and the main parameters (position, intensity, width, asymmetry factor) of each line are discussed. The research aims to a better identification of graphene related nanostructures isolated or dispersed within polymeric matrices by Raman spectroscopy.

<sup>1</sup>FAPESP (Grant 2013/20218-0) and CNPq (Grant 141197/2014 5) for financial support, LAS/INPE and LEFE/UNESP for collaboration.

**T1.00069 Study of near surface Nitrogen vacancy center (NV<sup>-</sup>) neutralization in diamond<sup>1</sup>**, ABU NAIM RAKIB AHMED, ARTHUR NEWELL, DONTRAY DOWDELL, DEBORAH SANTAMORE, Delaware State Univ — The performance of nitrogen vacancy based sensors strongly depends on the population of NV<sup>-</sup> near the diamond surface. The magnetic sensing capabilities of NV<sup>-</sup> diamonds are diminished as the NV<sup>-</sup> becomes neutralized and turns into NV<sup>0</sup>, where NV<sup>0</sup> represents the neutralized charge state of NV<sup>-</sup>. A theoretical calculation is performed to obtain the electron transfer rate between the NV<sup>-</sup> and surface molecules using the Marcus theory of electron transfer where reorganization energy and electronic wave function coupling are considered. The electronic wave function coupling is determined using the density functional theory method. Band structure simulation is also performed to confirm the NV<sup>-</sup> neutralization at the surface due to surface termination. The electron transfer rate is investigated for various surface terminations (hydrogen, oxygen). Moreover, an investigation of the stability of the NV<sup>-</sup> at different depths relative to the surface is conducted. This work provides the ratio of NV<sup>-</sup> to (NV<sup>0</sup>+NV<sup>-</sup>) at equilibrium, which demonstrates the effect of surface termination and contamination on NV<sup>-</sup> neutralization and also depicts surface properties of NV<sup>-</sup> diamonds.

<sup>1</sup>National Science Foundation(NSF Grant: DMR-1505641)

**T1.00070 Electronic structure of novel charge transfer compounds: application of Fermi orbital self-interaction corrected density functional theory<sup>1</sup>**, TORSTEN HAHN, Institute for Theoretical Physics, TU Freiberg, 09599 Freiberg, Germany, FLORIAN RCKERL, Institute for Solid State Research, IFW-Dresden, P.O. Box 270116, DE-01171 Dresden, Germany, SIMON LIEBING, Institute for Theoretical Physics, TU Freiberg, 09599 Freiberg, Germany, MARK PEDERSON, Department of Chemistry, Johns Hopkins University, Baltimore, Maryland 21218, USA — We present our experimental and theoretical results on novel Picene/F4TCNQ and Manganese-Phthalocyanine/F4TCNQ donor / acceptor systems. We apply the recently developed Fermi-orbital based approach for self-interaction corrected density functional theory (FO-SIC DFT) to these materials and compare the results to standard DFT calculations and to experimental data obtained by photoemission spectroscopy. We focus our analysis on the description of the magnitude of the ground state charge transfer and on the details of the formed hybrid orbitals. Further, we show that for weakly bound donor / acceptor systems the FO-SIC approach delivers a more realistic description of the electronic structure compared to standard DFT calculations. [1] M. R. Pederson, A. Ruzsinszky, and J. P. Perdew, J. Chem. Phys. 140, 121103 (2014). [2] M. R. Pederson, J. Chem. Phys. 142, 064112 (2015).

<sup>1</sup>Support by DFG FOR1154 is greatly acknowledged.

**T1.00071 Au nanoparticles improve amorphous carbon to be gas sensors**, KENG-WEN LIU, JIAN-HENG LEE, HSIUNG CHOU, TZU-CHING LIN, SI-TING LIN, Dept. of Physics, NSYSU, Kaohsiung 804, Taiwan, SHIH-JYE SUN COLLABORATION<sup>1</sup> — In order to make the amorphous carbon possess the gas sensing capability transferring some sp<sup>3</sup> orbits to sp<sup>2</sup> is necessary. It is proposed that the metallic materials having a large charge exchange with sp<sup>3</sup> carbon orbits are being catalysts to transfer the carbon orbits. We found embedding gold nanoparticles to the amorphous carbon will induce many compact sp<sup>2</sup> orbits around the nanoparticles, which make the amorphous carbon be the candidate material for the gas sensors. The orbits of amorphous carbon near the interface of Au nanoparticles can be changed from sp<sup>3</sup> to compact sp<sup>2</sup> to reduce the surface energy of Au nanoparticles. Meanwhile, our molecular dynamics simulation has confirmed the fact, when an Au nanoparticle is embedded in the amorphous carbon system the ratio of sp<sup>2</sup> orbits increases dramatically. Similar results also have been confirmed from the Raman spectrum measurements. We controlled the carrier transport by changing the hopping barriers formed by amorphous carbon matrix between the Au nanoparticles to modify the resistance. These nanocomposites exhibit a superior sensitivity to NH<sub>3</sub> at room temperature as well as good reproducibility and short response/recovery times, which could have potential applications in gas sensors.

<sup>1</sup>Dept. of Applied Physics, NUK, Kaohsiung, Taiwan.

## T1.00072 INSULATORS AND DIELECTRICS —

**T1.00073 Spin-charge separation of edge zero modes in one dimension**, ZHANG DANBO, WANG ZIDAN, Department of Physics, The University of HongKong — We propose a new type of edge zero modes that exhibit spin-charge separation, which can be realized at the boundaries in an exotic one dimensional topological matter that is both fermionic Haldane insulator and topological superconductor. We give a lattice model to illustrate the nature of edge zero modes, both from bosonization and mean-field analysis. Finally, We find that Haldane phase of spin-1 chain also owns spin-charge separation of edge zero modes when mapped into fermionic system by Jordan-Wigner transformation.

**T1.00074 Triggering Incipient Ferroelectricity in Calcium Copper Titanate (CaCu<sub>3</sub>Ti<sub>4</sub>O<sub>12</sub>) ceramics through partial B-site substitution with Te<sup>4+</sup> ion.**, NABADYUTI BARMAN, student, K.B.R VARMA, Retired — Double perovskite structured dielectric ceramic CaCu<sub>3</sub>Ti<sub>4-x</sub>Te<sub>x</sub>O<sub>12</sub> (CCTTO) ( $x = 0, 0.05, 0.1, 0.15, 0.2$ ) was fabricated from the powder obtained by conventional solid state synthetic route. The room temperature XRD patterns for the  $x = 0, 0.05, 0.075$  modified samples were confirmed to possess a single phase with cubic space group  $Im\bar{3}$  by Rietveld refinement. But, the Rietveld refinement performed on XRD patterns recorded for the compositions corresponding to  $x = 0.1, 0.15, 0.2$  shows the coexistence of the cubic phase (space group  $Im\bar{3}$ ;  $a = 7.4065\text{\AA}$ ) and tetragonal phase (space group  $I4/mcm$ ;  $a = 7.369\text{\AA}$  and  $c = 6.967\text{\AA}$ ). The dielectric properties of these ceramics were studied over a wide frequency (40Hz–2MHz) and temperature range (30–400K). The Te<sup>4+</sup> doped samples (CCTTO) exhibited dielectric permittivity ( $\epsilon_r$ ) value of  $\sim 23\text{--}33 \times 10^3$  which is more than twice that of undoped CCTO ( $\sim 11 \times 10^3$ ) at 1kHz. A decreasing trend in dielectric permittivity with increasing temperature, a signature of incipient ferroelectricity, was observed for all the samples. Barrett's formula was invoked to rationalize the dielectric permittivity variation as a function of temperature. The incipient ferroelectric behavior is correlated with soft phonon mode observed in temperature dependent Raman Spectroscopic studies. .

**T1.00075 Electric and Magnetic Characterization of patterned La<sub>0.6</sub>Sr<sub>0.4</sub>MnO<sub>3</sub>/SrTiO<sub>3</sub>/Si junctions using strained SrTiO<sub>3</sub> as a Ferroelectric Barrier.**, PARISA JALILI SHAFIGHI, RYAN COTTIER, DANIEL A CURRIE, BARRY D KOEHNE, Texas State university, San Marcos, ANDREW JOHNSON, JOSHUA P VEAZEY, Hope College, Holland, MI, NIKOLETA THEODOR-POULOU, Texas State university, San Marcos, TEXAS STATE UNIVERSITY, SAN MARCOS, TX TEAM, HOPE COLLEGE, HOLLAND, MI TEAM — Controlling a magnetic device via electrical means is a sought-after goal for technological devices and can be achieved through magnetoelectric coupling between ferroelectric and ferromagnetic materials. We investigate such as possibility through a by epitaxially growing a magnetic oxide, La<sub>0.6</sub>Sr<sub>0.4</sub>MnO<sub>3</sub> (LSMO) as an active magnetic electrode on a ferroelectric oxide, strained SrTiO<sub>3</sub> (STO) on Si. STO thin films grown on Si are compressively strained (1.7 %) and can be ferroelectric at T=300 K when less than 5nm thick. LSMO is ferromagnetic up to 340 K (in bulk), has an in-plane crystal constant of  $a = 0.3870\text{ nm}$ , and is closely lattice matched to STO ( $a = 0.3905\text{ nm}$ ) with a 0.9% in-plane tensile strain. Since STO is compressively strained in Si, an even smaller lattice mismatch is expected between LSMO and STO/Si. We investigate the epitaxial growth of LSMO/STO/Si and electrical characteristics in a capacitor type structure fabricated using photolithography as a function of Temperature and Magnetic Field. Acknowledgements: Support by the NSF-Career grant, DMR-1255629, Hope College Frissel Research Fund, NSF-MRI Grant, CHE-1126462 is gratefully acknowledged.

**T1.00076 Observation of ferroelectricity at room temperature in  $\sim 1\text{ nm}$  thick conducting BaTiO<sub>3- $\delta$</sub>** , SEUNGRAN LEE, KRISS, Daejeon 305-350, Rep. of Korea, L. BAASANFORJ, Uni. of Sci. and Tech., Daejeon 305-350, Rep. of Korea, JUNGWON CHANG, Dept. of Display and Semiconductor Physics, Korea University, Sejong 339-700, Rep. of Korea, INWOONG HWANG, Dept. of Physics, Chungnam Nat'l Uni., Daejeon 305-764, Rep. of Korea, JUNGRAE KIM, CCES-IBS, Seoul 151-742, Rep. of Korea, SEUNGBO SHIM, KRISS, Daejeon 305-350, Rep. of Korea, JONGHYUN SONG, Dept. of Physics, Chungnam Nat'l Uni., Daejeon 305-764, Rep. of Korea, JINHEE KIM, KRISS, Daejeon 305-350, Rep. of Korea — Efforts to search for new and multi-functionalities in thin-film systems have led important findings of unknown phenomena and functionality which do not appear in bulk systems. As film growth technique is advanced, one can decrease the film thickness even thinner down to  $\sim \text{nm}$ , its unique physical properties are still appearing. For example, the superconducting metallic state of an LaAlO<sub>3</sub>/SrTiO<sub>3</sub> (LAO/STO) heterostructure was found where LAO is about 3-4 unit cells (uc). An SrRuO<sub>3</sub> film exhibited its ferromagnetic metallicity down to 4-6 uc; a few years later, its ferromagnetism was found to be disappeared at 2-3 uc. Meanwhile, theoretical methods have predicted existence of ferroelectrical properties mostly in prototype ferroelectric BaTiO<sub>3</sub> (BTO): 3-6 uc. However, experimental verification to find such predicted thickness was hindered by large leakage current. Here we observed that  $\sim 1\text{ nm}$ -thick conducting BTO fillms show ferroelectric switching at room temperature (RT), and BTO films are fully-strained on LAO/STO heterostructures thicker than 5 nm thickness. Our experimental results will enlarge applicable functional oxide devices for future applications.

**T1.00077 Optical Properties and Electronic Transitions of  $\text{YbFe}_2\text{O}_4$  Thin Films**<sup>1</sup>, JOSH HINZ, MICHELLE PASCOLINI, RAM RAI, Physics Department, SUNY Buffalo State, 1300 Elmwood Ave., Buffalo, NY 14222 — We present growth, structural, optical and electronic properties of Ytterbium-Iron-oxide,  $\text{YbFe}_2\text{O}_4$ , thin films.  $\text{YbFe}_2\text{O}_4$  exhibits the unique physical properties due to the presence of  $\text{Fe}^{2+}$  and  $\text{Fe}^{3+}$  valence states within the triangular lattice structure. We prepared the compound by a solid state reaction starting with stoichiometric proportion of  $\text{Yb}_2\text{O}_3$ ,  $\text{Fe}_2\text{O}_3$ , and  $\text{FeO}$ . The material was then deposited on c-axis sapphire substrates using a reactive electron beam deposition technique to produce ~100 nm thick films. Absorption, reflectance, and transmittance of the  $\text{YbFe}_2\text{O}_4$  films were measured in the temperature range of 10 – 450 K. The optical spectra contain Fe d to d on-site transitions as well as O 2p to Fe 3d, Yb 6s, and Yb 5d charge-transfer transitions. In addition, the optical spectra exhibit strong temperature dependence, indicating evidence of a structural distortion of the crystal structure at ~180 K as well as a magnetic transition at ~250 K. The detail analysis of the optical data in comparison with theoretical studies will be presented.

<sup>1</sup>National Science Foundation (DMR-1406766)

**T1.00078 Structure and Magnetic Properties of Rare Earth Doped Transparent Alumina**, KRISTA LIMMER, MAHESH NEUPANE, TANYA CHANTAWANSRI, US Army Rsch Lab - Aberdeen — Recent experimental studies of rare earth (RE) doped alumina suggest that the RE induced novel phase-dependent structural and magnetic properties [1]. Motivated by these efforts, the effects of RE doping of alpha and theta alumina on the local structure, magnetic properties, and phase stability have been examined in this first principles study. Although a direct correlation between the magnetic field dependent materials properties observed experimentally and calculated from first principles is not feasible because of the applied field and the scale, the internal magnetic properties and other properties of the doped materials are evaluated. The RE dopants are shown to increase the substitutional site volume as well as increasingly distort the site structure as a function of ionic radii. Doping both the alpha (stable) and theta (metastable) phases enhanced the relative stability of the theta phase. The energetic doping cost and internal magnetic moment were shown to be a function of the electronic configuration of the RE-dopant, with magnetic moment directly proportional to the number of unpaired electrons and doping cost being inversely related. [1] Pavlacka, Robert, et al. Ceramic Transactions 252: 3, 2015.

**T1.00079 Magnetic and Ferroelectric Anisotropy in Multiferroic  $\text{FeVO}_4$** <sup>1</sup>, EHAB ABDELHAMID, Wayne State U, AMBESH DIXIT, IIT Jodhpur, KENTA KIMURA, TSUYOSHI KIMURA, Osaka U, ONATTU JAYAKUMAR, Bhabah Atomic Research Ctr, VAMAN NAIK, U of Michigan-Dearborn, RATNA NAIK, GAVIN LAWES, BORIS NADGORN, Wayne State U —  $\text{FeVO}_4$  has been studied as a model system for understanding the magnetoelectric interaction mechanisms in low symmetry multiferroics. Triclinic  $\text{FeVO}_4$  is characterized by two antiferromagnetic phase transitions, occurring at  $T_{N1}$  = 22 K and  $T_{N2}$  = 15 K, with the latter transition signaling a break in the space inversion symmetry, accompanied by the development of a non-collinear magnetic order which induces ferroelectricity. Earlier measurements on polycrystalline  $\text{FeVO}_4$  doped with magnetic (Cr and Mn) as well as non magnetic (Zn) dopants indicate the stability of the two antiferromagnetic transition temperatures. In this work, single crystals of both undoped and doped  $\text{FeVO}_4$  were grown from flux. To track the changes in lattice parameters induced by changing the doping concentration (measured by EDAX), XRD and Raman spectra were obtained. By recording the magnetization along two different crystal orientations, we were able to confirm the easy magnetic axis in this structure. Finally, we obtain the crystal's ferroelectric polarization along two different directions in an attempt to further understand the mechanism responsible for the ferroelectric transition.

<sup>1</sup>This work is supported by the NSF under DMR-1306449

**T1.00080 Anomalous enhancement of Neel temperature and magnetic coupling for  $\text{Bi}_{0.9}\text{Ca}_{0.1}\text{FeO}_{3-\delta}$  and  $\text{Bi}_{0.9}\text{Pb}_{0.1}\text{FeO}_{3-\delta}$** , GOPESHWAR-DHAR DWIVEDI, KUNG-SHANG YANG, BO-YU CHEN, HSIUNG CHOU<sup>1</sup>, Dept. of Physics, NSYSU, Kaohsiung 804, Taiwan — Temperature dependent neutron diffraction patterns of the Ca-doped  $\text{BiFeO}_3$  and Pb-doped  $\text{BiFeO}_3$  show that their Neel temperatures ( $T_N$ ) increase to 710 K and 680 K, while pure  $\text{BiFeO}_3$  has a  $T_N$  ~643 K. X-ray absorption spectra clearly shows that there is no evidence of mixed valence states despite divalent cation doping in trivalent Bi-sites. X-ray photoemission spectroscopy study revealed that divalent doping has introduced oxygen vacancies in the system. Oxygen deficiency plays a significant role in contracting Fe-O bond length in  $\text{FeO}_6$  octahedra and hence increasing the Fe-O-Fe bond angle in  $\text{Bi}_{0.9}\text{Ca}_{0.1}\text{FeO}_{3-\delta}$  and  $\text{Bi}_{0.9}\text{Pb}_{0.1}\text{FeO}_{3-\delta}$ . The decreased Fe-O bond length and increased Fe-O-Fe bond angle favors the Goodenough-Kanamori-Anderson (GKA) coupling. The GKA coupling increases the magnetic interaction between the spins and hence increases the  $T_N$ . Additionally, doping of divalent cations ( $\text{Ca}^{2+}$  and  $\text{Pb}^{2+}$ ) results in the destruction of cycloidal spin structure and formation of a simple antiferromagnetic (AFM) structure. This structure can easily be canted near the heterogeneous interface with a ferromagnetic layer to induce the Dzyaloshinskii-Moriya (DM) interaction and enhance the magneto-electric (M-E) coupling.

<sup>1</sup>Corresponding Author

**T1.00081 Phononic Structure Relationships in the Subgroup Phases of Ferroelectric  $\text{Ca}_3\text{Mn}_2\text{O}_7$** , ELVIS SHOKO, EMAN AL DAWOOD, UDO SCHWINGENSCHLOGL, PSE Division, KAUST, Saudi Arabia — The Ruddlesden-Popper (RP) compound,  $\text{Ca}_3\text{Mn}_2\text{O}_7$ , exhibits hybrid improper ferroelectric (FE) behavior in its  $A2_1am$  phase. However, a new phase (space group  $Acaa$ ), co-existing with the FE phase (200-320 K) and exhibiting negative thermal expansion (NTE) was recently discovered. This discovery highlighted the complexity of the phase relationships in the subgroup structure of  $\text{Ca}_3\text{Mn}_2\text{O}_7$ . Successful exploitation of RP compounds for FE applications depends on a clear understanding of the phononic relationships among the different relevant subgroup phases. Accordingly, we have used density functional theory (DFT) to map out the total energy landscape for the principal subgroup phases relative to the tetragonal phase. In order to elucidate the interrelationships of the soft phonon modes among the different subgroup phases, we performed lattice dynamics and quasi-harmonic approximation calculations. In addition, the latter calculations enabled us to extract mode Gruneisen parameters leading to new insights into the NTE behavior of  $\text{Ca}_3\text{Mn}_2\text{O}_7$ . The implications of our findings are discussed in the context of the potential of RP compounds as FE materials.

**T1.00082 Signatures of Soft Phonons in Impedance Spectroscopy of Barium Titanate Colloidal Solutions**, SCOTT TAN, GRAHAM KRAHN, Pomona College, RICHARD HASKELL, Harvey Mudd College, TODD MONSON, Sandia National Laboratories — Barium titanate (BTO) is a widely used dielectric material in capacitor technologies due to a high bulk dielectric constant between 1500-2000 [1] at room temperature. Although bulk BTO has been extensively studied, it is still not entirely clear how varying BTO nanoparticle size affects the dielectric constant, particularly for non-sintered discrete nanoparticles. The most widely accepted and agreed upon behavior is that smaller BTO particles have lower dielectric constants due to lower tetragonality. However, Wada et al. reported that the BTO dielectric constant reached a high value of ~5000 near a small particle size of ~140 nm. This anomaly was attributed to the soft phonon, which reached a minimum frequency at the particle size of ~140 nm when observed in FIR reflection measurements [2]. The soft phonon explanation for the anomaly observed by Wada et al. implies that the measured value of the dielectric constant will depend on the frequency of the applied electric field when performing impedance measurements. Herein, we present an equivalent circuit model to fit BTO colloidal solution impedance spectra, which accounts for a distribution of capacitance values as a function of applied electric field frequency. This model fits reasonably well to experimental measurements obtained via impedance spectroscopy, which suggests that the soft phonon contribution to the dielectric constant is observed in the impedance spectra for BTO colloidal solutions.

**T1.00083 High-Mobility Sm-Doped Bi<sub>2</sub>Se<sub>3</sub> Ferromagnetic Topological Insulators and Robust Exchange Coupling**, FENGQI SONG, TAISHI CHEN, XUEFENG WANG, Nanjing Univ — Here we prepare a new type of diluted magnetic semiconductor (Sm<sub>x</sub>Bi<sub>1-x</sub>)<sub>2</sub>Se<sub>3</sub>Te<sub>y</sub>. It reaches an anisotropic ferromagnetic phase at x=0.05, which exhibits a Curie temperature of around 50K and a typical coercive field of 0.05T. Its magnetic strength and carrier density can be tuned by controlling the dopant ratio of Sm and Te separately. Robust ferromagnetism is demonstrated by the fact that electronic control makes no significant influence on the Curie temperature. The density functional theory calculation supports the ferromagnetism origin from the Sm atoms. The carrier density is ~10<sup>18</sup>/cm<sup>3</sup> and the mobility is over 18000cm<sup>2</sup>/V s with the pronounced Shubnikov de Haas oscillations. This suggests it is a high-mobility candidate of magnetic topological insulators. (*Advan. Mater.* 201501254(2015))

**T1.00084 Gate-modulated magnetotransport and anomalous quantum oscillations in Dirac semimetal Cd<sub>3</sub>As<sub>2</sub> nanowires**, LIXIAN WANG, CAIZHEN LI, DAPENG YU, ZHIMIN LIAO, State Key Laboratory for Mesoscopic Physics, Department of Physics, Peking University — Magnetotransport studies of three-dimensional (3D) relativistic electrons in Dirac semimetals is critical for identifying exotic topological phenomena and quantum transport. Using gate-modulation method, we conducted systematic transport measurements over our fabricated Cd<sub>3</sub>As<sub>2</sub> nanowire based devices under a variable magnetic field. We observe an obvious ambipolar-field-effect as tuning the gate-voltage bias without applied field and distinctive MR behaviors at different gate-voltage bias with applied field. Remarkably, anomalous quantum oscillations occur at high fields, which may be in close relationship to the sought-after Fermi-arc surface state in Dirac semimetals. The presence of anomalous oscillations may suggest that Cd<sub>3</sub>As<sub>2</sub> nanomaterials with a gate-tunable Fermi-surface may be a promising candidate as an excellent platform to explore the elusive surface state in topological semimetals.

**T1.00085 Identification of topological surface states in (Bi<sub>1-x</sub>Sb<sub>x</sub>)<sub>2</sub>Te<sub>3</sub> alloy films**, J.C. WALRATH, V.A. STOICA, A.S. CHANG, YEN-HSIANG LIN, WEI LIU, L. ENDICOTT, R. CLARKE, C. UHER, R.S. GOLDMAN, Univ of Michigan - Ann Arbor — Topological insulators (TIs) have emerged as an exciting class of quantum materials, with an insulating bulk and spin-momentum-locked topologically-protected surface states, making them desirable for spintronics and other applications. Recently, tunable surface to bulk conduction has been demonstrated in ternary TI alloys (Bi<sub>1-x</sub>Sb<sub>x</sub>)<sub>2</sub>Te<sub>3</sub>, providing an ideal candidate for TI spintronic devices. Although room-temperature topological surface transport is desirable for device applications, direct detection of topological surface states at room temperature has yet to be demonstrated in (Bi<sub>1-x</sub>Sb<sub>x</sub>)<sub>2</sub>Te<sub>3</sub> systems. Here, we use scanning tunneling microscopy and spectroscopy (STM/STS) to characterize the band structure of (Bi<sub>1-x</sub>Sb<sub>x</sub>)<sub>2</sub>Te<sub>3</sub> alloy films and directly detect the presence of topological surface states at room temperature. We will discuss the thickness and composition dependence of the band structure, including the Fermi level energy, Dirac point, and carrier type, comparing STM/STS and macroscopic transport data.

**T1.00086 Microstructural and magneto-transport characterization of Bi<sub>2</sub>Se<sub>x</sub>Te<sub>3-x</sub> topological insulator thin films grown by pulsed laser deposition method<sup>1</sup>**, ZHENGHE JIN, RAJ KUMAR, FRANK HUNTE, JAY NARAYAN, KI WOOK KIM, North Carolina State Univ, NORTH CAROLINA STATE UNIVERSITY TEAM — Bi<sub>2</sub>Se<sub>x</sub>Te<sub>3-x</sub> topological insulator thin films were grown on Al<sub>2</sub>O<sub>3</sub> (0001) substrate by pulsed laser deposition (PLD). XRD and other structural characterization measurements confirm the growth of the textured Bi<sub>2</sub>Se<sub>x</sub>Te<sub>3-x</sub> thin films on Al<sub>2</sub>O<sub>3</sub> substrate. The magneto-transport properties of thick and thin films were investigated to study the effect of thickness on the topological insulator properties of the Bi<sub>2</sub>Se<sub>x</sub>Te<sub>3-x</sub> films. A pronounced semiconducting behavior with a highly insulating ground state was observed in the resistivity vs. temperature data. The presence of the weak anti-localization (WAL) effect with a sharp cusp in the magnetoresistance measurements confirms the 2-D surface transport originating from the TSS in Bi<sub>2</sub>Se<sub>x</sub>Te<sub>3-x</sub> TI films. A high fraction of surface transport is observed in the Bi<sub>2</sub>Se<sub>x</sub>Te<sub>3-x</sub> TI thin films which decreases in Bi<sub>2</sub>Se<sub>x</sub>Te<sub>3-x</sub> TI thick films. The Cosine ( $\theta$ ) dependence of the WAL effect supports the observation of a high proportion of 2-D surface state contribution to overall transport properties of the Bi<sub>2</sub>Se<sub>x</sub>Te<sub>3-x</sub> TI thin films. Our results show promise that high quality Bi<sub>2</sub>Se<sub>x</sub>Te<sub>3-x</sub> TI thin films with significant surface transport can be grown by PLD method to exploit the exotic properties of the surface transport in future generation spintronic devices.

<sup>1</sup>This work was supported, in part, by National Science Foundation ECCS-1306400 and FAME

**T1.00087 Discovery of the first Weyl fermion semimetal and topological Fermi arcs in TaAs<sup>1</sup>**, SUYANG XU, ILYA BELOPOLSKI, NASSER ALIDOUST, MADHAB NEUPANE, GUANG BIAN, Princeton University, CHENGLONG ZHANG, Peking University, RAMAN SANKAR, National Taiwan University, GUOQING CHANG, National University of Singapore, ZHUJUN YUAN, Peking University, CHENGCHENG LEE, SHIN-MING HUANG, National University of Singapore, HAO ZHENG, JIE MA, DANIEL SANCHEZ, Princeton University, BAKKAI WANG, ARUN BANSIL, Northeastern University, FANGCHENG CHOU, National Taiwan University, PAVEL SHIBAYEV, Princeton University, HSIN LIN, National University of Singapore, SHUANG JIA, Peking University, M. ZAHID HASAN, Princeton University — Weyl semimetals have opened a new era in condensed matter physics and materials science. They host Weyl fermions as emergent quasiparticles and admit a topological classification that protects Fermi arc surface states on the boundary. This unusual electronic structure has deep analogies with particle physics and leads to unique topological properties. We report the experimental discovery of the first Weyl semimetal, TaAs. We directly observe the Weyl fermions and the Fermi arcs in a TaAs single crystal and demonstrate its topological character. Our work opens the field for studying of Weyl fermions in table-top experiments.

<sup>1</sup>The work at Princeton and Princeton-led ARPES measurements were supported by the Gordon and Betty Moore Foundations EPIQS Initiative through grant GBMF4547 (Hasan) and by U.S. Department of Energy DE-FG-02-05ER46200.

**T1.00088 Condensation bottleneck as the driver of pseudogap physics in cuprates<sup>1</sup>**, R.S. MARKIEWICZ, I.G. BUDA, P. MISTARK, A. BANSIL, Northeastern Univ — We extend our previous GW calculations on cuprates [T. Das, R.S. Markiewicz, and A. Bansil, *Advances in Physics* 63, 151-266 (2014)] to include vertex corrections via self-consistent renormalization. We find that the antiferromagnetic transition is bottlenecked, as a continuous manifold of competing q-vectors attempts to soften at the same time. The resulting extended range of short-range order strongly resembles pseudogap physics. We discuss the strikingly different phenomena found for different cuprates, and try to determine their origins.

<sup>1</sup>Work supported by the U.S. Department of Energy.

**T1.00089 Magnetism in Olivine-type LiCo<sub>1-x</sub>Fe<sub>x</sub>PO<sub>4</sub> Cathode Materials: Bridging Theory and Experiment**, VIJAY SINGH, YELENA GERSHINSKY, MONICA KOSA, MUDIT DIXIT, DAVID ZITOUN, DAN THOMAS MAJOR, Department of Chemistry, Bar-Ilan University, Ramat-Gan, Israel, DR. DAVID ZITOUN COLLABORATION — We present a non-aqueous sol-gel synthesis of olivine type LiCo<sub>1-x</sub>Fe<sub>x</sub>PO<sub>4</sub> compounds (x = 0.00, 0.25, 0.50, 0.75, 1.00). The magnetic properties of the olivines are measured experimentally and calculated using first-principles theory. Specifically, the electronic and magnetic properties are studied in detail with standard density functional theory (DFT), as well as by including spin-orbit coupling (SOC), which couples the spin to the crystal structure. We find that the Co<sup>2+</sup> ions exhibit strong orbital moment in the pure LiCoPO<sub>4</sub> system, which is partially quenched upon substitution of Co<sup>2+</sup> by Fe<sup>2+</sup>. Interestingly, we also observe a non-negligible orbital moment on the Fe<sup>2+</sup> ion. We underscore that the inclusion of SOC in the calculations is essential to obtain qualitative agreement with the observed effective magnetic moments. Additionally, Wannier functions were used to understand the experimentally observed rising trend in the Néel temperature, which is directly related to the magnetic exchange interaction paths in the materials. We suggest that out of layer M – O – P – O – M magnetic interactions (J<sub>⊥</sub>) are present in the studied materials.

**T1.00090 Electronic and magnetic properties of double-perovskite  $(\text{La}_{1-x}\text{Sr}_x)_2\text{CuIrO}_6$  compounds**, S. X. ZHANG, W. K. ZHU, Indiana University, Bloomington, W. TONG, High Magnetic Field Laboratory, Chinese Academy of Sciences, PO-HAN LEE, National Taiwan Normal University, JEN-CHUAN TUNG, China Medical University, YIN-KOU WANG, National Taiwan Normal University, L. LING, High Magnetic Field Laboratory, Chinese Academy of Sciences, M. STARR, J. M. WANG, Indiana University, Bloomington, H. D. ZHOU, University of Tennessee, CHI-KEN LU, National Taiwan Normal University — Double perovskite oxides that combine 3d and 5d transition metal elements offer a model system to study novel electronic and magnetic states arising from the interplay of strong electron correlations and spin-orbit couplings (SOCs). In this work, we studied the electronic and magnetic properties of a double perovskite iridate  $\text{La}_2\text{CuIrO}_6$  and its hole-doped compounds  $(\text{La}_{1-x}\text{Sr}_x)_2\text{CuIrO}_6$ . Magnetic susceptibility measurements suggest that the Ir sublattice and the Cu sublattice both form antiferromagnetic order but at two different temperatures. Two-dimensional magnetism that was reported in many other Cu-based double-perovskites is not observed in our samples, indicating the existence of Cu-Ir interaction despite a weak orbital mixing. Sr-doping is shown to decrease the magnetic ordering temperatures and enhance the electrical conductivity. Density functional theory (GGA+SOC+U) calculations suggest that an isolated band is generated above the Fermi level as a result of strong SOC and U. The exchange coupling constants between transition metal ions are estimated by calculating the total energies for various magnetic ground states with expanded unit cells.

**T1.00091 Van der Waals Epitaxy of Ultrathin Halide Perovskites**, YIPING WANG, YUNFENG SHI, JIAN SHI, Department of Material Science and Engineering, Rensselaer Polytechnic Institute — We present our understanding, with  $\text{CH}_3\text{NH}_3\text{PbX}_3$  as a model system, on the 2D van der Waals growth and kinetics of 3D parent materials. We show the successful synthesis of ultrathin (sub-10 nm), large scale (a few tens of  $\mu\text{m}$ ) single crystalline 2D perovskite thin films on layered mica substrate by van der Waals (VDW) epitaxy. Classical nucleation and growth model explaining conventional epitaxy has been modified to interpret the unique 2D results under VDW mechanism. The generalization of our model shows that a 3D crystal with low cohesive energy tends to favor the 2D growth while the one with strong cohesive energy has less kinetic window. With Monte Carlo simulations, we show that the fractal 2D morphology in perovskite precisely manifests the kinetic competition between VDW diffusivity and thermodynamic driving force, a unique phenomenon to VDW growth, suggesting a fundamental limit on the morphology stability of the 2D form of a 3D material. On the other hand, our single crystal thin film growth results and subsequent cryogenic study in the iodide perovskite provide a perfect resource for the exploration of its complex optical and electronic properties and unveiling the origins of its popularity in the energy conversion field.

**T1.00092 Exciton spin dynamics in  $\text{MAPbI}_3$  measured by Hanle effect<sup>1</sup>**, WILLIAM TALMADGE, University of Utah Department of Physics and Astronomy, RUIZHI WANG, University of Utah Department of Physics and Astronomy, Nanjing University of Science and Technology, PATRICK ODENTHAL, NATHAN GUNDLACH, CHUANG ZHANG, DALI SUN, ZEEV VALY VARDENY, YAN (SARAH) LI, University of Utah Department of Physics and Astronomy — The organic-inorganic hybrid perovskites have emerged as a highly promising class of semiconductors for photovoltaic applications. The properties responsible for the high photoconversion efficiency are under extensive investigation. There have; however, been fewer investigations of spin-dependent effects in this class of materials. We present energy dependent photoinduced Faraday rotation in polycrystalline thin film  $\text{CH}_3\text{NH}_3\text{PbI}_3$ , which benefit from the band structure and optical selection rules. The Faraday rotation spectrum follows the exciton absorption band at low temperatures, indicating its excitonic origin. Through the Hanle effect, based on Faraday rotation, we found the coexistence of two spin components at 4 K, which was confirmed through time resolved measurements. Research supported by the NSF-MRSEC (DMR 1121252) at the University of Utah.

<sup>1</sup>Research supported by the NSF-MRSEC (DMR 1121252) at the University of Utah.

**T1.00093 Majorana transport in superconducting nanowire with Rashba and Dresselhaus spin-orbit couplings**, JIABIN YOU, The University of Hong Kong, XIAO-QIANG SHAO, Northeast Normal University, QING-JUN TONG, The University of Hong Kong, A H CHAN, C H OH, National University of Singapore, VLATKO VEDRAL, University of Oxford — The tunneling experiment is a key technique for detecting Majorana fermion (MF) in solid state systems. We use Keldysh non-equilibrium Green function method to study two-lead tunneling in superconducting nanowire with Rashba and Dresselhaus spin-orbit couplings. A zero-bias dc conductance peak appears in our setup which signifies the existence of MF and is in accordance with previous experimental results on  $\text{InSb}$  nanowire. Interestingly, due to the exotic property of MF, there exists a hole transmission channel which makes the currents asymmetric at the left and right leads. The ac current response mediated by MF is also studied here. To discuss the impacts of Coulomb interaction and disorder on the transport property of Majorana nanowire, we use the renormalization group method to study the phase diagram of the wire. It is found that there is a topological phase transition under the interplay of superconductivity and disorder. We find that the Majorana transport is preserved in the superconducting-dominated topological phase and destroyed in the disorder-dominated non-topological insulator phase.

**T1.00094 Chiral Topological Superconductor and Half-Integer Conductance Plateau from Quantum Anomalous Hall Plateau Transition**, QUAN ZHOU, JING WANG, BIAO LIAN, SHOUCENG ZHANG, Stanford Univ, ZHANG'S GROUP TEAM — We propose to realize a two-dimensional chiral topological superconducting (tsc) state from the quantum anomalous hall plateau transition in a magnetic topological insulator thin film through the proximity effect to a conventional s-wave superconductor. The optimal condition for realizing such chiral tsc is to have inequivalent superconducting pairing amplitudes on top and bottom surfaces of the doped magnetic topological insulator. We further propose several transport experiments to detect the chiral tsc. The conductance will be quantized into a half-integer plateau at the coercive field in this hybrid system. In particular, with the point contact formed by a superconducting junction, the conductance oscillates between  $e^2/h$  and  $e/h$  with the frequency determined by the voltage across the junction.

**T1.00095 Creation of Dirac cones in two-dimensional  $\text{HgTe}$  honeycomb lattices produced by gate voltage**, HUA-HUA FU, SHU-TING PING, HUI WANG, RUQIAN WU, University of California, Irvine —  $\text{HgTe}$  is the first 2D topological insulator that was confirmed experimentally. In this material, it is well known that  $\text{HgTe}$  quantum well manifests as a topological insulator only when the parameter  $M$ , which is determined by the energy difference between  $E_1$  and  $H_1$  bands, is negative ( $M < 0$ ). In this study, we demonstrate that the topological feature can still be obtained in the  $\text{HgTe}$  quantum well with  $M > 0$ , if we construct a honeycomb mask on 2D  $\text{HgTe}$  and apply gate voltages. The newly developed topological state has very large and controllable band gaps and can be used for the realization of various topological properties such as fraction Chern insulator and a fractional quantum spin Hall effect. It should be stressed that the newly developed Dirac cones is not ascribed to the band inversion but is driven by the honeycomb mask. Obviously, this idea can be extended to other materials and devices.

**T1.00096 SdH oscillations and pressure effect of the Weyl semimetal NbAs**, YONGKANG LUO, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, N. J. GHIMIRE, Argonne National Laboratory, Argonne, Illinois 60439, USA, M. WARTENBE, HONGCHUL CHOI, M. NEUPANE, R. D. MCDONALD, E. D. BAUER, JIANXIN ZHU, J. D. THOMPSON, F. RONNING, Los Alamos National Laboratory, Los Alamos, NM 87545, USA — Via angular Shubnikov-de Hass (SdH) quantum oscillations measurements, we determine the Fermi surface topology of NbAs. The SdH oscillations consist of two frequencies: 20.8 T ( $\alpha$ -pocket) and 15.6 T ( $\beta$ -pocket). The analysis shows that the  $\beta$ -pocket has a Berry phase of  $\pi$  and a small effective mass 0.033  $m_0$ , indicative of a nontrivial topology; whereas the  $\alpha$ -pocket has a trivial Berry phase of 0 and a heavier effective mass 0.066  $m_0$ . Subtle changes can be seen in the  $\rho_{xx}(T)$  profiles with pressure up to 2.31 GPa. The Fermi surfaces undergo an anisotropic evolution under pressure, while the topological features of the two pockets remain unchanged. Specific heat measurements reveal a small Sommerfeld coefficient  $\gamma_0 = 0.09(1)$  mJ/(mol $\cdot$ K<sup>2</sup>) and a large Debye temperature,  $\Theta_D = 450(9)$  K, confirming a “hard” crystalline lattice. The Kadowaki-Woods ratio and a suppressed transport scattering rate are also studied. **References:** [1] N. J. Ghimire *et al.*, JPCM **27**, 152201 (2015) [2] Y. Luo *et al.*, arXiv: 1506.01751 (2015) [3] Y. Luo *et al.*, arXiv: 1510.08538 (2015)

**T1.00097 Weak Antilocalization Effect in Metallic  $\text{Bi}_2\text{Te}_3$  Topological Insulator**, K. SHRESTHA, TcSUH and Department of Physics, University of Houston, 3201 Cullen Blvd., Houston, Texas 77204, USA, M. CHOU, Department of Materials and Optoelectronic Science, National Sun Yat-Sen University, Taiwan, D. GRAF, National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32310, USA, H. D. YANG, Department of Physics, National Sun Yat-Sen University, Taiwan, B. LORENZ, PAUL C. W. CHU<sup>1</sup>, TcSUH and Department of Physics, University of Houston, 3201 Cullen Blvd., Houston, Texas 77204, USA — We have observed weak antilocalization effect in the metallic  $\text{Bi}_2\text{Te}_3$  single crystals having different bulk carrier densities. The angle dependence of weak antilocalization with respect to the direction of the magnetic field showed the surface states dominating in the samples having lower carrier concentration. The surface states dominance in weak antilocalization does not depend on the nature of the bulk charge carriers (p or n-type). Using the Hikami-Larkin-Nagaoka (HLN) formula, we have found the number of conduction channels is smaller in the samples having lower carrier concentration.

<sup>1</sup>Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA 94720, USA

**T1.00098 Ultrafast terahertz spectroscopy study of Kondo insulating thin film  $\text{SmB}_6$ : evidence for an emergent surface state**<sup>1</sup>, JINGDI ZHANG, Univ of California - San Diego, JIE YONG, ICHIRO TAKEUCHI, RICHARD GREENE, University of Maryland, College Park, RICHARD AVERITT, Univ of California - San Diego — We utilize terahertz time domain spectroscopy to investigate thin films of the heavy fermion compound  $\text{SmB}_6$ , a prototype Kondo insulator. Temperature dependent terahertz (THz) conductivity measurements reveal a rapid decrease in the Drude weight and carrier scattering rate at  $T^* = 20$  K, well below the hybridization gap onset temperature (100 K). Moreover, a low-temperature conductivity plateau (below 20K) indicates the emergence of a surface state with an effective electron mass of  $0.1m_e$ . Conductivity dynamics following optical excitation are also measured and interpreted using Rothwarf-Taylor (R-T) phenomenology, yielding a hybridization gap energy of 17 meV. However, R-T modeling of the conductivity dynamics reveals a deviation from the expected thermally excited quasiparticle density at temperatures below 20K, indicative of another channel opening up in the low energy electrodynamics. Taken together, these results suggest the onset of a surface state well below the crossover temperature (100K) after long-range coherence of the f-electron Kondo lattice is established.

<sup>1</sup>JZ and RDA acknowledge support from DOE - Basic Energy Sciences under Grant No. DE-FG02-09ER46643, under which the THz measurements and data analysis were performed. JY, IT and RLG acknowledge support from ONR N00014-13-1-0635 and NSF DMR 1410665.

**T1.00099 Topological insulator with negative spin-orbit coupling**, XIAN-LEI SHENG, Univ of Delaware, ZHIJUN WANG, RUI YU, HONGMING WENG, ZHONG FANG, XI DAI, Institute of Physics, Chinese Academy of Sciences, KEY LABORATORY OF CONDENSED MATTER THEORY AND COMPUTATION TEAM — Based on the first-principles calculations, we reveal that  $\text{TlN}$ , a simple binary compound with Wurtzite structure, is a three-dimensional (3D) topological insulator (TI) with effectively negative spin-orbit coupling  $\lambda_{eff} < 0$ , which makes it distinguished from other TIs by showing opposite spin-momentum locking effect in its surface states. The sign of  $\lambda_{eff}$  depends on the hybridization between N-2p and Tl-5d states, and can be tuned from negative to positive by lattice strain or chemical substitution, which drive the system into a Dirac semimetal with 3D Dirac cones in its bulk states. Such topological phase transition can be realized by electronic mechanism without breaking any crystal symmetry.

## T1.00100 COMPLEX STRUCTURED MATERIALS, INCLUDING GRAPHENE —

**T1.00101 Bosonic Dirac materials in two dimensions**, SAIKAT BANERJEE, Nordic Institute for Theoretical Physics, Sweden, JONAS FRANSSON, ANNICA BLACK-SCHAFER, Uppsala University, Sweden, HANS GREN, Royal Institute of Technology, Sweden, ALEXANDER BALATSKY, Nordic Institute for Theoretical Physics, Sweden — We examine the low energy effective theory of phase oscillations in a two-dimensional granular superconducting sheet where the grains are arranged in honeycomb lattice structure. Two different types of collective phase oscillations are obtained, which are analogous to the massive Leggett and massless Bogoliubov-Anderson-Gorkov modes in a two-band superconductor. It is shown that the spectra of these collective bosonic modes cross each other at the  $K$  and  $K'$  points in the Brillouin zone and form a Dirac node. Dirac node dispersion of bosonic excitations is representative of Bosonic Dirac Materials (BDM). We show that the Dirac node is preserved in presence of an inter-grain interaction, despite induced changes of the qualitative features of the two collective modes. Finally, breaking the sublattice symmetry by choosing different on-site potentials for the two sublattices leads to a gap opening near the Dirac node, in analogy with Fermionic Dirac materials.

**T1.00102 Black Arsenic-Phosphorus: Layered Anisotropic Infrared Semiconductors with Highly Tunable Compositions and Properties**, BILU LIU, CHONGWU ZHOU, University of Southern California — 2D layered materials with diverse properties have attracted significant interest in the past decade. The layered materials discovered so far have covered a wide, yet discontinuous electromagnetic spectral range from semimetallic graphene, insulating boron nitride, to semiconductors with bandgaps from middle infrared to visible light. Here, we introduce new layered semiconductors, black arsenic-phosphorus (b-AsP), with highly tunable chemical compositions and electronic and optical properties. Transport and infrared absorption studies demonstrate the semiconducting nature of b-AsP with tunable bandgaps, ranging from 0.3 to 0.15 eV. These bandgaps fall into long-wavelength infrared (LWIR) regime and cannot be readily reached by other layered materials. Moreover, polarization-resolved infrared absorption and Raman studies reveal in-plane anisotropic properties of b-AsP. This family of layered b-AsP materials extend the electromagnetic spectra covered by 2D layered materials to the LWIR regime, and may find unique applications for future all 2D layered material based devices. Ref. Liu, B., et al., Black Arsenic-Phosphorus: Layered Anisotropic Infrared Semiconductors with Highly Tunable Compositions and Properties. Adv. Mater., 2015, 27, 4423-4429.

**T1.00103 High free carrier density in aluminum adsorbed graphene**, YU-TSUNG LIN, MING-FA LIN, Department of Physics, National Cheng Kung University — Electronic properties of graphene are enriched by aluminum adsorption on surface. The Al adsorbate could be used in n-type transfer doping in graphene. From the first-principle density functional calculations, performed by Vienna ab initio simulation package, there are lots of free conduction electrons in the distorted Dirac-cone structure. Charges transferred from Al to C atoms are about 1.24 e, almost irrespective of the concentration and distribution of the adatoms. A high carrier density is estimated to be  $\sim 6 \times 10^{-14} / \text{cm}^2$  for a ratio of Al/C = 12.5%. Such carriers mainly originate from the hybridization of Al 3s and C 2p<sub>z</sub> orbitals, as clearly indicated from the orbital-projected density states, charge distributions and atom-dominated energy bands. Aluminum adsorbed graphene is predicted to have the highest free carriers density except for Al/C  $\geq 25\%$  compared with the other adatom-adsorbed systems.

**T1.00104 Zigzag phosphorene nanoribbons: one dimensional resonant tunnelling in two dimensional atomic crystals**, CARLOS PAEZ, ANA PEREIRA, University of Campinas, DARIO BAHAMON, Mackenzie Presbyterian University, PETER SCHULZ, University of Campinas — We theoretically investigate phosphorene zigzag nanoribbons as a platform for constriction engineering. In the presence of a constriction at one of the edges, quantum confinement of edge protected states reveals breit-wigner-like resonant tunneling, if the edge is uncoupled to the other. If the constriction is narrow enough to promote coupling between edges, it gives rise to fano-like as well as anti-resonances in the transmission spectrum. These effects are shown to mimic an atomic chain like behavior in a two dimensional atomic crystal.

**T1.00105 Room-Temperature, Low-Barrier Boron Doping of Graphene**, SHIXUAN DU, Institute of Physics, Chinese Academy of Sciences — Doping graphene with boron has been difficult because of high reaction barriers. Here, we describe a low-energy reaction route derived from first-principles calculations and validated by experiments. We find that a boron atom on graphene on a ruthenium(0001) substrate can replace a carbon by pushing it through, with substrate attraction helping to reduce the barrier to only 0.1 eV, implying that the doping can take place at room temperature. High-quality graphene is grown on a Ru(0001) surface and exposed to B<sub>2</sub>H<sub>6</sub>. Scanning tunneling microscopy/spectroscopy and X-ray photoelectron spectroscopy confirmed that boron is indeed incorporated substitutionally without disturbing the graphene lattice. (L.D. Pan et al., Nano Lett. 2015, 15, 6464. In collaboration with Lida Pan, Yande Que, Hui Chen, Dongfei Wang, Jun Li, Chengmin Shen, Wende Xiao, Hongjun Gao in CAS, and S. Pantellides in Vanderbilt University.)

**T1.00106 Peculiarities of sliding friction in graphene, graphene fluoride, graphite: Comparison of experiment with atomistic simulations**, LIUDMYLA BARABANOVA, JEFFREY MCCAUSLAND, ALPER BULDUM, SERGEI LYUKSYUTOV, University of Akron — Friction is the major source of energy dissipation at the nanoscale. We use atomic force microscopy (AFM) to study slide friction based on analysis of trace-minus-retrace (TMR) signals. To obtain the signals a directional dependence of the sliding friction using a rotational technique was used at the edges and interiors of the samples graphene (G), graphene fluoride (GF), and graphite. The friction coefficient experimental results were based on a methodology assuming orthotropic friction and found to be in the range of  $10^{-3}$  to  $10^{-1}$  over all samples. Supplementing experimental measurements, we also performed atomistic modeling and simulations to investigate tribological properties of G including the edges. Molecular dynamics simulations and geometry optimization calculations were carried and compared with experimental measurements. It is suggested that the atoms at the apex of the asperities and at the graphene edges have important effect on friction.

**T1.00107 Recognition of DNA sequencing through binding of nucleobases to graphene**, VALENTINA ZAFFINO, Univ of Central Florida — Graphene is one of the most promising materials in nanotechnology. Its large surface to volume ratio, high conductivity and electron mobility at room temperature are outstanding properties for use in DNA sensors. For this study, we used Density Functional Theory (DFT), with and without the inclusion of van der Waals (vdW) interactions, to investigate the adsorption of nucleobases (cytosine, guanine, adenine, thymine, and uracil) on pristine graphene and graphene with defects (Divacancy and Stone-Wales). We investigated the performance of two types of vdW-DF functional (optB86b-vdW and rPW86-vdW), as well as the PBE functional, and their description of the adsorption geometry and electronic structure of the nucleobase-graphene systems. The inclusion of defects results in an increase in binding energy, closer adsorption of the molecule to graphene and greater buckling in both the graphene structure and nucleobase.

**T1.00108 Orientationally Misaligned Zipping of Lateral Graphene and Boron Nitride Nanoribbons with Minimized Strain Energy and Enhanced Half-Metallicity<sup>1</sup>**, JIANG ZENG, Univ of Sci & Tech of China, WEI CHEN, Harvard University, PING CUI, Univ of Sci & Tech of China, DONG-BO ZHANG, Beijing Computational Science Research Center, ZHENYU ZHANG, Univ of Sci & Tech of China — Lateral heterostructures of two-dimensional materials may exhibit various intriguing emergent properties. Yet when specified to the orientationally aligned heterojunctions of zigzag graphene and hexagonal boron nitride (hBN) nanoribbons, realizations of the high expectations on their properties encounter two standing hurdles. First, the rapid accumulation of strain energy prevents largescale fabrication. Secondly, the pronounced half-metallicity predicted for freestanding graphene nanoribbons is severely suppressed. By properly tailoring orientational misalignment between zigzag graphene and chiral hBN nanoribbons, here we present a facile approach to overcome both obstacles. Our first-principles calculations show that the strain energy accumulation in such heterojunctions is significantly diminished for a range of misalignments. More strikingly, the half-metallicity is substantially enhanced from the orientationally aligned case, back to be comparable in magnitude with the freestanding case. The restored half-metallicity is largely attributed to the recovered superexchange interaction between the opposite heterojunction interfaces. The present findings may have important implications in eventual realization of graphene-based spintronics.

<sup>1</sup>This work was supported by the National Natural Science Foundation of China and the National Key Basic Research Program of China.

**T1.00109 Oscillatory behavior of the surface reduction process of multilayer graphene oxide at room temperature<sup>1</sup>**, DMITRY VOYLOV, Univ of Tennessee, Knoxville, ILIA IVANOV, Oak Ridge National Laboratory, VALERII BYKOV, Emanuel Institute of Biochemical Physics RAS, SVETLANA TSYBENOVA, Moscow City Teacher Training University, IGOR MERKULOV, Oak Ridge National Laboratory, SERGEI KUROCHKIN, Institute of Problems of Chemical Physics RAS, ADAM HOLT, Univ of Tennessee, Knoxville, ALEXANDR KISLIUK, Oak Ridge National Laboratory — The graphene oxide (GO) is one of 2D materials which continues to be studied intensively since it is thought can be used as a precursor of graphene. Recently, it was found that the chemical composition of multilayer GO is metastable on the time scale of one month even at room temperature. The observed changes in chemical composition were attributed to a reduction process controlled by the in-plane diffusion of functional groups which progresses through radical reactions. Here we report the observation of oscillatory oxidation-reduction (redox) reactions on the surface of multilayer GO films at room temperature. The redox reactions exhibited damped oscillatory behavior with a period of about 5 days and found to be dependent on the time elapsed from GO deposition. The kinetic behavior of the processes and observed metastability of the surface functional groups are adequately described by two models involving reactions between functional groups of GO and reactant diffusion.

<sup>1</sup>US team acknowledges partial financial support from the Division of Materials Science and Engineering, U.S. Department of Energy, Office of Basic Energy Sciences.

**T1.00110 Atomistic Simulation Studies on the Friction of 2D materials**, MINWOONG JOE, CHANGGU LEE, Department of Mechanical Engineering and Center for Human Interface Nano Technology (HINT), Sungkyunkwan University — Frictional properties of two-dimensional (2D) layered materials including graphene, MoS<sub>2</sub>, NbSe<sub>2</sub>, and h-BN, have been revealed using atomic force microscopy (AFM) [1]. All the materials exhibit similar trends on friction: the thicker the sheet the lower the friction is. Puckering effect has been suggested as the primary mechanical reason for this thickness-dependent behaviors. Despite this novel findings, detailed atomic-scale processes during tip sliding against such atomically thin sheets are not fully understood yet. In this work, we provide a detailed study of the role of the buried interface between tip and surface on atomic friction using molecular dynamics (MD) simulation. We investigate the magnitude of puckering under various tip and surface conditions such as tip size and surface orientation, to unravel its effect on friction. Our systematic approach could provide a comprehensive understanding of friction phenomena at atomic level.

[1] C. Lee et al. *Science* **328** (2010) 76

**T1.00111 Transferring graphene onto hydrated "soft" substrates using a modified H<sub>2</sub> bubbling method<sup>1</sup>**, W. PIERRE, M. BLADES, P. VENDOLA, S. JEDLICKA, S.V. ROTKIN, Lehigh University — Graphene has many applications, most of which require its deposition onto a specific substrate. Several methods exist for transferring large areas of graphene. However, there is a lack of existing techniques for proper transfer onto soft hydrated substrates. We demonstrate a method for transferring a large wrinkle-free area of graphene onto soft substrates using a modified bubbling technique. Widefield microscopy was used to characterize the results.

<sup>1</sup>NSF ECCS-1509786

**T1.00112 Effect of the sample mounting geometry on the grain size of single-crystalline transition-metal dichalcogenide monolayers grown by chemical vapor deposition**, ZHENG YANG, BO HSU, University of Illinois at Chicago, DEPARTMENT OF ELECTRICAL AND COMPUTER ENGINEERING TEAM — In this presentation, it is reported that the local pressure near the surface of the substrate plays a significant role affecting the single crystal grain size of two-dimensional (2D) transition-metal dichalcogenide  $\text{MX}_2$  ( $\text{M}=\text{Mo}, \text{W}$ ;  $\text{X}=\text{S}, \text{Se}$ ) monolayers in addition to other regular growth parameters such as growth chamber pressure, temperature, and gas flow rates etc during the chemical vapor deposition growth. Different sample mounting geometries (such as substrate facing up, facing down, sandwiching) and vapor trapping techniques (such as vapor trapping tube) to introduce qualitatively various local pressure have been employed in the growth to systematically study this effect. The grain size, optical, and electrical properties of 2D  $\text{MX}_2$  monolayer samples grown at different local pressures are compared. It is observed that the enhanced local pressure facilitates larger single crystal grain size and higher quality of the 2D  $\text{MX}_2$  monolayers. The size of the single-crystalline  $\text{MX}_2$  monolayers achieved by this method were comparable to the literature reported largest size.

**T1.00113 Mechanisms of Bowtie- and Star-Shaped  $\text{MX}_2$  Nanoisland Formation**, VASILII I. ARTYUKHOV, ZHILI HU, ZHUHUA ZHANG, BORIS I. YAKOBSON, Rice University — A large number of experimental studies over the last few years observed the formation of unusual highly symmetric polycrystalline twinned nanoislands of transition metal dichalcogenides, resembling bowties or stars. Here we analyze their morphology in terms of equilibrium and growth shapes. We propose a mechanism for their formation via collision of concurrently growing islands and validate the theory with phase-field simulations. Finally, we use first-principles calculations to propose an explanation of the predominance of high-symmetry polycrystals with 60-degree lattice misorientation angles.

**T1.00114 Metal Contact Formation and Substrate Ferroelectric Poling: Effective Means of Determining  $\text{MoS}_2$  Transport Properties**, LUDWIG BARTELS, JOSEPH MARTINEZ, ARIANA NGUYEN, MICHAEL GOMEZ, EDWIN PRECIADO, VELVETH KLEE, MICHAEL VALENTIN, I-HSI LU, DAVID BARROSO, University of California Riverside, THOMAS SCOTT, PETER DOWBEN, University of Nebraska- Lincoln — Monolayer transition metal dichalcogenides (TMDs) are of rising interest due to their direct band gap at the single-layer limit and pronounced spin splitting in the valence band. Metal contact formation to such materials is a persistent issue yet it holds tremendous opportunity for improving TMD transport properties: simply through their composition, metal contacts can increase the very low carrier numbers in single-layer films leading to significant shifts of the Fermi energy. X-ray photoelectron spectroscopy (XPS) measurements of the charge transfer during metal contact formation reveal the TMD valence band edge to approach the Fermi level underneath the contact, so that TMD devices resemble *pnp*-junctions. We employ a combination of scanning photocurrent microscopy (SPCM) and surface acoustic spectroscopy on ferroelectric substrates to ascertain our findings. SPCM measurements allow us to probe the impact of electrical contacts on the photoconductivity of the materials. In contrast, surface acoustic spectroscopy allows access to the transport properties of the material even in the absence of contacts. The combination of these technique sheds new light on the band alignment in TMD materials between contacts and on ways to manipulate it.

**T1.00115 Substrate induced phase transformation of monolayer transition metal dichalcogenides**, SHUDUN LIU, University of Louisville, XIAOJUN FU, ZHENYU ZHANG, WENGUANG ZHU, University of Science and Technology of China — Using density functional theory calculations, we investigate the effects of a metal substrate on the structural and electronic properties of a monolayer of transition metal dichalcogenide (TMD). We find that a suitable choice of substrate can induce a transformation of the phase of the monolayer from 2H to 1T. We will discuss the impact of the results on some earlier studies of TMD/metal contacts as well as potential applications of our system in catalysis.

**T1.00116 HYDROGENATED GRAPHENE- METAL OXIDE NANOHYBRIDS: AN INVENTIVENESS PLINTH FOR SENSING DEVICES**, P BARANEEDHARAN, S. RAMAPRABHU, Indian Institute of Technology Madras — Graphene- a two dimensional sheet of  $\text{sp}^2$  hybridized carbon atoms has been considered as promising materials in sensor design for detection of target molecule. Charge carriers in graphene obey linear dispersion relation and it behaves like mass less relativistic particles which act as base for enhanced electron transport. Thus the electrons move ballistically without scattering giving higher mobility even at room temperature. Further, the presence of oxygen containing functional group and crystal defects assisted via hydrogenation process take vital part in electrochemical adsorption of electro active species and catalyses the same. Though issues with selectivity, stability and sensitivity are limited for several nanostructured metal oxides sensing, the hybrid system started its effective role in design of sensing platform. Thus considering the potential important of hydrogenated graphene -metal oxide systems, a nanohybrid system is developed and its structural, morphological and optical properties were understood using respective characterization tool. Further, the prepared hybrid nanosystem used as a platform for bimolecule detection, where the sensor exhibits higher range of sensitivity and selectivity.

**T1.00117 Bias dependent transport property of defective phosphorene.**<sup>1</sup>, M FAROOQ, ARQUM HASHMI, pukyong National University, CHANYONG HWANG, KRISS, JISANG HONG, pukyong National University — Phosphorene is receiving great research interests because of its peculiar physical properties. Nonetheless, no systematic studies on the transport properties modified due to defects have been performed. Here, we present the electronic band structure, defect formation energy and bias dependent transport property of various defective systems. We found that the defect formation energy is much less than that in graphene. The defect configuration strongly affects the electronic structure. The band gap vanishes in single vacancy layers, but the band gap reappears in divacancy layers. Interestingly, a single vacancy defect behaves like a p-type impurity for transport property. Unlike the common belief, we observe that the vacancy defect can contribute to greatly increasing the current. Along the zigzag direction, the current in the most stable single vacancy structure was significantly increased as compared with that found in the pristine layer. In addition, the current along the armchair direction was always greater than along the zigzag direction and we observed a strong anisotropic current ratio of armchair to zigzag direction.

<sup>1</sup>This research was supported by Basic Science Research Program through the National Research

**T1.00118 Low-temperature optical spectroscopy of single-layer transition metal dichalcogenides**, GERD PLECHINGER, PHILIPP NAGLER, CHRISTIAN SCHÜLLER, TOBIAS KORN, Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D-93040 Regensburg, Germany — In recent years, layered materials beyond graphene have attracted immense interest in the scientific community. Among those, particularly the semiconducting transition metal dichalcogenides (TMDCs) in their monolayer form are in the focus of the current research due to their intriguing optical properties and their potential application in valleytronic-based devices. The optical properties are governed by excitonic features, even at room temperature. The excitons in monolayer TMDCs have unusually large binding energies due to the two-dimensional carrier confinement and weak dielectric screening. Here, we investigate the photoluminescence spectra of monolayer TMDCs at low temperatures. We present clear evidence for the existence of biexcitons in monolayer  $\text{WS}_2$ , exhibiting a superlinear behavior in excitation-power-dependent measurements. Applying a gate-voltage in a FET-configuration, we can identify charge-neutral and negatively charged excitons (trions) in the optical spectrum of different TMDCs. The trion binding energies range in the order of 30 meV. The evolution of the excitonic peaks under the application of external magnetic fields give further insight into the internal structure of these materials.

**T1.00119 Valley polarization and coherence in atomically thin tungsten disulfide via optical spectroscopy**, BAIREN ZHU, The University of Hong Kong, HUALING ZENG, The Chinese University of Hong Kong, JUNFENG DAI, South University of Science and Technology of China, ZHIRUI GONG, XIAODONG CUI, The University of Hong Kong — Atomically thin group-VI transition metal dichalcogenides (TMDC) has been emerging as a family of intrinsic 2-dimensional crystals with a sizeable bandgap, opening a potential avenue for ultimate electronics and optoelectronics. Besides, the characteristic structural inversion symmetry breaking in monolayers leads to non-zero but contrasting Berry curvatures and orbital magnetic moments at K/K' valleys. These features provide an opportunity to manipulate electrons' additional internal degrees of freedom, namely the valley degree of freedom, making monolayer TMDC a promising candidate for the conceptual valleytronics. Here, our experimental approach on valley dependent circular dichroism in monolayer and bilayer WS<sub>2</sub> via optical spectroscopy are elaborated. Consequently, the polarization of photoluminescence inherits that of excitations, circularly and linearly polarized, confirming the valley dependent selectivity rule. However, the valley polarization and valley coherence in bilayer WS<sub>2</sub> owing to the coupling of spin, valley and layer degrees of freedom, are anomalously robust compared with monolayer WS<sub>2</sub>. We propose potential mechanisms of the anomalous behavior in WS<sub>2</sub> bilayers.

**T1.00120 Optical nano-imaging of waveguide exciton polaritons in transition-metal dichalcogenides**, ZHE FEI, Iowa State University, MARIE SCOTT, University of Washington, DAVID GOSZTOLA, Argonne National Laboratory, JONATHAN FOLEY, William Paterson University, JIAQIANG YAN, DAVID MANDRUS, Oak Ridge National Laboratory, HAIDAN WEN, Argonne National Laboratory, PENG ZHOU, DAVID ZHANG, Fudan university, YUGANG SUN, JEFFREY GUEST, STEPHEN GRAY, Argonne National Laboratory, WENZHONG BAO, Fudan university, GARY WIEDERRECHT, Argonne National Laboratory, XIAODONG XU, University of Washington — Exciton polaritons, which are collective oscillations of photons and excitons in semiconductors, trigger tremendous research interests in both fundamental physics and technological applications. Previous studies retain to spectroscopic studies of exciton polaritons confined in microcavities. Here, we report on optical nano-imaging study of waveguide exciton polaritons of thin flakes of transition-metal dichalcogenides (TMDCs) using the near-field scanning optical microscopy. The observed polaritons are formed by strong coupling between waveguide photons and A excitons in TMDCs. The wavelength of these exciton polaritons can reach as low as 300 nm. By tuning the laser frequency, we are able to map the entire polariton dispersion both above and below the A exciton energy. Further analysis indicates that polaritons in the lower-energy branch have a propagation length over many microns while the modes in the upper-energy branch are strongly damped due to the Landau damping.

**T1.00121 ABSTRACT WITHDRAWN** —

**T1.00122 Anisotropic Electron transport and device applications of atomically thin ReS<sub>2</sub>**, ERFU LIU, YAJUN FU, YAOJIA WANG, YANQING FENG, HUIMEI LIU, XIANGANG WAN, WEI ZHOU, BAIGENG WANG, JUNWEN ZENG, Nanjing University, CHING-HWA HO, YING-SHENG HUANG, National Taiwan University of Science and Technology, HONGTAO YUAN, HAROLD Y. HWANG, YI CUI, Stanford University, DINGYU XING, FENG MIAO, Nanjing University — Semiconducting two-dimensional transition metal dichalcogenides are emerging as top candidates for post-silicon electronics. While most of them exhibit isotropic behavior, lowering the lattice symmetry could induce anisotropic properties, which are both scientifically interesting and potentially useful. In this talk, we will present atomically thin rhenium disulfide (ReS<sub>2</sub>) flakes with unique distorted 1T structure, which exhibit in-plane anisotropic properties. We first fabricated mono- and few-layer ReS<sub>2</sub> field effect transistors, which exhibit competitive performance with large current on/off ratios (~10<sup>7</sup>) and low subthreshold swings (100 mV dec<sup>-1</sup>). The observed anisotropic ratio along two principle axes reaches up to 3.1. Furthermore, we successfully demonstrated an integrated digital inverter with good performance by utilizing two ReS<sub>2</sub> anisotropic field effect transistors, suggesting the promising implementation of large-scale two-dimensional logic circuits. Recent results on ultra-high responsivity (as high as 88,600 A W<sup>-1</sup>) phototransistors based on few-layer ReS<sub>2</sub> will also be discussed. Our results underscore the unique properties of two-dimensional semiconducting materials with low crystal symmetry for future electronic and optoelectronic applications.

**T1.00123 Nonlinear dynamics of the normal and superfluid dipolariton gas in transition-metal dichalcogenide-based heterostructures**, GERMAN KOLMAKOV, NYC College of Technology, CUNY, TIM BYRNES, New York University, ANDY HE, ROMAN YA. KEZERASHVILI, NYC College of Technology, CUNY — Propagation of a dipolariton quantum gas in normal and superfluid states in a patterned microcavity in the presence of an external electric field is studied. The double layer transition-metal dichalcogenide structure is embedded into the microcavity. The dipolaritons are formed as a superposition of direct and indirect excitons in the layers and cavity photons. By numerically solving the Boltzmann equation for a gas of interacting dipolaritons in a normal state at room temperatures and the Gross-Pitaevskii equation for a dipolariton Bose-Einstein condensate in superfluid state at low temperatures we show that the dipolariton flow can be controlled by the electric field in the cavity. We also numerically studied the dipolariton propagation in channels of various geometries in the cavity and determine conditions when the dipolariton flow can be guided in the channels.

**T1.00124 Tunable valley polarization of quantum confined excitons in WSe<sub>2</sub>**, SAJAL DHARA, CHITRALEEMA CHAKRABORTY, KENNETH GOODFELLOW, NICK VAMIVAKAS, Univ of Rochester — The discovery of single photon emitters in two dimensional transition metal dichalcogenides opens up a new research direction in the field of two-dimensional layered materials. In order to understand the origin of the quantum confinement that is responsible for these localized excitonic states we perform polarization resolved optical measurements. The quantum dots are embedded in a diode-like device to control the quantum dot energy levels via the quantum confined Stark effect. In addition to applied electric field, an external magnetic field is also used to control the quantum dot exciton properties. In this work we present our findings that sheds light on the symmetry of the confinement potential. The observed extent of valley polarization indicates quantum confined exciton's valley degree of freedom protection from environmental disturbances.

**T1.00125 Phonons in Stabilized B or N doped graphene**, GIRIJA DUBEY, York College-CUNY, NY11451, SARITA MANN, POOJA RANI, VIJAY JINDAL, Department of Physics, Panjab University, Chandigarh 160014, India — Based on *Ab-initio* density functional perturbation theory, we have investigated various doped B and N based graphene sheets by raising their concentrations upto 50% of the host carbon. Although the doped structures seem to stabilize in 2-D configurations, but the resulting Phonon frequencies do not confirm the stability as the transverse modes above critical concentrations of B and N tend to result in negative eigenvalues. This essentially requires strained 2-D sheets when doped above such critical concentrations. We find the results of phonons and thermodynamics very interesting and attempt to report these in strained lattices. The motivation to do such a calculation results from our primary goal to address the issue of heat dissipation rate in the devices based on designable electronic and optical properties of such doped graphene reported already.

**T1.00126 Multi-Level Memory Effect of CVD Graphene Transferred on SiO<sub>2</sub> by Controlled Hydron Adsorption at Interface<sup>1</sup>**, SUNGCHUL JUNG, JUNHYOUNG KIM, HOON HAHN YOON, HAN BYUL JIN, GAHYUN CHOI, JUNG-YONG LEE, Ulsan Natl Inst of Sci & Tech, DAEJIN EOM, Korea Research Institute of Standards and Science, KIBOG PARK, Ulsan Natl Inst of Sci & Tech — Memory effect of graphene based on the Fermi-level shift driven by external electric field has been studied in various ways. There have been several experimental reports exploring the fabrication of two-level memory devices relying on the hysteresis loop of channel current vs. gate voltage of Graphene/SiO<sub>2</sub>/Si field effect transistor (FET). This channel current hysteresis has been explained by the motion of the water molecules trapped between graphene and SiO<sub>2</sub> insulator. In this study, we fabricated a CVD-grown graphene FET on a SiO<sub>2</sub>/Si substrate and found four different channel conductivity states tunable by varying the applied gate voltage pulse. It is noticed that the stabilization of reset state (lowest conductivity state) is one of the challenging issues in fabricating memory devices with graphene FET. We found that the stabilization of reset state can be achieved by positioning the Fermi-level in reset state as close to the charge neutrality point as possible during read-out. We propose one easy way to ensure the proper positioning of the reset state Fermi-level, which is to apply a constant gate voltage during read-out. Our study demonstrates the possibility of fabricating graphene-based multi-bit memory devices.

<sup>1</sup>Supported by NRF in South Korea (2013R1A1A2007070)

**T1.00127 Gate-tunable tunneling resistance in graphene/topological insulator vertical junctions<sup>1</sup>**, LIANG ZHANG, 1 State Key Laboratory for Mesoscopic Physics, Department of Physics, Peking University, Beijing 100871, P.R. China, YUAN YAN, State Key Laboratory for Mesoscopic Physics, Department of Physics, Peking University, Beijing 100871, P.R. China, HAN-CHUN WU, School of Physics, Beijing Institute of Technology, Beijing, 100081, P.R. China, ZHI-MIN LIAO, DA-PENG YU, State Key Laboratory for Mesoscopic Physics, Department of Physics, Peking University, Beijing 100871, P.R. China — The emergence of graphene-based vertical heterostructures, especially stacked by various layered materials, opens up new promising possibilities for investigations and applications. The junction based on two famous Dirac materials, graphene and topological insulator, Bi<sub>2</sub>Se<sub>3</sub>, can considerably enlarge the family of van der Waals heterostructures, while the experimental approach to obtain controllable interface of these junctions is still a challenge. Here we show the experimental realization of the vertical heterojunction between Bi<sub>2</sub>Se<sub>3</sub> and monolayer graphene. The tunneling-mediated quantum oscillations are identified to arise from several two-dimensional conducting layers. The electrostatic field induced by back gate voltage, as well as the magnetic field, is applied to tailor the available density of states near the Fermi surface. We observe exotic gate-tunable tunneling resistance in high magnetic field, which is attributed to semimetal-quantum Hall insulator transition in the underlying graphene.

<sup>1</sup>This work was supported by MOST (Nos. 2013CB934600, 2013CB932602) and NSFC (Nos. 11274014, 11234001).

**T1.00128 Theory of hot electron photoemission from graphene**, LAY KEE ANG, SHIJUN LIANG, Singapore University of Technology and Design — Motivated by the development of Schottky-type photodetectors, some theories have been proposed to describe how the hot carriers generated by the incident photon are transported over the Schottky barrier through the internal photoelectric effect. One of them is Fowler's law proposed as early as 1931, which studied the temperature dependence of photoelectric curves of clean metals. This law is very successful in accounting for mechanism of detecting photons of energy lower than the band gap of semiconductor based on conventional metal/semiconductor Schottky diode. With the goal of achieving better performance, graphene/silicon contact-based- graphene/WSe<sub>2</sub> heterostructure-based photodetectors have been fabricated to demonstrate superior photodetection efficiency. However, the theory of how hot electrons is photo-excited from graphene into semiconductor remains unknown. In the current work, we first examine the photoemission process from suspended graphene and it is found that traditional Einstein photoelectric effect may break down for suspended graphene due to the unique linear band structure. Furthermore, we find that the same conclusion applies for 3D graphene analog (e.g. 3D topological Dirac semi-metal). These findings are very useful to further improve the performance of graphene-based photodetector, hot-carrier solar cell and other kinds of sensor.

**T1.00129 Memristive Phenomena in Polycrystalline Single Layer MoS<sub>2</sub>**, VINOD SANGWAN, DEEP JARIWALA, IN-SOO KIM, KAN-SHENG CHEN, TOBIN MARKS, LINCOLN LAUHON, MARK HERSAM, Northwestern University, HERSAM LABORATORY TEAM<sup>1</sup> — Recently, a new class of layered two-dimensional semiconductors has shown promise for various electronic applications. In particular, ultrathin transition metal dichalcogenides (e.g. MoS<sub>2</sub>) present a host of attractive features such as high carrier mobility and tunable band-gap. However, available growth methods produce polycrystalline films with grain-boundaries and point defects that can be detrimental in conventional electronic devices. In contrast, we have developed unconventional device structures that exploit these defects for useful electronic functions.[1] In particular, we observe grain-boundary mediated memristive phenomena in single layer MoS<sub>2</sub> transistors. Memristor current-voltage characteristics depend strongly on the topology of grain-boundaries in MoS<sub>2</sub>. A grain boundary directly connecting metal electrodes produces thermally assisted switching with dynamic negative differential resistance, whereas a grain boundary bisecting the channel shows non-filamentary soft-switching. In addition, devices with intersecting grain boundaries in the channel show bipolar resistive switching with high on/off ratios up to ~10<sup>3</sup>. [1] Furthermore, the gate electrode in the field-effect geometry can be used to control the absolute resistance of the on and off states. Correlated electrostatic force microscopy, photoluminescence, and Raman microscopy reveal the role of sulfur vacancies in the switching mechanism. Refs: 1. Sangwan et al., *Nature Nanotech*, 10 403 (2015)

<sup>1</sup>This abstract is replacing MAR16-2015-004166 that had exceeded the character limit.

**T1.00130 Resonance frequency shifts due to quantized electronic states in atomically thin NEMS**, CHANGYAO CHEN, Argonne National Lab, VIKRAM DESHPANDE, Department of Physics and Astronomy, University of Utah, MIK-ITO KOSHINO, Department of Physics, Tohoku University, SUNWOO LEE, Department of Electrical Engineering, Columbia University, ALEXANDER GONDARENKO, Department of Mechanical Engineering, Columbia University, ALLAN MACDONALD, Department of Physics, University of Texas, Austin, PHILIP KIM, Department of Physics, Harvard University, JAMES HONE, Department of Mechanical Engineering, Columbia University — The classic picture of the force exerted on a parallel plate capacitor assumes infinite density of states (DOS), which implies identical electrochemical and electrostatic potential. However, such assumption can breakdown in low-dimensional devices where the DOS is finite or quantized. Here we consider the mechanical resonance shift of a nanoelectromechanical (NEMS) resonator with small DOS, actuated and detected capacitively at fixed electrochemical potential. We found three leading correction terms to the classical picture: the first term leads to the modulation of static force due to the variation in chemical potential, and the second and third terms are related to the static and dynamic changes in spring constants, caused by quantum capacitance. The theory agrees well with recent experimental findings from graphene resonator in quantum Hall regimes, where the chemical potential and quantum capacitance are tuned by magnetic field, while the gate voltage is kept constant.

**T1.00131 A theoretical design of graphene-based spin field-effect transistors**, LIXUE LIU, University of Science and Technology of China, SHUDUN LIU, University of Louisville, ZHENYU ZHANG, WENGUANG ZHU, University of Science and Technology of China — The search for a feasible design of graphene-based materials for spintronics applications has been intensified in recent years. Encouraged by recent experimental achievements, here we propose a new scheme to realize graphene-based spin field-effect transistors. The new design is constituted of a half-hydrogenated graphene nanoroad embedded in a fully-hydrogenated graphene. Using first-principles density function theory calculations, we demonstrate that such a design can convert non-magnetic pristine graphene into a bipolar ferromagnetic semiconductor. More importantly, the magnetism of such a nanoroad is very robust: independent of its width and orientation. We also discuss the stability of such nanoroads, as well as a simple design of an all-electric controlled device for generation and detection of a fully spin-polarized electric current.

**T1.00132 Control of Rewriteable Doping Patterns in Graphene/Boron Nitride Heterostructures**, SALMAN KAHN, JAIRO VELASCO JR., DILLON WONG, JUWON LEE, HSIN ZON TSAI, University of California - Berkeley, LONG JU, Cornell University, LILI JIANG, ZHIWEN SHI, PAUL ASHBY, University of California - Berkeley, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, ALEX ZETTL, FENG WANG, MICHAEL CROMMIE, University of California - Berkeley — Spatial control of charge doping in 2D materials is a prerequisite for designing future electronic devices and understanding novel physics. Electrostatic gating and chemical doping are two of the most common methods to achieve this. However, these approaches suffer from complicated fabrication processes that introduce impurities, change material properties irreversibly, and lack flexibility. Here we introduce a new method for patterning rewriteable doping profiles using an STM tip by way of local tip-voltage-induced ionization of defects in a BN substrate. We characterize these spatial doping patterns through local probe and transport techniques. This technique enables many novel device designs for 2D materials, including atomically thin p-n junctions and rewriteable memory devices.

**T1.00133 Effects of interface oxygen vacancies at the FeSe/SrTiO<sub>3</sub> interface**, MINGXING CHEN, D. F. AGTERBERG, L. LIAN, MICHAEL WEINERT, Univ of Wisconsin, Milwaukee — The effects of oxygen vacancies on the electronic bands at the interface of between monolayer and bilayer FeSe and SrTiO<sub>3</sub> are investigated by first-principles supercell calculations. Unfolded bands derived from the *k*-projection method reveal that the oxygen vacancy not only provides electron doping to the interface FeSe layer, but also significantly renormalizes the width of the Fe-3*d* band near the Fermi level for the checkboard antiferromagnetic (AFM) state. However, the effects of the oxygen vacancies on the electronic properties of the top layer of bilayer FeSe are limited. The *k*-projected bands for the checkboard AFM state are in good agreement with ARPES results.

**T1.00134 ABSTRACT WITHDRAWN —**

**T1.00135 Even-dimensional topological semimetals under disorders**, X. J. HUANG, Y. X. ZHAO, Z. D. WANG, The Univ of Hong Kong — A topological theory of even-dimensional, chiral symmetry-preserving topological semimetal, which is known as the counterpart of Weyl semimetal, is developed in this work. We show that, in presence of disorder, an anisotropic topological  $\theta$ -term emerges in the action of effective non-linear sigma model, meanwhile, an anisotropic Chern character term in terms of  $U(1)$  gauge response theory, which gives the electromagnetic response, whose stability against disorders is ensured by the former topological  $\theta$ -term, has also been derived. Moreover, it is found that this topological semimetal can be included in the family of topological quantum matter preserving chiral symmetry. The relations of this topological semimetal to odd-dimensional topological insulator and even-dimensional Dirac fermion are revealed in both effective non-linear sigma model and gauge theory. And importantly, above results can be applied to graphene if we set dimension  $d = 2$  and thus reveal the topological character of this kind of 2-dimensional topological semimetal with two Dirac cones with opposite chiralities.

**T1.00136 Supercurrent in the quantum Hall regime**, MING-TSO WEI, Duke Univ, FRANCOIS AMET, Appalachian State University, CHUNG-TING KE, Duke Univ, IVAN BORZENETS, University of Tokyo, JIYINGMEI WANG, Duke Univ, KEJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, RUSSELL DEACON, Center for Emergent Matter Science, RIKEN, MICHIOHISA YAMAMOTO, University of Tokyo, YURIY BOMZE, Duke Univ, SEIGO TARUCHA, University of Tokyo, GLEB FINKELSTEIN, Duke Univ — Combining superconductivity and the quantum Hall (QH) effect is a promising route for creating new types of topological excitations. Despite this potential, signatures of superconductivity in the quantum Hall regime remain scarce, and a superconducting current through a QH weak link has so far eluded experimental observation. Here we demonstrate the existence of a novel type of Josephson coupling through a QH region at magnetic fields as high as 2 Tesla. The supercurrent is mediated by states encompassing QH edge channels, which are flowing on opposite sides of the sample. The edges are coupled together by the hybrid electron-hole modes at the interfaces between the QH region and the superconducting contacts. These chiral modes, which share some features with Majorana modes, are formed when electron and hole edge states are mixed by the superconductor.

**T1.00137 Cooper pairing protected by spin-valley locking in two-dimensional superconductivity on MoS<sub>2</sub>**, YU SAITO, The University of Tokyo, YASU HARU NAKAMURA, Kyoto University, MOHAMMAD BAHRAMY, The University of Tokyo, YOSHIMITSU KOHAMA, ISSP, JIANTING YE, The University of Tokyo, YUICHI KASAHARA, Kyoto University, MASASHI TOKUNAGA, ISSP, TSUTOMU NOJIMA, Tohoku University, YUICHI YANASE, Kyoto University, YOSHIHIRO IWASA, The University of Tokyo — MoS<sub>2</sub> is an archetypal layered semiconductor; monolayer shows out-of-plane spin polarization at the K-points due to intrinsic Zeeman-type spin-orbit coupling (SOC) derived from its in-plane broken inversion symmetry. By ionic-liquid gating, almost all carriers are confined only to topmost layer, realizing two-dimensional superconductivity in this system [1]. We reported the first observation of a huge in-plane upper critical field of about 52 T and a clear saturating behaviour in the low temperatures using pulsed magnetic fields up to 55 T [2]. From first-principles-based tight binding supercell calculations followed by realistic numerical calculations of  $H_{c2}$  based on the subband structure, we revealed that this unusual behavior is due to the moderately large Zeeman-type spin splitting of 13 meV at the Fermi level (vicinity of the K points) [3]. This forces Cooper pairs to be completely aligned to out-of-plane direction by spin-valley locking effect, thereby causing the dramatic enhancement of the Pauli limit. Our calculation also indicates that even if the carrier density and then spin splitting (9–15 meV) at the Fermi level changes, the Pauli limit is predominantly controlled by both the Zeeman-type SOI and  $T_c$ , and the contribution of Rashba-type SOI is negligibly small. [3]. [1] Y. Saito et al. <http://meetings.aps.org/link/BAPS.2014.MAR.T52.8> [2] Y. Saito, et al. <http://meetings.aps.org/link/BAPS.2015.MAR.G11.11> [3] Y. Saito et al. Nature Phys. doi: 10.1038/nphys3580. (arXiv:1506.04146).

**T1.00138 Highly anisotropic Dirac fermions in square graphynes**, LIZHI ZHANG, Univ of Electronic Sci & Tech / University of Utah, ZHENGFEI WANG, University of Science and Technology of China, JIANSHEG RAO, ZIHENG LI, WULIN HUANG, ZHIMING WANG, Univ of Electronic Sci & Tech, SHIXUAN DU, HONGJUN GAO, Institute of Physics, Chinese Academy of Sciences, FENG LIU, University of Utah — Recently, there have been intense search of new 2D materials, and one especially appealing class of 2D materials is the all-carbon allotropes of Dirac materials. Here, we predict a new family of 2D carbon allotropes, square graphynes (S-graphynes) that exhibit highly anisotropic Dirac Fermions, using first-principle calculations within density functional theory. The equal-energy contour of their 3D band structure shows a crescent shape, and the Dirac crescent has varying Fermi velocities from  $0.6 \times 10^5$  to  $7.2 \times 10^5$  m/s along different *k* directions. Near the Fermi level, the Dirac crescent can be nicely expressed by an extended 2D Dirac model Hamiltonian. Furthermore, tight-binding band fitting reveals that the Dirac crescent originates from the next-nearest-neighbor interactions between C atoms. Our findings enrich the Dirac physics founded in other 2D Dirac systems, and offer a new design mechanism for creating Dirac band by tuning the interaction range. We envision that the highly anisotropic Dirac crescent may be exploited in all-carbon-based electronic devices for manipulating anisotropic electron propagation.

**T1.00139 Microwave Irradiation on Halloysite-Polypropylene Nanocomposites**, OMAR ESPINO, BRIAN YUST, DORINA CHIPARA, Univ of Texas, Pan American, PULLICKEL AJAYAN, ALIN CHIPARA, Rice University, MIRCEA CHIPARA, Univ of Texas, Pan American, UTRGV COLLABORATION, RICE COLLABORATION — Halloysite is an unique cylindrical nanoclay characterized by poor electrical and thermal conductivity, which may become the filler of choice for the reinforcement of polymeric matrix, where electrical or thermal insulation are required. The main limits in the use of halloysite as replacement for carbon nanotube (CNT) are: 1. Smaller aspect ratio as halloysites are typically shorter than CNTs. 2. Smaller Young modulus of halloysites compared with CNTs. 3. Reduced thermal stability due to the loss of water upon heating. A research on halloysite dispersed within isotactic polypropylene is reported. To improve the interface between the halloysite and the polymeric matrix a microwave irradiation step has been considered. The local heating of the halloysite nanotubes is mediated by the absorbed/structural water content of the nanoclay. Nanocomposites loaded by various amounts of halloysite ranging from 0 % to 20 % wt. have been prepared by melt mixing by using a Haake RheoMixer. The as obtained nanocomposites have been subjected to microwave irradiation at 75 W in an Anton Paar Monowave 300 system and various irradiation times ranging from 5, 10, 15, 30, 45, and 60 minutes. The effect of microwave irradiation has been studied by Raman and FTIR spectroscopy

**T1.00140 On the Radial Breathing Mode in SWCNTs dispersed within PVC**, FERNANDO FLOR, The University of Texas Rio Grande Valley, PULLICKEL AJAYAN, ALIN CHIPARA, Rice University, KAREN LOZANO, DORINA CHIPARA, The University of Texas Rio Grande Valley, ROBERT VAJTAI, Rice University, MIRCEA CHIPARA, The University of Texas Rio Grande Valley, UTRGV-RICE COLLABORATION — The Radial Breathing Mode (RBM) is an unique set of Raman lines, characterized by shifts smaller than  $500\text{ cm}^{-1}$ , assigned to vibrations that affect the diameter of carbon nanotubes. The position of the RBM lines is inversely proportional to the diameter of nanotubes. RBM was reported in Single Walled Carbon Nanotubes (SWCNTs) and Double Walled Carbon Nanotubes. This mode is very sensitive being frequently used to obtain information regarding the stress transfer from the polymeric matrix. Nanocomposites have been prepared by loading the polyvinylchloride (PVC) purchased from Sigma Aldrich with SWCNTs from Cheap Tubes Inc., by melt mixing, using Haake Rheomix equipped with two counter rotating screws. The concentration of SWCNTs dispersed within PVC ranged from 0 % wt. up to 20 % wt. The as recorded spectra have been deconvoluted into several individual lines characterized by an extended Breit-Wigner-Fano line shape. A full analysis of the Raman spectra of the polymeric matrix and of the matrix is reported with emphasize on the RBM features. The spectra have been recorded by using a Renishaw InVia spectrometer equipped with Eclipse filters that allow the recording of Raman lines starting from about  $25\text{ cm}^{-1}$ .

**T1.00141 First Principles Study of Carbyne Structural Stability<sup>1</sup>**, KEVIN KWON<sup>2</sup>, COLIN HOLMES<sup>3</sup>, KI CHUL KIM<sup>4</sup>, SEUNG SOON JANG<sup>5</sup>, Georgia Institute of Technology — Carbyne is composed of linear sp-hybridized carbon bonds and yields promising results to surpass graphene's mechanical and electrical properties. Carbyne has two semi-stable conformations: Polyyne (alternating triple and single bonds) and Polycumulene (repeating double bonds). This study investigated the stability of these forms at infinite chain lengths by using periodic boundary conditions. Geometric optimization was performed via DFT calculations using DMol3 and PBE GGA functional group. Each configuration's chain was stretched or compressed until the most stable form – lowest energy – was obtained. After comparing the energies, the most stable form alternated between Polyyne and Polycumulene as the number of carbon atoms within each boundary increased. Polyyne was the most stable form for odd number of carbons and Polycumulene was the most stable for even number of carbons. Finally, K-point sampling was increased in the direction of the chain axis to obtain a more accurate depiction of structural stability. As the number of k-points increased, the Polycumulene structure became more stable compared to Polyyne.

<sup>1</sup>School of Materials Science and Engineering, Georgia Institute of Technology

<sup>2</sup>Undergraduate Researcher

<sup>3</sup>Undergraduate Researcher

<sup>4</sup>Graduate Student Researcher Assistant

<sup>5</sup>Head Research Advisor

**T1.00142 Monoclonal Antibodies Attached to Carbon Nanotube Transistors for Paclitaxel Detection**, WONBAE LEE, CALVIN LAU, MARK RICHARDSON, ARITH RAJAPAKSE, GREGORY WEISS, PHILIP COLLINS, Univ of California - Irvine, UCI, MOLECULAR BIOLOGY AND BIOCHEMISTRY COLLABORATION, UCI, DEPARTMENTS OF PHYSICS AND ASTRONOMY COLLABORATION — Paclitaxel is a naturally-occurring pharmaceutical used in numerous cancer treatments, despite its toxic side effects. Partial inhibition of this toxicity has been demonstrated using weakly interacting monoclonal antibodies (3C6 and 8A10), but accurate monitoring of antibody and paclitaxel concentrations remains challenging. Here, single-molecule studies of the kinetics of antibody-paclitaxel interactions have been performed using single-walled carbon nanotube field-effect transistors. The devices were sensitized with single antibody attachments to record the single-molecule binding dynamics of paclitaxel. This label-free technique recorded a range of dynamic interactions between the antibody and paclitaxel, and it provided sensitive paclitaxel detection for pM to nM concentrations. Measurements with two different antibodies suggest ways of extending this working range and uncovering the mechanistic differences among different antibodies.

**T1.00143 Observation of dopant-induced impurity states in bottom-up graphene nanoribbons**, ZAHRA PEDRAMRAZI, CHEN CHEN, TOMAS MARANGONI, RYAN CLOKE, TING CAO, STEVEN LOUIE, FELIX FISCHER, MICHAEL CROMMIE, Univ of California - Berkeley — Graphene nanoribbons (GNRs) provide a means for inducing energy gaps in graphene and are a promising candidate for many nanotechnological applications. New bottom-up fabrication techniques allow the structure of GNRs to be tuned with atomic precision, thus providing new opportunities for modifying their electronic structure. Here we report the synthesis of bottom-up armchair GNRs (AGNRs) with isolated substitutional boron-dopant centers; thus creating localized impurity states in the GNR. These impurities are realized via dilute doping of pristine n=7 AGNRs with sparse boron-containing monomer units, resulting in uniform-width n=7 AGNR segments where only two carbon atoms have been substitutionally replaced by boron atoms. Scanning tunneling microscopy (STM) and spectroscopy (STS) were performed to study the electronic structure of these AGNR impurity systems, enabling us to observe localized mid-gap impurity states.

**T1.00144 *In Situ* Characterization of Nanostructures Using Rayleigh Scattering<sup>1</sup>**, BISWAJIT SANTRA, MIKHAIL N. SHNEIDER, ROBERTO CAR, Princeton University, Princeton, USA — Controlling selective growth of nanotubes has posed a considerable challenge over the last two decades. A crucial step to overcoming such hurdle is to gain detailed knowledge of the early stage of nanomaterial syntheses for which *in situ* measurements are required. Laser-based probes, such as Rayleigh scattering (RS), can potentially characterize the shape and size of nanoparticles *in situ*. The intensity of RS in a gas mixed with nanoparticles is proportional to the polarizabilities of the constituent particles, therefore, theoretical spectroscopy can complement such measurements. Here, we employed time-dependent density functional theory to compute the frequency-dependent polarizabilities of various nanostructures and predicted the corresponding RS intensity and depolarization. We found that with increasing length and asymmetry of the nanostructures the longitudinal polarizability exhibited characteristic resonances leading to measurable signatures in the RS intensity and depolarization. Also by considering gas-particle mixtures at estimated experimental conditions for nanoparticle synthesis on the periphery of an arch, we predict that *in situ* characterization of a few nanometer long particles with concentration as low as one particle per million is feasible using RS.

<sup>1</sup>This work was supported by U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

**T1.00145 Giant Rashba spin-orbit splitting in  $n-p$  codoped graphene<sup>1</sup>**, SHIFEI QI, YINGPING YANG, Shanxi Normal University, ZHENHUA QIAO, University of Science & Technology of China, XIAOHONG XU, Shanxi Normal University, INSTITUTE OF MATERIALS CHEMISTRY TEAM, ICQD TEAM — Enhancement of the spin-orbit coupling (SOC) in graphene may lead to various topological phenomena and also find applications in spintronics. However, increasing the SOC strength in graphene without drastically affecting the basic physical properties is proving extremely difficult. Here, we propose a new approach, based on compensated  $n-p$  codoping, that can simultaneously address all the main shortcomings associated with single-element adsorption in graphene, effectively resulting in giant Rashba spin-orbit splitting. Our proposal is to deposit strong SOC adatoms with outer shell  $p$  electrons, acting as  $n$ -type dopants, onto already  $p$ -doped (e.g., by B) graphene. We found that: (1) the electrostatic attraction between the  $n$ - and  $p$ -type dopants effectively enhances the adsorption of the metal adatoms and suppress their undesirable clustering, (2) considerable ( $\sim 130$  meV) Rashba-type SO splitting can be achieved in the graphene  $\pi$  bands, (3) the charge compensated nature and mutually screening each other of the  $n-p$  codopants helps to preserve the Dirac nature of the charge carriers, and (4) the B doping effect together with intrinsic induced SOC by adatom also lead the codoped system open about 20  $\sim$  90 meV band gap.

<sup>1</sup>NSFC 11104173, 61434002 and 51025101

**T1.00146 Flexible, Transparent and Conductive Carbon Nanotube Aerogels /PEDOT:PSS Electrodes created by Top-bottom Fabrication**, PATRICIA M. MARTINEZ, Univ of Texas, Dallas, ANDREA CERDAN PASARAN, University of Guanajuato, ANVAR ZAKHIDOV, Univ of Texas, Dallas, UNIVERSITY OF GUANAJUATO, MEXICO COLLABORATION — The sheets of Carbon Nanotubes (CNT) have proven to be a good substitute for ITO. To improve their conductivity and increase optical transparency we have created composites which incorporate silver nanowires or other evaporated metals. Coating CNT/metals with PEDOT:PSS is important for creating hole transport/electron barrier layer functionality, but it is not easy to achieve using PEDOT:PSS solutions due to the hydrophobicity of CNT. We report a new top-to-bottom approach for the fabrication of highly flexible, transparent and conductive carbon nanotube-based electrodes using PDMS as a substrate. A uniform and smooth layer of approximately 50 nm of PEDOT:PSS was spin coated on top of a PDMS stamp followed by the deposition of vapor densified freestanding Multiwall Carbon Nanotube (MWNT) aerogels. An incorporation of silver nanowires, silver or Aluminum thin layer can be sprayed or evaporated on top of the freestanding MWNT aerogels in order to lower the sheet resistance even further. The PDMS substrate is drop cast on top of the configuration then the PDMS stamp is lifted-up. The PEDOT:PSS layer is selectively deposited on top of the MWNT only. The composite electrodes can be laminated on photovoltaic devices and on LEDs.

**T1.00147 Computational design of metal-organic frameworks with paddlewheel-type secondary building units**, UDO SCHWINGENSCHLOGL, MAXIM V. PESKOV, NEJIB MASGHOUNI, PSE Division, KAUST, Thuwal 23955, Saudi Arabia — We employ the TOPOS package to study 697 coordination polymers containing paddlewheel-type secondary building units. The underlying nets are analyzed and 3 novel nets are chosen as potential topologies for paddlewheel-type metal organic frameworks (MOFs). Dicarboxylate linkers are used to build basic structures for novel isorecticular MOF series, aiming at relatively compact structures with a low number of atoms per unit cell. The structures are optimized using density functional theory. Afterwards the Grand Canonical Monte Carlo approach is employed to generate adsorption isotherms for CO<sub>2</sub>, CO, and CH<sub>4</sub> molecules. We utilize the universal forcefield for simulating the interaction between the molecules and hosting MOF. The diffusion behavior of the molecules inside the MOFs is analyzed by molecular dynamics simulations.

**T1.00148 Structural, Electronic and Magnetic Properties of Ti<sub>1+x</sub>FeSb and TiFe<sub>0.75</sub>M<sub>0.25</sub>Sb (M= Ni, Mn) Heusler Alloys**, SAID AL AZAR, Basic Sciences Department, Dar Al Uloom University, Riyadh, Saudi Arabia, AHMAD MOUSA, Department of Basic Sciences, Middle East University, Amman, Jordan — Density functional theory calculations based on full potential linearized augmented plane-wave (FPLAPW) plus local orbital method in the framework of GGA-PBE, as embodied in the WIEN2k code, is used to investigate the structural, electronic and magnetic properties of intermetallic Ti<sub>1+x</sub>FeSb Heusler compounds, where ( $x = i/4$ ,  $i = -3, -2, -1, 0, 1, 2, 3, 4$ ) and the TiFe<sub>0.75</sub>M<sub>0.25</sub>Sb (M = Ni, Mn) quaternary semi-Heusler compounds. Moreover, the modified Becke-Johnson exchange potential, as a semi-local method, was employed to predict the band-gap more precisely. We examined the site preference of the parent compound TiFeSb and varying the electron concentration by doping or removing a Ti atom. It is found that they play a crucial role in physical properties of these material systems. The lattice parameters and spin magnetic moment calculated were consistent with the previous experimental and theoretical data available. Moreover, alloys with  $x < 0$  are found to exhibit a ferrimagnetic phase, and the alloy with  $x = 0.25$  exhibit a non-magnetic properties, whereas the rest have shown ferromagnetic phase. The band-structure analysis of Ti<sub>1.75</sub>FeSb, Ti<sub>2</sub>FeSb and TiFe<sub>0.75</sub>Ni<sub>0.25</sub>Sb alloys suggested that they could be a ferromagnetic half-metallic members with band-gaps 0.67, 0.41 and 0.54 eV, respectively.

**T1.00149 Stability of Carbyne: First Principles Approach**, KEVIN KWON, COLIN HOLMES, SEUNG SOON JANG, School of Materials Science and Engineering, Georgia Institute of Technology 771 Ferst Drive, Atlanta, GA 30332-0245 — Over the last decade, carbon based nanomaterials have gained attention due to the discovery of graphene and its extraordinary properties. This has inspired new research into other carbon allotropes to obtain their unique properties. Carbyne is one such allotrope composed of linear sp-hybridized carbon bonds that has promising results and characteristics to surpass graphene's mechanical strength and possess novel electrical properties. It has two semi-stable conformations: Polyyne (alternating triple and single bonds) and Polycumulene (repeating double bonds). We investigated the stability of these forms with infinite chain lengths by employing periodic boundary conditions. Geometric optimization was performed using DMol3 with GGA PBE. After comparing the energies, the most stable form alternated between Polyyne and Polycumulene as the number of carbon atoms within each boundary increased; furthermore, every odd carbon atoms showed Polyyne as the most stable form, while every even number of carbon atoms showed Polycumulene as the most stable form. Considering k-point sampling resulted in the Polycumulene structure being the most stable as the number of k-points increased.

**T1.00150 Development and Validation of Polarized Models for Peptide-Graphene Interactions**, HENDRIK HEINZ, AMANDA GARLEY, NABANITA SAIKIA, University of Colorado - Boulder, STEPHEN BARR, GARY LEUTY, RAJIV BERRY, Air Force Research Laboratory — Biosensor technologies require the understanding of interactions between organic and inorganic materials to tune electric response functions, such as peptide assembly on graphitic substrates. Laboratory characterization of specific interactions and molecular assembly of such biomolecules in atomic resolution remains challenging. These methods can be complemented by molecular simulations and quantum-mechanical analysis of band gaps and expected conductivity. We improved common dispersive interatomic potentials for graphite and graphene to include pi electron density at virtual sites. The new models reproduce experimental X-ray structure, density, cleavage energy, hydration energy, and contact angles. As a result we have improved existing models which gave the wrong sign of hydration energies and deviations on the order of 30% in other properties. The parameters are embedded in CHARMM, CVFF, TEAM-AMBER, and other common force fields as part of the INTERFACE force field. An analysis of binding residues, binding energies, conformations, and dynamic information of molecular mobility on the surfaces will be presented.

**T1.00151 Accurate prediction of the refractive index of polymers using first principles and data modeling**, MOHAMMAD ATIF FAIZ AFZAL, CHONG CHENG, JOHANNES HACHMANN, State Univ of NY - Buffalo — Organic polymers with a high refractive index (RI) have recently attracted considerable interest due to their potential application in optical and optoelectronic devices. The ability to tailor the molecular structure of polymers is the key to increasing the accessible RI values. Our work concerns the creation of predictive *in silico* models for the optical properties of organic polymers, the screening of large-scale candidate libraries, and the mining of the resulting data to extract the underlying design principles that govern their performance. This work was set up to guide our experimentalist partners and allow them to target the most promising candidates. Our model is based on the Lorentz-Lorenz equation and thus includes the polarizability and number density values for each candidate. For the former, we performed a detailed benchmark study of different density functionals, basis sets, and the extrapolation scheme towards the polymer limit. For the number density we devised an exceedingly efficient machine learning approach to correlate the polymer structure and the packing fraction in the bulk material. We validated the proposed RI model against the experimentally known RI values of 112 polymers. We could show that the proposed combination of physical and data modeling is both successful and highly economical to characterize a wide range of organic polymers, which is a prerequisite for virtual high-throughput screening.

**T1.00152 Nanoscale Characterization of Organometal Trihalide Perovskite using Photothermal Induced Resonance (PTIR) Technique**, JUNGSEOK CHAE, ANDREA CENTRONE, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, YONGBO YUAN, YUCHUAN SHAO, QI WANG, ZHENG GUO XIAO, QINGFENG DONG, JINSONG HUANG, Department of Mechanical and Materials Engineering, University of Nebraska-Lincoln — Further improvement of the performance of organometal trihalide perovskites (OTP) solar cells can be aided by nanoscale characterization. Photothermal induced resonance (PTIR), is a novel scanning probe method that enable measuring vibrational and electronic absorption maps and spectra with a resolution as high as 20 nm. In this presentation, the chemical composition and bandgap of OTP thin films was characterized with PTIR: 1) to identify the origin of the switchable photovoltaic effect and 2) to quantify the local chloride content in mixed-halide perovskites. PTIR vibrational maps recorded in correspondence of methyl ammonium ions (MA<sup>+</sup>) for a as prepared lateral structure solar cell were uniform but displayed stronger intensity in proximity of the cathode after electric poling. Those measurements provide the first direct proof of ion electron migration in OTP devices. Because chloride incorporation modifies the bandgap in MAPbI<sub>3</sub>-xCl<sub>x</sub> perovskites, PTIR electronic maps and spectra were used to extract the local chloride content as a function of annealing. Results show that the as-prepared sample consist of a mixture of Cl-rich and Cl-poor phases that evolves into a homogenous Cl-poorer phase upon annealing. This measurement suggests that Cl<sup>-</sup> is progressively expelled from the film.

**T1.00153 High Pressure Raman Spectroscopic Studies on CuInTe<sub>2</sub> Quantum Dots<sup>1</sup>**, HOWARD YANXON, RAVHI KUMAR, University of Nevada Las Vegas - HiPSEC, HIPSEC - UNIVERSITY OF NEVADA LAS VEGAS TEAM — High pressure Raman spectroscopy studies were performed on CuInTe<sub>2</sub> Quantum Dots (QD) up to 7.7 GPa. At ambient conditions, the Raman modes of the QD loaded into a high-pressure diamond anvil cell (DAC) were observed at 125.1 cm<sup>-1</sup> (A<sub>1</sub> mode) and 142.8 cm<sup>-1</sup> (B<sub>2</sub> or E mode). As the pressure increases, the A<sub>1</sub> mode starts to split above 2 GPa and shifts to the left as indication of a structural change. A pressure-induced phase transition was observed around 2.9 GPa due to the collapse of the modes with the appearance of a new Raman peaks. The phase transition observed in our experiments compare well with the characteristics of bulk and larger nanoparticles. Further, it could be concluded that the phase transition pressure observed mainly depends on the particle size.

<sup>1</sup>H.Y. thanks McNair foundation for fellowship award. He also acknowledges Melanie White, Jason Baker and Phuc Tran for help in the experiments. He thanks Michael Pravica for using the Raman facility.

**T1.00154 Tunneling spectroscopy of multi-shell carbon fullerenes<sup>1</sup>**, KEITH DOORE, MATT COOK, ERIC CLAUSEN, TIM KIDD, ZHIPENG YE, GAIHUA YE, RUI HE, ANDREW STOLLENWERK, University of Northern Iowa — Carbon allotropes such as fullerenes and nanotubes have generated considerable interest due possible exploitation of their mechanical and electrical properties for practical applications. Carbon onions are a type of fullerene consisting of multiple spherically concentric shells of curved graphitic sheets. Compared to single-shell fullerenes, few studies have been directed toward understanding the structural and electrical properties of carbon onions. Because carbon onions have proven difficult to fabricate in a controlled method, most of these studies have focused on synthesis methods. In this study, we investigate the electrical properties of carbon onions using a scanning tunneling microscope. Carbon onions were fabricated using ultrasonic agitation to break down isopropanol facilitated by a MoS<sub>2</sub> catalyst. Particles suspended in the remaining solution were deposited onto atomically flat HOPG substrates. Scanning tunneling spectroscopy indicate that carbon onions can exhibit both metallic and semiconducting properties, similar to carbon nanotubes.

<sup>1</sup>This work was supported in part by the National Science Foundation, Grants No. DMR-1206530 and No. DMR- 1410496.

**T1.00155 Electro-optical properties of a bilayer  $\beta$ -graphyne<sup>1</sup>**, MÓNICA PACHECO, UNIVERSIDAD TECNICA FEDERICO SANTA MARIA, ALEJANDRO LEÓN, UNIVERSIDAD DIEGO PORTALES — Graphynes (GYs) are graphene-like structures that can be constructed by replacing some bonds = C = C = in graphene by acetylenic linkages, - C  $\equiv$  C - [1]. According to first-principles calculations [2] the so-called  $\beta$ -graphyne, has a Dirac cone not located at the K and K' points of the Brillouin zone but on lines between the high symmetry  $\Gamma$  and M points. In a previous work we show that a bilayer of  $\beta$ -graphyne can be metal or semiconductor, depending on the staking. An electric field applied perpendicular to the layers has remarkable effects on the electronic properties of this structure. We have found that the field can close the gap in the case of semiconductor bilayers [3]. In this work we perform a theoretical study of the electro-optical properties of a bilayer  $\beta$ -graphyne. Calculations are based on density functional theory (DFT) method. The indirect and direct band gap of the optimized lattice parameters is calculated by ABINIT. Finally, the dielectric function of the bilayer  $\beta$ -graphyne is calculated. Our results show that the optical properties of this type of graphyne are strongly anisotropic and that the optical band gap can be tuned by means of an external electric field. [1] Baughman RH et al., Chem. Phys., 87 (1987) 6687. [2] Malko D et al., Phys. Rev. Lett., 108 (2012) 086804 [3] León A, Pacheco M, Chem. Phys. Lett., 620 (2015) 67

<sup>1</sup>FONDECYT N 1151316

**T1.00156 ABSTRACT WITHDRAWN —**

**T1.00157 Reactivity of Graphene Investigated by Density-Functional Theory<sup>1</sup>**, HIMADRI SONI, JULIAN GEBHARDT, ANDREAS GRUNG, Friedrich-Alexander Universität Erlangen-Nürnberg, CHAIR OF THEORETICAL CHEMISTRY TEAM — Using spin-polarized density-functional theory, we study the adsorption and reaction of hydrogen and fluorine with graphene. Graphene has a bipartite lattice with two different sublattices and hence, due to Lieb's theorem, the inequality between two sublattices should lead to a net magnetic moment upon adsorption of hydrogen or fluorine. Our calculations using density-functional theory with the generalized gradient approximation predict a magnetic moment of 1 B for a single hydrogen adsorbed on graphene but not for a single fluorine atom adsorbed on graphene. Switching to hybrid density-functional theory with the HSE functional [1], we obtain a magnetic moment of 1 B for a single fluorine atom adsorption on graphene. This is in line with work of Kim et al. [2], who also found in density-functional theory calculations with the HSE exchange-correlation functional spin-polarization for a fluorine adatom on graphene. Here, we present a systematic study of the reactivity and relevant adsorption mechanism for single-sided graphene, i.e., a graphene sheet which is accessible by an adsorbate from only one side with hydrogen and fluorine using hybrid density-functional theory. References 1) AV Krukau et al., J. Chem. Phys. 125,224106(2006) 2) H-J Kim et al., Phys. Rev B 87,174435(2013)

<sup>1</sup>German Research Council (DFG) by the Collaborative Research Center 953

**T1.00158 Electronic structures of hybrid graphene/boron nitride nanoribbons with hydrogen adsorption<sup>1</sup>**, CHI-HSUAN LEE, CHIH-KAI YANG, National Chengchi University — Electronic properties of hybrid graphene/boron nitride nanoribbons are investigated using density functional calculations. It is found that hydrogen adsorption on a graphene nanoribbon alters band structures drastically. Furthermore, H-vacancy chains and lines can effectively shape the conduction properties. Influences of edge atoms with nonzero magnetic moments and the interface between B and N are also prominent in the electronic structures.

<sup>1</sup>This work was supported by the Ministry of Science and Technology of the Republic of China under grant number MOST 104-2112-M-004-003

**T1.00159 Role of Cooperative Interactions in the Intercalation of Heteroatoms between Graphene and a Metal Substrate**, SHIXUAN DU, Institute of Physics, Chinese Academy of Sciences — Graphene, a two-dimensional crystal of carbon atoms packed in a honeycomb structure, has many promising mechanical, electrical, and optical properties. The intercalation of heteroatoms between graphene and a metal substrate has been studied intensively over the past few years, due to its effect on the graphene properties, and as a method to create vertical heterostructures. Various intercalation processes have been reported with different combinations of heteroatoms and substrates. In this talk, I will present the investigation of the key processes governing the intercalation of heteroatoms between graphene and a substrate by combining atomic-scale characterization with density functional theory (DFT). Si intercalation between graphene and Ru(0001) is chosen as a test bed. We elucidate the role of cooperative interactions between heteroatoms, graphene, and substrate. By combining scanning tunneling microscopy with density functional theory, the intercalation process is confirmed to consist of four key steps, involving creation of defects, migration of heteroatoms, self-repairing of graphene, and growth of an intercalated monolayer. Other combinations of heteroatoms (such as Ni, Pd and Pt) and substrates (such as Ir(111) and SiC(0001)) are also investigated to support the generality of our study. Both theory and experiments indicate that this mechanism applies also to other combinations of heteroatoms and substrates. (G. Li et al., J. Am. Chem. Soc. 137 (2015) 7099. In collaboration with G. Li, H.T. Zhou, L.D. Pan, Y. Zhang, L. Huang, W.Y. Xu, and H.J. Gao in CAS, Min Ouyang in MU, and A.C. Ferrari in U. Cambridge.)

**T1.00160 Optical properties of AAB-stacked trilayer graphene.**, CHIH-WEI CHIU, Department of Physics, National Kaohsiung Normal University, Taiwan, RONG-BIN CHEN, Center of General Studies, National Kaohsiung Marine University, Taiwan, MING-FA LIN, Department of Physics, National Cheng Kung University, Taiwan, YUAN-CHENG HUANG, Center for General Education, Kao Yuan University, Taiwan — The band structures and optical properties of AAB-stacked trilayer graphenes (AAB-TLG) are calculated by the tight-binding model and gradient approximation. There are one pair of parabolic bands and two pairs of wavy bands at low energy, and three pairs of saddle points at the middle energy. At zero electric field, 3<sup>2</sup> excitation channels exist in both the low and middle frequencies, and cause the very rich joint density of states (JDOS). However, the structures in the JDOS do not appear in the absorption spectra completely. In the spectra, due to the velocity metric elements, the transitions between the same pair only make the slight contributions in the low frequency, except for the transition between the pair of the lowest bands. Furthermore, three transitions with the similar energies at the saddle points peaks lead to a strong peak in the middle frequency. The energy dispersions and the energy spacing exhibit obvious variations with the change of the electric field, and thus the absorption spectra..

**T1.00161 A new way of describing the Dirac bands in graphene**, GREGORY KISSINGER, SASHI SATPATHY, University of Missouri-Columbia — We develop a new way of describing the electronic structure of graphene, by treating the honeycomb lattice as a network of one-dimensional quantum wires. The electrons travel as free particles along these quantum wires and interfere at the three-way junctions formed by the carbon atoms. The model generates the linearly dispersive Dirac cone band structure as well as the chiral nature of the pseudo-spin sublattice wave functions. When vacancies are incorporated, we find that it also reproduces the well known zero mode states. This simple approach might have advantages over other methods for some applications, such as in analyzing electronic transport through graphene nanoribbons. In addition, this finding suggests new ways of constructing Dirac band materials in the laboratory by nano-patterning for investigating Dirac fermions.

**T1.00162 Electronic and geometrical properties of monoatomic and diatomic 2D honeycomb lattices. A DFT study<sup>1</sup>**, NGELA ROJAS, RAFAEL REY, KAREN FONSECA, Universidad Nacional de Colombia, GRUPO DE FÍSICA E INFORMÁTICA CUNTA TEAM — Since the discovery of graphene by Geim and Novoselov at 2004, several analogous systems have been theoretically and experimentally studied, due to their technological interest. Both monoatomic lattices, such as silicene and germanene, and diatomic lattices (h-GaAs and h-GaN) have been studied. Using Density Functional Theory we obtain and confirm the chemical stability of these hexagonal 2D systems through the total energy curves as a function of interatomic distance. Unlike graphene, silicene and germanene, gapless materials, h-GaAs and h-GaN exhibit electronic gaps, different from that of the bulk, which could be interesting for the industry. On the other hand, the ab initio band structure calculations for graphene, silicene and germanene show a non-circular cross section around K points, at variance with the prediction of usual Tight-binding models. In fact, we have found that Dirac cones display a dihedral group symmetry. This implies that Fermi speed can change up to 30% due to the orientation of the wave vector, for both electrons and holes. Traditional analytic studies use the Dirac equation for the electron dynamics at low energies. However, this equation assumes an isotropic, homogeneous and uniform space.

<sup>1</sup>Authors would like to thank the División de Investigación Sede Bogotá for their financial support at Universidad Nacional de Colombia. A. M. Rojas-Cuervo would also like to thank the Colciencias, Colombia.

**T1.00163 Magneto-optical transitions in bilayer graphene nanoribbons<sup>1</sup>**, HSIEN-CHING CHUNG, MING-FA LIN, Natl Cheng Kung Univ — We utilize the tight-binding theory to study the magneto-optical transitions in bilayer graphene nanoribbons. The magneto-absorption spectra highly depend on the stacking, edge orientation, ribbon width, and strength of magnetic field. The competition between the magnetic quantization and lateral confinement results in the coexistence of edge-dependent selection rules and magneto-absorption selection rule. The magneto-electronic properties, including energy dispersions, density of states, and wave functions, are also discussed in detail.

<sup>1</sup>One of us (Hsien-Ching Chung) thanks Ming-Hui Chung and Su-Ming Chen for financial support. This work was supported in part by the National Science Council of Taiwan under grant number NSC 102-2112-M-006-007-MY3.

**T1.00164 Semiconducting graphene nanoribbon fabricated by gate-controlled, edge-selective photo-oxidation of graphene.**, MORIHIRO MATSUMOTO, RYO NOUCHI, Nanoscience and Nanotechnology Research Center, Osaka Prefecture University, Sakai 599-8570, Japan — Graphene is attracting much attention for its ultrahigh carrier mobility, and is expected as the next generation material which makes high speed communication possible. However, since graphene has no bandgap, its conductivity cannot be turned completely off. Thus, pristine graphene cannot be used as a transistor in logic applications, where high on/off current ratios are required. It is known that narrow graphene nanoribbons with nanometer-scale widths show semiconducting characteristics with sufficiently large bandgap [1]. In this presentation, we propose and demonstrate a new method to fabricate graphene nanoribbons at room temperature in air. We have found that ultraviolet(UV)-induced photochemical reactions can be controlled by a configuration of a field effect transistor, and graphene edges are selectively photo-oxidized by the UV irradiation under a negative gate voltage and a finite drain voltage [2]. By means of this gate-controlled, edge-selective photo-oxidation, we succeeded to improve the on/off ratio from 2.7 to 43 at room temperature. [1] Y. W. Son, M. L. Cohen, and S. G. Louie, Phys. Rev. Lett. **97**, 216803 (2006). [2] N. Mitoma and R. Nouchi, Appl. Phys. Lett. **103**, 201605 (2013).

**T1.00165 Controllably Inducing and Modeling Optical Response from Graphene Oxide**, NICHOLAS LOMBARDO, Central Connecticut State University, ANTON NAUMOV, Texas Christian University — Graphene, a novel 2-dimensional  $sp^2$ -hybridized allotrope of Carbon, has unique electrical and mechanical properties. While it is naturally a highly conductive zero band gap semiconductor, graphene does not exhibit optical emission. It has been shown that functionalization with oxygen-containing groups elicits an opening of band gap in graphene. In this work, we aim to induce an optical response in graphene via controlled oxidation, and then explore potential origins of its photoluminescence through mathematical modeling. We employ timed ozone treatment of initially non-fluorescent reduced graphene oxide (RGO) to produce graphene oxide (GO) with specific optical properties. Oxidized material exhibits substantial changes in the absorption spectra and a broad photoluminescence feature, centered at 532 nm, which suggests the appearance of a band gap. We then explore a number of possible mechanisms for the origin of GO photoluminescence via PM3 and ab initio calculations on a functionalized single sheet of graphene. By adjusting modeling parameters to fit experimentally obtained optical transition energies we estimate the size of the  $sp^2$  graphitic regions in GO and the arrangement of functional groups that could be responsible for the observed emission.

**T1.00166 Plasmon-polaritonic bands in sequential doped graphene superlattices<sup>1</sup>**, FELIPE RAMOS-MENDIETA, Departamento de Investigación en Física, Universidad de Sonora, MARTHA PALOMINO-OVANDO, Facultad de Ciencias Físico-Matemáticas, Benemérita Universidad Autónoma de Puebla, ALEJANDRO HERNÁNDEZ-LÓPEZ, Facultad de Ciencias Físico-Matemáticas, Benemérita Universidad Autónoma de Puebla, IVÁN FUENTECILLA-CÁRCAMO, Facultad de Ciencias Físico-Matemáticas, Benemérita Universidad Autónoma de Puebla — Doped graphene has the extraordinary quality of supporting two types of surface excitations that involve electric charges (the transverse magnetic surface plasmons) or electric currents (the transverse electric modes). We have studied numerically the collective modes that result from the coupling of surface plasmons in doped graphene multilayers. By use of structured supercells with fixed dielectric background and inter layer separation, we found a series of plasmon-polaritonic bands of structure dependent on the doping sequence chosen for the graphene sheets. Periodic and quasiperiodic sequences for the graphene chemical potential have been studied. Our results show that transverse magnetic bands exist only in the low frequency regime but transverse electric bands arise within specific ranges of higher frequencies. Our calculations are valid for THz frequencies and graphene sheets with doping levels between 0.1 eV and 1.2 eV have been considered.

<sup>1</sup>AHL and IFC acknowledge fellowship support from CONACYT México

**T1.00167 Localization properties of graphene Landau levels: The role of edge states**, DANIEL SOLIS, Instituto de Física IFGW, Universidade Estadual de Campinas, CARLOS PAEZ, PETER SCHULZ, ANA PEREIRA, Faculdade de Ciências Aplicadas FCA, Universidade Estadual de Campinas, Limeira — The observation of the quantum Hall effect for graphene in 2005 represented an important landmark, proving the genuine two-dimensional nature of graphene. Here we use a tight-binding approach to investigate the localization properties of quantum Hall edge states of graphene flakes with sharp edges. In order to identify which wave function is concentrated in the edges, or distributed in the bulk, we defined a quantity named "Edge Fraction", indicating the fraction of electronic probability densities over the atomic sites at distances from the edges limited to twice the magnetic length  $l_B$ . We also calculate separately the fraction of the wave function amplitude over zigzag or armchair edges, observing an interesting and clear pattern for different energies between consecutive Landau levels. The edge states are manifested in the presence of states among the Landau levels. Here we explored the interplay of different square lattices sizes and disorder in the localization properties of the system. We observed that size variation do not affect the behavior of the Edge Fraction. Also it was found that exist a dependence between the behavior of the Edge Fraction for the armchair and zigzag contribution with respect to disorder.

**T1.00168 STRONGLY CORRELATED SYSTEMS, INCLUDING QUANTUM FLUIDS AND SOLIDS** —

**T1.00169 Optical Signatures of Weyl Points in TaAs**, BING XU, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100190, China, YAOMIN DAI, Center for Integrated Nanotechnologies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA, LINGXIAO ZHAO, KAI WANG, RUN YANG, WEI ZHANG, JINYUN LIU, HONG XIAO, GENFU CHEN, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100190, China, A. J. TAYLOR, D. A. YAROTSKI, R. P. PRASANKUMAR, Center for Integrated Nanotechnologies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA, XIANGGANG QIU, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100190, China — We present a systematic study of both the temperature and frequency dependence of the optical response in TaAs, a material that has recently been realized to host the Weyl semimetal state. Our study reveals that the optical conductivity of TaAs features a narrow Drude response alongside a conspicuous linear dependence on frequency. The width of the Drude peak decreases upon cooling, following a  $T^2$  temperature dependence which is expected for Weyl semimetals. Two linear components with distinct slopes dominate the 5-K optical conductivity. A comparison between our experimental results and theoretical calculations suggests that the linear conductivity below  $\sim 230 \text{ cm}^{-1}$  is a clear signature of the Weyl points lying in very close proximity to the Fermi energy.

**T1.00170 Theoretical analysis of high-resolution X-ray absorption spectra and 2p-3d resonant X-ray emission spectra of CeO<sub>2</sub>** , HIRONORI TONAI, Osaka Prefecture University, NAOMI KAWAMURA, MASAICHIRO MIZUMAKI, JASRI/SPRing-8, TAKAYUKI UOZUMI, Osaka Prefecture University — The 3d and 4f systems show various attractive phenomena due to strong electron correlations. The X-ray core-level spectroscopy, such as X-ray absorption spectroscopy (XAS), is an efficient technique to investigate electronic states of the systems. Recent years, the experimental techniques have been rapidly developing, and, especially, the progress in the experimental resolution has enabled us to observe fine spectral features. For example, a pioneering work was made by K. Hmlinen et al.[1] Recently, we performed high-resolution XAS experiments (partial fluorescence yield; PFY) and observed a peak corresponding to 2p-4f quadrupole transition around the pre-edge region of the L<sub>3</sub>-edge of CeO<sub>2</sub>. Conventionally, X-ray spectra have been analyzed using a phenomenological impurity Anderson model (IAM). However, such a simplified model does not seem to be appropriate for analysis of high-resolution spectrum because of possible ambiguities from the choice of adjustable parameters included. Thus we constructed an IAM framework combined with a first principle band calculation. In this meeting, we report experimental results and theoretical analysis for the PFY spectrum and 2p-3d resonant X-ray emission spectroscopy. [1] K. Hmlinen et al., PRL 67 (1991) 2850.

**T1.00171 The 4f multipole ordering effect on core-level spectroscopies of Ce intermetallics** , NORIMASA SASABE, HIRONORI TONAI, TAKAYUKI UOZUMI, Osaka Prefecture University — The 3d transition metal compounds and 4f rare earth compounds show attractive phenomena, such as superconductivity and Kondo effect, due to strong electron correlations among localized 3d and 4f electrons. Especially, multipole ordering of orbital and/or spin in 4f and 5f compounds are attracting much attention these years. For example, CeB<sub>6</sub> is known to show antiferro-quadrupolar (AFQ) ordering below 3.2K. X-ray core-level spectroscopy is an efficient technique to investigate the electronic states of strongly correlated systems. Recent years, experimental techniques have been rapidly developing and, especially, the progress in experimental resolution has enabled us to observe fine spectral features, which were not formerly observed. These advantages will enable us to observe spectral fine features related with the multipole ordering. In this study, we discuss multipole ordering effects on X-ray spectra for CeB<sub>6</sub>, especially paying attention on the polarization dependence. In order to simulate the electronic state of CeB<sub>6</sub> with the multipole ordering, we use an impurity Anderson model including realistic valence structure and a simplified RKKY interaction.

**T1.00172 Twisted Boundary Conditions for Lattice Monte Carlo Simulations** , JOSEPH PAKI, EMANUEL GULL, University of Michigan, SIMMONS MANY BODY PHYSICS COLLABORATION — Numerical simulations for spatially correlated lattice models have made progress via Dynamical Mean Field Theory and Dynamical Cluster Approximation, but are still hindered by a computational cost that scales exponentially with lattice size. We present a method of addressing finite size errors in a computationally efficient manner by running simulations with twisted boundary conditions. Averaging over these boundary conditions allows for thermodynamic extrapolation of physical quantities of interest without the cost associated with large system simulations.

**T1.00173 Structural and Magnetic Phase Coexistence in Oxygen Deficient Perovskites (Sr,Ca)FeO<sub>2.5+δ</sub>** , J. P. CARLO, M. E. EVANS, J. A. ANCZARSKI, J. OCK, K. BOYD, J. R. POLICHEMI, I. A. LEAHY, W. VOGEL, A. J. VIESCAS, G. C. PAPAETHYMIU, Villanova University — A variety of compounds crystallize into perovskite and similar structures, making them versatile laboratories for many phenomena and applications, including multiferroicity, superconductivity, and photovoltaics. Oxygen-deficient perovskites ABO<sub>x</sub> have attracted interest for use in fuel cells and related applications due to high oxygen mobility and the possibility of charge disproportionation. Vast chemical flexibility is obtained through reductions in lattice symmetry and rotation/distortion of the BO<sub>6</sub> octahedra, as well as ordering of oxygen vacancies. We have synthesized and studied the structural and magnetic properties of oxygen-deficient perovskites (Sr,Ca)FeO<sub>2.5+δ</sub> using x-ray diffraction and Mossbauer spectroscopy. While the ideal perovskite has  $\delta = 0.5$ , this requires Fe<sup>4+</sup>, and hence strongly oxidizing environments. When grown in air, Fe<sup>3+</sup> is favored, yielding  $\delta \approx 0$ . SrFeO<sub>2.5+δ</sub> exhibits cubic symmetry and paramagnetism at 300K, but CaFeO<sub>2.5+δ</sub> crystallizes into the orthorhombic brownmillerite structure, and is magnetically ordered at 300K. In the doped intermediaries we find coexistence of cubic/paramagnetic and orthorhombic/magnetic phases over a wide range of Ca content.

<sup>1</sup>Financial support from the Villanova Undergraduate Research Fellowship program and the Research Corporation for Science Advancement.

**T1.00174 ABSTRACT WITHDRAWN —**

**T1.00175 Introducing a New Capability at SSRL: Resonant Soft X-ray Scattering** , JUN-SIK LEE, HOYOUNG JANG, DONGHUI LU, SSRL/SLAC National Accelerator Laboratory, CHI-CHANG KAO, SLAC National Accelerator Laboratory — Stanford Synchrotron Radiation Lightsource (SSRL) at SLAC recently developed a setup for the resonant soft x-ray scattering (RSXS). In general, the RSXS technique uniquely probes not only structural information, but also chemical specific information. This is because this technique can explore the spatial periodicities of charge, orbital, spin, and lattice with spectroscopic aspect. Moreover, the soft x-ray range is particularly relevant for a study of soft materials as it covers the K-edge of C, N, F, and O, as well as the L-edges of transition metals and M-edges of rare-earth elements. Hence, the RSXS capability has been regarded as a very powerful technique for investigating the intrinsic properties of materials such as quantum- and energy-materials. The RSXS capability at the SSRL composes of in-vacuum 4-circle diffractometer. There are also the fully motorized sample-motion manipulations. Also, the sample can be cooled down to 25 K via the liquid helium. This capability has been installed at BL 13-3, where the photon source is from elliptically polarized undulator (EPU). Covering the photon energies is from 230 eV to 1400 eV. Furthermore, this EPU system offers more degree of freedoms for controlling x-ray polarizations (linear and circular). Using the advance of controlling x-ray polarization, we can also investigate a morphology effect of local domain/grain in materials. The detailed introduction of the RSXS end-station and several results will be touched in this poster presentation.

**T1.00176 Electric-field-driven resistive switching in dissipative Hubbard model** , JIAJUN LI, State Univ of NY - Buffalo, CAMILLE ARON, Princeton University, GABRIEL KOTLIAR, Rutgers University, JONG HAN, State Univ of NY - Buffalo — Understanding of solids driven out of equilibrium by external fields has been one of the central goals in condensed matter physics for the past century and is relevant to nanotechnology applications such as resistive transitions. We study how strongly correlated electrons on a dissipative lattice evolve from equilibrium when driven by a constant electric field, focusing on the extent of the linear regime and hysteretic non-linear effects at higher fields. We access the non-equilibrium steady states, non-perturbatively in both the field and the electronic interactions, by means of a non-equilibrium dynamical mean-field theory in the Coulomb gauge. The linear response regime is limited by Joule heating effects and breaks down at fields orders of magnitude smaller than the quasi-particle energy scale. For large electronic interactions, strong but experimentally accessible electric fields can induce a resistive switching by driving the strongly correlated metal into a Mott insulator. Hysteretic I-V curves suggest that the non-equilibrium current is carried through a spatially inhomogeneous metal-insulator mixed state.<sup>1</sup>

[1] J. Li, C. Aron, G. Kotliar, J. E. Han, Phys. Rev. Lett. **114**, 226403 (2015)

**T1.00177 Unconventional but tunable phase transition above the percolation threshold by two-layer conduction in electroless-deposited Au nanostructures on silicon substrate<sup>1</sup>**, SEUNG-HOON LEE, Department of Physics, Pukyong National University, SEONGPIL HWANG, Department of Advanced Materials Chemistry, Korea University, JAW-WON JANG<sup>2</sup>, Department of Physics, Pukyong National University — Previous research has shown that disorder, dislocation, and carrier concentration are the main factors impacting transitions in the traditional metal–insulator transition (MIT) and metal–semiconductor transition (MST). In this study, it is demonstrated that a non-traditional MST governed by two-layer conduction is possible by tuning the conducting channel of one layer of the two-layer conduction system. By means of the electroless deposition method we produced Au nanostructures (AuNFs) on p-type silicon (p-Si) as the two-layer conduction system, controlling AuNF coverage (Au%) below and above the percolation threshold (pc). Even when the AuNF coverage percentage is larger than pc, the resistivities of the AuNFs on p-Si show MST as the temperature increases. We present a conduction model based upon two predominant parallel conduction channels by AuNFs and p-Si in the present paper. In the results, we show how the temperature of the MST is tuned from 145 to 232 K as Au% is changed from 82.7 to 54.3%.

<sup>1</sup>Supported by Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (no. 2013K1A3A1A32035429 and 2015R1A1A1A05027681)

<sup>2</sup>Corresponding Author

**T1.00178 Fractal nature of metallic and insulating domain configurations in nearly grain-boundary-free VO<sub>2</sub>/TiO<sub>2</sub> thin films**, AHRUM SOHN, Ewha womans university, TERUO KANKI, HIDEKAZU TANAKA, Osaka university, DONG-WOOK KIM, Ewha womans university — We investigated evolution of the surface work function ( $W_S$ ) maps of epitaxial 15-nm-thick VO<sub>2</sub>/TiO<sub>2</sub> thin films using Kelvin probe force microscopy (KPFM) measurements while the film undergoes the metal–insulator transition (MIT). The metallic and insulating domains coexist in the VO<sub>2</sub> thin films during the transition, since the MIT is the first-order phase transition. Nearly grain-boundary-free samples allowed observation of metallic and insulating domains with distinct  $W_S$  values, throughout the transition. Each domain allowed us to obtain real space domain maps with nanoscopic spatial resolution. The two-dimensional percolation model well explained the relationship between the metallic domain fraction and the measured the resistivity. The domain maps also suggested that the percolation clusters formed a fractal surface.

**T1.00179 On metal-insulator transition in cubic fullerides**, NAOYA IWAHARA, LIVIU CHIBOTARU, Theory of Nanomaterials Group, Katholieke Universiteit Leuven — The interplay between degenerate orbital and electron correlation is a key to characterize the electronic phases in, for example, transition metal compounds [1,2] and alkali-doped fullerides [3]. Besides, the degenerate orbital couples to spin and lattice degrees of freedom, giving rise to exotic phenomena. Here, we develop the self-consistent Gutzwiller approach for the simultaneous treatment of the Jahn-Teller effect and electron correlation, and apply the methodology to reveal the nature of the ground electronic state of fullerides [4]. For small Coulomb repulsion on site  $U$ , the fulleride is quasi degenerate correlated metal. With increase of  $U$ , we found the quantum phase transition from the metallic phase to JT split phase. In the latter, the Mott transition (MT) mainly develops in the half-filled subband, whereas the empty and the completely filled subbands are almost uninvolved. Therefore, we can qualify the metal-insulator transition in fullerides as an orbital selective MT [2] induced by JT effect. [1] Y. Tokura and N. Nagaosa, Science **288**, 462 (2000). [2] A. Koga, *et al.*, Phys. Rev. Lett. **92**, 216402 (2004). [3] O. Gunnarsson, Rev. Mod. Phys. **69**, 575 (1997). [4] N. Iwahara and L. F. Chibotaru, Phys. Rev. B **91**, 035109 (2015).

**T1.00180 Vanadium dioxide thin films prepared on silicon by low temperature MBE growth and ex-situ annealing<sup>1</sup>**, PIA HOMM, BART VAN BILZEN, MARIELA MENGHINI, JEAN-PIERRE LOCQUET, KU Leuven, TODORA IVANOVA, LUIS SANCHEZ, PABLO SANCHIS, Universidad Politécnica de Valencia — Vanadium dioxide (VO<sub>2</sub>) is a material that shows an insulator to metal transition (IMT) near room temperature. This property can be exploited for applications in field effect devices, electro-optical switches and nonlinear circuit components. We have prepared VO<sub>2</sub> thin films on silicon wafers by combining a low temperature MBE growth with an ex-situ annealing at high temperature. We investigated the structural, electrical and optical characteristics of films with thicknesses ranging from 10 to 100 nm. We have also studied the influence of the substrate cleaning. The films grown with our method are polycrystalline with a preferred orientation in the (011) direction of the monoclinic phase. For the films produced on silicon with a native oxide, an IMT at around 75 °C is observed. The magnitude of the resistance change across the IMT decreases with thickness while the refractive index at room temperature corresponds with values reported in the literature for thin films. The successful growth of VO<sub>2</sub> films on silicon with good electrical and optical properties is an important step towards the integration of VO<sub>2</sub> in novel devices.

<sup>1</sup>The authors acknowledge financial support from the FWO project G052010N10 and EU-FP7 SITOGA project. PH acknowledges support from Becas Chile - CONICYT.

**T1.00181 Magnetic-order-driven topological transition in the Haldane-Hubbard model.**, HUITAO SHEN, WEI ZHENG, ZHONG WANG, HUI ZHAI, Tsinghua Univ — We study the Haldane model with on-site repulsive interactions at half-filling. We show that the mean-field Hamiltonian with magnetic order effectively modifies parameters in the Haldane Hamiltonian, such as sublattice energy difference and phase in next nearest hopping. As interaction increases, increasing of magnetic order corresponds to varying these parameters and consequently, drives topological transitions. At the mean-field level, one scenario is that the magnetic order continuously increases, and inevitably, the fermion gap closes at the topological transition point. Beyond the mean-field, fluctuation induced interaction can further open up the gap, rendering a first-order transition. Another scenario is a first-order transition at mean-field level across which a canted magnetic order develops discontinuously, avoiding the fermion gap closing. We find that both scenarios exist in the phase diagram of the Haldane-Hubbard model. Our predication is relevant to recent experimental realization of the Haldane model in cold atom system.

**T1.00182 Dilute magnetic topological semiconductors**, KYOUNG-MIN KIM, YONG-SOO JHO, KI-SEOK KIM, POSTECH — Replacing semiconductors with topological insulators, we propose the problem of dilute magnetic topological semiconductors. Performing the renormalization group analysis for an effective field theory, where doped magnetic impurities give rise to a spatially modulated random axion term, we find a novel insulator-metal transition from either a topological or band insulating phase to an inhomogeneously distributed Weyl metallic state with such insulating islands, where extremely broad distributions of ferromagnetic clusters combined with strong spin-orbit interactions are responsible for the emergence of randomly distributed Weyl metallic islands. Since electromagnetic properties in a Weyl metal are described by axion electrodynamics, the role of random axion electrodynamics in transport phenomena casts an interesting problem beyond the physics of percolation in conventional disorder-driven metal-insulator transitions.

**T1.00183 Confinement transition of  $Z_2$  gauge theory coupled to fermions. A sign problem free quantum Monte Carlo study.** , SNIR GAZIT, University of California, Berkeley, MOHIT RANDERIA, The Ohio State University, ASHVIN VISHWANATH, University of California, Berkeley — In two space dimensions, the  $Z_2$  lattice gauge theory is known to undergo a zero temperature confinement to de-confinement quantum phase transition . In this work, we study how this transition is modified in the presence of lattice fermions which are minimally coupled to the  $Z_2$  gauge field. This may be viewed as an extreme version of the BEC-BCS transition where fermions are confined in the strong coupling phase. We investigate both a square lattice model with a large fermi surface and Dirac fermions realized on a  $\pi$  flux and honeycomb lattices. The models are found to be free of the numerical sign problem for all fermion density. In addition, we introduce a numerical method to stochastically incorporate the Gauss law constraint in a quantum Monte Carlo (QMC) simulation. The phase diagram as a function of the model parameters, chemical potential and temperature is determined by means of a large scale determinant QMC.

## **T1.00184 MOVED TO V27.015 —**

**T1.00185 Angle dependence of Shubnikov-de Haas effect of filled skutterudite compounds  $\text{CeOs}_4\text{Sb}_{12}$  and  $\text{NdOs}_4\text{Sb}_{12}$** <sup>1</sup>, P.-C. HO, Califor. State U., Fresno, J. SINGLETON, F. F. BALAKIREV, NHMFL/LANL, M. B. MAPLE, UC San Diego, T. YANAGISAWA, Hokkaido U., Jpn. — Intriguingly the three filled skutterudite compounds  $\text{CeOs}_4\text{Sb}_{12}$ ,  $\text{PrOs}_4\text{Sb}_{12}$ , and  $\text{NdOs}_4\text{Sb}_{12}$  span the range from the Kondo insulator to a 1K antiferromagnetic (AFM) order, a 1.85K unconventional superconductor (SC), to a 1K mean-field type ferromagnet (FM), indicating that they reside near quantum critical points of AFM and FM with unconventional SC induced within this regime. Therefore, understanding the Fermi surfaces of  $\text{NdOs}_4\text{Sb}_{12}$  and  $\text{CeOs}_4\text{Sb}_{12}$  becomes crucial in elucidating the superconducting pairing mechanism in  $\text{PrOs}_4\text{Sb}_{12}$ . Penetration depths of single crystals of  $\text{CeOs}_4\text{Sb}_{12}$  and  $\text{NdOs}_4\text{Sb}_{12}$  were measured for temperatures down to 1.3 K and magnetic fields up to 60 tesla by using proximity detection oscillators in the Pulsed Field Facility at NHMFL/LANL. Angle dependence of Shubnikov-de Haas oscillations was detected for rotating the field with respect to the crystalline orientations [010] and [0-10]. The results indicate that  $\text{LaOs}_4\text{Sb}_{12}$ ,  $\text{PrOs}_4\text{Sb}_{12}$  and  $\text{NdOs}_4\text{Sb}_{12}$  have similar Fermi surfaces. The Fermi surface of  $\text{CeOs}_4\text{Sb}_{12}$  is rather isotropic and is much different from the other three compounds.

<sup>1</sup>Research at CSU-Fresno is supported by NSF DMR-1506677; at UCSD by NSF DMR-1206553 and US DOE DE-FG02-04ER46105; at NHMFL by DOE, NSF, and FL; at Hokkaido U by Grant-In-Aid No. 2600342,Jpn.

**T1.00186 Dipolar glass and strong magneto-electric coupling within a purely organic system** , ADAM BERLIE, ISIS Neutron and Muon Source, Science and Technology Facilities Council, UK, IAN TERRY, Department of Physics, Durham University, UK, YUN LIU, Research School of Chemistry, Australian National University, Australia, MAREK SZABLEWSKI, Department of Physics, Durham University, UK — There is much interest in the search for novel materials that show ferroelectric as well as magneto-electric coupling, such as that observed in multiferroics. Within organic based materials the electronic polarisation can come from a charge distribution across a molecule or molecules and so one must search for systems that have a electronic (and magnetic) dipole that is intrinsic. One such material is tetraethylammonium bis-7,7,8,8-tetracyanoquinodimethane ( $\text{TEA}(\text{TCNQ})_2$ ) which is a charge transfer system where there is a single electron delocalised across a TCNQ dimer. We show that dielectric measurements yield anomalies at the Peierls structural distortion and on going through the spin-Peierls transition. In both cases the electric response is glassy and at low temperature the corresponding magnetic measurements evidence the strong magneto-electric coupling within the material showing analogies to spin glass systems.

**T1.00187 Epitaxial  $\text{Ni}/\text{VO}_2$  heterostructures on Si (001)** , SRINIVASA RAO SINGAMANENI, GABRIELLE FOLEY, JOHN PRATER, JAY NARAYAN, North Carolina State University —  $\text{VO}_2$  is a strongly correlated oxide, undergoes a first order metal-insulator (MIT) well above the room temperature 340K. Previous works have shown that the stress associated with structural changes across MIT,  $\text{VO}_2$  can produce significant changes in magnetic properties of over layer ferromagnetic films such as Ni. This control of the magnetic properties could be very important to many technological applications. However, the current use of r-sapphire as substrate can be restrictive in the microelectronics industry. The previous works focused their studies on polycrystalline Ni and  $\text{VO}_2$  films, which do not allow the precise controlling of the associated properties due to poor reproducibility of polycrystalline films. We have investigated the magnetic and electronic properties of  $\text{Ni}/\text{VO}_2$  films when epitaxially integrated on Si (001) by pulsed laser deposition using domain matching epitaxy paradigm. Ni was grown both in nanoscale islands and layered form. The XRD results showed that the Ni,  $\text{VO}_2$  and YSZ layers were grown epitaxially in single out of plane orientations. We found that the hysteresis in resistance vs. temperature curves in  $\text{VO}_2$  thin films was retained even when it is in close proximity with the Ni layer which helped confirm that  $\text{VO}_2$  layer preserves its characteristic features, revealed the fingerprint magnetic features of Ni layer. We will present and discuss our comprehensive experimental findings.

**T1.00188 Exact sign structure and variational wave function of t-J chain and ladder** , QING-RUI WANG, ZHENG ZHU, Tsinghua Univ, YANG QI, Perimeter Institute, D. N. SHENG, California State University, Northridge, ZHENG-YU WENG, Tsinghua Univ — The motion of a doped hole in the anti-ferromagnetic spin background generally induces a many-body phase shift, which is identified by an exact sign structure of the t-J model known as the phase string. We find that the characteristic momentum structure, the one dimensional (1D) Luttinger liquid behavior, the quantum phase interference of the hole under a periodic boundary condition, and the breakdown of Landau's quasiparticle description can all be attributed to it. Based on the exact sign structure, we introduce a variational wave function for the t-J model and calculate physical properties such as the momentum distribution, quasiparticle weight, and hole distribution of the single-hole 1D and ladder system in detail using Monte Carlo (MC) method. An excellent agreement is found between the MC and Density Matrix Renormalization Group results.

**T1.00189 Experimental Apparatus to Observe Dynamical Manifestations of Hamiltonian Monodromy** , M. PERRY NEREM, DANIAL SALMON, JOHN DELOS, SETH AUBIN, William & Mary Coll — An experiment to observe a topological change in a classical system with nontrivial monodromy is presented. Monodromy is the study of the topological behavior of a system as it evolves along a closed path. If the system does not return to the initial topological state at the end of the circuit, that system exhibits nontrivial monodromy. Such a topological change has been predicted in certain mechanical systems, but has not yet been observed experimentally. One such system is a family of paths in a cylindrically symmetric champagne-bottle potential, with a classically forbidden region centered at the origin. We constructed this system with a long spherically symmetric pendulum and a permanent magnet attached at the end. Magnetic fields from coils are used to create the potential barrier and the external forces to drive the pendulum about a monodromy circuit. A loop of initial conditions, that is initially on one side of the forbidden region, is driven smoothly about this circuit such that it continuously evolves into a loop that surrounds the forbidden region. We will display this phenomena through numerical simulations and hopefully experimental measurement.

**T1.00190 Elastoconductivity measurements as a probe of broken mirror symmetries** , PATRIK HLOBIL, Karlsruhe Institute of Technology, AKASH V. MAHARAJ, PAVAN HOSUR, MAXWELL C. SHAPIRO, IAN R. FISHER, SRINIVAS RAGHU, Stanford University — We propose the possible detection of broken mirror symmetries in correlated two-dimensional materials by elastotransport measurements. Using linear response theory we calculate the shearconductivity  $\Gamma_{xx,xy}$ , defined as the linear change of the longitudinal conductivity  $\sigma_{xx}$  due to a shear strain  $\epsilon_{xy}$ . This quantity can only be non-vanishing when in-plane mirror symmetries are broken and we discuss how candidate states in the cuprate pseudogap regime (e.g. various loop current or charge orders) may exhibit a finite shearconductivity. We also provide a realistic experimental protocol for detecting such a response, including the specific form of the elastoresistance for broken tetragonal symmetry.

**T1.00191 Casimir effect mechanism of pairing between fermions in the vicinity of a magnetic quantum critical point**, YAROSLAV KHARKOV, UNSW, Sydney, Australia, OLEG P SUSHKOV TEAM — We consider two spin 1/2 fermions in a two-dimensional magnetic system that is close to the  $O(3)$  magnetic quantum critical point (QCP) which separates magnetically ordered and disordered phases. Focusing on the disordered phase in the vicinity of the QCP, we demonstrate that the criticality results in a strong long range attraction between the fermions, with potential  $V(r) \propto -1/r^\alpha$ ,  $\alpha \approx 0.75$ , where  $r$  is separation between the fermions. The mechanism of the enhanced attraction is similar to Casimir effect and corresponds to multi-magnon exchange processes between the fermions. While we consider a model system, the problem is originally motivated by recent experimental establishment of magnetic QCP in hole doped cuprates under the superconducting dome at doping of about 10%. We suggest the mechanism of magnetic critical enhancement of pairing in cuprates.

**T1.00192 Application of the Debye formula to the computation of x-ray diffraction patterns of nanostructured diffusion couples<sup>1</sup>**, CHARLES CHEUNG, BRIAN KELLY, KARL UNRUH, MATTHEW DECAMP, Department of Physics and Astronomy, University of Delaware — Time resolved optical pump/x-ray probe techniques have made it possible to acquire x-ray diffraction patterns corresponding to very early diffusion times in nanostructured diffusion couples. The analysis of these diffraction patterns, however, is complicated by significant line broadening and other finite size effects that appear in samples containing a relatively small number of scatterers. In order to better quantify these issues, x-ray diffraction patterns have been calculated by the direct application of the Debye formula to core/shell and thin film diffusion couples. In particular a series of diffraction patterns have been calculated as a function of the sample size and composition profile determined from the appropriate solutions to Fick's second law. The results of these calculations have been used to guide the interpretation of the measured diffraction patterns of Pt/Ni core/shell nanoparticles and Pt/Ni thin film multilayers.

<sup>1</sup>This material is based upon work supported by the National Science Foundation under Grant No. 1410076

## **T1.00193 SUPERCONDUCTIVITY —**

**T1.00194 All-metal superconducting planar microwave resonator<sup>1</sup>**, MATT HORSLEY, SERGEY PEREVERZEV, JONATHAN DUBOIS, STEPHAN FRIEDRICH, DONGXIA QU, STEVE LIBBY, VINCENZO LORDI, GIANPAOLO CAROSI, WOLFGANG STOEFFL, GEORGE CHAPLINE, OWEN DRURY, Lawrence Livermore National Laboratory, QUANTUM NOISE IN SUPERCONDUCTING DEVICES TEAM — There is common agreement that noise and resonance frequency jitter in superconducting microwave planar resonators are caused by presence of two-level systems, or fluctuators, in resonator materials- in dielectric substrate, in superconducting and dielectric layers and on the boundaries and interfaces. Scaling of noise with device dimensions indicate that fluctuators are likely concentrated around boundaries; physical nature of those fluctuators remains unclear. The presence of dielectrics is not necessary for the superconducting device functionality, and one can ask question about properties of all-metal device, where dielectric substrate and oxide films on metal are absent. Resonator made from of thin conducting layer with cuts in it is usually called slot line resonator. We report on the design, fabrication and initial testing of multiple split rings slot line resonator made out of thin molybdenum plate.

<sup>1</sup>This work is being funded as part of a three year strategic initiative (LDRD 16-SI-004) to better understand noise in superconducting devices

**T1.00195 Normal state above the upper critical field in Fe<sub>1+y</sub>Te<sub>1-x</sub>(Se,S)<sub>x</sub>.**, AIFENG WANG, Brookhaven National Laboratory, ERIK KAMPERT, Hochfeld-Magnetlabor Dresden (HLD), H. SAADAOUI, H. LUETKENS, Paul Scherrer Institute, RONGWEI HU, Brookhaven National Laboratory, E. MORENZONI, Paul Scherrer Institute, J. WOSNITZA, Hochfeld-Magnetlabor Dresden (HLD), CEDOMIR PETROVIC, Brookhaven National Laboratory — We have investigated characteristics of the normal state above the upper critical field ( $H_{c2}$ ) in Fe<sub>1.14</sub>Te<sub>0.7</sub>Se<sub>0.3</sub>, Fe<sub>1.02</sub>Te<sub>0.61</sub>Se<sub>0.39</sub>, Fe<sub>1.05</sub>Te<sub>0.89</sub>Se<sub>0.11</sub>, and Fe<sub>1.06</sub>Te<sub>0.86</sub>S<sub>0.14</sub>. Superconductivity is suppressed in high magnetic fields above 60 Tesla, allowing for the insight into normal state below the superconducting transition temperature ( $T_c$ ). We show that Fe<sub>1.14</sub>Te<sub>0.7</sub>Se<sub>0.3</sub> and Fe<sub>1.02</sub>Te<sub>0.61</sub>Se<sub>0.39</sub> resistivity above the  $H_{c2}$  is metallic as  $T \rightarrow 0$ , just like the normal state resistivity above  $T_c$ . On the other hand, Fe<sub>1.05</sub>Te<sub>0.89</sub>Se<sub>0.11</sub> and Fe<sub>1.06</sub>Te<sub>0.86</sub>S<sub>0.14</sub> normal state resistivity is nonmetallic as  $T \rightarrow 0$ , reflecting the normal state resistivity above  $T_c$ . These results suggest that conductivity of normal states above  $H_{c2}$  is connected with the details of crystal structure inhomogeneity.

**T1.00196 Observation of Superconducting Fluctuations above  $T_c$  in underdoped BaFe<sub>2-x</sub>Ni<sub>x</sub>As<sub>2</sub>**, WEI ZHANG, HUIQIAN LUO, RUI ZHANG, XINGYE LU, BING XU, KAI WANG, RUN YANG, JINYUN LIU, Institute of Physics, Chinese Academy of Sciences, HAO YANG, College of Physics, Optoelectronics and Energy Collaborative Innovation Center of Suzhou Nano Science and Technology, Soochow University, XIANGGANG QIU, Institute of Physics, Chinese Academy of Sciences, INSTITUTE OF PHYSICS, CHINESE ACADEMY OF SCIENCES TEAM, COLLEGE OF PHYSICS, OPTOELECTRONICS AND ENERGY COLLABORATIVE INNOVATION CENTER OF SUZHOU NANO SCIEN TEAM — Angular dependent torque measurements have been performed on the electron doped iron pnictide superconductors BaFe<sub>2-x</sub>Ni<sub>x</sub>As<sub>2</sub> with a series Ni doping ( $0.03 \leq x \leq 0.3$ ). In the superconducting state, an irreversibility, as the evidence for the pinning of vortex, is observed between the torque measured with increasing and decreasing angle. Our results in underdoped sample ( $x = 0.065$ ) show that the irreversible torque signal can survive up to a temperature  $T_{irr}$  well above the superconducting transition temperature  $T_c$ , suggesting the existence of superconducting fluctuations (SCF) above  $T_c$ . The Ni doping dependent phase diagram both for  $T_{irr}$  and  $T_c$  with a strong SCF region in the underdoped samples, is summarized based on our results.

**T1.00197 Persistence of Dirac Node near Antiferromagnetic-to-Superconducting Phase Boundary in Ba(Fe<sub>1-x</sub>Co<sub>x</sub>)<sub>2</sub>As<sub>2</sub>**, HITOSHI TAKITA, NAOYA KISHIMOTO, YOUSUKE NAKASHIMA, Hiroshima University, AKIHIRO INO, MASASHI ARITA, HIROHUMI NAMATAME, MASAKI TANIGUCHI, Hiroshima Synchrotron Radiation Center, YOSHIHIRO AIURA, IZUMI HASE, HIROSHI EISAKI, KUNIHIRO KIHOU, CHUL-HO LEE, AKIRA IYO, National Institute of Advanced Science and Technology, MASAMICHI NAKAJIMA, Osaka University, SHIN-ICHI UCHIDA, University of Tokyo, HIROSHIMA UNIVERSITY TEAM, HIROSHIMA SYNCHROTRON RADIATION CENTER TEAM, NATIONAL INSTITUTE OF ADVANCED SCIENCE AND TECHNOLOGY TEAM, OSAKA UNIVERSITY TEAM, UNIVERSITY OF TOKYO TEAM — Since the ground state of iron-pnictides changes from an antiferromagnetic (AF) phase to a superconducting (SC) phase, the evolution of electronic structure has attracted much attention. However, systematic investigation has been hindered by the intricate multiple bands arising from the orbital degree of freedom of iron 3d states. Here we performed a polarization-dependent ARPES study of Ba(Fe<sub>1-x</sub>Co<sub>x</sub>)<sub>2</sub>As<sub>2</sub> across the AF-SC phase boundary. The doping-dependence of ARPES spectra has shown that the Dirac node reported in the AF phase of BaFe<sub>2</sub>As<sub>2</sub> persists in  $x = 0.04$  near the AF-SC phase boundary, and that it disappears in the SC phase of  $x = 0.05$ . We parametrized the cone-like dispersion in  $x = 0.04$ . The polarization-dependence of our ARPES spectra is consistent with the view that the Dirac node is protected by Berry phase arising from orbital degree of freedom under the inversion symmetry.

**T1.00198 Unconventional superconductivity in  $\text{CaFe}_{0.85}\text{Co}_{0.15}\text{AsF}$  evidenced by torque measurements**, HONG XIAO, Center for High Pressure Science and Technology Advanced Research, X. J. LI, G. MU, T. HU, Shanghai Institute of Microsystem and Information Technology — Out-of-plane angular dependent torque measurements were performed on  $\text{CaFe}_{0.85}\text{Co}_{0.15}\text{AsF}$  single crystals. Abnormal superconducting fluctuation, featured by enhanced diamagnetism with magnetic field, is detected up to about 1.5 times superconducting transition temperature  $T_c$ . Compared to cuprate superconductors, the fluctuation effect in iron-based superconductor is less pronounced. Anisotropy parameter  $\gamma$  is obtained from the mixed state torque data and it is found that  $\gamma$  shows both magnetic field and temperature dependence, pointing to multiband superconductivity. The temperature dependence of penetration depth  $\lambda(T)$  suggests unconventional superconductivity in  $\text{CaFe}_{0.85}\text{Co}_{0.15}\text{AsF}$ .

**T1.00199 High- $T_c$  Superconductivity and Raman Scattering Study of the phonon properties of electron doped (transition metal, rare-earth) - Oxygen-Free  $\text{CaFeAsF}$  and compared with  $\text{RFeAsO}$  system.**, KALYAN SASMAL, VIKTOR HADJIEV, C.W(PAUL) CHU, Texas Center for Superconductivity & Dept of Physics, University of Houston, TX, USA — Quaternary  $\text{CaFeAsF}$  has  $\text{ZrCuSiAs}$ -type structure,  $(\text{RO})^{\delta+}$  layer in  $\text{RFeAsO}$  replaced by  $(\text{CaF})^{\delta+}$  layer, with tetragonal ( $P4/nmm$ )-orthorhombic ( $Cmma$ ) phase transition at 134K, while magnetic order, SDW sets in at 114K. Partial replacement of Fe with Co/Ni is direct electron doping to  $(\text{FeAs})^{\delta+}$  layer.  $T_c \sim 15\text{K}$  in  $\text{CaFe}_{0.9}\text{Ni}_{0.1}\text{AsF}$ . Substitution of rare earth metal for alkaline earth metal suppresses anomaly in resistivity & induces superconductivity.  $T_c \sim 52\text{K}$  in  $\text{Ca}_{0.5}\text{Pr}_{0.5}\text{FeAsF}$ . Characterized by resistivity, susceptibility, XRD & EDX-SEM. Upper critical field estimated from magneto resistance. Bulk superconductivity proved by DC magnetization. Hall coefficient  $R_H$  revealed hole-like charge carriers in parent compound  $\text{CaFeAsF}$ , while electron-type ( $R_H$  in normal state is  $-Ve$ ) for  $\text{Ca}_{0.5}\text{Pr}_{0.5}\text{FeAsF}$ . Evolution of Raman active phonons of  $\text{Ca}_{1-x}\text{Pr}_x\text{FeAsF}$  measured with polarized Raman spectroscopy at room temperature from  $ab$  surfaces of impurity-free microcrystals. Spectra exhibit sharp phonon lines on very weak electronic scattering background. Frequency and symmetry of Raman phonons involving out-of-plane atomic vibrations are found at  $162.5\text{ cm}^{-1}$  ( $A1g$ , Pr),  $201\text{ cm}^{-1}$  ( $A1g$ , As),  $215.5\text{ cm}^{-1}$  ( $B1g$ , Fe),  $265\text{ cm}^{-1}$  ( $Eg$ , Fe) and  $334\text{ cm}^{-1}$  ( $B1g$ , F) for  $\text{Ca}_{0.5}\text{Pr}_{0.5}\text{FeAsF}$ . Observations are compared with  $\text{RFeAsO}$  unconventional superconductors also possibly related to magnetic fluctuations

**T1.00200 Functional renormalization group study of the pairing symmetry and pairing mechanism in iron-selenide superconductors**, YUAN-YUAN XIANG, HoHai University, QIANG-HUA WANG, Nanjing University — In iron-selenide superconductors only electron-like Fermi pockets survive, challenging the  $s_{\pm}$  pairing based on the quasi-nesting between the electron and hole pockets (as in iron arsenides). By functional renormalization group study we show that an in-phase  $s$ -wave pairing on the electron pockets is realized. The pairing mechanism involve two competing driving forces: the strong C-type spin fluctuations cause attractive pair scattering between and within electron pockets via Cooperon excitations on the virtual hole-like pockets, while the G-type spin fluctuations cause repulsive pairing scattering. The latter effect is however weakened by the hybridization splitting of the electron-like pockets. The in phase  $s$ -wave pairing symmetry is consistent with the existing experiments.

**T1.00201 Electronic structure of the titanium-based oxypnictide superconductor  $\text{Ba}_{0.95}\text{Na}_{0.05}\text{Ti}_2\text{Sb}_2\text{O}$  and direct observation of its charge density wave order**, QI SONG, JUAN JIANG, YAJUN YAN, ZIRONG YE, MINGQIANG REN, SHIYONG TAN, XIAOHAI NIU, BINPING XIE, TONG ZHANG, DONGLAI FENG, Fudan Univ — The unconventional superconducting ground state usually emerges in proximity to a spin or charge ordering state, such as that in cuprates, iron-based superconductors and layered chalcogenides. This unique character offers a platform for searching unconventional superconductivity in analogous layered compounds. Recently, superconductivity has been achieved in  $\text{Ba}_{1-x}\text{Na}_x\text{Ti}_2\text{Sb}_2\text{O}$  with maximum  $T_c$  at 5.5 K, which makes this material more interesting. Here we perform high resolution angle-resolved photoemission spectroscopy and scanning tunneling microscopy studies on the titanium-based oxypnictide superconductor  $\text{Ba}_{0.95}\text{Na}_{0.05}\text{Ti}_2\text{Sb}_2\text{O}$ . The electronic structure shows both multi-orbital and three-dimensional nature, consistent with the theoretical calculations. The observed Fermi surface is well nested along the  $(\pi, \pi)$  direction, which might probably be the driving force of the CDW transition. This is further proved by the scanning tunneling microscopy result, which directly observed a CDW wave vector at  $(\pi, \pi)$  direction. However, due to the weak CDW coupling, we didn't observe the CDW gap here. Our results give a comprehensive picture of the electronic structure and direct observation of the CDW order in  $\text{Ba}_{0.95}\text{Na}_{0.05}\text{Ti}_2\text{Sb}_2\text{O}$

**T1.00202 ABSTRACT WITHDRAWN —**

**T1.00203 Dynamic Stimulation of Superconductivity with Resonant Terahertz Phonons**, ALAN M. KADIN, Princeton Junction, NJ, STEVEN B. KAPLAN, Estes Park, CO — Can superconductivity be induced at a temperature far above the equilibrium critical temperature  $T_c$ ? While small enhancements were observed many years ago and associated with nonequilibrium electron distributions, it is proposed here that much larger enhancements (up to a factor of two in temperature) may be possible by generation of coherent phonons at appropriate resonant frequencies comparable to the gap frequency, in the terahertz range. These phonon standing waves may induce real-space electron localization that forms the basis for superconducting coherence within a novel model of superconductivity [1,2]. This concept may be generalized to dynamic stimulation using coherent spin waves for non-phonon mediated superconductors such as the cuprates. Several experiments to test this are proposed. [1] S.B. Kaplan and A.M. Kadin (2012), "Superconductivity via Two-Phase Condensation of Localized Electrons", <http://absimage.aps.org/image/MAR12/MWS.MAR12-2011-002491.pdf> [2] A.M. Kadin (2009), "Superconductivity without Pairing?," <http://arxiv.org/abs/0909.2901>.

**T1.00204 Break the electron- hole balance and pressure induced superconductivity in Tungsten Ditelluride.<sup>1</sup>**, FENGQI SONG, XING-CHEN PAN, Nanjing Univ — Tungsten ditelluride has garnered immense interest due to the recent discovery of titanic unsaturated magnetoresistance up to 60 Tesla and its possible topological metal nature. The titanic unsaturated magnetoresistance is attributed to the perfect compensation between the opposite carriers in this material. Motivated by the small and sensitive Fermi surface of 5d electronic orbitals, we break the electron-hole balance by the application of high pressure. Superconductivity sharply appears at the pressure of 2.5 GPa, quickly reaching a maximum critical temperature of 7 K at around 16.8 GPa, and followed by a monotonic decrease in  $T_c$  with increasing pressure exhibiting the typical dome-shaped superconducting phase. What's more, linear magnetoresistance dominates the transport behavior under high pressure instead of semi-classical parabolic magnetoresistance, like in other topological metals. Reference: Nature Commun. 6, 7805 (2015), arXiv 1505, 07968.

<sup>1</sup>The authors would like to thank the National Key Projects for Basic Research in China, the National Natural Science Foundation of China, the NSF of Jiangsu Province, the PAPD project, and the Fundamental Research Funds for the Central Universities.

**T1.00205 Photoemission spectra of charge density wave states in cuprates**, WEI-LIN TU, Department of Physics, National Taiwan University, PENG-JEN CHEN, TING-KUO LEE, Institute of Physics, Academia Sinica — Angle-resolved photoemission spectroscopy (ARPES) experiments have reported many exotic properties of cuprates, such as Fermi arc at normal state, two gaps at superconducting state and particle-hole asymmetry at the antinodal direction[1]. On the other hand, a number of inhomogeneous states or so-called charge density waves (CDW) states have also been discovered in cuprates by many experimental groups. The relation between these CDW states and ARPES spectra is unclear. With the help of Gutzwiller projected mean-field theory[2], we can reproduce the quasiparticle spectra in momentum space. The spectra show strong correspondence to the experimental data with afore-mentioned exotic features in it. \pard1. I. Vishik et al, PNAS 109, 18332-18337(2012).. Wei-Lin Tu and Ting-Kuo Lee, arXiv: 1505.07728(2015).

**T1.00206 Quantum creep in a highly crystalline two-dimensional superconductor** , YU SAITO, The University of Tokyo, YUICHI KASAHARA, Kyoto University, JIANTING YE, University of Groningen, YOSHIHIRO IWASA, The University of Tokyo, TSUTOMU NOJIMA, Tohoku University — Conventional studies on quantum phase transitions, especially on superconductor-insulator or superconductor-metal-insulator transitions have been performed in deposited metallic thin films such as Bismuth or MoGe. Although the techniques of thin films deposition have been considerably improved, unintentional disorder such as impurities and deficiencies, generating the pinning centers, seems to still exist in such systems. The mechanical exfoliated highly crystalline two-dimensional material can be a good candidate to realize a less-disordered 2D superconductor with extremely weak pinning, combined with transfer method or ionic-liquid gating. We report on the quantum metal, namely, magnetic-field-induced metallic state observed in an ion-gated two-dimensional superconductor based on an ultra-highly crystalline layered band insulator, ZrNCl [1]. We found that the superconducting state is extremely fragile against external magnetic fields; that is, zero resistance state immediately disappears, once an external magnetic field switches on. This is because the present system is relatively clean and the pinning potential is extremely weak, which cause quantum tunneling and flux flow of vortices, resulting in metallic ground state. [1] Y. Saito et al. Science 350, 409-413 (2015).

**T1.00207 Negative Oxygen Isotope Effect on the Static Spin Stripe Order in  $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$  ( $x = 1/8$ )** , ZURAB GUGUCHIA, RUSTEM KHASANOV, Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, Switzerland, MARKUS BENDELE, Physik-Institut der Universität Zurich, Zurich, Switzerland, EKATERINA POMJAKUSHINA, KAZIMIERZ CONDER, Laboratory for Developments and Methods, Paul Scherrer Institut, Switzerland, ALEXANDER SHENGELAYA, Department of Physics, Tbilisi State University, Tbilisi, Georgia, HUGO KELLER, Physik-Institut der Universität Zurich, Zurich, Switzerland — Cuprate high temperature superconductors (HTS's) are characterized by a complex interplay between lattice, charge, and spin degrees of freedom. One of the remarkable phases is a self-organized charge/spin structure, which is known as "stripes" and is observed in some cuprates near 1/8 doping. The microscopic origin of the stripe phase is still unclear at present. We report large negative oxygen-isotope ( $^{16}\text{O}/^{18}\text{O}$ ) effects (OIE's) on the static spin-stripe ordering temperature  $T_{\text{so}}$  and the magnetic volume fraction  $V_{\text{m}}$  in  $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$  ( $x = 1/8$ ) observed by means of muon spin rotation experiments [1]. The corresponding OIE exponents were found to be  $\alpha_{T_{\text{so}}} = -0.57(6)$  and  $\alpha_{V_{\text{m}}} = -0.71(9)$ , which are sign reversed to  $\alpha_{T_{\text{c}}} = 0.46(6)$  measured for the superconducting transition temperature  $T_{\text{c}}$ . This indicates that the electron-lattice interaction is involved in the stripe formation and plays an important role in the competition between bulk superconductivity and static stripe order in the cuprates. [1] Z. Guguchia et. al., Phys. Rev. Lett. 113, 057002 (2014).

**T1.00208 Calculation of the superconducting transition temperature of a graphene layer doped with titanium and palladium.** , GERARDO VAZQUEZ, FERNANDO MAGANA, OSIRIS SALAS-TORRES, Instituto de Física, UNAM — We explore the structural interactions between graphene and transition metals such as palladium (Pd) and titanium (Ti) and the possibility of inducing superconductivity in a graphene sheet in two cases, one by doping its surface with palladium atoms sit on the center of the hexagons of the graphene layer and other by covering the graphene layer with two layers of titanium metal atoms. The results here were obtained from first-principles density functional theory in the local density approximation. The Quantum-Espresso package was used with norm conserving pseudopotentials. All of the structures considered were relaxed to their minimum energy configuration. Phonon frequencies were calculated using the linear-response technique on several phonon wave-vector mesh. The electron-phonon coupling parameter was calculated with several electron momentum k-mesh. The superconducting critical temperature was estimated using the Allen-Dynes formula with  $\mu^* = 0.1 - 0.15$ . We note that palladium and titanium are good candidate materials to show a metal-to-superconductor transition. We thank Dirección General de Asuntos del Personal Académico de la Universidad Nacional Autónoma de México, partial financial support by Grant IN-106514 and we also thank Miztli Super-Computing center the technical assistance.

**T1.00209 Formation of As-As bond and its effect on absence of superconductivity in the collapsed tetragonal phase of  $\text{Ca}_{0.86}\text{Pr}_{0.14}\text{Fe}_2\text{As}_2$ : An optical spectroscopy study** , RUN YANG, XIANGGANG QIU, Institute of Physics, Chinese Academy of Sciences, INSTITUTE OF PHYSICS, CHINESE ACADEMY OF SCIENCES TEAM, HIGH MAGNETIC FIELD LABORATORY, CHINESE ACADEMY OF SCIENCES TEAM — The temperature dependence of in-plane optical conductivity has been investigated for  $\text{Ca}_{0.86}\text{Pr}_{0.14}\text{Fe}_2\text{As}_2$ , which shows a structural transition from tetragonal (T) to collapsed tetragonal (cT) phase at  $T_{\text{cT}} \sim 73$  K. Upon entering the cT phase, drastic change characterized by the formation of a midinfrared peak near  $3200 \text{ cm}^{-1}$  (0.4 eV) in the optical conductivity is observed. Analysis of the spectral weight reveals reduced electron correlation after the cT phase transition. Based on the calculated band structure and simulated optical conductivity, we attribute the new feature around 0.4 eV to the formation of an interlayer As-As bond. The As-As bond strongly affects the Fe-As hybridizations and, in turn, drastically changes the  $\text{Ca}_{0.86}\text{Pr}_{0.14}\text{Fe}_2\text{As}_2$  into a nonmagnetic Fermi liquid system without bulk superconductivity in the cT phase.

## T1.00210 METALS AND ALLOYS —

**T1.00211 Structural  $\gamma$ - $\varepsilon$  phase transition in Fe-Mn alloys: a CPA+DMFT study<sup>1</sup>** , ALEXANDER BELOZEROV, SERGEY SKORNYAKOV, ALEXANDER POTERYAEV, VLADIMIR ANISIMOV, Institute of Metal Physics, 620137 Yekaterinburg, Russia — We study the  $\gamma$ - $\varepsilon$  structural transition in paramagnetic Fe-Mn alloys for Mn content from 10 to 20 at.% using CPA+DMFT method. This method employs the coherent potential approximation (CPA) combined with the dynamical mean-field theory (DMFT). The material-specific Hamiltonians in the Wannier function basis are obtained by density functional theory. The electronic correlations are found to play a crucial role in this transition. The calculated transition temperature decreases with increasing Mn content and is in a good agreement with experiment. We demonstrate that in contrast to the  $\alpha$ - $\gamma$  transition in pure iron, the  $\gamma$ - $\varepsilon$  transition in Fe-Mn alloys is driven by a combination of kinetic and Coulomb energies. The latter is found to be responsible for the decrease of the  $\gamma$ - $\varepsilon$  transition temperature with Mn content.

<sup>1</sup>The study was supported by the grant of the Russian Scientific Foundation (project no. 14-22-00004).

**T1.00212 An ab initio study of the structure and dynamics of bulk liquid Ag and its liquid-vapor interface.** , BEATRIZ GONZALEZ DEL RIO, LUIS ENRIQUE GONZALEZ TESEDO, DAVID JOSE GONZALEZ FERNANDEZ, Fisica Teorica, Atomica y Optica, Universidad de Valladolid — Several static and dynamic properties of bulk liquid Ag at a thermodynamic state near its triple point have been calculated by means of *ab initio* molecular dynamics simulations. The calculated static structure shows a very good agreement with the available experimental data. The dynamical structure reveals collective density excitations with an associated dispersion relation which points to a small positive dispersion. Results are also reported at a slightly higher temperature in order to study the structure of the free liquid surface. The ionic density profile shows an oscillatory behaviour with two different wavelengths, as the spacing between the outer and first inner layer is different from that between the other inner layers.

**T1.00213 Optical pump/x-ray probe studies of lattice parameter evolution in Pt nanoparticles due to sintering and grain growth**<sup>1</sup>, BRIAN KELLY, AARON LOETHER, Department of Physics and Astronomy, University of Delaware, ANTHONY DICHARA, ROBERT HENNING, Advanced Photon Source, Argonne National Laboratory, KARL UNRUH, MATTHEW DECAMP, Department of Physics and Astronomy, University of Delaware — An *in-situ* optical pump/x-ray probe technique has been developed to study the evolution in the lattice parameter of nanometer-sized Pt particles as a function of the particle size during sintering and grain growth. In particular, the lattice parameter of the as-prepared nanoparticles was observed to be about 0.4% smaller than the corresponding bulk value in good agreement with the value expected for isolated spherical particles subject only to a simple surface stress. As the as-prepared nanoparticles sinter and grow as a result of the photo-thermal irradiation, however, the evolution in the lattice parameter reflects the effects of both an increasing grain size and the evolving particle-particle interface. As a result, the lattice parameter does not evolve monotonically with increasing grain size.

<sup>1</sup>This material is based upon work supported by the National Science Foundation under Grant No. 1410076.

## T1.00214 MAGNETISM —

**T1.00215 The Magnetism of  $Mn_{2-x}Fe_xB$  Alloys : First-Principles Calculations**, PO-HAN LEE, Affiliated Senior High School of National Taiwan Normal University, Taipei, Taiwan, SHIH-WEI WANG, Stevenson School, Pebble Beach, CA USA, CHAO-YANG LIN, Department of Electrical Engineering, National Tsing Hua University, Hsinchu, Taiwan, KUANG-LING CHEN, Department of Electrical and Computer Engineering, Cornell University, NY USA, HSUAN-AN HSIA, Affiliated Senior High School of National Taiwan Normal University, Taipei, Taiwan, KUANG-YU CHEN, Department of Physics, National Taiwan University, Taipei, Taiwan, PANG-YU LIU, Department of Engineering and System Science, National Tsing Hua University, Hsinchu, Taiwan, KE-BENG CHEN, Department of Law, National Taiwan University, Taipei, Taiwan, EN-HUI LIU, Center for Nanotechnology, Materials Science and Microsystems, National Tsing Hua University, Hsinchu, Taiwan — Magnetic, electronic and structural properties of  $Mn_{2-x}Fe_xB$  ( $0 \leq x \leq 2$ ) are investigated by the First principles calculations with the virtual crystal approximation (VCA) based on the density-functional theory (DFT) with generalized gradient approximation (GGA). Although both of  $Mn_2B$  and  $Fe_2B$  have the same electronic structure of I4/MCM with different lattice constants, the former is anti-ferromagnetic and the latter ferromagnetic. All calculations, based on the four types of magnetic states of NM (non-magnetic), FM (ferromagnetic), AFM1 and AFM2 (anti-ferromagnetic), illustrate that there is a critical point of magnetic phase transition occurred at  $x$  as 0.5 from AFM2 to FM state under the condition of the lowest energy. Results are also in agreement with the Stoner model within the range of FM state.

**T1.00216 Magnetic Nanoparticles in Non-magnetic CNTs and Graphene**<sup>1</sup>, MOSES KAYONDO, DEREJE SEIFU, Morgan State University, PHYSICS — Magnetic nanoparticles were embedded in non-magnetic CNTs and graphene matrix to incorporate all the advantages and the unique properties of CNTs and graphene [1]. Composites of CNTs and graphene with magnetic nanoparticles may offer new opportunities for a wide variety of potential applications such as magnetic data storage, magnetic force microscopy tip, electromagnetic interference shields, thermally conductive films, reinforced polymer composites, transparent electrodes for displays, solar cells, gas sensors, magnetic nanofluids, and magnetically guided drug delivery systems. Magnetic nanoparticles coated CNTs can also be used as an electrode in lithium ion battery to replace graphite because of the higher theoretical capacity. Graphene nanocomposites, coated with magnetic sensitive nanoparticles, have demonstrated enhanced magnetic property. 1. D. Seifu, S. Neupane, L. Giri, S. P. Karna, H. Hong, and M. S. Seehra, "Multilayered graphene acquires ferromagnetism in proximity with magnetite particles", Appl. Phys. Lett., **106**, 212401, (2015).

<sup>1</sup>We would like to acknowledge support by NSF-MRI-DMR-1337339.

**T1.00217 Ferromagnetic  $Fe_2CrAl$  Nanowires**<sup>1</sup>, RAJENDRA DULAL, BISHNU DAHAL, IAN L PEGG, JOHN PHILIP, The Catholic University of America — Heusler alloy  $Fe_2CrAl$  (FCA) nanowires were grown on silicon substrates. Nanowires have diameters in the range 50 to 200 nm and lengths up to 100  $\mu$ m. They exhibit cubic  $L_{21}$  and  $A_2$  type structure with a space group,  $Pm\bar{3}m$ . Magnetic characterization reveals that they display ferromagnetic behavior and has a Curie temperature above 400 K. Magnetic behavior of FCA nanowires is different from the reported bulk behavior. Bulk FCA with  $L_{21}$  structure has a Curie temperature around 274 K.

<sup>1</sup>National Science Foundation under ECCS-0845501 and NSF-MRI, DMR-0922997

**T1.00218 Magnetic Properties of 3D Printed Toroids**, LINDSEY BOLLIG, AUSTIN OTTO, PETER HILPISCH, GREG MOWRY, BRITTANY NELSON-CHEESEMAN, School of Engineering, University of St. Thomas, RENEWABLE ENERGY AND ALTERNATIVES LAB (REAL) TEAM — Transformers are ubiquitous in electronics today. Although toroidal geometries perform most efficiently, transformers are traditionally made with rectangular cross-sections due to the lower manufacturing costs. Additive manufacturing techniques (3D printing) can easily achieve toroidal geometries by building up a part through a series of 2D layers. To get strong magnetic properties in a 3D printed transformer, a composite filament is used containing Fe dispersed in a polymer matrix. How the resulting 3D printed toroid responds to a magnetic field depends on two structural factors of the printed 2D layers: fill factor (planar density) and fill pattern. In this work, we investigate how the fill factor and fill pattern affect the magnetic properties of 3D printed toroids. The magnetic properties of the printed toroids are measured by a custom circuit that produces a hysteresis loop for each toroid. Toroids with various fill factors and fill patterns are compared to determine how these two factors can affect the magnetic field the toroid can produce. These 3D printed toroids can be used for numerous applications in order to increase the efficiency of transformers by making it possible for manufacturers to make a toroidal geometry.

**T1.00219 Electro-magneto-thermal characterization of ferromagnetic thin films.**, SANDEEP KUMAR, DAVIL GARCIA, Univ of California - Riverside — In this work we report electro-magneto-thermal characterization of ferromagnetic multilayer thin films. These thin films include Co/Pd, Co/Pt and CoFeB/MgO multilayers. We carried out in-situ focused magneto optic Kerr effect based hysteresis measurement while the specimen was under DC bias to ascertain the electro-magnetic behavior. These experiments are then supplemented with in-situ transmission electron microscope studies to verify the microstructural changes. We also report thermal conductivity measurements using 3-omega method. Thermal conductivity measurements suggest thermo-magnetic resistance due to spin scattering at the interfaces in multilayer thin films.

**T1.00220 Brillouin Light Scattering study of the rotatable magnetic anisotropy in exchange biased bilayers of Ni<sub>81</sub>Fe<sub>19</sub>Ir<sub>20</sub>Mn<sub>80</sub>**, ROBERTO RODRIGUEZ, Pontificia Universidad Catlica de Chile, ALEXANDRE OLIVEIRA, Univ. Fed. Rio Grande do Norte, BR-59072970 Natal, RN, Brazil, FRANCISCO ESTRADA, OBED SANTOS, ANTONIO AZEVEDO, SERGIO REZENDE, Universidade Federal de Pernambuco, 50670-901, Recife, PE, Brasil. — It is known that when a ferromagnet (FM) is in atomic contact with an antiferromagnet (AF) the exchange coupling between the FM and AF spins at the interface induces a unidirectional anisotropy in the ferromagnetic film. This effect is known as exchange bias (EB). Despite the large amount of research on this topic there are still several aspects of the EB mechanism that are not well understood. One of this aspects is the origin of the rotatable anisotropy in polycrystalline AFs. By means of Brillouin Light Scattering (BLS) measurements, we investigated the dependence of the rotatable anisotropy field  $H_{RA}$  and exchange field  $H_E$  with the magnitude of the external magnetic field ( $H_0$ ) in FM/AM bilayers of Ni<sub>81</sub>Fe<sub>19</sub>(10nm)/Ir<sub>20</sub>Mn<sub>80</sub>(t<sub>AF</sub>). We developed an algorithm to numerically fit the in-plane angular dependence of the magnon frequency, at a fixed value of  $H_0$  measured by BLS. From the fit parameters we were able to investigate  $H_{RA}$  and  $H_E$  dependency on  $H_0$ . The results reveal that  $H_{RA}$  value depends on  $H_0$ , so we argue that AF grain distribution at the interface is partially modified by the applied field strength. Contrary to this, the relation between  $H_E$  and  $H_0$  is not straightforward, remaining constant at high values of  $H_0$ .

**T1.00221 Atomic structure prediction of Zr-Co and Hf-Co nanoclusters using the evolutionary algorithm**, NABIL AL-AQTASH, The Hashemite University, RENAT SABIRIANOV, University of Nebraska at Omaha — Nanostructures of Hf-Co and Zr-Co rare earth free magnetic material that exhibit a high room-temperature energy product. In our study, the evolutionary algorithm coupled with density functional (DFT) method is used to identify the global energy minimum atomic structure of Zr-Co and Hf-Co clusters. Using evolutionary crystal structure optimization algorithm, as implemented in USPEX, we studied the atomic structure, binding energies, magnetic properties, and anisotropy of Zr<sub>x</sub>Co<sub>y</sub> and Hf<sub>x</sub>Co<sub>y</sub> (x=1,2 and y=5,7,11) clusters. A set of metastable and global minimum atomic structures are identified. Several new lower energy configurations were identified for Zr<sub>2</sub>Co<sub>11</sub>, Zr<sub>1</sub>Co<sub>5</sub>, Zr<sub>1</sub>Co<sub>7</sub>, Hf<sub>2</sub>Co<sub>11</sub>, Hf<sub>1</sub>Co<sub>5</sub> and Hf<sub>1</sub>Co<sub>7</sub> clusters by our calculations. We discussed the magnetic interaction between the atoms of the clusters which is critical in finding the lowest energy structure. Our calculation show that Zr-Co and Hf-Co have ferromagnetic coupling and large magnetization. We will also discuss the magnetocrystalline anisotropy (MAE) variation in these clusters.

**T1.00222 Magneto-electric control of magnetization in a chain of circular nanomagnets as new paradigm for ultra low power binary information propagation.**, MOHAMMAD SALEHI-FASHAMI, University of Delaware, MAMUN AL-RASHID, Virginia Commonwealth University, WEI-YANG SUN, PAUL NORDEEN, University of California, Los Angeles, SUPRIYO BANDYOPADHYAY, Virginia Commonwealth University, GREGORY CARMAN, University of California, Los Angeles, JAYASIMHA ATULASIMHA, Virginia Commonwealth University — Elliptical nanomagnets with bi stable magnetization states are traditionally employed for dipole coupled Bennett clocked nanomagnetic logic. Logic bits are propagated down a chain of nanomagnets by sequentially rotating their magnetizations with an electric field [1]. In this talk, we present for the first time, the notion of replacing elliptical nanomagnets with circular nanomagnets that have no inherent shape anisotropy. The circular nanomagnets would develop bi stable magnetization orientations with the application of an electrical field to induce in-plane strain anisotropy. This new strategy provides two significant advantages for nanomagnetic logic applications: (i) re-orienting the magnetizations does not require overcoming a shape-anisotropy energy barrier and hence the electric field needed to reorient is reduced, leading to lower energy dissipation in the clocking process, and (ii) scalability to dimensions substantially smaller than what presently exists becomes possible. [1] J. Atulasimha and S. Bandyopadhyay, Appl. Phys. Lett., 97, 173105 (2010). This work was supported by NSF CAREER grant CCF-1253370 and by FAME, one of six centers of STARnet, Semiconductor Research Corporation program sponsored by MARCO and DARPA.

**T1.00223 The impact of substrate stimulated functional interface on magnetic and magneto-transport signature of martensitic transformation in NiMnIn shape memory alloy<sup>1</sup>**, R. SABIRIANOV, University of Nebraska Omaha, A. SOKOLOV, University of Nebraska Lincoln, E. KIRIANOV, A. ZLENKO, Lincoln South West High School, A. QUETZ, A. ARYAL, S. PANDEY, I. DUBENKO, N. ALI, Southern Illinois University, S. STADLER, Louisiana State University, N. AL-AQTASH, Hashemite University — We study the impact of the substrate on the martensite transformation of Ni-Mn-In thin films by Hall resistance measurements and discuss it using density functional theory calculations. Similarly to the bulk systems, thin films grown on MgO exhibit the martensitic transformation accompanied by large magnetoresistance and a sign reversal of the ordinary as well as anomalous Hall coefficient. Martensite transition temperature of films grown on (100) surface of MgO is near 170K, while the films grown on (111) surface of MgO show the change of Hall coefficient at 110K. The calculated total energy difference between FM austenite and FiM martensite states in Ni<sub>2</sub>Mn<sub>1.5</sub>In<sub>0.5</sub> film on MgO (001) substrate (with Ni/MgO interface) is 0.20eV per NiMnIn f.u., compared to 0.24eV in the bulk at the same equilibrium lattice parameters, i.e. when film is “unstrained”. When lattice parameters of Ni<sub>2</sub>Mn<sub>1.5</sub>In<sub>0.5</sub>/MgO are of those of MgO substrate, i.e. when the film experiences strong bi-axial tensile strain  $\Delta a/a = 2.4\%$ , the energy difference is 0.08eV per NiMnIn f.u. These results clearly indicate strong interplay between lattice strain/stress and the relative stability martensite and austenite phase

<sup>1</sup>The work is supported by NSF

**T1.00224 Ferromagnetic properties of manganese doped iron silicide.**, ANGEL RUIZ-REYES, LUIS F. FONSECA, University of Puerto Rico, RENAT SABIRIANOV, University of Nebraska at Omaha — We report the synthesis of high quality Iron silicide (FeSi) nanowires via Chemical Vapor Deposition (CVD). The materials exhibits excellent magnetic response at room temperature, especially when doped with manganese showing values of  $2.0 \times 10^{-4}$  emu for the Fe<sub>x</sub>Mn<sub>y</sub>Si nanowires. SEM and TEM characterization indicates that the synthesized nanowires have a diameter of approximately 80nm. MFM measurements present a clear description of the magnetic domains when the nanowires are doped with manganese. Electron Diffraction and XRD measurements confirms that the nanowires are single crystal forming a simple cubic structure with space group P213. First-principle calculations were performed on (111) FeSi surface using the Vienna ab initio simulation package (VASP). The exchange correlations were treated under the Ceperley-Alder (CA) local density approximation (LDA). The Brillouin Zone was sampled with 8x8x1 k-point grid. A total magnetic moment of about 10  $\mu_B$  was obtained for three different surface configuration in which the Iron atom nearest to the surface present the higher magnetization. To study the effect of Mn doping, Fe atom was replaced for a Mn. Stronger magnetization is presented when the Mn atom is close to the surface. The exchange coupling constant have been evaluated calculating the energy difference between the ferromagnetic and anti-ferromagnetic configurations.

**T1.00225 Effect of Milling Time on the Blocking Temperature of Nanoparticles of Magnetocaloric Gd<sub>5</sub>Si<sub>4</sub>.**, RAVI HADIMANI, Iowa State University, SHALBH GUPTA, Ames Laboratory, US Department of Energy, SHANE HARSTAD, Iowa State University, VITALIJ PECHARSKY, Ames Laboratory, US Department of Energy, DAVID JILES, Iowa State University, DAVID C JILES TEAM, VITALIJ PECHARSKY COLLABORATION — Extensive research has been done on giant magnetocaloric material Gd<sub>5</sub>(Si<sub>x</sub>Ge<sub>1-x</sub>)<sub>4</sub> to improve adiabatic temperature/isothermal entropy change. However, there have been only a few reports on fabrication of nanostructure/nanoparticles that can be used to tune various properties by changing the length scale. Recently we have reported fabrication of room temperature ferromagnetic nanoparticles of Gd<sub>5</sub>Si<sub>4</sub> using high energy ball milling. These nanoparticles have potential applications in biomedical engineering such as better T<sub>2</sub> MRI contrast agents and in hypothermia. Here we report the effect of milling time on the blocking temperature, micro-structure, crystal structure, and magnetic properties of these nanoparticles. Magnetization vs. temperature at an applied field of 100 Oe is measured for all the ball milled samples. Bulk Gd<sub>5</sub>Si<sub>4</sub> has a transition temperature of  $\approx 340$  K. There are two phase transitions observed in the nanoparticles, one near 300 K corresponding to the Gd<sub>5</sub>Si<sub>4</sub> phase and another between 75-150 K corresponding to Gd<sub>5</sub>Si<sub>3</sub>. Zero Field Cooling (ZFC) and Field Cooling (FC) were measured. The blocking temperatures for the nanoparticles increase with decrease in milling time.

**T1.00226 Magnetic and optical properties of Co-doped and Mn-doped ZnO nanocrystalline particles.** , ABDEL ALSMADI, B. SALAMEH, Kuwait University, M. SHATNAWI, The Hashimite University, G. ALNAWASHI, The Hashemite University, I. BSOU, Al al-Bayt University — We carried out a systematic study on the effect of Co doping and Mn doping on the structural, magnetic and optical properties of ZnO nanocrystalline particles, using x-ray diffraction, x-ray photoelectron spectroscopy (XPS), Quantum Design PPMS-9 magnetometry, and Ultra Violet-Visible spectroscopy. The  $\text{Zn}_{1-x}\text{Co}_x\text{O}$  and  $\text{Zn}_{1-x}\text{Mn}_x\text{O}$  nanoparticles with  $0 \leq x \leq 0.1$  were successfully prepared by the formal solid-state reaction method. The XPS results and the XRD analysis with full structural Rietveld refinement reveal that both structures have hexagonal wurtzite structure. For all Co-doped ZnO nanoparticles under investigation, the field dependence of the magnetization curves exhibits ferromagnetic behavior with relatively small coercive fields at room temperature. In addition, we found a signature for antiferromagnetic ordering between the Co ions. For the Mn-doped ZnO nanoparticles, we observed ferromagnetic behavior only below 50 K. We also observed a strong correlation between the magnetic and optical behavior of the Co-doped ZnO nanoparticles. Optical diffuse reflectance and absorption spectra exhibit a red shift at room temperature in the absorption band edge with increasing Co-doping. The red shift is attributed to the *sp-d* exchange interaction between free charge carriers in ZnO band and the localized magnetic moments.

**T1.00227 Investigation of the Magnetic Properties of Ni-implanted ITO Thin Films<sup>1</sup>** , FIGEN AY, BEKIR AKTAS, Gebze Technical University, Department of Physics, RUSTEM KHAIBULLIN, VLADIMIR NUZHIDIN, Kazan Physical-Technical Institute of RAS, BULAT RAMEEV, Gebze Technical University, Department of Physics; Kazan Physical-Technical Institute of RAS — Commercially available ITO thin films on fused silica substrates were implanted with 40 keV  $\text{Ni}^+$  ions to fluences of  $(0.5, 1.0 \& 1.5) \times 10^{17}$  ions/cm<sup>2</sup> at room temperature. XRR measurements show that the thickness of the implanted films ( $\sim 28.5$  nm) does not change noticeably with the fluence, while the surface roughness increases essentially. SEM and EDX studies revealed a highly non-uniform distribution of Ni atoms. Room temperature ferromagnetism was observed in the samples with fluences of  $(1.0 \& 1.5) \times 10^{17}$  ions/cm<sup>2</sup>. VSM hysteresis curves and FMR signal point to the formation of a ferromagnetic near-surface layer in the implanted films due to agglomeration of closely-spaced metal Ni nanoparticles. The filling factor of the Ni ferromagnetic phase in the granular magnetic layer was estimated from the FMR results. Super- and para- magnetic phases were observed in the temperature dependence of magnetization by VSM. Superparamagnetic phase is attributed to the Ni nanoparticles located in deeper regions near the film/substrate interface, while paramagnetic phase is related to the impurity centers. For the samples with fluences of  $(1.0 \& 1.5) \times 10^{17}$  ions/cm<sup>2</sup> average sizes of the superparamagnetic nanoparticles were calculated from the blocking temperatures  $T_B$  observed in thermo-magnetic dependences.

<sup>1</sup>TÜBITAK, grant No. 114F359 TÜBITAK / RFBR joint project program, grant No. 213M524 / 14-02-91374-cT-a. RAS Programme No.32

**T1.00228 Magnetization reversal in the orthochromite  $\text{Y}_0.5\text{Gd}_0.5\text{CrO}_3$ .**<sup>1</sup> , ALEJANDRO DURAN, Centro de Nanociencias y nanotecnología-UNAM, ROBERTO ESCUDERO, RAUL ESCAMILLA, FRANCISCO MORALES, Instituto de Investigaciones en Materiales-UNAM, EDUARDO VERDIN, Departamento de Física-UNISON — Complex oxide of transition metal with perovskite structure represent fascinating playground for basic solid state research: new electronics and exotic ground states emerge via the competing interplay like spin, orbital, charge as well as lattice degree of freedom. Accordingly, orthochromites are not exception to the rule. In these compounds have been found ferroelectric polarization, spin reorientation transition along with the characteristic behavior known as; magnetization reversal (MR) consisting that a characteristic temperature,  $T^*$ , the system becomes diamagnetic. In this work, the magnetic behavior of the equimolar  $\text{Y}_0.5\text{Gd}_0.5\text{CrO}_3$  composition was studied. Negative magnetization was observed at  $T^* \sim 70$  K in FC mode, and applied field of 100 Oe. The characteristic hysteresis loop in the M-H graph of the pristine sample disappears for a wide range of temperature below of  $T_N$ , and the characteristic spin reorientation is shifted from 14 K in  $\text{GdCrO}_3$  to 5 K for  $\text{Y}_0.5\text{Gd}_0.5\text{CrO}_3$ . The negative magnetization is explained according the model that take into account the anisotropic and antisymmetric exchange interaction between Gd+3 – Cr+3 sublattice.

<sup>1</sup>A.D. and R.E. thanks to grants by DGAPA-PAPIIT, IN103213 and IN 106014 respectively.

**T1.00229 Investigation of Low Temperature Non-Linear Magnetization Behavior in Al and Ga- Substituted  $\text{La}_{0.4}\text{Bi}_{0.6}\text{MnO}_3$  Manganites.** , VIJAYLAKSHMI DAYAL, PUNITH KUMAR V, Maharaja Institute of Technology-Mysore, RAVI HADIMANI, DAVID JILES, Iowa State University, DAVID C JILES TEAM, VIJAYLAKSHMI DAYAL COLLABORATION — Low temperature magnetization measurements have been carried out for the samples containing Al and Ga at B-site in  $\text{La}_{0.4}\text{Bi}_{0.6}\text{MnO}_3$  manganites. The magnetization (M) vs. T(K) data shows strong ferromagnetic behavior with highest magnetization of 6.45 emu/g for  $\text{La}_{0.4}\text{Bi}_{0.6}\text{Mn}_{0.95}\text{Al}_{0.05}\text{O}_3$  and 5.40 emu/g for  $\text{La}_{0.4}\text{Bi}_{0.6}\text{Mn}_{0.90}\text{Ga}_{0.10}\text{O}_3$  samples respectively for an applied magnetic field of  $H=100$  Oe at  $T=20$  K. Similarly at  $T=20$  K for  $\text{La}_{0.4}\text{Bi}_{0.6}\text{Mn}_{0.95}\text{Ga}_{0.05}\text{O}_3$  the highest magnetization ( $M_S$ ) was found to be 5.44 emu/g and for  $\text{La}_{0.4}\text{Bi}_{0.6}\text{Mn}_{0.90}\text{Ga}_{0.10}\text{O}_3$  the  $M_S$  is 5.05 emu/g. The decrease in magnetization with both Al and Ga substitution produces magnetic dilution with increasing concentrations. Both Al and Ga substituted samples exhibit non-linear behavior in their magnetization ( $M_{NL}$ ) curves around 40–120 K due to the frustrations arising from mismatch in their magnetic spin arrangements. The quantity non linear susceptibility,  $\chi_{NL} = -M_{NL}/H$ , diverges as the temperature approaches the frustrated region  $T_f$  from above (i.e.  $T_C$ ). Further from  $d\chi_{NL}/dT$  vs. T(K) plots and critical analysis with unusual critical exponent's  $\gamma$  and  $\beta$  gives an experimental evidence for the observed non linearity and magnetic frustration.

**T1.00230 Tunnel Magneto Resistance of Fe/Insulator/Fe** <sup>1</sup> , DENNIS ARYEE, DEREJE SEIFU, Morgan State University, PHYSICS — Tri-layer thin films of Fe/Insulator/Fe were synthesized using magnetron DC/ RF sputtering with MgO insulator and  $\text{Bi}_2\text{Te}_3$  topological insulators as middle buffer layer. The multi-layered samples thus produced were studied using in-house built magneto-optic Kerr effect (MOKE) instrument, vibrating sample magnetometer (VSM), torque magnetometer (TMM), AFM, MFM, and magneto-resistance (MR). This system, that is Fe/Insulator/Fe on MgO(100) substrate, is a well-known tunnel magneto resistance (TMR) structure often used in magnetic tunnel junction (MTJ) devices. TMR effect is a method by which MTJs are used in developing magneto-resistive random access memory (MRAM), magnetic sensors, and novel logic devices. The main purpose behind this research is to measure the magnetic anisotropy of Fe/Insulator /Fe structure and correlate it to magneto-resistance [1]. In this presentation, we will present results from MOKE, VSM, TMM, AFM, MFM, and MR studies of Fe/Insulator/Fe on MgO(100). [1] A. Newman, S. Khatriwada,, S. Neupane, D. Seifu, "Nano Wires of Fe/MWCNTs and Nanometric Thin Films of Fe/MgO", J. of Appl. Phys., **117**, 144302 (2015).

<sup>1</sup>We would like to acknowledge support by NSF-MRI-DMR-1337339.

**T1.00231 Integration of Multifunctional Epitaxial Oxide Heterostructures with Si(001)** , SRINIVASA RAO SINGAMANENI, JOHN PRATER, JAY NARAYAN, North Carolina State University — Multifunctional heterostructures exhibit a wide range of functional properties, including colossal magneto-resistance, multiferroic behavior, and spin, charge, and orbital ordering. However, putting this functionality to work remains a challenge. To date, most of the previous works reported in the literature have dealt with heterostructures deposited on closely lattice matched (using lattice matching epitaxy-LME) insulating substrates such as  $\text{DyScO}_3$ ,  $\text{NdGaO}_3$ , MgO,  $\text{SrTiO}_3$  and MBE-grown STO buffered Si(100). This presentation discusses the major advances in the integration of multifunctional oxide materials onto ubiquitous silicon semiconductor platform reported<sup>1–6</sup> in the recent past by the presenting authors using a novel thin film growth approach, called 'domain matching epitaxy'(DME), which minimizes the strain and nucleation of unwanted defects. The DME paradigm has been used across the large misfit scale (7–25%). Of particular interest, thin film heterostructures including two-phase multiferroics such as  $\text{BiFeO}_3$ (BFO)/ $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$  (LSMO),  $\text{BaTiO}_3$ (BTO)/LSMO, and LSMO/SrRuO<sub>3</sub>(SRO). These significant materials advancements may herald a flurry of exciting new advances in CMOS-compatible multifunctional devices.<sup>1</sup> S. S. Rao, et al., Nano Letters **13**, 5814 (2013); J. Appl. Phys., **116**, 094103 (2014); J. Appl. Phys., **116**, 224104 (2014); J. Appl. Phys., **117**, 17D908 (2015); <sup>5</sup>J. Appl. Phys., **117**, 17B711 (2015); <sup>6</sup>Current Opinion in Solid State and Materials Science. **19**, 301-304 (2015).

**T1.00232 Untangling the contributions of cerium- and iron- sublattices to the magnetism of Ce-doped yttrium iron garnet.** , GERVASI HERRANZ, BLAI CASALS, MARINA ESPINOLA, RAFAEL CICHELO, JOSEP FONTCUBERTA, Institut de Ciència de Materials de Barcelona ICMA-B-CSIC, Campus UAB, 08193 Bellaterra, Spain, STEPHAN GEPRAGS, MATTHIAS OPEL, RUDOLF GROSS, Walther-Meiner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — The remarkable magnetic properties of yttrium iron garnets (YIGs) underpin the use of these materials in a broad scope of spintronic and photonic applications. In particular, the addition of rare-earth metals in the structure enhances to a great extent the magneto-optical activity, which is beneficial for the development of nonreciprocal devices for communication along optical fibers. Yet, the physical mechanisms that lead to the observed enhanced gyrotropic response of doped YIG are not fully unveiled. Here we present a methodology based on magneto-optical spectroscopy that may be instrumental to better understand the optical response of these materials. In particular, we have exploited the wavelength selectivity of magneto-optics to identify a range of frequencies at which one can unravel the individual contributions to the magnetism and gyrotropic response arising from the individual cerium and iron sublattices. The approach outlined here paves the way to assess quantitatively the effect on the optical properties of rare-earth incorporation into YIG, providing an instrumental methodology towards tailoring the functional properties of YIG.

**T1.00233 Growth of EuO films on Si using Pulsed Laser Deposition<sup>1</sup>** , VIVEK S. JAIN, GAURAB RIMAL, JINKE TANG, Department of Physics & Astronomy, University of Wyoming — Epitaxial monolayers of europium monoxide (EuO) deposited on silicon (Si) wafers are suited for spintronic applications such as adding spin filter tunneling and spin current to Si technology, and for probing phenomena like Anomalous Hall effect and Topological Hall effect. However, the innate chemical reactivity of europium (Eu) and Si prevents a direct synthesis of EuO by pulsed laser deposition technique, without significant contamination of the EuO/Si interface and degradation of the EuO thin film. Silicon oxides ( $\text{SiO}_{2-\delta}$ ) on the surface of Si substrates, partial pressure of oxygen ( $\text{O}_2$ ) gas and water vapors in the vacuum chamber act as contaminants. Techniques like standard wet etching process, thermal annealing, and decomposition of  $\text{SiO}_{2-\delta}$  by the bombardment of metal ions, and their effectiveness is studied using the X-Ray diffraction (XRD) system. Our goal is one-process in situ integration of spin-functional magnetic oxides seamless on Si wafers. Also the mechanism for the ferromagnetic order in oxygen-deficient europium monoxide ( $\text{EuO}_{1-x}$ ) at temperatures higher than 69K (the Curie temperature of stoichiometric EuO) remains controversial. We have investigated the magnetization of  $\text{EuO}_{1-x}$  thin films prepared via PLD as a function of (emu) vs (K)

<sup>1</sup>Wyoming EPSCoR

**T1.00234 Room temperature ferromagnetism of Cr-doped  $\text{In}_2\text{O}_3$  bi-layer consisted of a triangular crystal-amorphous interface** , DAI-JHEN JHONG, BO-YU CHEN, CHUN-YU HSU, YAUN-CHAO LIANG, HSIUNG CHOU<sup>1</sup>, Department of Physics, NSYSU, Kaohsiung 804, Taiwan —  $\text{In}_2\text{O}_3$  film is a very conductive and can be modified to exhibit room temperature ferromagnetism upon doping of Cr. In this study, we developed a method, based on the RF power, to control the Cr-doped  $\text{In}_2\text{O}_3$  (CIO) thin-films to form a crystalline phase, at a high power region, or an amorphous phase, at a low power region. When the RF power is set at a medium power, the CIO film self-assemble into a two layers system consisted of crystalline and amorphous layers with interface manifests zig-zag feature. The two layer system has a saturation magnetization  $M_s$ , of  $\sim 0.27$  to  $\sim 1.78$  emu/c.c. with increase of Cr-doping content. In contrast, the  $M_s$  of the amorphous films are  $\sim 0.45$  emu/c.c independent of Cr content. Electron energy loss spectroscopy (EELS) measurements suggested that Cr existed in mixed oxidation states in all films. The Cr with lower oxidation state prefers crystalline structure, while the higher oxidation state Cr prefers an amorphous structure. Due to this charge imbalance, a transport of charge across the interface originates the ferromagnetic interaction, and hence, we observe enhanced  $M_s$  in crystal-amorphous interface system.

<sup>1</sup>Corresponding Author

**T1.00235 Two phase multiferroics for voltage-induced entropy change with application in near-room-temperature refrigeration<sup>1</sup>** , PRAKASH GIRI, University of Nebraska - Lincoln, DHANANJAY KUMAR, North Carolina Agricultural and Technical State University, CHRISTIAN BINEK, University of Nebraska-Lincoln — The demand for environmental friendly, cost-effective and energy efficient cooling drives the emerging technology of magnetic refrigeration at room temperature. We fabricate a two phase multiferroic  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3/\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3\text{-PbTiO}_3(001)$  via pulsed laser deposition for application in advanced near room-temperature refrigeration and miniature cooling devices. The key innovation rests on utilizing the magnetocaloric effect in zero applied magnetic fields. The magnetocaloric effect of the composite is activated purely by electric field. We utilize strain originating from stress which is voltage-induced via the inverse piezoelectric effect of PMN-PT. The strain is carried over into the adjacent LSMO thin film thus changing its magnetic order. The voltage-induced variation in magnetization leads to change in isothermal entropy when the experiment is carried out in contact with a thermostat and gives correspondingly rise to an adiabatic temperature change when heat exchange is suppressed.

<sup>1</sup>This project is supported by NSF through Nebraska MRSEC DMR-1420645.

**T1.00236 Enhanced Magnetic Proximity Effect at Ferromagnetic Insulator / Magnetic Topological Insulator Interface** , MINGDA LI, CUI-ZU CHANG, MIT, BRIAN KIRBY, NIST, MICHELLE E. JAMER, Northeastern University, WENPING CUI, Boston College, LIJUN WU, Brookhaven National Lab, PENG WEI, MIT, YIMEI ZHU, Brookhaven National Lab, DON HEIMAN, Northeastern University, JU LI, JAGADEESH MOODERA, MIT, MIT TEAM, NIST TEAM, NORTHEASTERN UNIVERSITY COLLABORATION, BOSTON COLLEGE COLLABORATION, BROOKHAVEN NATIONAL LAB COLLABORATION — Magnetic proximity effect at magnetic insulator / topological insulator interface provides a promising approach to realize low-dissipation quantum devices. However, the commonly used magnetic insulators have in-plane anisotropy hence cannot magnetize topological insulator. Here we report an enhancement of proximity exchange coupling in ferromagnetic insulator / magnetic topological insulator  $\text{EuS} / \text{Sb}_{2-x}\text{V}_x\text{Te}_3$  hybrid heterostructure, where proximity effect is enhanced by a factor of 3 through the Vanadium doping. Moreover, an artificial antiferromagnetic-like structure is created between two strong ferromagnets, which may account for the proximity effect enhancement. The interplay between the proximity effect and doping in hybrid heterostructure provides insights into the engineering of magnetic ordering.

**T1.00237 Structural and magnetic properties of epitaxial  $\text{FeMn}_2\text{O}_4$  film on  $\text{MgO}$  (100).** , THIET DUONG VAN, THI MINH HAI NGUYEN, ANH PHUONG NGUYEN, DUNG DANG DUC, ANH TUAN DUONG, QUANG NGUYEN VAN, SUNGLAE CHO, Univ of Ulsan —  $\text{FeM}_2\text{X}_4$  spinel structures, where  $M$  is a transition metal and  $X$  is oxygen or sulfur, are candidate materials for spin filters, one of the key devices in spintronics. On the other hand, the electronic and magnetic properties of these spinel structures could be modified via the control of cation distribution. Among the spinel oxides, iron manganese oxide is one of promising materials for applications.  $\text{FeMn}_2\text{O}_4$  shows inverse spinel structure above 390 K and ferrimagnetic properties below the temperature. In this work, we report on the structural and magnetic properties of epitaxial  $\text{FeMn}_2\text{O}_4$  thin film on  $\text{MgO}(100)$  substrate. The reflection high energy electron diffraction (RHEED) and X-ray diffraction (XRD) results indicated that films were epitaxially grown on  $\text{MgO}(100)$  without the impurity phases. The valence states of Fe and Mn in the  $\text{FeMn}_2\text{O}_4$  film were carried out using x-ray photoelectron spectrometer (XPS). The magnetic properties were measured by vibrating sample magnetometer (VSM), indicating that the samples are ferromagnetic at room temperature. The structural detail and origin of magnetic ordering in  $\text{FeMn}_2\text{O}_4$  will be discussed.

**T1.00238 Study of Magnetic and Electric Properties in  $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$  Thin Film**<sup>1</sup>, ISABEL ARANGO, JOHN ORDOEZ, ALBA AVILA, WILSON LOPERA, MARIA GOMEZ, None, THIN FILM GROUP TEAM<sup>2</sup>, DEPARTMENT OF ELECTRICAL AND ELECTRONIC ENGINEERING COLLABORATION<sup>3</sup> —  $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$  (LSMO) is the most interesting compound of the manganite perovskite family due to its Curie temperature above 300K that makes its remarkable properties desirable for practical applications. However, it is well known that ferromagnetic properties weaken when dimensions are reduced. We have grown LSMO thin films by sputtering DC in pure oxygen atmosphere on  $\text{SrTiO}_3$  (STO) and  $\text{LaAlO}_3$  (LAO) substrates at temperature of 830 C. From x-ray diffraction analysis, we have found the Bragg peaks of LSMO thin films around (002) reflection, indicating a textured growth. We have characterized the morphology of the samples by atomic force microscopy. LSMO thin film was patterned using standard UV photolithography. Dependence of resistivity with temperature shows a behavior typical of ferromagnetic system with metal-insulator transition above 300 K. The electrical properties of the structured will be contrasted with thin film. We carried out isothermal resistance and magnetization versus applied magnetic field loops to characterize the samples. We study the dependence of magnetic transport properties with film thickness of 25nm and path size (5 micron) for potential applications like magnetic sensors.

<sup>1</sup>Thanks to "CENM.

<sup>2</sup>Universidad del Valle

<sup>3</sup>Universidad de los andes

**T1.00239 A Focker-Planck description of the spin Seebeck effect**, GUILLERMO REYES, JUAN ADRIAN REYES, Universidad Nacional de Mexico, Instituto de Fisica — Thermally driven spin-wave spin current in a ferromagnetic material FM and the resulting electric signal in a metal probe placed on the FM are theoretically investigated by considering a thermally fluctuating spin at the interface of a FM-metal junction. We develop an analytical formulation to establish a Focker Plank equation for the probability distribution as a function of magnetization components of the material, for calculating the spin Seebeck signal detected by the metal probe, which converts spin current to charge current by the inverse spin Hall effect. The spin current is induced in the metal probe via an exchange interaction when the metal senses the temperature gradient.

**T1.00240 Ferromagnetic thickness dependence of current-driven spin-orbit torques in different ferromagnetic and heavy metal bilayers**, JUN WU, University of Delaware, XIN FAN, University of Denver, TAO WANG, YUNPENG CHEN, Q. JOHN XIAO, University of Delaware — The spin-orbit torques in ferromagnetic (FM) and heavy metal (HM) bilayers have attracted extensive research interests recently because of the rich physical phenomena and potential applications. We measured the effective fields of field-like torques in Ni/Pt, NiFe/Pt and CoFeB/Pt bilayer systems by the second-order planar Hall effect. When the FM layers are less than 2nm, the effective fields increase rapidly with decreasing the FM layer thickness for all three different FM layers. Among the three FMs, the effective field in Ni is largest, followed by NiFe, then CoFeB. Above 2nm, the effective fields decrease much slower with increasing the FM layer thickness and level off to the Orested field due to the current in the Pt layer. Through FM layer thickness dependence of the field-like torque study, we found that the spin dephasing length in the FM layer, which is related to the scattering in FM layer, plays an important role in determining the magnitude of field-like spin-orbit torque in FM/HM bilayers.

**T1.00241 Thermal conductivity of magnetic insulators with strong spin-orbit coupling**<sup>1</sup>, GEORGIOS STAMOKOSTAS, PANTELEIMON LAPAS, GREGORY A. FIETE, Physics department, Univ of Texas, Austin — We study the influence of spin-orbit coupling on the thermal conductivity of various types of magnetic insulators. In the absence of spin-orbit coupling and orbital-degeneracy, the strong-coupling limit of Hubbard interactions at half filling can often be adequately described in terms of a pure spin Hamiltonian of the Heisenberg form. However, in the presence of spin-orbit coupling the resulting exchange interaction can become highly anisotropic. The effect of the atomic spin-orbit coupling, taken into account through the effect of magnon-phonon interactions and the magnetic order and excitations, on the lattice thermal conductivity of various insulating magnetic systems is studied. We focus on the regime of low temperatures where the dominant source of scattering is two-magnon scattering to one-phonon processes. The thermal current is calculated within the Boltzmann transport theory.

<sup>1</sup>We are grateful for financial support from NSF Grant DMR-0955778.

**T1.00242 spin pumping occurred under nonlinear spin precession**, HENGAN ZHOU, XIAOLONG FAN, Lanzhou University, LI MA, SHIMING ZHOU, Tongji University, DESHENG XUE, Lanzhou University — Spin pumping occurs when a pure-spin current is injected into a normal metal thin layer by an adjacent ferromagnetic metal layer undergoing ferromagnetic resonance, which can be understood as the inverse effect of spin torque, and gives access to the physics of magnetization dynamics and damping. An interesting question is that whether spin pumping occurring under nonlinear spin dynamics would differ from linear case. It is known that nonlinear spin dynamics differ distinctly from linear response, a variety of amplitude dependent nonlinear effect would present. It has been found that for spin precession angle above a few degrees, nonlinear damping term would present and dominated the dynamic energy/spin-moment dissipation. Since spin pumping are closely related to the damping process, it is interesting to ask whether the nonlinear damping term could be involved in spin pumping process. We studied the spin pumping effect occurring under nonlinear spin precession. A device which is a Pt/YIG microstrip coupled with coplanar waveguide was used. High power excitation resulted in spin precession entering in a nonlinear regime. Foldover resonance lineshape and nonlinear damping have been observed. Based on those nonlinear effects, we determined the values of the precession cone angles, and the maximum cone angle can reach a values as high as 21.5 degrees. We found that even in nonlinear regime, spin pumping is still linear, which means the nonlinear damping and foldover would not affect spin pumping process.

**T1.00243 Spin Hall and spin Nernst effects: temperature dependence**, ANNA DYRDAL, JOZEF BARNAS, Faculty of Physics, Adam Mickiewicz University, ul. Umultowska 85, 61-614 Poznan, Poland, VITALII DUGAEV, Department of Physics and Medical Engineering, Rzeszow University of Technology, al. Powstancow Warszawy 6, 35-959 Rzeszow, Poland — We have considered temperature dependence of spin Hall and spin Nernst effect in two-dimensional electron gas with spin-orbit interaction of Rashba type [arXiv:1510.03080]. In our considerations we have employed the approach based on the Matsubara Green functions. The formalism used in the case of electric field as a driving force was subsequently adopted to the situation of a spin current driven by a temperature gradient. To achieve this, we have used the concept of an auxiliary vector field. Such a description gives the possibility to consider all mechanisms leading to the spin Hall and spin Nernst effect on equal footing and also their behavior at finite temperatures. Both spin Hall and spin Nernst conductivities were calculated in the approximation including the vertex correction. The total spin Hall conductivity, including vertex correction, has been shown to vanish exactly in the whole temperature range. Thus, our results extend the earlier ones to an arbitrary temperatures. In turn, the total spin Nernst conductivity remains finite when the vertex corrections are included. Using the Ioffe-Regel localization criterion, we have also estimated the range of parameters where the calculated results for the spin Hall and spin Nernst conductivities are applicable.

**T1.00244 Non-equilibrium spin polarization and spin-orbit torque induced by electric field and temperature gradient in a magnetized two-dimensional electron gas with Rashba spin-orbit interaction** , ANNA DYRDAL, JOZEF BARNAS, Adam Mickiewicz University, ul. Umultowska 85, 61-614 Poznan, Poland, VITALII DUGAEV, Department of Physics and Medical Engineering, Rzeszow University of Technology, al. Powstancow Warszawy 6, 35-959 Rzeszow, Poland — We have considered theoretically temperature dependence of non-equilibrium spin polarization of electrons that appears in a magnetized two-dimensional electron gas with Rashba spin-orbit interaction due to external electric field and/or temperature gradient. To do this we have employed the approach based on the Matsubara Green function formalism. We analyzed in detail variation of the induced spin polarization with position of the Fermi level, temperature, and Rashba coupling constant. Moreover, we analyzed the temperature dependence of the electrically and thermally induced spin polarization in the temperature regime, where the spin relaxation time can be assumed constant (independent of temperature). In contrast to the case of nonmagnetic Rashba gas, all three components of the induced spin polarization are now nonzero. The induced spin-polarization is exchange-coupled to the local equilibrium magnetization and therefore exerts a torque on the magnetization vector. We have considered in detail the temperature behavior of spin-orbit torque induced by electric field and by temperature gradient for specific relative orientation of the magnetization and electric field or temperature gradient, respectively.

**T1.00245 Cross-tunneling and phonon bottleneck effects in the relaxation phenomena of the XY pyrochlore antiferromagnet  $\text{Er}_2\text{Ti}_2\text{O}_7$ .**<sup>1</sup> , MARTIN ORENDÁČ, P. J. Šafárik University, Košice, Slovak republic, KATARINA TIBENSKÁ, Technical University, Košice, Slovak Republic, JOZEF STREČKA, JANA ČISÁROVÁ, VLADIMÍR TKÁČ, ALŽBETA ORENDÁČOVÁ, ERIK ČIŽMÁR, P. J. Šafárik University, Košice, Slovak republic, JAN PROKLEŠKA, VLADIMÍR SECHOVSKÝ, Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic — Multiple time-scale relaxation dynamics are revealed by alternating-current (ac) susceptibility measurements of a single crystal of  $\text{Er}_2\text{Ti}_2\text{O}_7$  studied at high temperatures ( $k_B T \gg J/k_B$ ) and in a wide-range of static magnetic fields. The analysis of the frequency dependence of the ac susceptibility revealed the existence of two relaxation mechanisms identified as an Orbach process with a pronounced effect of phonon bottleneck and cross-tunneling. The origin of the phonon bottleneck is attributed to a resonant phonon trapping. The relevance of the obtained results for relaxation phenomena found in other rare-earth pyrochlores, studied under similar conditions, is discussed.

<sup>1</sup>The work was supported by projects APVV-14-0073 and ITMS 26220120005

**T1.00246 Characterization of defect structures on triangular antiferromagnet  $\text{PdCrO}_2$  using scanning tunneling microscopy and spectroscopy** , JINOH JUNG, KAIST , WON-JUN JANG, IBS CAPP, HYUN WOO CHOI, SEOKHWAN CHOI, KAIST, JONG MOK OK, POSTECH, DONG HYUN SON, KAIST, HWAN SOO SUH, SAIT, JUN SUNG KIM, POSTECH, JHINHWAN LEE, KAIST — Frustrated magnetic systems have received significant attentions due to the possibility as source of ferroelectricity. We studied atomic structures and electronic structures of defects in two dimensional triangular-lattice antiferromagnet  $\text{PdCrO}_2$  using scanning tunneling microscopy and spectroscopy (STM / STS). In  $\text{CrO}_2$  layers and Pd layers, atomic resolution STM images showed distinguishable defects and differential conductance images showed unusual standing wave patterns. We identified the origin of defect structures using STS measurements, atomic ball model analysis and Density Functional Theory (DFT) calculations. Atomic structure analysis of defects gives the opportunity to understand a ground state of frustrated magnetic materials.

**T1.00247 Imaging Magnetic Order and Frustration on Distinct Sublattices in Artificial Quasicrystals**<sup>1</sup> , BARRY FARMER, Department of Physics and Astronomy, University of Kentucky, ANDREW BALK, Center for Nanoscale Science and Technology, National Institute of Standards and Technology. Maryland Nanocenter, University of Maryland, VINAYAKA BHAT, Technical University of Munich, ERIC TEIPEL, NATHAN SMITH, Department of Physics and Astronomy, University of Kentucky, JOHN UNGURIS, Center for Nanoscale Science and Technology, National Institute of Standards and Technology, JEFFREY TODD HASTINGS, Department of Electrical and Computer Engineering, University of Kentucky, LANCE DE LONG, Department of Physics and Astronomy, University of Kentucky — Scanning electron microscopy with polarization analysis (SEMPA) was used to acquire direct images of as-grown magnetization textures for Permalloy thin films patterned into Penrose P2 tilings (P2T). Simulations yield a low-energy manifold of textures composed of two distinct, perfectly ordered sublattices and two sublattices that remain frustrated. As-grown P2T samples exhibited large domains of the two ordered sublattices in the room-temperature SEMPA images. Higher resolution Monte Carlo simulations based on long-range dipolar interactions predict the two frustrated sublattices will order. These results indicate 3<sup>rd</sup> generation P2T will offer the first example of magnetic order in a quasicrystalline material.

<sup>1</sup>Research at University of Kentucky supported by U.S. Department of Energy grant no. DE-FG02-97ER-45653, and U.S. National Science Foundation grant no. DMR-1506979.

**T1.00248 Itinerant Ferromagnetism in Rashba Spin-Orbit Coupled Semiconductors** , WEIZHE LIU, School of Physics, University of New South Wales, Sydney, Australia, ROLAND WINKLER, Department of Physics, North Illinois University, De Kalb, USA, ULRICH ZUELICKE, School of Chemical and Physical Sciences, Victoria University of Wellington, New Zealand, ROBERT JOYNT, Department of Physics, University of Wisconsin-Madison, Madison, USA, DIMITRIE CULCER, School of Physics, University of New South Wales, Sydney, Australia — We theoretically studied the itinerant ferromagnetism in the Rashba spin-orbit coupled 2D electron system by oppositely shifting the two spin-split Fermi surfaces, on condition that electric current vanishes. We found that the system is stable for the infinitesimal displacements only if  $r_s$  is smaller than around 10. But when  $r_s$  becomes much larger than 10, the system becomes unstable at the original state, and finally we obtained another stable state with nonzero spin polarisation.

**T1.00249 Magnetic torque measurements in a chiral magnet  $\text{CrNb}_3\text{S}_6$**  , JUNICHIRO YONEMURA, Osaka Prefecture Univ, TAKANORI KIDA, DAICHI YOSHIZAWA, Osaka Univ, YUSUKE KOSAKA, JUN AKIMITSU, SADAFUMI NISHIHARA, KATSUA INOUE, Hiroshima Univ, JUNICHIRO KISHINE, The Open Univ of Japan, MASAYUKI HAGIWARA, Osaka Univ, YOSHIIHIKO TOGAWA, Osaka Prefecture Univ — Chiral magnetic orders emerge in a particular class of magnetic materials with a chiral crystal structure. As a consequence of the competition between Heisenberg exchange and Dzyaloshinskii-Moriya (DM) interactions in the presence of external magnetic field, chiral helimagnetic order (CHM) formed at zero magnetic field transforms into a nonlinear magnetic superlattice called chiral soliton lattice (CSL) under magnetic fields perpendicular to the chiral axis. The CSL consists of forced ferromagnetic (FM) regions periodically partitioned by chiral soliton kinks of spins. The period of the CSL increases gradually with increasing magnetic field. The CSL is the ground state and exhibits a phase transition into forced FM state above the critical field. To understand the nature of the phase transition, it is important to examine thermodynamic quantities such as magnetization. Furthermore, it is interesting to explore the possibility of the discretization of such physical quantities in a finite CSL system. In this talk, we will present the development of magnetic torque measurement method using micro cantilever in order to precisely measure the magnetization of a micro-sized sample and a set of experimental data obtained by magnetic torque measurements performed in chiral magnet  $\text{CrNb}_3\text{S}_6$ . Hysteresis and stepped behavior of magnetization observed are discussed.

### T1.00250 Realization of Ground State Artificial Skyrmion Lattices at Room Temperature ,

DUSTIN A. GILBERT, BRIAN B. MARANVILLE, ANDREW J. BALK, BRIAN J. KIRBY, DANIEL T. PIERCE, JOHN UNGURIS, JULIE A. BORCHERS, National Institute of Standards and Technology, PETER FISCHER, Lawrence Berkeley National Laboratory, KAI LIU, University of California, Davis — Artificial skyrmion lattices stable at ambient conditions offer a convenient and powerful platform to explore skyrmion physics and topological phenomena and motivates their inclusion in next-generation data and logic devices. In this work we present direct experimental evidence of artificial skyrmion lattices with a stable ground state at room temperature [1]. Our approach is to pattern vortex-state Co nanodots (560 nm diameter) in hexagonal arrays on top of a Co/Pd multilayer with perpendicular magnetic anisotropy; the skyrmion state is prepared using a specific magnetic field sequence. Ion irradiation has been employed to suppress PMA in the underlayer and allow imprinting of the vortex structure from the nanodots to form skyrmion lattices, as revealed by polarized neutron reflectometry. Circularity control is realized through Co dot shape asymmetry, and confirmed by microscopy and FORC magnetometry. The vortex polarity is set during the field sequence and confirmed by magnetometry. Spin-transport studies further demonstrate a sensitivity to the skyrmion spin texture. Work supported by NSF (DMR-1008791, ECCS-1232275 and DMR-1543582). [1]. D. A. Gilbert, et al, Nat. Commun. 6, 8462 (2015)].

### T1.00251 Unexpected observation of splitting of skyrmion phase in Zn doped $\text{Cu}_2\text{OSeO}_3$ ,

HUNG-DUEN YANG, HUNG-CHENG WU, KAKALA-DEVI CHANDRASEKHAR, TIEN-YU WEI, TA-YE CHEN, Department of Physics, National Sun Yat-Sen University, Kaohsiung, 804 Taiwan, HELMUTH BERGER, Institute of Physics of Complex Matter, Ecole Polytechnique Federal de Lausanne, CH-1015 Lausanne, Switzerland — Polycrystalline  $(\text{Cu}_{1-x}\text{Zn}_x)_2\text{OSeO}_3$  ( $0 \leq x \leq 0.2$ ) samples were characterized by X-ray diffraction. The effect of Zn doping upon saturation magnetization ( $M_S$ ) indicates that the Zn favors to occupying Cu(II) square pyramid crystallographic site. The Zn doping concentration is found to greatly affect the  $M$ - $T$  and  $\chi'_{ac}$ - $T$ . The skyrmion phase has been inferred from the  $\chi'_{ac}$ - $H$  data, and then indicated within the  $H$ - $T$  phase diagrams for various Zn doping concentrations. The striking and unexpected observation is that the skyrmion phase region becomes split upon Zn doping concentration. Interestingly, second conical boundary accompanied by second skyrmion phase was also observed from  $d\chi'_{ac}/dH$  vs.  $H$  curves. Atomic site disorder created by the chemical doping modulates the delicate magnetic interactions via changes in the Dzyaloshinskii-Moriya (DM) vector of distorted Cu(II) square pyramid, thereby splitting of skyrmion phase might occurred. These findings illustrate the potential of using chemical and atomic modification for tuning the temperature and field dependence of skyrmion phase of  $\text{Cu}_2\text{OSeO}_3$ .

### T1.00252 Vanadyl Phthalocyanine ( $\text{C}_{32}\text{H}_{16}\text{N}_8\text{VO}$ ): a near-perfect molecular paramagnet , z.

WANG, M.S. SEEHRA, Department of Physics and Astronomy, West Virginia University — Transition-metal-doped phthalocyanines (TMPc, TM = Mn, Fe, Co, Ni, and Cu) are semiconductors with interesting photoconductive properties and so have potential applications in optoelectronic devices [1]. TMPc are planar molecules with the TM atom at the center bound to four N atoms and forming a linear chain along the monoclinic b-axis. Recent magnetic studies reported in CuPc, CoPc, and MnPc show that the exchange coupling between the TM ions are either ferromagnetic as in MnPc [2] or antiferromagnetic as in CuPc [3] and CoPc [4]. In contrast to TMPc, VOPc has a five-coordinate square pyramidal structure with a single electron associated with  $\text{VO}^{2+}$  ion [5]. Here we report results from detailed investigations of the magnetic properties of powder sample of VOPc X-ray diffraction of which shows it to be triclinic. Temperature dependence of magnetization  $M$  from 2 K to 300 K in  $H = 1$  kOe fits the Curie-Weiss (CW) law with  $\theta = 0$  K,  $\mu = 1.665\mu_B$  and  $g = 1.922$  for spin  $S = 1/2$  which indicates VOPc is paramagnetic without any exchange coupling between  $\text{VO}^{2+}$  ions, quite different from CuPc, CoPc and MnPc. Also,  $M$  vs.  $H$  data (up to 90 kOe) at 2 K, 5 K, 10 K, 25 K, 50 K, 100 K, and 300 K fit well with the Brillouin function variation for  $S = 1/2$ , again confirming perfect paramagnetism in VOPc. [1]S.Heutz et al. Adv. Mater.19, 3618 (2007). [2]J.E.Brumboiu et al, J. Phys. Chem. A. 118, 927(2014). [3]Z.Wang et al, IEEE Trans. Magn. 51, 2700104(2015). [4]M.Serri et al, Nature Commun. 5, 3079(2014). [5]H.Adler et al, J. Phys. Chem. C. 119, 8755 (2015).

**T1.00253 Quantum mechanical forces in the presence of spin and rotational states of nano-magnets ,** GWANG-HEE KIM, Sejong Univ — We study nanomagnets that are free to rotate about their anisotropy and display quantum mechanical forces originated from quantum tunneling between classically degenerate magnetic states. Employing superpositions of spin and rotational states, we show that such forces can exist in the presence of a microwave field and a static magnetic field with a gradient. The optimal conditions for the observation of the oscillating force with quantum beats are presented.

**T1.00254 How to probe transverse magnetic anisotropy of a single-molecule magnet by electronic transport?**<sup>1</sup> , M. MISIORNY, Chalmers UT, Sweden and Adam Mickiewicz Univ., Poland, E. BURZURI, R. GAUDENZI, Delft UT, The Netherlands, K. PARK, Virginia Tech, USA, M. LEIJNSE, Lund Univ., Sweden, M. WEGEWIJS, FZ Jülich, Germany and RWTH Aachen, Germany, J. PAASKE, Univ. of Copenhagen, Denmark, A. CORNIA, Univ. of Modena and Reggio Emilia, Italy, H. VAN DER ZANT, Delft UT, The Netherlands — We propose an approach for *in-situ* determination of the transverse magnetic anisotropy (TMA) of an individual molecule by electronic transport measurements, see Phys. Rev. B **91**, 035442 (2015). We study a Fe4 single-molecule magnet (SMM) captured in a gateable junction, a unique tool for addressing the spin in different redox states of a molecule. We show that, due to mixing of the spin eigenstates of the SMM, the TMA significantly manifests itself in transport. We predict and experimentally observe the pronounced intensity modulation of the Coulomb peak amplitude with the magnetic field in the linear-response transport regime, from which the TMA parameter  $E$  can be estimated. Importantly, the method proposed here does not rely on the small induced tunnelling effects and, hence, works well at temperatures and electron tunnel broadenings by far exceeding the tunnel splittings and even  $E$  itself. We deduce that the TMA for a single Fe4 molecule captured in a junction is substantially larger than the bulk value.

<sup>1</sup>Work supported by the Polish Ministry of Science and Education as Iuventus Plus project (IP2014 030973) in years 2015-2016.

### T1.00255 Micromagnetic Simulation for Exploring Spin-wave Filtering Effects<sup>1</sup> ,

CHAO MA, XIANGYIN LI, TOBIAS STUECKLER, Fert Beijing Research Institute, School of Electronics and Information Engineering, Beihang University, Beijing, China, SHENGDA WANG, Technical University Munich, PEDRAM KHALILI, KANG L. WANG, Department of Electrical Engineering, University of California, Los Angeles, California, WEISHENG ZHAO, HAIMING YU, Fert Beijing Research Institute, School of Electronics and Information Engineering, Beihang University, Beijing, China, FERT BEIJING RESEARCH INSTITUTE TEAM, DEVICE RESEARCH LABORATORY COLLABORATION, TECHNICAL UNIVERSITY LABORATORY COLLABORATION — Spin wave propagation in periodical magnetic structures has been studied in experiments and simulations over last few years and offers potential applications in spin wave filters. We conduct simulation studies on the band gap structure of three types of structures for potential spin filter applications: first, antidot lattice based on yttrium iron garnet (YIG); second, magnonic crystal with iron dots embedded in YIG film; third, grating coupler formed by iron dots above YIG film. We found that the width and frequency position of band gap vary among these different structures. In addition, we investigate spin filter properties depend on the geometry parameters of the periodic pattern, e.g. lattice period, dot diameter. Such studies can be helpful for the realization of the spin filter device with optimized periodical structure and geometry parameters using nanotechnology.

<sup>1</sup>NSF China under Grant No. 11444005

**T1.00256 Propagating spin waves in YIG micro-channel on Silicon** , JILEI CHEN, PING CHE, SA TU, Fert Beijing Research Institute, School of Electronics and Information Engineering, Beihang University, Beijing, China, YAN ZHANG, JUN QIN, LEI BI, State Key Laboratory of Electronic Thin Films and Integrated Devices, University of Electronic Science and Technology of China, Chengdu, China, CHUANPU LIU, ZHIMIN LIAO, DAPENG YU, State Key Laboratory for Mesoscopic Physics, School of Physics, Peking University, Beijing, China, HAIMING YU, Fert Beijing Research Institute, School of Electronics and Information Engineering, Beihang University, Beijing, China, FERT BEIJING RESEARCH INSTITUTE TEAM, UNIVERSITY OF ELECTRONIC SCIENCE AND TECHNOLOGY OF CHINA TEAM, PEKING UNIVERSITY COLLABORATION — Recently the utilization of spin waves in the field of information processing has been widely developed because it is free of Joule heat dissipation and beneficial to miniaturization of the magnon based devices. Here we study spin waves in yttrium iron garnet (YIG) with a low damping property. The YIG film is fabricated on silicon substrate using pulsed laser deposition and the measured FMR linewidth is only a few Gauss. Using ebeam lithography, we are able to pattern the YIG film into a micro-channel and integrate sub-meter waveguides to generate and detect spin waves of wavelength down to  $1\mu\text{m}$  or below. We show results of propagating spin waves in the YIG micro-channel measured by the  $S_{12}$  parameter of the vector network analyzer.

**T1.00257 User-friendly software for modeling collective spin wave excitations<sup>1</sup>** , STEVEN HAHN, PETER PETERSON, RANDY FISHMAN, GEORG EHLERS, Oak Ridge National Laboratory — There exists a great need for user-friendly, integrated software that assists in the scientific analysis of collective spin wave excitations measured with inelastic neutron scattering. SpinWaveGenie is a C++ software library that simplifies the modeling of collective spin wave excitations, allowing scientists to analyze neutron scattering data with sophisticated models fast and efficiently. Furthermore, one can calculate the four-dimensional scattering function  $S(\mathbf{Q}, E)$  to directly compare and fit calculations to experimental measurements. Its generality has been both enhanced and verified through successful modeling of a wide array of magnetic materials. Recently, we have spent considerable effort transforming SpinWaveGenie from an early prototype to a high quality free open source software package for the scientific community.

<sup>1</sup>S.E.H. acknowledges support by the Laboratory's Director's fund, ORNL. Work was sponsored by the Division of Scientific User Facilities, Office of Basic Energy Sciences, US Department of Energy, under Contract no. DE-AC05-00OR22725 with UT-Battelle, LLC.

**T1.00258 Field-driven domain wall motion in ferromagnetic nanowires with Dzyaloshinskii-Moriya interaction** , ZHUO FENGJUN, SUN ZHOUSHOU, College of Physics, Optoelectronics and Energy & Jiangsu Key Laboratory of Thin Films, Soochow University, China — Field-driven domain-wall (DW) motion in ferromagnetic nanowires with easy- and hard-axis anisotropies was studied theoretically and numerically in the presence of the Dzyaloshinskii-Moriya interaction (DMI) based on the Landau-Lifshitz-Gilbert equation. We proposed a new trial function and found the exact solution for the DW motion along a uniaxial nanowire driven by an external magnetic field. A new strategy was suggested to speed up the DW motion in a uniaxial magnetic nanowire with large DMI parameters. In the presence of the hard-axis anisotropy, we found that the breakdown field and velocity of the DW motion was strongly affected by the strength and sign of the DMI parameter under external fields. The work may be useful for future magnetic information storage devices based on the DW motion.

**T1.00259 Ultralow field magnetization reversal of two-body Stoner particles system<sup>1</sup>** , FEI LI, XIAOFENG LU, RUJUN TANG, Z. Z. SUN, Soochow Univ — Magnetic mechanism of nanoparticles has attracted explosive attention in the development of modern information industry. On the base of Landau-Lifshitz-Gilbert equation, we studied the magnetization reversal in a system of two Stoner particles with uniaxial anisotropies and static magnetic interaction. Using micromagnetic simulation, two typical geometrical configurations of perpendicular (PERP) and parallel (PARA) configuration where the diameter of each particle is 20nm are considered. We found that when the separation between two particles has 23nm in PERP configuration ultralow switching field strength, 17mT can be realized, which satisfies the zero-field condition in our previous works[J. Appl. Phys. 109, 104303(2011)] according to the chosen parameters of cobalt material. For other separation values the switching field are multiple of lowest field. However, in PARA configuration the switching field changes with the separation faintly. This two-body system considered in our work might be implement as a composite information bit and our results offer further possibilities for its applications in information storage and/or fast magnetic response.

<sup>1</sup>Ultralow field magnetization reversal of two-body Stoner particles system

**T1.00260 Static Magnetic Properties of Films Measured by Means of Angular Perturbative Magnetoresistance** , ALEXANDRE OLIVEIRA, ABNER MELO, RICARDO DA COSTA, CARLOS CHESMAN, Universidade Federal do Rio Grande do Norte — In this work we introduced a new technique to measure magnetic anisotropies and magnetoelectrical properties, such as Anisotropic Magnetoresistance (AMR) and Giant Magnetoresistance (GMR) amplitudes. The Perturbative Magnetoresistance (PMR) consist of a regular collinear four probe magnetoresistance set up with an AC magnetic field ( $h_{ac}$ ) applied perpendicular to the DC ( $H_{dc}$ ) one.  $h_{ac}$  amplitude is about 1.0 Oe and oscillate at 270 Hz. We successfully interpreted the signal response from the voltage measured by lock-in amplifier and proposed a model based on energy minimization to extract magnetic anisotropies, AMR and GMR amplitudes. Measuring the in-plane angular dependency of PMR signal we were able to identify the usual magnetic anisotropy, such as uniaxial, unidirectional and cubic. Taking into account the perturbative nature of this technique (small  $h_{ac}$  amplitude and low frequency), we argue that angular PMR can be used to investigate some dynamic magnetic effects where static technique can not provide such information. A distinct feature of angular PMR is the capability to be used in saturated and non-saturated regime, so revealing magnetic properties dependency on applied field strength. We addressed the Rotatable Anisotropy as an example in this work.

**T1.00261 New mechanism of kinetic exchange interaction induced by strong magnetic anisotropy** , NAOYA IWAHARA, LIVIU CHIBOTARU, Theory of Nanomaterials Group, Katholieke Universiteit Leuven — It is well known that the kinetic exchange interaction between single-occupied magnetic orbitals (s-s) is always antiferromagnetic, while between single- and double-occupied orbitals (s-d) is always ferromagnetic and much weaker. Here we show that the exchange interaction between strongly anisotropic doublets of lanthanides, actinides and transition metal ions with unquenched orbital momentum contains a new s-d kinetic contribution equal in strength with the s-s one [1]. In noncollinear magnetic systems, this s-d kinetic mechanism can cause an overall ferromagnetic exchange interaction which can become very strong for transition metal ions. The importance of the s-d kinetic interaction and the possibility of the ferromagnetic interaction are confirmed in some existing complexes on the basis of the density functional theory calculations. [1] N. Iwahara and L. F. Chibotaru, arXiv:1502.04180.

**T1.00262 Itinerant ferromagnetism in fermionic systems with  $SP(2N)$  symmetry** , WANG YANG, CONGJUN WU, University of California San Diego — The Ginzburg-Landau free energy of systems with  $SP(2N)$  symmetry describes a second order phase transition on the mean field level, since the Casimir invariants of the  $SP(2N)$  group can be only of even order combinations of the generators of the  $SP(2N)$  group. This is in contrast with systems having the  $SU(N)$  symmetry, where the allowance of cubic term generally makes the phase transition into first order. In this work, we consider the Hertz-Millis type itinerant ferromagnetism in an interacting fermionic system with  $SP(2N)$  symmetry, where the ferromagnetic orders are enriched by the multi-component nature of the system. The quantum criticality is discussed near the second order phase transition point.

**T1.00263 Partially Screened Edgemagnetoplasmons**, MEHMET GOKSU, Millersville University — We present a study of edgemagnetoplasmons in a partially-screened system of electrons on a helium surface. We compare experiment results with Fetter's theory fits the mode frequency versus field and screening parameter for small magnetic fields. Fetter's theory fits the mode frequency versus field and screening parameter for small magnetic fields. Deviations at larger fields occur near the point where the penetration length becomes shorter than the width of the density profile at the sample perimeter. At larger fields, the mode frequencies are in reasonable agreement with the theoretical predictions of Volkov and Mikhailov. The linewidths are in fair qualitative agreement with their theory.

**T1.00264 First-principles investigation of transient spin transfer torque in magnetic layers**, ZHIZHOU YU, JIAN WANG, The Univ of Hong Kong — By employing the nonequilibrium Green's function (NEGF) method, the transient current-induced spin transfer torque (STT) of the magnetic layered system is investigated based on the density functional theory (DFT). The computational cost of the transient STT is huge due to the dense mesh of  $k$ -sampling for the layered system. In order to speed up the calculation, the Hamiltonian of leads is replaced by the complex absorbing potential (CAP) so that the Green's function can be cast into the wide-band form. After employing the Padé spectrum decomposition, the energy integrals in the formalism of transient electric current and STT, including that of the Fermi distribution function, can be analytically calculated by the theorem of residue, which dramatically reduces the computational complexity of the transient STT. As an application, the NEGF-DFT-CAP formalism with the Padé approximation is implemented to study the transient electric current and current-induced STT of Co/Cu/Co trilayers under an upward pulse of bias with different rotating angles of magnetization direction between two leads. The oscillation behavior is obtained for the transient STT when it approaches the steady state.

**T1.00265 Generalized non-Local Resistance Expression and its Application in F/N/F Spintronic Structure with Graphene Channel**<sup>1</sup>, HUAZHOU WEI, SHIWEI FU, China University of Petroleum - Beijing — We report our work on the spin transport properties in the F/N/F(ferromagnets/normal metal/ferromagnets) spintronic structure from a new theoretical perspective. A significant problem in the field is to explain the inferior measured order of magnitude for spin lifetime. Based on the known non-local resistance formula and the mechanism analysis of spin-flipping within the interfaces between F and N, we analytically derive a broadly applicable new non-local resistance expression and a generalized Hanle curve formula. After employing them in the F/N/F structure under different limits, especially in the case of graphene channel, we find that the fitting from experimental data would yield a longer spin lifetime, which approaches its theoretical predicted value in graphene.

<sup>1</sup>The authors acknowledge the financial support by China University of Petroleum-Beijing and the Key Laboratory of Optical Detection Technology for Oil and Gas in this institution.

**T1.00266 Theoretical Study on Twofold and Fourfold Symmetric Anisotropic Magnetoresistance Effect**, SATOSHI KOKADO, Graduate School of Integrated Science and Technology, Shizuoka University, MASAKIYO TSUNODA, Graduate School of Engineering, Tohoku University — We theoretically study the twofold and fourfold symmetric anisotropic magnetoresistance (AMR) effect [1]. We first extend our previous model [2] to a model including the crystal field effect [1]. Using the model, we next obtain an analytical expression of the AMR ratio, i.e.,  $AMR(\phi) = C_0 + C_2 \cos(2\phi) + C_4 \cos(4\phi)$ , with  $C_0 = C_2 - C_4$  [1]. Here,  $\phi$  is the relative angle between the magnetization direction and the electric current direction and  $C_2$  ( $C_4$ ) is a coefficient of the twofold (fourfold) symmetric term. The coefficients  $C_2$  and  $C_4$  are expressed by a spin-orbit coupling constant, an exchange field, a crystal field, and s-s and s-d scattering resistivities. Using this expression, we analyze the experimental results for Fe<sub>4</sub>N [3], in which  $|C_2|$  and  $|C_4|$  increase with decreasing temperature. The experimental results can be reproduced by assuming that the tetragonal distortion increases with decreasing temperature.

[1] S. Kokado *et al.*, J. Phys. Soc. Jpn. **84** (2015) 094710.

[2] S. Kokado *et al.*, J. Phys. Soc. Jpn. **81** (2012) 024705.

[3] M. Tsunoda *et al.*, Appl. Phys. Express **3** (2010) 113003.

**T1.00267 Dynamical correlation functions of the transverse Ising model with next-nearest-neighbor interactions**, P. R. C. GUIMARES, Universidade Federal de Viosa, Minas Gerais, Brazil, J. A. PLASCAK, University of Georgia, Athens - GA, USA, O. F. DE ALCANTARA BONFIM, University of Portland, Portland, Oregon, USA, J. FLORENCIO, Universidade Federal Fluminense, Niteri, RJ, Brazil — We investigate the effects of next-nearest-neighbor (NNN) interactions on the dynamics of the one-dimensional spin-1/2 transverse Ising model in the high temperature limit. Using exact diagonalization of finite chains, we obtain the time-dependent transverse correlation function and the corresponding spectral density for a tagged spin. Our results for chains of 13 spins with periodic boundary conditions produce results which are valid in the infinite-size limit. In general we find that the NNN coupling produces slower dynamics accompanied by an enhancement of the central mode behavior. Even in the case of a strong transverse field, if the NNN coupling is sufficiently large there is a crossover from collective mode to central mode behavior. We also obtain several recurrences for the continued fraction representation of the relaxation function.

**T1.00268 Precise quantum control on solid-state spins**, JIANPEI GENG, University of Science and Technology of China — Precise quantum control is of great importance for quantum information processing, high resolution spectroscopy, and quantum metrology. One of the key obstacles to realizing precise quantum control on solid-state spins is the noises arising from both environment and control field. Here, we design a composite pulse to realize precise quantum control on a single electron spin in diamond by suppressing the effect of both noises simultaneously. The control is experimentally demonstrated to be with a low error rate of 4.8E-5. We improve quantum optimal control method to realize precise two-qubit quantum control on a system comprised by a single electron spin and <sup>14</sup>N nuclear spin. With the improved quantum optimal control method, we design a pulse sequence for CNOT gate to suppress the noises simultaneously. The error rate of CNOT gate is measured to be 8E-3. To the best of our knowledge, the control we have realized stands for the state of art in precise quantum control on solid-state spins.

**T1.00269 Micromagnetic Simulation of Amorphous TbFeCo Thin Films with Self Exchange Bias**<sup>1</sup>, CHUNG MA, XIAOPU LI, JIWEI LU, JOSEPH POON, Univ of Virginia — Amorphous ferrimagnetic TbFeCo thin films are found to exhibit self exchange bias effect near compensation temperature by magnetic hysteresis loop measurement. Atom probe tomography, scanning transmission electron microscopy, and energy dispersive spectroscopy mapping have revealed two nanoscale amorphous phases with different Tb concentrations distributed within the amorphous films. The observed exchange anisotropy originates from the exchange interaction between the two nanoscale amorphous phases. Here, we present a computational model of TbFeCo with two nanoscale amorphous phases using micromagnetic simulation. To obtain a structure similar to the two nanoscale amorphous phases, two kinds of cells with different Tb concentration are distributed within the simulated space. Each cell contains separated Tb and FeCo components, forming two antiferromagnetically coupled sublattices. Using this model, we show exchange bias effect near compensation temperature, in agreement with experimental results. The effect can be tuned by controlling the microstructure and composition.

<sup>1</sup>The work was supported by the Defense Threat Reduction Agency grant.

**T1.00270 Spin-to-charge-current conversion in yttrium iron garnet-graphene hybrid structure<sup>1</sup>**, JOAQUIM MENDES, Universidade Federal de Vicosa, OBED ALVES SANTOS, Universidade Federal de Pernambuco, LEONEL MEIRELES, RODRIGO LACERDA, Universidade Federal de Minas Gerais, LUIS VILELA-LEO, FERNANDO MACHADO, ROBERTO RODRIGUEZ-SUREZ, ANTONIO AZEVEDO, SERGIO REZENDE, Universidade Federal de Pernambuco — The use of graphene in spintronic devices depends, among other things, on its ability to convert a spin excitation into an electric charge signal, a phenomenon that requires a spin-orbit coupling (SOC). In this work we report the observation of two effects that show the existence of SOC in large-area CVD grown single-layer graphene (SLG) deposited on a single crystal film of the ferrimagnetic insulator yttrium iron garnet (YIG). The first is a magnetoresistance of graphene induced by the magnetic proximity effect with YIG. The second is the detection of a DC voltage along the graphene layer resulting from the conversion of the spin current generated by spin pumping from microwave driven FMR into charge current. We interpret the spin-to-charge conversion as arising from the inverse Rashba-Edelstein effect (IREE) made possible by the extrinsic spin-orbit coupling in graphene. These observations show that spin orbit coupling can be extrinsically enhanced in graphene by the proximity effect with a ferromagnetic layer. This result opens new possibilities for the use of graphene in spintronic devices with unique functionalities.

<sup>1</sup>Research supported in Brazil by the agencies CNPq, CAPES, FINEP, FAPEMIG, FACEPE, and in Chile by FONDECYT No. 1130705

**T1.00271 Magnetic Anisotropy and Crystalline Electric Field in Quaternary Intermetallic Compounds.<sup>1</sup>**, W. C. LEE, Dept. of Physics, Sookmyung Women's Univ. Seoul 140-742 — All isostructural compounds  $RNi_2B_2C$  ( $R=Er, Ho, Dy$ ) show some magnetic transitions in magnetization isotherms at certain applied magnetic fields and temperatures above and below Neel and superconducting temperatures ( $T_N, T_C$ ) where  $T_N/T_C$  varies from 0.57 to 1.66 for  $ErNi_2B_2C$  and  $DyNi_2B_2C$ . By using theoretical group analysis of  $D_{4h}$  ( $I_4/mmm$ ) to the energy level scheme of crystalline electric field of magnetization isotherms anisotropy at various temperatures, we have obtained some possible ground state energy levels such as singlet  $\Gamma_4$  and first excited doublet state  $\Gamma_5$  in addition to another excited singlet  $\Gamma_1$ . Our crystalline electric field energy scheme analysis shows some qualitative agreement between theoretical calculation and experiments at high magnetic fields regime only, which means the interplay between antiferromagnetism and superconductivity should be included.

<sup>1</sup>Magnetic Anisotropy and Crystalline Electric Field in Quaternary Intermetallic Compounds.

**T1.00272 Tailoring of  $SmCo_5$  for optimal structure, magnetic anisotropy, and reduced criticality<sup>1</sup>**, DURGA PAUDYAL, R. CHOUHAN, The Ames Laboratory, Iowa State University, Ames, IA 50011, K. A. GSCHNEIDNER, JR., The Ames Laboratory and Department of Materials Science and Engineering, Iowa State University, Ames, IA 50011 —  $SmCo_5$  forms hexagonal  $CaCu_5$ -type structure with three non-equivalent sites: Sm (1a), Co (2c), and Co (3g). Sm lies in the middle of the Co (2c) hexagonal layers. Advanced density functional theory calculations employing Hubbard model show crystal field split localized Sm 4f states, which are responsible for the large part of the magnetic anisotropy exhibited by this system. In addition, the hexagonal Co (2c) layers help enhancing the anisotropy. Due to the partially quenched Sm 4f orbital moment, there is a net Sm 4f moment, which also helps enhancing magnetic moment. The substitution of some of the Sm sites by Nd adds Nd 4f multiplet thereby enhancing crystal field split 4f states and overall magnetic moment. The substitution of Co (2c) by Fe is preferred over Co (3g) but the compound becomes chemically unstable. The criticality issues could be addressed by substituting abundant Ce.

<sup>1</sup>This work is supported by the Critical Materials Institute, an Energy Innovation Hub funded by the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, Advanced Manufacturing Office.

**T1.00273 Rare-earth element based permanent magnets: a theoretical investigation<sup>1</sup>**, RAJIV K CHOUHAN, DURGA PAUDYAL, Ames Laboratory, U S department of Energy, Iowa State University, Ames, IA 50011 — Permanent magnetic materials with large magnetization and high magnetocrystalline anisotropy are important for technical applications. In this context rare-earth (R) element based materials are good candidates because of their localized 4f electrons. The 4f crystal field splitting provides large part of magnetic anisotropy depending upon the crystal environment. The d spin orbit coupling of alloyed transition metal component provides additional anisotropy.  $RCo_5$  and its derivative  $R_2Co_{17}$  are known compounds for large magnetic anisotropy. Here we have performed electronic structure calculations to predict new materials in this class by employing site substitutions. In these investigations, we have performed density functional theory including on-site electron correlation (DFT+U) and L-S coupling calculations. The results show that the abundant Ce substitution in R sites and Ti/Zr substitutions in some of the Co sites help reduce criticality without substantially affecting the magnetic moment and magnetic anisotropy in these materials.

<sup>1</sup>This work is supported by the Critical Materials Institute, an Energy Innovation Hub funded by the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, Advanced Manufacturing Office.

**T1.00274 Magnetostrictive stress reconfigurable thin film resonators in vacuum**, PETER FINKEL, US Naval Research Laboratory — The magnetic response of microdevices is significantly enhanced at structural resonance allowing for improved sensitivity and signal-to-noise ratio. The magnetic field resolution of these devices can be further improved when operating in vacuum due to an increase in mechanical quality factor. In this work, free-standing thin film CoFe bridge resonators have been fabricated and investigated. A strong magnetic field dependence of the fundamental resonance frequency is a function of magnetic field orientation due to a large unidirectional anisotropy. Under vacuum, a quality factor of up to 25 times greater than at atmosphere was revealed as well as an increased magnetic field sensitivity. Such stress reconfigurable sensors offer the possibility of broadband sensing with high resolution, and may therefore represent a new approach to fully integrated resonant magnetic field sensing technology.

**T1.00275 Heisenberg antiferromagnetic chain with multiple spin 1/2 particles of different flavors per site<sup>1</sup>**, SOLOMON F. DUKI, YI-KUO YU, NCBI/NLM/NIH — Motivated by the discoveries of quasi-1D magnetic systems, we studied a quantum mechanical spin lattice system consisting of a one-dimensional antiferromagnetic Heisenberg chain. In this system we considered M spin 1/2 particles of different flavors per site, and the low-lying states, ground state included, of the Hamiltonian was solved numerically using the exact diagonalization method for finite cluster sizes. We have also obtained the corresponding solutions for systems of the same chain length but with one spin M/2 particle per site. The low energy spectra of both systems are then compared. For  $M=2$  and  $M=3$ , our result shows that the two spin chain systems (one spin M/2 per site vs. M spin 1/2 of different flavors per site) have the same excitation spectra at low energy and the number of overlapped states increases as the size of the cluster increases. The observed overlap also indicates that low energy excitations of the M flavored spin 1/2 chain system selects the high spin states, effectively satisfying the Hund's Rule even though the system does not possess the orbital angular momentum.

<sup>1</sup>This work was supported by the Intramural Research Program of the National Library of Medicine at the National Institutes of Health.

**T1.00276 Comparison of Magnetic Behavior in Nanostructured and Bulk-Crystalline  $\text{Mn}_x\text{TaS}_2$** <sup>1</sup>, PAUL SHAND, LUCAS BEVING, MATTHEW FLEMING, PAYTON BURKEN, TIM KIDD, LAURA STRAUSS, University of Northern Iowa, CHIH-WEI CHEN, EMILIA MOROSAN, Rice University — The magnetic behavior of nanostructured  $\text{Mn}_x\text{TaS}_2$  for several different Mn concentrations  $x$  have been studied and a magnetic phase diagram obtained. For  $x$  values between 0.15 (the lowest measured) and 0.19, the nanostructured system shows cluster-glass behavior as evidenced by spin relaxation well described by the Vogel-Fulcher-Tammann law as well as aging effects in the dc magnetization and ac susceptibility. For  $x$  values between 0.19 and 0.24, nanostructured  $\text{Mn}_x\text{TaS}_2$  displays re-entrant cluster-glass characteristics, with transitions from paramagnetism to ferromagnetism at higher temperature and ferromagnetism to cluster glass at lower temperature. The tricritical point where all three phases converge seems to be close to  $x = 0.19$ . Results for single-crystal  $\text{Mn}_x\text{TaS}_2$  from the literature show single transitions: paramagnetism to ferromagnetism for  $x = 0.25$  and paramagnetism to cluster glass for  $x$  values in the range 0.02–0.1. For comparable  $x$  values, Curie temperatures seem to be slightly higher and cluster-glass transition temperatures slightly lower in the nanostructures. Bulk crystalline samples with Mn concentrations in the range 0.1–0.25 are currently being studied to more comprehensively compare the magnetic phase diagrams.

<sup>1</sup>Supported by NSF grant DMR 1206530

**T1.00277 Effects of disorder in the  $\text{Sr}_2\text{FeMoO}_6$  double perovskite via first principles calculations.**, O. NAVARRO, A.M. REYES, Unidad Morelia, Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, Y. ARREDONDO, Escuela Nacional de Estudios Superiores, Unidad Morelia, Universidad Nacional Autónoma de México — First principles calculations were done in the double perovskite  $\text{Sr}_2\text{FeMoO}_6$  regarding the effects of cationic disorder and electronic correlation in the ground-state properties such as spin polarization and magnetic moment. We used the Generalized Gradient Approximation (GGA) method including a U Hubbard term. Disorder is introduced via atomic substitution with a ratio of 25% and 12.5%. It is found a magnetic saturation of 2.22 $\mu_B$  and 2.99 $\mu_B$  for 25% and 12.5% of disorder respectively, in agreement with neutron magnetic scattering experiments. The half-metallic behavior of the above double perovskite remains only for a 12.5% of disorder.

**T1.00278 Magnetic Properties of Single-Crystal and Polycrystalline YIG Films Using a Custom Broad-Band FMR System**, SCOOTER JOHNSON, HARVEY NEWMAN, SANGHOON SHIN, EVAN GLASER, Naval Research Laboratory — We present a comparison of ferromagnetic resonance data acquired from single-crystal and polycrystalline yttrium iron garnet thick films deposited by liquid phase epitaxy and aerosol deposition, respectively. Data were taken using a custom broad-band measurement system consisting of a 1.2 T dc magnet and a 40 GHz vector network analyzer, which is used to track the ferromagnetic resonance signal up to 40 GHz. Ferromagnetic resonance data of the films were also taken using a high-sensitivity cavity system operating at 9.5 GHz. We include details on the experimental configuration and include an empirical conversion scheme relating frequency-swept to field-swept linewidths obtained from analysis of  $S$ -parameter data. Our results show that using these complementary measurement techniques can provide insight into dynamic magnetization characteristics of ferromagnetic materials.

**T1.00279 Alternatives to Rare Earth Permanent Magnets for Energy Harvesting Applications**<sup>1</sup>, HELENA KHAZDOZIAN, RAVI HADIMANI, DAVID JILES, Department of Electrical and Computer Engineering, Iowa State University — Direct-drive permanent magnet generators (DDPMGs) offer increased reliability and efficiency over the more commonly used geared doubly-fed induction generator, yet are only employed in less than 1 percent of utility scale wind turbines in the U.S. One major barrier to increased deployment of DDPMGs in the U.S. wind industry is NdFeB permanent magnets (PMs), which contain critical rare earth elements Nd and Dy. To allow for the use of rare earth free PMs, the magnetic loading, defined as the average magnetic flux density over the rotor surface, must be maintained. Halbach cylinders are employed in 3.5kW Halbach PMGs (HPMGs) of varying slot-to-pole ratio to concentrate the magnetic flux output by a lower energy density PM over the rotor surface. We found that for high pole and slot number, the increase in magnetic loading is sufficient to allow for the use of strontium iron oxide hard ferrite PMs and achieved rated performance. Joule losses in the stator windings were found to increase for the hard ferrite PMs due to increased inductance in the stator windings. However, for scaling of the HPMG designs to 3MW, rated performance and high efficiency were achieved, demonstrating the potential for elimination for rare earth PMs in commercial scale wind turbines.

<sup>1</sup>This work was supported by the National Science Foundation under Grant No. 1069283 and a Barbara and James Palmer Endowment at Iowa State University

**T1.00280 Triple Halo Coil: Development and Comparison with Other TMS Coils**<sup>1</sup>, PRIYAM RASTOGI, RAVI HADIMANI, DAVID JILES, Electrical and Computer Engineering, Iowa State University — Transcranial Magnetic Stimulation (TMS) is a non-invasive stimulation technique that can be used for the treatment of various neurological disorders such as Parkinson's Disease, PTSD, TBI and anxiety by regulating synaptic activity. TMS is FDA approved for the treatment of major depressive disorder. There is a critical need to develop deep TMS coils that can stimulate deeper regions of the brain without excessively stimulating the cortex in order to provide an alternative to surgical methods. We have developed a novel multi-coil configuration called "Triple Halo Coil" (THC) that can stimulate deep brain regions. Investigation of induced electric and magnetic field in these regions have been achieved by computer modelling. Comparison of the results due to THC configuration have been conducted with other TMS coils such as "Halo Coil", circular coil and "Figure of Eight" coil. There was an improvement of more than 15 times in the strength of magnetic field, induced by THC configuration at 10 cm below the vertex of the head when compared with the "Figure of Eight" coil alone.

<sup>1</sup>Carver Charitable Trust

**T1.00281 Anomalous Hall effect sensors based on magnetic element doped topological insulator thin films**, YAN NI, Iowa State University, ZHEN ZHANG, Purdue University, IKENNA NLEBEDIM, Ames Laboratory, U.S. Department of Energy, DAVID JILES, Iowa State University — Anomalous Hall effect (AHE) is recently discovered in magnetic element doped topological insulators (TIs), which promises low power consumption highly efficient spintronics and electronics. This discovery broadens the family of Hall effect (HE) sensors. In this work, both HE and AHE sensor based on Mn and Cr doped  $\text{Bi}_2\text{Te}_3$  TI thin films will be systematically studied. The influence of Mn concentration on sensitivity of  $\text{Mn}_x\text{Bi}_{2-x}\text{Te}_3$  HE sensors will be discussed. The Hall sensitivity increase 8 times caused by quantum AHE will be reported. AHE sensor based on Cr-doped  $\text{Bi}_2\text{Te}_3$  TI thin films will also be studied and compared with Mn doped  $\text{Bi}_2\text{Te}_3$  AHE sensor. The influence of thickness on sensitivity of  $\text{Cr}_x\text{Bi}_{2-x}\text{Te}_3$  AHE sensors will be discussed. Ultrahigh Hall sensitivity is obtained in Cr doped  $\text{Bi}_2\text{Te}_3$ . The largest Hall sensitivity can reach 2620  $\Omega/\text{T}$  in sensor which is almost twice higher than that of the normal semiconductor HE sensor. Our work indicates that magnetic element doped topological insulator with AHE are good candidates for ultra-sensitive Hall effect sensors.

**T1.00282 Enhanced Response of Magneto-active Elastomers by Anisotropy**, SAMUEL LOFLAND, CHRIS KASSNER, CHRIS ROTELLA, WILLIAM RIEGER, ROBERT WALKO, PAUL HORNUNG, STEVE KUTSKA, Department of Physics, Rowan University — We have investigated the magnetostriction of magneto-active elastomers which have random or aligned packing and magnetic filler particles of varying aspect ratios. We have systematically also varied the volume fraction. In general, we find that the response is a complex function of both particle aspect ratio as well as volume fraction. While for any given aspect ratio, there is a maximum in the magnetostriction as a function of volume fraction, for a given volume fraction, there is a local minimum for spherical particles. That is, stubby rods and thick disks show maximal response. We discuss these results in terms of competition between the magnetic dipole interactions, magnetic torque, and elastic response.

**T1.00283 Surface magnetic properties and magnetoimpedance of Co-rich amorphous and nanocrystalline  $(\text{Co}_{1-x}\text{Fe}_x)_{89}\text{Zr}_7\text{B}_4$  ribbons with oxide layer formed by long-term exposure to air**, TATIANA EGGERS, Dept. of Physics, Univ. of South Florida, ALEX LEARY, MICHAEL MCHENRY, Materials Science and Engineering, Carnegie-Mellon University, IVAN SKORVANEK, Institute of Experimental Physics, Slovak Academy of Sciences, HARIHARAN SRIKANTH, MANH-HUONG PHAN, Department of Physics, University of South Florida, Tampa — The surface magnetic properties and magnetoimpedance (MI) of amorphous and nanocrystalline  $(\text{Co}_{1-x}\text{Fe}_x)_{89}\text{Zr}_7\text{B}_4$  melt-spun ribbons with  $x = 0, 0.025, 0.05$  &  $0.1$  was investigated. A 540C heat treatment for 1 hour under a 2 T transverse field formed a large volume fraction of nanocrystalline phases in the ribbons, in addition to a well-defined transverse anisotropy indicated by x-ray diffraction and magneto-optical Kerr effect microscopy. After the heat treatment, the ribbon samples were exposed to open air for an extended period of time producing a visible oxide layer on the surfaces. High frequency magnetoimpedance measurements in the driving frequency range of 1-1000 MHz were made to characterize the potential impact of the surface oxide layer on the ac magnetization process. Unique field-dependent behavior of the real and imaginary components of the MI was found in nanocrystalline ribbons with higher Co content ( $x \geq 0.05$ ), showing multiple peaks above 50 MHz driving current.

**T1.00284 Interface and surface effects on Magnetic Properties in FeRh**, PERIHAN AKSU, ADEM PARABAS, FIKRET YILDIZ, gebze technical university department of physics —  $\text{Fe}_x\text{Rh}_{1-x}$  alloy systems has different magnetic properties depending of composition and temperature. When  $x$  is around 0.5, it is antiferromagnetic at room temperature and has phase transition around 370K from antiferromagnetic to ferromagnetic ordering. Due to this property, the FeRh alloy has a big potential for technological applications. In this study, effects of growing parameters, using buffer and cap layers on magnetic ordering and on phase transition have been studied. All films were grown on  $\text{MgO}(100)$  surface by sputter technique at different substrate temperatures. Rh and Pt were deposited on substrate as buffer and cap layer. Structural properties of the film were investigated by X-ray diffraction. Magnetization measurements were performed as a function of temperature by PPMS. And FMR spectra were registered and the results were analyzed for the ferromagnetic phases. Magnetization measurements showed that growing temperature has noteworthy effect on magnetic properties and structure of FeRh thin films. Depending of growth temperature, ferromagnetic and antiferromagnetic ordered samples were observed at room temperature. Phase transition also was controlled successfully by using buffer and cap layers.

**T1.00285 Analysis of ringing due to magnetic core materials used in pulsed nuclear magnetic resonance applications**, NEELAM PRABHU GAUNKAR, CAJETAN NLEBEDIM, RAVI HADIMANI, Iowa State Univ, IRFAN BULU, YI-QIAO SONG, Schlumberger-Doll Research Division, MANI MINA, DAVID JILES, Iowa State Univ — Oil-field well logging instruments employ pulsed nuclear magnetic resonance (NMR) techniques and use inductive sensors to detect and evaluate the presence of particular fluids in geological formations. Acting as both signal transmitters and receivers most inductive sensors employ magnetic cores to enhance the quality and amplitude of signals recorded during field measurements. It is observed that the magnetic core also responds to the applied input signal thereby generating a signal ('ringing') that interferes with the measurement of the signals from the target formations. This causes significant noise and receiver dead time and it is beneficial to eliminate/suppress the signals received from the magnetic core. In this work a detailed analysis of the magnetic core response and in particular loading of the sensor due to the presence of the magnetic core is presented. Pulsed NMR measurements over a frequency band of 100 kHz to 1MHz are used to determine the amplitude and linewidth of the signals acquired from different magnetic core materials. A lower signal amplitude and a higher linewidth are vital since these would correspond to minimal contributions from the magnetic core to the inductive sensor response and thus leading to minimized receiver dead time.

**T1.00286 Ground State of the One Dimensional Heisenberg Model with  $NNN$  Interactions**, J.D. MANCINI, Kingsborough Community College, V. FESSATIDIS, Fordham University, S.P. BOWEN, J. MALY, Chicago State University, R.K. MURAWSKI, Drew University — A great number of insights into a variety of complex physical many-body systems have been gleaned from the study of the one-dimensional Heisenberg model. There exists a number of quasi one-dimensional inorganic compounds such as  $\text{TTF}-\text{C}_6\text{H}_4(\text{CF}_3)_4$ ,  $\text{SRCu}_2\text{O}_3$ ,  $\text{VO}_2\text{P}_2\text{O}_7$  and  $\text{CuGeO}_3$  for which this Hamiltonian system is relevant. For this work we shall study the one-dimensional Heisenberg Model with nearest, next nearest and next -next nearest interactions. The Hamiltonian is given by:

$$H = J_1 \sum_k \mathbf{S}_k \cdot \mathbf{S}_{k+1} + J_2 \sum_k \mathbf{S}_k \cdot \mathbf{S}_{k+2} + J_3 \sum_k \mathbf{S}_k \cdot \mathbf{S}_{k+3}$$

where  $\mathbf{S}_k$  represents the spin 1/2 operator along a chain of  $N$  sites and periodic boundary conditions is assumed for the closed chain. We note that it is further possible to describe the Coulomb interaction subject to the Pauli exclusion principle for two quantum dots an  $XY$  model. Here we shall study the ground-state energy as well as the energy gap of this system using both a Lanczos (tridiagonal) scheme as well as a generalized Moments approach.

**T1.00287 Ground-State of the Bose-Hubbard Model**, J.D. MANCINI, Kingsborough Community College, V. FESSATIDIS, Fordham University, S.P. BOWEN, Chicago State University, R.K. MURAWSKI, Drew University, J. MALY, Kingsborough Community College — The Bose-Hubbard Model represents a simple theoretical model to describe the physics of interacting Boson systems. In particular it has proved to be an effective description of a number of physical systems such as arrays of Josephson arrays as well as dilute alkali gases in optical lattices. Here we wish to study the ground-state of this system using two disparate but related moments calculational schemes: the Lanczos (tridiagonal) method as well as a Generalized moments approach. The Hamiltonian to be studied is given by (in second-quantized notation):

$$H = -t \sum_{\langle i,j \rangle} b_i^\dagger b_j + \frac{U}{2} \sum_i n_i (n_i - 1) - \mu \sum_i n_i.$$

Here  $i$  is summed over all lattice sites, and  $\langle i,j \rangle$  denotes summation over all neighboring sites  $i$  and  $j$ , while  $b_i^\dagger$  and  $b_i$  are bosonic creation and annihilation operators.  $n_i = b_i^\dagger b_i$  gives the number of particles on site  $i$ . Parameter  $t$  is the hopping amplitude, describing mobility of bosons in the lattice. Parameter  $U$  describes the on-site interaction, repulsive, if  $U > 0$ , and attractive for  $U < 0$ .  $\mu$  is the chemical potential. Both the ground-state energy and energy gap are evaluated as a function of  $t$ ,  $U$  and  $\mu$ .

**T1.00288 Atomic structure prediction of Zr-Co and Hf-Co nanoclusters using the evolutionary algorithm.**, AHMAD ALSAAD, Department of Physics, Jordan university of sci. & Technology, Irbid 22110, Jordan, NABIL AL-AQTASH, Department of Physics, The Hashemite University, Zarqa 13133, Jordan, RENAT SABIRIANOV, Department of Physics, University of Nebraska at Omaha, 6001 Dodge St., Omaha, NE, USA — Nanostructures of Hf-Co and Zr-Co rare earth free magnetic materials exhibit a high room-temperature energy product. In our study, the evolutionary algorithm coupled with density functional theory (DFT) is used to identify the global energy minimum atomic structures of Zr-Co and Hf-Co clusters. Using evolutionary crystal structure optimization algorithm, as implemented in USPEX, we studied the atomic structure, binding energies, magnetic properties, and anisotropy of  $\text{Zr}_x\text{Co}_y$  and  $\text{Hf}_x\text{Co}_y$  ( $x=1,2$  and  $y=5,7,11$ ) clusters. A set of metastable and global minimum atomic structures are identified. Several new lower energy configurations were identified for  $\text{Zr}_2\text{Co}_{11}$ ,  $\text{Zr}_1\text{Co}_5$ ,  $\text{Zr}_1\text{Co}_7$ ,  $\text{Hf}_2\text{Co}_{11}$ ,  $\text{Hf}_1\text{Co}_5$  and  $\text{Hf}_1\text{Co}_7$  clusters by our calculations. We discussed the magnetic interaction between the atoms of the clusters which is critical in finding the lowest energy structure. Our calculations show that Zr-Co and Hf-Co clusters have ferromagnetic coupling and large magnetization. Magnetocrystalline anisotropy energies (MAE) of these clusters were also found to be large.

## T1.00289 POSTDEADLINE —

**T1.00290 Analytical Phase Equilibrium Function for Mixtures Obeying Raoult's and Henry's Laws<sup>1</sup>**, ROBERT HAYES, North Carolina State University — When a mixture of two substances exists in both the liquid and gas phase at equilibrium, Raoult's and Henry's laws (ideal solution and ideal dilute solution approximations) can be used to estimate the gas and liquid mole fractions at the extremes of either very little solute or solvent. By assuming that a cubic polynomial can reasonably approximate the intermediate values to these extremes as a function of mole fraction, the cubic polynomial is solved and presented. A closed form equation approximating the pressure dependence on mole fraction of the constituents is thereby obtained. As a first approximation, this is a very simple and potentially useful means to estimate gas and liquid mole fractions of equilibrium mixtures. Mixtures with an azeotrope require additional attention if this type of approach is to be utilized.

<sup>1</sup>This work paid for under NRC-HQ-84-14-G-0059

**T1.00291 Oxide double quantum dot - an answer to the qubit problem?**, SUDHAKAR YARLAGADDA<sup>1</sup>, AMIT DEY, Saha Institute of Nuclear Physics, Kolkata — We propose that oxide-based double quantum dots with only one electron (tunnelling between the dots) can be regarded as a qubit with little decoherence; these dots can possibly meet future challenges of miniaturization. The tunnelling of the  $e_g$  electron between the dots and the attraction between the electron and the hole on adjacent dots can be modelled as an anisotropic Heisenberg interaction between two spins with the total z-component of the spins being zero. We study two anisotropically interacting spins coupled to optical phonons; we restrict our analysis to the regime of strong coupling to the environment, to the antiadiabatic region, and to the subspace with zero value for  $S_{zT}$  (the z-component of the total spin). In the case where each spin is coupled to a different phonon bath, we assume that the system and the environment are initially uncorrelated (and form a simply separable state) in the polaronic frame of reference. By analyzing the polaron dynamics through a non-Markovian quantum master equation, we find that the system manifests a small amount of decoherence that decreases both with increasing nonadiabaticity and with enhancing strength of coupling  $g$ .

<sup>1</sup>Recently I got an invitation to visit Argonne National Lab from Jan./2106 to end of March/2016. I thought I would give a talk at APS March meeting. Please accept the submission.

**T1.00292 Chiral projected entangled-pair state with topological order<sup>1</sup>**, SHUO YANG, Perimeter Institute for Theoretical Physics, Waterloo, ON, N2L 2Y5, Canada, THORSTEN WAHL, HONG-HAO TU, Max-Planck Institute for Quantum Optics, Hans-Kopfermann-Str. 1, D-85748 Garching, Germany, NORBERT SCHUCH, JARA Institute for Quantum Information, RWTH Aachen University, D-52056 Aachen, Germany, J. IGNACIO CIRAC, Max-Planck Institute for Quantum Optics, Hans-Kopfermann-Str. 1, D-85748 Garching, Germany — We show that projected entangled-pair states (PEPS) can describe chiral topologically ordered phases. For that, we construct a simple PEPS for spin-1/2 particles in a two-dimensional lattice. We reveal a symmetry in the local projector of the PEPS that gives rise to the global topological character. We also extract characteristic quantities of the edge conformal field theory using the bulk-boundary correspondence.

<sup>1</sup>EU projects SIQS and QALGO, the Alexander von Humboldt foundation, the Government of Canada through Industry Canada, and the Province of Ontario through the Ministry of Economic Development & Innovation

**T1.00293 OIST - A New Model of Graduate Education.**, NEIL CALDER, Okinawa Institute of Science and Technology — I would present the Okinawan Institute of Science and Technology Graduate University. The Graduate University offers outstanding opportunities for students looking to study for a Ph.D. I would outline what makes OIST different from other Graduate Schools and explain the opportunities for students but also the posts open for Faculty. The Okinawa Institute of Science and Technology is an interdisciplinary graduate school offering a 5-year PhD program in Science. Over half of the faculty and students are recruited from outside Japan, and all education and research is conducted entirely in English.

**T1.00294 Controlling Surface Chemistry of Gallium Liquid Metal Alloys to Enhance their Fluidic Properties**, NAHID ILYAS, BRAD CUMBY, ALEXANDER COOK, MICHAEL DURSTOCK, CHRISTOPHER TABOR, Air Force Research Laboratory, MATERIALS AND MANUFACTURING DIRECTORATE TEAM — Gallium liquid metal alloys (GaLMAs) are one of the key components of emerging technologies in reconfigurable electronics, such as tunable radio frequency antennas and electronic switches. Reversible flow of GaLMA in microchannels of these types of devices is hindered by the instantaneous formation of its oxide skin in ambient environment. The oxide film sticks to most surfaces leaving unwanted metallic residues that can cause undesired electronic properties. In this report, residue-free reversible flow of a binary alloy of gallium (eutectic gallium indium) is demonstrated via two types of surface modifications where the oxide film is either protected by an organic thin film or chemically removed. An interface modification layer (alkyl phosphonic acids) was introduced into the microfluidic system to modify the liquid metal surface and protect its oxide layer. Alternatively, an ion exchange membrane was utilized as a sponge-like channel material to store and slowly release small amounts of HCl to react with the surface oxide of the liquid metal. Characterization of these interfaces at molecular level by surface spectroscopy and microscopy provided with mechanistic details for the interfacial interactions between the liquid metal surface and the channel materials.

**T1.00295 Hellmann-Feynman Forces within the DFT+U in Wannier functions basis**, DMITRY NOVOSELOV, DMITRY KOROTIN, VLADIMIR ANISIMOV, Institute of Metal Physics — The most general way to describe localized atomic-like electronic states in strongly correlated materials is to use Wannier functions. In the present paper we continue development of widely-used DFT+U method with the Wannier function basis set and propose a technique to calculate Hubbard contribution to atomic forces. The technique was implemented as a part of plane-waves pseudopotential code Quantum-ESPRESSO and tested on two compounds: charge transfer insulator NiO with cubic crystal structure and correlated metal SrVO<sub>3</sub> with perovskite structure.

**T1.00296 Generation of nondegenerate narrow-band photon pairs for hybrid quantum network**, JIAN WANG, PENGYINJIE LV, JINMING CUI, BIHENG LIU, JIANSUN TANG, YUNFENG HUANG, CHUANFENG LI, GUANGCAN GUO, Univ of Sci & Tech of China — In a hybrid quantum network, the linking two types of quantum nodes through photonic channels requires excellent matching of the central frequency and bandwidth between both nodes and their interfacing photons. However, pre-existing photon sources cannot fulfill this requirement. Using a novel conjoined double-cavity strategy, we report the generation of nondegenerate narrow-band photon pairs by cavity-enhanced spontaneous parametric down-conversion. The central frequencies and bandwidths of the signal and idler photons are independently set to match with trapped ions and solid-state quantum memories. With this source we achieve the bandwidths and central frequencies of 4 MHz at 935 nm and 5 MHz at 880 nm for the signal and idler photons, respectively, with a normalized spectral brightness of 4.9/s/MHz/mW. Due to its ability to be independently locked to two different wavelengths, the conjoined double-cavity is universally suitable for a hybrid quantum network consisting of various quantum nodes.

**T1.00297 Optimization of the profile of a pulsed slow positron beam extracted from a buffer-gas positron trap for the production of a variable energy positronium beam<sup>1</sup>**, R. GLADEN, Univ of Texas at Arlington, K. MICHISHIO, L. CHIARI<sup>2</sup>, Tokyo University of Science, N. OSHIMA, AIST, Tsukuba, Japan, Y. NAGASHIMA, Tokyo University of Science — In this poster we will present some details of steps taken to optimize the beam profile of a pulsed slow positron beam extracted from a buffer-gas positron trap. The beam will be employed for the production of a novel positronium beam by the acceleration and photodetachment of positronium negative ions [1, 2]. The TUS group is planning on using this beam to study positronium diffraction from solid surfaces, providing a unique neutral-particle spectroscopic method with several advantages over conventional neutral-particle spectroscopy, such as a reduced particle mass and, hence, the reduction of damage to the sample surface. [1] K. Michishio, et al. Phys. Rev. Lett. **106**, 153401 (2011) [2] K. Michishio, et al. Appl. Phys. Lett. **100**, 254102 (2012)

<sup>1</sup>This work was performed at the Tokyo University of Science. The visit of R. G. to the laboratory was sponsored in part by the NSF EAPSI fellowship and the JSPS Summer Program.

<sup>2</sup>1-3 Kagurazaka, Shinjuku, Tokyo, Japan

**T1.00298 Synthesis, Characterization and Electrochemical Analysis of Composite Cathode Material  $0.5\text{Li}_2\text{MnO}_3\text{-}0.25\text{LiMn}_2\text{O}_4\text{-}0.25\text{LiNi}_{0.5}\text{Mn}_{0.5}\text{O}_2$  for LIB applications.<sup>1</sup>**, MONICA LOPEZ DE VICTORIA, JIFI SHOJAN, LORAIN TORRES, RAJESH KATIYAR, VALERIO DORVILIEN, RAM KATIYAR, University of Puerto Rico — Structural stability, environment friendliness, low cost as well as good electrochemical performances are the major requirements for cathode materials.  $\text{Li}_2\text{MnO}_3$  based composite cathode materials are one of the widely investigated positive cathode materials due to their ability to provide high discharge capacity and good rate capability. We have synthesized layered- spinel composite cathode material  $0.5\text{Li}_2\text{MnO}_3\text{-}0.25\text{LiMn}_2\text{O}_4\text{-}0.25\text{LiNi}_{0.5}\text{Mn}_{0.5}\text{O}_2$  by sol-gel synthesis technique and surface characterized using XRD, Raman, SEM and EDX. Peaks corresponding to layered and spinel structures are identified by XRD and Raman studies. SEM images depict the nano-sized particles and EDX data confirms the presence of constituent transition metals and oxygen. Electrochemical studies were performed on coin cells, which were assembled in the Ar- filled glove box using Li as anode and spread material as cathode.  $\text{LiPF}_6$  with EC:DMC::1:2 ratio was used as the electrolyte. CV, EIS and charge discharge studies shows that the developed cathode material is a promising electrode for next generation Li ion batteries.

<sup>1</sup>Nasa Epscore Grant

**T1.00299 Propulsion and Levitation with a Large Electrodynamic Wheel**, NATHAN GAUL, HANNAH LANE, Northern Virginia Community College, Annandale, VA — We constructed an electrodynamic wheel using a motorized bicycle wheel with a radius of 12 inches and 36 one-inch cube magnets attached to the rim of the wheel. The radial magnetic field on the outside of the wheel was maximized by arranging the magnets into a series of Halbach arrays which amplify the field on one side of the array and reduce it on the other side. Rotating the wheel produces a rapidly oscillating magnetic field. When a conductive metal “track” is placed in this area of strong magnetic flux, eddy currents are produced in the track. These eddy currents create magnetic fields that interact with the magnetic fields from the electrodynamic wheel. The interaction of the magnetic fields produces lift and drag forces on the track which were measured with force gauges. Measurements were taken at a variety of wheel speeds, and the results were compared to the theoretical prediction that there should be a linear relationship between the lift and drag forces with increasing wheel speed. Partial levitation was achieved with the current electrodynamic wheel. In the future, the wheel will be upgraded to include 72 magnets rather than 36 magnets. This will double the frequency at which the magnetic field oscillates, increasing the magnetic flux. Electrodynamic wheels have applications to the transportation industry, since multiple electrodynamic wheels could be used on a vehicle to produce a lift and propulsion force over a conductive track.

**T1.00300 The Microwave Hall Effect Measured Using a Waveguide Tee**, WILLIAM JOHNSON, JOYCE COPPOCK, J. ROBERT ANDERSON, Univ of Maryland-College Park — We describe a simple microwave apparatus to measure the Hall effect in semiconductor wafers. This technique does not require contacts on the sample or the use of a resonant cavity. Our method consists of placing a semiconductor wafer into a slot in an X-band (8 - 12 GHz) waveguide series tee, injecting microwave power into the two opposite arms of the tee, and measuring the microwave output at the third arm. A magnetic field is applied perpendicular to the wafer and produces a microwave Hall signal that is linear in the magnetic field and which reverses phase when the magnetic field is reversed. The microwave Hall signal is proportional to the semiconductor mobility, which we compare for calibration purposes with d. c. mobility measurements obtained using the van der Pauw method. We obtain the resistivity by measuring the microwave reflection coefficient of the sample. We determine a calibration constant as a function of the ratio of thickness to skin depth for two and three inch silicon and germanium samples doped with boron or phosphorus. The measured mobilities ranged from 270 to 3000  $\text{cm}^2 / (\text{Vsec})$

**T1.00301 Adsorption of Water Molecule on Silicene-FE System**, GREGORIO RUIZ CHAVARRIA, UNIVERSIDAD AUTONOMA CHAPINGO — After graphene synthesis[1], there have been numerous studies on similar systems in two dimensions so, we have the borophene [2], germanene [3], silicene [4,5], phosphorene [6], etc. Following this line, I do a study that takes the silicene system at its starting point, system to which it add Fe atom. At first, the stability of SILICENE-Fe system is studied, which is stable. Then a water molecule is added to the SILICENE-Fe system, which is captured, as is bounded to the Fe atom. To make this study I used Functional Density Theory, Born-Openheimer Approximation, Atomic Pseudopotentials and Molecular Dynamics.

[1] Novoselov, K.S.;Geim, A.K. et al, Science, **306** , 666 (2004).

[2] Yang, X., et al, PRB,**77**, 041402(R) (2008).

[3] Bianco, E., et al, ACS Nano, **7**, 4414 (2013).

[4] Kamal, C, et al, J.Phys.: Condens. Matter, **25**, 085508 (2013).

[5] Drummond, N.P., et al, PRB,**85**, 075423 (2012).

[6] Liang, L., et al, Nanolett., **14**, 6400 (2014).

**T1.00302 Effect of immersion in simulated body environment on mechanical properties of twist-oriented poly(lactic acid) screws.**, MASATO SAKAGUCHI, SATOSHI KOBAYASHI, Tokyo metropolitan university, COMPOSITE ENGINEERING LAB COLLABORATION — Poly(lactic acid) (PLA) has been applied to bone fixation devices, since it has high biocompatibility. In order to apply PLA device to a higher loaded part, mechanical properties of PLA have been improved by uniaxial drawing. However, mechanical properties along the other loading direction than the drawing direction such as torsion were not improved. Therefore, surgeon should be carefully conducted not to brake the reinforced PLA screw when tightening. In this study, screw is focused on as a bone fixation device. In order to improve torsional strength of a PLA screw, twist-orientation method was developed. PLA screw is prepared through a series of routes including casting, extrusion drawing, twist-orientation and forging. This screw was immersed in the phosphate buffered solution for 0, 8, 16 and 24 weeks, then shear strength, orientation function, crystallinity and molecular weight were measured. As a result, twist-orientation improves the initial torsional strength of PLA screw without the decrease in initial shear strength. In addition, the shear strength on twist-oriented screw is equivalent that of non-twist oriented screw during immersion until 24 weeks. This result shown that the twist-orientation does not decrease shear strength after immersion.

### **T1.00303 Lift to Drag Ratio Analysis in Magnetic Levitation with an Electrodynamic Wheel<sup>1</sup>**

, ANGEL GUTARRA-LEON, VINCENT CORDREY, WALERIAN MAJEWSKI, Northern Virginia Comm Coll — Our experiments explored inductive magnetic levitation (MagLev) using simple permanent magnets and conductive tracks. Our investigations used a circular Halbach array with a 1 Tesla variable magnetic field on the outer rim of the ring. Such a system is usually called an Electrodynamic Wheel (EDW). Rotating this wheel around a horizontal axis above or below a flat conducting surface should induce eddy currents in said surface through the variable magnetic flux. The eddy currents produce, in turn, their own magnetic fields, which interact with the magnets of the EDW. We constructed a four-inch diameter Electrodynamic Wheel using twelve Neodymium permanent magnets and demonstrated that the magnetic interactions produce both lift and drag forces on the EDW. These forces can be used for levitation and propulsion of the EDW to produce magnetic levitation without coils and complex control circuitry. We achieved full levitation of the non-magnetic aluminum and copper plates. Our results confirm the expected behavior of lift to drag ratio as proportional to  $(L/R)\omega$ , with L and R being the inductance and resistance of the track plate, and  $\omega$  being the angular velocity of the magnetic flux.

<sup>1</sup>Supported by grants from the Virginia Academy of Science, Society of Physics Students, Virginia Community College System, and the NVCC Educational Foundation.

### **T1.00304 Electromigration in focused ion beam deposited tungsten single nanowires<sup>1</sup>**

, PABITRA MANDAL, BIPUL DAS<sup>2</sup>, A. K. RAYCHAUDHURI, S. N. Bose National Center for Basic Sciences, Salt lake, Kolkata-98, India — As the focused ion beam induced deposited (FIBID) nanowires (NWs) of W, Pt are being used in nanoelectronic technology to connect individual nanodevices, repairing damaged interconnects in integrated circuit (IC), electromigration study in FIBID-NWs has become essential. Briefly, when a thin conductor, like metallic Al, Cu interconnects in an IC chip carry quite high current density  $\sim 10^{12}$  A/m<sup>2</sup>, ions or atoms start migrating. Such migration causes void and hillock formation leading to interconnect discontinuity, short circuit and ultimately IC failure. Our electromigration study in single FIBID-NWs of W reveals that failure in NWs of width and thickness  $\approx 100$  nm occurs typically at  $10^{11}$  A/m<sup>2</sup>. Most notably, void and hillock always form in opposite polarity compared to typical metallic NWs. Such distinctly new outcome is explained via electromigration driven by direct force (ionic charge\*electric field) opposed to wind force driven migration observed in metallic NWs. As FIBID-NWs are composite in nature, different species (e.g., Ga, W and C) migrate with different degree and direction depending on their oxidation state, leading to redistribution of species across NW length and formation of a Ga rich hillock.

<sup>1</sup>S. N. Bose National Centre for Basic Sciences, Block-JD, Sector-III, Salt Lake, Kolkata-98, India

<sup>2</sup>Present address: National Changhua University of Education, Jin-De Road, Changhua 500, Taiwan

### **T1.00305 Robust surface states in epitaxial Bi(111) thin films**

, KAI ZHU, XIAOFENG JIN, Physics department of Fudan University — Bulk Bi a prototype semimetal with trivial electronic band topology. Unanticipatedly, we show the Altshuler-Aronov-Spivak and Aharonov-Bohm effects in epitaxial Bi(111) thin films. Meanwhile, we clearly identify the interaction of the top and bottom surface states via quantum tunneling by the electrical conductance and weak anti-localization measurements. These results have significantly enriched our understanding about the electronic structure of Bi, which might be helpful for clearing up some of its longstanding subtle issues.

### **T1.00306 Ternary Synaptic Plasticity Arising from Memdiode Behavior of TiOx Single Nanowire<sup>1</sup>**

, DESHUN HONG, YUANSHA CHEN, JIRONG SUN, BAOGEN SHEN, Chinese Academy of Sciences, Beijing, GROUP 3 OF MAGNETISM LABORATORY, BEIJING NATIONAL LABORATORY FOR CONDENSED MATTER PHYSICS TEAM — Electric field-induced resistive switching (RS) effect has been widely explored as a novel nonvolatile memory over the past few years. Recently, the RS behavior with continuous transition has received considerable attention for its promising prospect in neuromorphic simulation. Here, the switching characteristics of a planar-structured TiOx single nanowire device were systematically investigated. It exhibited a strong electrical history-dependent rectifying behavior that was defined as a "memdiode". We further demonstrated that a ternary synaptic plasticity could be realized in such a TiOx nanowire device, characterized by the resistance and photocurrent responses. For a given state of the memdiode, a conjugated memristive characteristic and a distinct photocurrent can be simultaneously obtained, resulting in a synchronous implementation of various Hebbian plasticities with the same temporal order of spikes. These intriguing properties of TiOx memdiode provide a feasible way toward the designing of multifunctional electronic synapses as well as programmable artificial neural network

<sup>1</sup>This work has been partially supported by the National Basic Research of China (2013CB921700), the "Strategic Priority Research Program (B)" of the Chinese Academy of Sciences (XDB07030200) and the National Natural Science Foundation of China (11374339)

### **T1.00307 Formation of silicene-germanene heterostructures by Ge deposition on epitaxial silicene**

, YUTO AWATANI, ANTOINE FLEURENCE, YUKIKO YAMADA-TAKAMURA, Japan Advanced Institute of Science and Technology — Silicene and germanene are two dimensional honeycomb sheets composed of Si and Ge atoms. Epitaxial silicene and germanene form spontaneously on ZrB2(0001) thin films grown on Si(111) [1] and Ge(111) [2] substrates and can be identified by (2X2)- and ( $\sqrt{3}X\sqrt{3}$ )-reconstruction of ZrB2(0001) respectively. In the present work, we demonstrate that silicene-germanene heterostructures can be formed by deposition of Ge on epitaxial silicene and by subsequent annealing. LEED and STM analysis revealed the growth of the following Si-Ge structures depending on preparation conditions. (1): After annealing at 830 K, (2X2)- and ( $\sqrt{3}X\sqrt{3}$ )-reconstructed areas existed side by side, which suggests that a two-dimensional silicene-germanene heterostructures is formed. (2): After annealing at 1070 K, the surface is (2X2)-reconstructed, with a heterogeneous atomic contrast different from silicene which suggests the incorporation of Ge atoms in the silicene lattice. (3): After annealing this mixed Si-Ge layer at 830 K, a ( $2\sqrt{3}X2\sqrt{3}$ )-reconstruction is observed, in agreement with the overlapping of ( $\sqrt{3}X\sqrt{3}$ )- and (2X2)-reconstructed layers. The structure is presumably a silicene-germanene heterostack structure. [1] A.Fleurence, et al., Phys. Rev. Lett. 108 245501(2012). [2] A.Fleurence, et al., APS March Meeting 2016.

### **T1.00308 Analysis of magnetic anisotropy on BaTiO3/La2/3Sr1/3MnO3 bilayers**

, JOHN EDWARD ORDONEZ, MARIA E GOMEZ, PEDRO PRIETO, Univ del Valle Cali, GRUPO DE PELICULAS DELGADAS TEAM — We have deposited BTO/LSMO bilayers as a possible route to design systems with artificial magnetoelectric coupling. We maintain a fixed ferroelectric layer thickness (tBTO= 100 nm) and ferromagnetic layer (tLSMO = 25 nm). We analyze the influence of direction substrate on electrical and magnetic properties of manganite. From XRD we found that the BTO layer for STO(001) growth textured with almost two different distribution of domains (c domains in plane and out-plane) with cBTO=4.108 Å and LSMO layer growth textured with cLSMO=3.855 Å. Interestingly, for STO(110) and STO(111) the BTO layer and LSMO layer the growth is textured with cBTO=4.037 Å and cBTO=4.018 Å while LSMO growth is also textured with cLSMO=3.867 Å and cLSMO=3.858 Å, respectively. Magnetization with temperature curves shows a ferromagnetic transition for all bilayers at room temperature with a magnetization between 280-320 emu/cm3. Measures of anisotropy at 300 K show a change in magnetic anisotropy for bilayer growth on STO(001) from biaxial magnetic ordering (LSMO/STO) to uniaxial magnetic ordering (bilayer), probably due to BTO layer influence on magnetic properties on LSMO layer. This work has been supported by "Colciencias-CENM Research Project CI7917-CC 10510 contract 0002-2013 and CI 7978.

**T1.00309 The anomalous Hall effect of Fe(001) in ultrathin film regime**, LIN WU, XIAOFENG JIN, Physics Department, Fudan University — The anomalous Hall effect (AHE) in ultrathin film regime is investigated in Fe(001)(1 nm-3 nm) epitaxial on MgO(001). We find the intrinsic anomalous Hall conductivity (AHC) is reducing when the thickness decreasing. The reduction of the intrinsic AHC is interpreted as modification of electronic band structure of iron through boundary confinement. We also observe localization correction to longitudinal resistivity, while the anomalous Hall resistivity of different temperature can be figured out by a set of variable skew scattering coefficients and a constant side-jump contribution. The analysis indicates that localization correction has a significant impact on skew scattering but little on side-jump.

**T1.00310 Unusual magnetic properties of superconducting Bi/Ni bilayers**, HEXIN ZHOU, XIAOFENG JIN, Fudan University, JIN GROUP TEAM — Superconductivity and ferromagnetism are two incompatible phenomena. However, the interaction between them attracts numerous physicists' interests for both theoretical and experimental purposes. Recently, increasing experimental discoveries reveal unconventional effects in superconductor and ferromagnet hybrids, which stimulates a new field called superconducting spintronics. In present work, we report various intriguing magnetic properties of an unexpected superconducting bilayer consisting of non-superconducting Bi and ferromagnetic Ni. A large spontaneous magnetization is induced when the temperature is decreased below the superconductivity transition temperature, which indicates a complex interaction between superconductivity and ferromagnetism in this bilayer. The zero field cooling results show normal Meissner effect while the field cooling results show paramagnetic Meissner effect. Besides, magnetic hysteresis loops in low temperatures show flux pinning and flux jumping effects. Our findings pave the way for exploring unconventional superconductivity coupled to ferromagnetism and potential applications in superconducting spintronics.

**T1.00311 Long-lived non-equilibrium states in a quantum-Hall Tomonaga-Luttinger liquid<sup>1</sup>**, TOSHIMASA FUJISAWA, KAZUHISA WASHIO, RYO NAKAZAWA, MASAYUKI HASHISAKA, Tokyo Inst of Tech - Tokyo, KOJI MURAKI, NTT Basic Research Laboratories, YASUHIRO TOKURA, Univ. Tsukuba — The existence of long-lived non-equilibrium states without showing thermalization, which has previously been demonstrated in time evolution of ultracold atoms (quantum quench), suggests the possibility of their spatial analogue in transport behavior of interacting electrons in solid-state systems. Here we report long-lived non-equilibrium states in one-dimensional edge channels in the integer quantum Hall regime. For this purpose, non-trivial binary spectrum composed of hot and cold carriers is prepared by an indirect heating scheme using weakly coupled counterpropagating edge channels in an AlGaAs/GaAs heterostructure. Quantum dot spectroscopy clearly reveals that the carriers with the non-trivial binary spectrum propagate over a long distance (5 - 10  $\mu\text{m}$ ), much longer than the length required for electronic relaxation (about 0.1  $\mu\text{m}$ ), without thermalization into a trivial Fermi distribution. This observation is consistent with the integrable model of Tomonaga-Luttinger liquid. The long-lived spectrum implies that the system is well described by non-interacting plasmons, which are attractive for carrying information for a long distance.

<sup>1</sup>This work was supported by the JSPS 26247051 and 15H05854, and Nanotechnology Platform Program of MEXT.

**T1.00312 A unified understanding of the thickness-dependent bandgap transition in hexagonal layered semiconductors**, JOONGOO KANG, DGIST, Daegu 711-873, Korea, LIJUN ZHANG, Jilin University, Changchun 130012, China, SU-HUAI WEI, Beijing Computational Science Research Center, Beijing 100094, China — Over the past few years, it has been recognized that a single layer of hexagonal two-dimensional semiconductors—such as hexagonal boron nitride (hBN) and transition metal dichalcogenides (TMDs)—has a direct bandgap, while it becomes an indirect semiconductor as the number of layers increases to two or more. Understanding and control of the direct-to-indirect bandgap transition (DIBT) of hexagonal layered semiconductors is of great scientific and technological importance, because the DIBT converts multilayer hBN or TMD into optically less active materials. Here, taking hBN and MoS<sub>2</sub> as examples, we provide a microscopic understanding of the DIBT of hexagonal layered semiconductors based on our symmetry analysis and direct first-principles calculations. Starting from a simple phenomenological explanation of the DIBT within the first-order perturbation theory of multilayer phases, we show how the bandgap transition arises from the selective orbital couplings in hexagonal layered semiconductors.

**T1.00313 Making Distinct Dynamical Systems Look Identical Spectrally**, ANDRE GONTIJO CAMPOS, DENYS BONDAR, RENAN CABRERA, HERSCHEL RABITZ, Princeton University — We use tracking control techniques to match the optical responses of distinct dynamical systems interacting with laser pulses in both quantum and classical regimes. As a result we provide illustrations where a variety of open and closed systems display the same optical response, demonstrating that the optical spectrum alone is not enough to uniquely characterize general dynamical systems. These findings have important implications in quantum inversion techniques encompassing both linear and nonlinear optics. Moreover, the presented results can be applied to designing materials with desired optical responses.

**T1.00314 Searching for Correlations with the HCO<sup>+</sup> 4-3 Molecular Spectra of Protostars<sup>1</sup>**, OGULCAN ACIKGOZ, SEDA BASTURK, Middle East Tech Univ — The assignment is based on HCO<sup>+</sup> J=4-3 spectral line molecular observations of protostars from the James Clerk Maxwell Telescope, which has the 15 m diameter dish and located in Mauna Kea, Hawaii, USA. Data of 20 protostars are taken from the public LOMASS database and analyzed. We looked for correlations between a few observational quantities.

<sup>1</sup> We thank Dr Umut Yildiz (NASA/JPL-Caltech) for providing data and his comments and support to our research project.

**T1.00315 Dependence of the Crossing Time on the Sequence Length in a Diploid Discrete-Time Mutation-Selection Model for a Finite Population<sup>1</sup>**, WONPYONG GILL<sup>2</sup>, Pusan Natl Univ — This study examined the crossing time in the diploid discrete-time mutation-selection model in a finite population for a range of dominance parameters and selective advantages by switching on a diploid, asymmetric, bridged landscape, from an initial state, a steady state in a diploid, bridged landscape. The dependence of the crossing time on the sequence length was examined for a fixed extension parameter, which was defined as the mean Hamming distance from the optimal allele of the initial steady state divided by the sequence length. The boundary between the deterministic and stochastic regions in the diploid discrete-time mutation-selection model was characterized using the same formula as that in the haploid discrete-time mutation-selection model. The crossing time in a finite population with various population sizes, dominance parameters and selective advantages began to deviate from the crossing time for an infinite population at the critical sequence length. The crossing time for a finite population in the stochastic region was found to be an exponentially increasing function of the sequence length, whose rate was unchanged, regardless of changes in the population size, dominance parameter and selective advantage with a fixed extension parameter.

<sup>1</sup>This work was supported by a 2-Year Research Grant of Pusan National University.

<sup>2</sup>Department of Physics, Busan, Korea 609-735

**T1.00316 Molecular Origins of Higher Harmonics in Large-Amplitude Oscillatory Shear Flow: Shear Stress Response**, PETER GILBERT, A. JEFFREY GIACOMIN, Chemical Engineering Department, Queen's University, ANDREW SCHMALZER, Chemical Diagnostics and Engineering, Los Alamos National Laboratory, R. B. BIRD, Chemical Engineering Department, University of Wisconsin - Madison — Recent work has focused on understanding the molecular origins of higher harmonics that arise in the shear stress response of polymeric liquids in large-amplitude oscillatory shear flow. These higher harmonics have been explained using only the orientation distribution of a dilute suspension of rigid dumbbells in a Newtonian fluid, which neglects molecular interactions and is the simplest relevant molecular model of polymer viscoelasticity [R.B. Bird et al., *J Chem Phys*, **140**, 074904 (2014)]. We explore these molecular interactions by examining the Curtiss-Bird model, a kinetic molecular theory that accounts for restricted polymer motions arising when chains are concentrated [Fan and Bird, *JNNFM*, **15**, 341 (1984)]. For concentrated systems, the chain motion transverse to the chain axis is more restricted than along the axis. This anisotropy is described by the link tension coefficient,  $\epsilon$ , for which several special cases arise:  $\epsilon = 0$  corresponds to reptation,  $\epsilon > 1/8$  to rod-climbing,  $1/2 \geq \epsilon \geq 3/4$  to reasonable shear-thinning predictions in steady simple shear flow, and  $\epsilon = 1$  to a dilute solution of chains. We examine the shapes of the shear stress versus shear rate loops for the special cases,  $\epsilon = (0, 1/8, 3/8, 1)$ , of the Curtiss-Bird model, and we compare these with those of rigid dumbbell and reptation model predictions.

**T1.00317 Micro-architected Composite Lattices with Tunable Negative Thermal Expansions**, QIMING WANG, University of Southern California — Solid materials with minimum or negative thermal expansion (NTE) have broad applications, from dental fillings to thermal-sensitive precision instruments. Previous studies on NTE structures were mostly focused on theoretically design and 2D experimental demonstrations. Here, aided with multimaterial projection micro-stereolithography, we experimentally fabricate multi-material composite lattices that exhibit significant negative thermal expansion in three directions and over a large range of temperature variations. The negative thermal expansion is induced by the structural interaction of material components with distinct thermal expansion coefficients. The NTE performance can be tuned over a large range by varying the thermal expansion coefficient difference between constituent beams and geometrical arrangement. Our experimental results match qualitatively with a simple scaling law and quantitatively consistently with computational models.

**T1.00318 Surface Tension of Methanol as a Function of cut-off Radius and Temperature Controllers.**<sup>1</sup>, ABDALLA OBEIDAT, ADNAN JARADAT, BUSHRA HAMDAN, JUST — Molecular dynamics is used to calculate the surface tension of van Leeuwen methanol. The van Leeuwen model of methanol is chosen over other models of methanol, since this model is widely used to study nucleation at low temperature. Usually, scientists use the cut-off radius to be three order of magnitude of segment diameter. In this study, we varied the cut-off radius to estimate the best cut-off at which the surface tension reaches its plateau. After deciding the best cut-off radius for van der Waals and Coulomb interactions (CUT-OFF and PME were used for Coulomb interaction), we varied the temperature controller (van-Housen, Berendsen, and v-rescale) to decide the best temperature controller to be used to study methanol. In all simulations, Gromacs is used at T=200-300K with periodic boundary conditions in all dimensions.

<sup>1</sup>JUST

**T1.00319 Geometrical design of self-phoretic colloids**<sup>1</sup>, AMIR NOURHANI, Penn State University, PAUL E. LAMMERT, Phys. Dept., Penn State University — Within a unified formalism we study the generic properties of self-phoretic particles for source-or-sink (such as self-diffusiophoresis and self-thermophoresis) and sink-and-source (such as self-electrophoresis) flux distribution across a continuous range of geometries from disk-like to sphere to rod-like shapes. We obtain new insights into the performance of self-phoretic particles as a function of the distribution of surface flux and their shape. Surprisingly, upon varying the geometry between the sphere and rod-like shape, the velocity is not simply an interpolation, but has a nonmonotonic dependent on particle geometry.

<sup>1</sup>This work was supported by the NSF under grants No. DMR-0820404 and DMR-1420620 through the Penn State Center for Nanoscale Science

**T1.00320 Effect of Graphene, Carbon Black, and Multi-wall Carbon Nano Tube as fillers on Dielectric Response Function of Polystyrene Matrix.**, ADNAN JARADAD, None, HIND ABU GHAZLEH COLLABORATION, HASSAN GHANEM COLLABORATION — A set of thin samples of three different fillers (graphene, carbon black, and multi-wall carbon nano-tubes) has been prepared in the laboratory. The thin composite films have different concentration of the filler (weight concentration). The dielectric response function of the prepared samples shows strong relaxation at high frequency (>500 KHz), the position of this peak is found to be a function of weight percent of the composite.

**T1.00321 ABSTRACT MOVED TO V40.003 —**

**T1.00322 SANG-a kernel density estimator incorporating information about the measurement error.**<sup>1</sup>, ROBERT HAYES<sup>2</sup>, North Carolina State University — Analyzing nominally large data sets having a measurement error unique to each entry is evaluated with a novel technique. This work begins with a review of modern analytical methodologies such as histogramming data, ANOVA, regression (weighted and unweighted) along with various error propagation and estimation techniques. It is shown that by assuming the errors obey a functional distribution (such as normal or Poisson), a superposition of the assumed forms then provides the most comprehensive and informative graphical depiction of the data set's statistical information. The resultant approach is evaluated only for normally distributed errors so that the method is effectively a Superposition Analysis of Normalized Gaussians (SANG). SANG is shown to be easily calculated and highly informative in a single graph from what would otherwise require multiple analysis and figures to accomplish the same result. The work is demonstrated using historical radiochemistry measurements from a transuranic waste geological repository's environmental monitoring program.

<sup>1</sup>This work paid for under NRC-HQ-84-14-G-0059

<sup>2</sup>Nuclear Engineering Department

**T1.00323 Interface enhanced superconductivity in single unit-cell FeSe films on SrTiO<sub>3</sub>(110)**, LILI WANG, Tsinghua University — The advent of enhanced superconductivity in FeSe/STO(001) has instigated great interests in other interfacial systems both experimentally and theoretically. To figure out the key role of substrate, STO(110) substrate is of great interest because it resembles STO(001) in high density subsurface oxygen vacancies but distinguishes itself by anisotropic in-plane lattice constants and dielectric constant. Here, we investigated molecular beam epitaxy growth of 1-UC FeSe films on STO(110) substrates and studied the superconducting properties by combined *in-situ* scanning tunneling spectroscopy (STS) and *ex-situ* transport measurement. By STS we observed a superconducting gap as large as 17 meV. Transport measurements on 1-UC FeSe/STO(110) capped with FeTe layers reveal superconductivity with an onset transition temperature ( $T_C$ ) of 31.6 K and an upper critical magnetic field of 30.2 T. We also find that  $T_C$  can be further increased by an external electric field, but the effect is weaker than that on STO(001) substrate. Our study highlights the important roles of interface related charge transfer and electron-phonon coupling in the high temperature superconductivity of FeSe/STO. References: [1] Q. Y. Wang, et al., Chin. Phys. Lett., **29**, 037402 (2012). [2] J. J. Lee et al., Nature **515**, 245 (2014).

**T1.00324 Micro-Structure of Iron in *Petroselinum crispum* and its dependence with the chemical nature of the soil.**<sup>1</sup>, SUNIL DEHIPAWALA, Queensborough Community College, PUBUDU SAMARASEKARA, RASIKA DAHANAYAKE, University of Peradeniya, LEUNG EDMUND, Queensborough Community College — The micro structure of the iron in *Petroselinum crispum* is investigated using synchrotron X-ray Absorption and Mossbauer spectroscopy. Plants were grown under controlled soil conditions with different pH, and iron concentrations. The correlation between the micro structure of the iron in *Petroselinum crispum* plants and the soil conditions were studied. Most of the iron present in the plants has the form  $\text{Fe}^{3+}$  or electron density at the site of the iron nucleus similar to that of  $\text{Fe}^{3+}$ . But the amount of iron absorbed by the plants depends on the soil conditions. These findings will help establish soil conditions necessary to increase  $\text{Fe}^{2+}$  intake by plants similar to the form of iron present in most supplements.

<sup>1</sup>Support for this project was provided by a PSC-CUNY Award, jointly funded by The Professional Staff Congress and The City University of New York.

**T1.00325 Numerical study of the butterfly effect on the solutions of the logistic difference equation using arbitrary significant digits**, JESUS RODRIGUEZ-NUNEZ, JESUS CASTILLO, Departamento de Investigacion en Fisica, Universidad de Sonora, MARTIN MOLINAR-TABARES, Organismo de Cuenca Noroeste, Comision Nacional del Agua — The solutions of the logistic difference equation when they are under the influence of the chaotic regime are very sensitive to initial conditions due to the butterfly effect. In this study we used arbitrary significant digits to generate solutions of the logistic difference equation under the influence of chaos, and a follow of its effects along each digit of the solutions was made. A large amount of significant digits to generate the solutions is necessary since it is the only way of naturally appreciating the implications of chaos on these solutions. We compared digit by digit the numerical solutions that were generated by several different initial conditions that contain modifications in a very far significant digit, with respect to the solution of another initial condition that was selected for a control solution. The results shown that it is possible to track the butterfly effect and easily predict the moment on which its effects will be noticeable.

**T1.00326 Experimental determination of fluxoid quantum's contribution to magnetic moment for force metrology**, JAE-HYUK CHOI, HEONHWA CHOI, YUN WON KIM, MIN-SEOK KIM, Korea Research Institute of Standards and Science, SOON-GUL LEE, Korea University Sejong Campus — Utilizing a cantilever torque-magnetometry equipped with fiber-scanning capability, we have executed precision measurements of the magnetic moment of a micron-sized Nb ring in superconducting state at  $T = 4$  K, which is a key element for sub-piconewton force standard previously suggested by some of the authors. The magnetic moments due to diamagnetic response and individual magnetic fluxoid have been independently determined with a resolution of sub-femto-Am<sup>2</sup>. Within the accuracy of the spring constant determined from a thermal noise method, the results are very consistent with the estimation by Brandt and Clems model that considers finite-penetration-depth effect.

**T1.00327 Analytical Phase Equilibrium Function for Mixtures Obeying Raoult's and Henry's Laws.**<sup>1</sup>, ROBERT HAYES, North Carolina State Univ — When a mixture of two substances exists in both the liquid and gas phase at equilibrium, Raoult's and Henry's laws (ideal solution and ideal dilute solution approximations) can be used to estimate the gas and liquid mole fractions at the extremes of either very little solute or solvent. By assuming that a cubic polynomial can reasonably approximate the intermediate values to these extremes as a function of mole fraction, the cubic polynomial is solved and presented. A closed form equation approximating the pressure dependence on mole fraction of the constituents is thereby obtained. As a first approximation, this is a very simple and potentially useful means to estimate gas and liquid mole fractions of equilibrium mixtures. Mixtures with an azeotrope require additional attention if this type of approach is to be utilized.

<sup>1</sup>This work supported in part by federal grant NRC-HQ-84-14-G-0059.

**T1.00328 Possible Unconventional superconductivity in  $\text{YCo}_{0.7}\text{C}_2$** , ORLANDO CIGARROA, Univ de Sao Paulo, PRISCILA FERRARI ROSA, University of California Irvine, LUIZ TADEU ELENIO, Univ de Sao Paulo, ZACHARY FISK, University of California Irvine, ANTONIO JEFFERSON DA SILVA MACHADO, Univ de Sao Paulo — Non-centrosymmetric superconductors as  $\text{CePt}_3\text{Si}$  [1,2] and sequicarbides  $(\text{La,Y})_2\text{C}_3$  [3] are remarkable examples of unusual properties displayed associated to unconventional pairing due to an antisymmetric spin-orbit coupling. Another interesting case is the family of compounds belonging to the  $\text{CeNiC}_2$  type structure, in which more than thirty stable compounds have found to crystallize in this structure. Here we report magnetization, resistivity, and heat capacity measurements on poly-crystalline samples of non-centrosymmetric  $\text{YCo}_{0.7}\text{C}_2$ , showing clear evidence of bulk superconductivity with a critical temperature of  $T_c = 4$  K. Interestingly the specific heat of the superconducting state deviates from conventional exponential temperature dependence, which is suggestive of possible unconventional superconducting behavior in  $\text{YCo}_{0.7}\text{C}_2$ , similar to that seen in the isostructural and isoelectronic superconductor  $\text{LaNiC}_2$  [4]. Besides, these results strongly suggest that this material is a strong candidate of multiband superconductivity.

References: [1] E. Bauer, G. Hilscher, H. Michor, C. Paul and P. Rogl, Phys. Rev. Lett. 92 (2004) 027003.

**T1.00329 Structural and electronic properties of atomically thin germanium selenide polymorphs**, ZIYU HU, Beijing Computational Science Research Center — Using comprehensive density functional theory calculations, we systematically investigate the structure, stability, and electronic properties of five polymorphs of GeSe monolayer, and highlight the differences in their structural and electronic properties. Our calculations show that the five free-standing polymorphs of GeSe are stable semiconductors.  $\beta$ -GeSe,  $\gamma$ -GeSe,  $\delta$ -GeSe, and  $\varepsilon$ -GeSe are indirect gap semiconductors, whereas  $\alpha$ -GeSe is a direct gap semiconductor. We calculated Raman spectra and scanning tunneling microscopy images for the five polymorphs. Our results show that the  $\beta$ -GeSe monolayer is a candidate for water splitting.

**T1.00330 Structure and Self-Assembly of Oligocarbonate-Fluorene End Functionalized Poly (ethylene glycol) ABA Triblock Polymer**, GUANGMIN WEI, VIVEK PRABHU, National Institute of Standards and Technology, SHRINIVAS VENKATARAMAN, YI YAN YANG, Institute of Bioengineering and Nanotechnology, The Nanos, Singapore, JAMES HEDRICK, IBM Almaden Research Center, California USA, VIVEK PRABHU TEAM, SHRINIVAS VENKATARAMAN, YI YAN YANG COLLABORATION, JAMES HEDRICK COLLABORATION — Hierarchical structures of oligocarbonate-fluorene end-functionalized poly(ethylene glycol) triblock copolymer  $(\text{P}(\text{F-TMC})_m\text{-PEG444-P}(\text{F-TMC})_m)$  were characterized by light scattering, atomic force microscopy, and Ultraviolet-visible spectroscopy in dilute regime in water, a poor solvent of F-TMC block. The evidence for pai-pai stacked of F-TMC block in self-assembled structure was provided. The self-assembly behavior is highly dependent on concentration and F-TMC block length, m. The presence of clusters dominates the population of scatterers once m is larger than 2, where there is no clear evidence of a separation of micelles and clusters. The molecular aggregation driven by F-TMC groups appears too strong to permit labile micelle-cluster dynamics as observed with  $m = 2$  and 1.2. The non-mean field scaling of the aggregation number, when compared to models for triblock copolymers, highlights the need for a molecular-based model to predict the self-assembly at low end-group numbers. In our case, the end-groups are oligomers, so the comparison to Flory scaling may not be justified.

this abstract is

replacing MAR16-2015-020422.

**T1.00331 Negative magnetization and exchange bias effect in  $\text{Ni}_{1.4}\text{Mn}_2\text{Ga}_{0.6}$** , ABDULLAH ALBAGAMI, MAHMUD KHAN, Miami University — Ni-Mn-X based Heusler alloys have attracted significant interest in recent years due to their multifunctional properties. Exchange bias (EB) is one such property that results from competing magnetic interactions in these alloys. The EB effect is typically observed in materials where ferromagnetic (FM) and antiferromagnetic (AFM) interactions co-exist. Since the discovery of EB effect in CoO (AFM) coated Co (FM) nanoparticles by Meikle John and Bean in 1956, a significant amount of research efforts have been made on this subject. Here, we have performed an experimental study on the magnetic and exchange bias properties of polycrystalline  $\text{Ni}_{1.4}\text{Mn}_2\text{Ga}_{0.6}$  alloy by X-ray diffraction, dc magnetization, and ac susceptibility measurements. The material exhibits a ferromagnetic Curie temperature of  $\sim 300$  K. The magnetization versus field data obtained at 5 K under zero field condition exhibits a double shifted hysteresis loop that disappears at higher temperatures. When the sample is cooled from room temperature to 5 K in applied magnetic fields, exchange bias is observed, whose magnitude is strongly dependent on the cooling field. A maximum exchange bias field of 730 Oe is observed under field cooling condition at 5 K. A negative magnetization is observed in the magnetization versus temperature data obtained at magnetic fields smaller than 75 Oe. The experimental results are explained in terms of the competing ferromagnetic and antiferromagnetic exchange interaction that exist in the materials due to the Mn atoms occupying multiple crystalline sites resulting in a spin glass-type frustrated ground state.

**T1.00332 Anomalous transport properties of  $\text{Ni}_2\text{Mn}_{1-x}\text{Cr}_x\text{Ga}$  Heusler alloys at the martensite-austenite phase transition**, JEFFREY BROCK, MAHMUD KHAN, Miami Univ — The Heusler alloy  $\text{Ni}_2\text{MnGa}$  exhibits a first order martensitic phase transition at  $T_M \approx 202$  K. During this transition, the high temperature cubic  $L2_1$  phase (austenite) of the alloy transforms to a low temperature phase (martensite) with a lower symmetry. In both stoichiometric and off-stoichiometric  $\text{Ni}_2\text{MnGa}$  based materials, jump-like anomalies are observed in the resistivity versus temperature data in the vicinity of  $T_M$ . The magnitude of the jump has been reported to vary from less than 1% to a few percent. This variation in the magnitude of resistivity change has been attributed to the difference in scattering on the vibrational motion of the lattice between the austenitic and martensitic phases and the reconstruction of the electronic structure. Although, several reports can be found in existing literature that discuss the change of resistivity of Heusler alloys at MPT, detailed study of a complete system that shows a systematic change of resistivity at MPT is missing. Here we report an experimental study on a series of  $\text{Ni}_2\text{Mn}_{1-x}\text{Cr}_x\text{Ga}$  Heusler alloys. A detailed study has been performed on this previously unexplored system by magnetization and transport measurements. Sharp step-like anomalies are observed in the resistivity data of the alloys, in the vicinity of the  $T_M$ , that changes dramatically with increasing Cr concentration. The magnitude of the jump in resistivity changes dramatically from less than 1 % to nearly 18 %. The results provide a further understanding of the mechanisms that may cause the change in resistivity in the vicinity of MPT.

**T1.00333 Information jet: Handling noisy big data from weakly disconnected network**, DEEDER AURONGZEB, Texas AM university, Department of Statistics. — Sudden aggregation (information jet) of large amount of data is ubiquitous around connected social networks, driven by sudden interacting and non-interacting events, network security threat attacks, online sales channel etc. Clustering of information jet based on time series analysis and graph theory is not new but little work is done to connect them with particle jet statistics. We show pre-clustering based on context can element soft network or network of information which is critical to minimize time to calculate results from noisy big data. We show difference between, stochastic gradient boosting and time series-graph clustering. For disconnected higher dimensional information jet, we use Kallenberg representation theorem (Kallenberg, 2005, arXiv: 1401.1137) to identify and eliminate jet similarities from dense or sparse graph.

**T1.00334 Scale Invariant Fluctuations of Proteins Native States<sup>1</sup>**, QIAN-YUAN TANG, YANG-YANG ZHANG, JUN WANG, WEI WANG, Collaborative Innovation Center of Advanced Microstructures, National Laboratory of Solid State Microstructure, Nanjing University, China, DANTE R CHIALVO, Consejo Nacional de Investigaciones Científicas y Tecnológicas (CONICET), Argentina — Long-range correlations in biological systems often hints for the presence of universal mechanism at work. Here we study protein native dynamics by analyzing a large set of structure ensembles determined by solution NMR. For proteins of diverse sizes, the average distance-dependent cross-correlation functions  $\phi(r)$  and its correlation length  $\xi_\phi$  are analyzed. The analysis uncovered the presence of nontrivial scaling in the proteins' equilibrium dynamics around native states. We show that the correlation length is proportional to the gyration radius of the molecule, implying that the motion of any residue could influence all the others, up to the entire molecule. In addition, it is found that certain shapes are favored, such that for any given protein size the folding process "chooses" the shape with the maximum susceptibility. These results suggest that the proteins native state is critical in the same sense with other slowly built self-organized critical systems, which once posed near the minimum of the energy landscape, preserve their dynamic flexibility.

<sup>1</sup>Supported by Natural Science Foundation of China (Grants 11334004, 11174133, 81421091) and National Basic Research Program of China (Grant 2013CB834100).

**T1.00335 Verwey transition of nano-sized magnetite crystals investigated by  $^{57}\text{Fe}$  NMR**, SUMIN LIM, BAEK SOON CHOI, SOON CHIL LEE, department of physics, KAIST, JAEYOUNG HONG, JISOO LEE, TAEHUN HYEON, Center for Nanoparticle Research, Institute for Basic Science (IBS), Seoul 151-742, Korea, TAEHUN KIM, JAEHONG JEONG, JE-GEUN PARK, Center for Correlated Electron Systems, Institute for Basic Science — It is well known that magnetite crystals undergo a metal-insulator transition at the Verwey transition temperature,  $T_V = 123$  K. In this work, we studied the Verwey transition of nano-sized crystals with  $^{57}\text{Fe}$  NMR. In the metallic state above  $T_V$ , the NMR spectrum shows a single sharp peak, which broadens below  $T_V$  indicating the Verwey transition. We measured the spectra of the nano-crystals with radii of 16 nm, 25 nm, and 40 nm and compared with that of a bulk. The transition temperature obtained from the NMR spectra depends on both the crystal size and crystallinity. When the crystal size decreases from bulk to 16 nm, the transition temperature drops from 123 K to 100 K. The transition temperature of the samples kept dry air decrease due to aging.

**T1.00336  $\text{Cr}^{3+}$  NMR for Multiferroic Chromium spinel  $\text{ZnCr}_2\text{Se}_4$** , SEJUN PARK, Department of Physics, KAIST, SANGIL KWON, Institute for Quantum Computing, University of Waterloo, SOONCHIL LEE, Department of Physics, KAIST, SEUNGHYUN KHIM, DILIP KUMAR BHOI, KEE HOON KIM, CENSCMR, Department of Physics and Astronomy, Seoul National University — Multiferroic systems including  $\text{ZnCr}_2\text{Se}_4$ , the chromium spinel with helical spin structure, have been in huge interest for decades due to its physical variety and applicability. In the temperature range between 21K and 80K, this material shows negative thermal expansion. Due to the bond frustration, the spins of the chromium ions order helically below the transition temperature, 21K, though the exchange constant tends to make a ferro-order. The anomalous  $1^{st}$  order-like magnetic transition is yet clarified and still an interesting topic. To probe microscopic origin of these features, we measured zero-field NMR of  $\text{Cr}^{3+}$  ions having nuclear spin 3/2. Six peaks were observed revealing Nuclear Quadrupole Resonance(NQR) and anisotropic hyperfine field at chromium sites. The NQR spectrum reveals that the structure is highly distorted below the magnetic transition temperature where the normal Jahn-Teller distortion is absent. Temperature dependence of the spectrum is also measured to obtain the magnetization as a function of temperature.

**T1.00337 Topological Analysis, Modeling, and Imaging of Gelatin-Based Hydrogels**, MAHO KOGA, Ward Melville High School, CLEMENT MARMORAT, MIRIAM RAFILOVICH, Stony Brook University, YISHAI TALMON, EYAL ZUSSMAN, ARKADII ARINSTEIN, Technion Institute of Technology — Gelatin is a component of natural biocompatible scaffolds used in tissue engineering constructs. However, due its supra-molecular structure, the mesh size is drastically larger compared to synthetic polymers having the same moduli, and therefore the Rubber Elastic Theory cannot be used to describe properties of gelatin. Gelatin forms distinct fibrils, bundles of triple helix chains, which form rigid areas. We experimented with two different gel moduli, made possible by varying the concentration of microbial transglutaminase (mTG). mTG forms permanent cross links and affects the morphology of the gelatin by changing the number of fibrils formed. Thus, the mesh size calculated from the Rubber Elastic Theory was much smaller than the actual size of the mesh, as measured from cryoscanning electron microscopy images and fluorescent bead particle migration. We also observed the en-mass migration behavior of dermal fibroblast cells as a function of the substrate rheological response. Our results will present the ability of the cells to sense the structure of the underlying substrate, as well as the absolute value of the modulus. Furthermore, the data will be interpreted in terms of a modified theoretical model, which takes into account the structure and mesh size of the gel.

**T1.00338 Charge transport in the organic doped spin-liquid candidate,  $\kappa$ -(ET)<sub>4</sub>Hg<sub>2.89</sub>Br<sub>8</sub>, under Pressure**, YUJI SUZUKI, JUN IBUKA, University of Tokyo, HIROSHI OIKE, RIKEN, KAZUYA MIYAGAWA, University of Tokyo, HIROMI TANIGUCHI, Saitama University, KAZUSHI KANODA, University of Tokyo — The family of layered organic conductors  $\kappa$ -(ET)<sub>2</sub>X plays an important role in the study of Mott physics, which is a major subject in the condensed matter physics. While most  $\kappa$ -(ET)<sub>2</sub>X compounds have half-filled bands and antiferromagnetic nature, the title compound  $\kappa$ -(ET)<sub>4</sub>Hg<sub>2.89</sub>Br<sub>8</sub> ( $\kappa$ -HgBr) is an exceptional doped system which is supposed to be the only doped spin-liquid candidate up to the present. The transport study under controlled pressure, which enables us to investigate this intriguing system with tuning the correlation strengths, revealed that  $\kappa$ -HgBr shows a transition or crossover from a non-Fermi liquid to a Fermi-liquid as pressure increases.<sup>1,2</sup> In the present work, we have carried out the detailed transport measurement under pressure for  $\kappa$ -HgBr with static magnetic fields applied normal to the conducting layers. I will discuss the in-plane and out-of-plane charge transport in normal and superconducting states in this doped spin-liquid candidate with variable electron correlation.

<sup>1</sup>H. Taniguchi *et al.*, J. Phys. Soc. Jpn. **76**, 113709 (2007).

<sup>2</sup>H. Oike *et al.*, Phys. Rev. Lett. **114**, 067002 (2015).

**T1.00339 Analytical Lower and Upper Bounds for the Threshold Surfaces of Quantum Error Correcting Codes**, RYUJI TAKAGI, THEODORE YODER, ISAAC CHUANG, Massachusetts Institute of Technology — If all the physical gates in a fault tolerant code construction have a failure probability below a certain value, the failure probability of the construction approaches zero after many concatenations. This value is called the threshold value of the code and lower bounds for it for various codes have been reported in the literature. However, these approaches do not take into account that the failure probability of each species of logical gate depends on that of many different species of physical gates, and that the distribution of logical failure probability depends on that of many different physical gates. How can we reconcile the interdependency of the failure probabilities of all the various species of gates? Direct simulation would be one of the possible ways to attack this question, but it would be difficult to be done at high concatenation levels because of the exponential growth of simulation time. Here, we deal with this question by instead considering a multidimensional space of the failure probabilities of the physical gates and study the set of points that approach zero error after a large number of concatenations. We present a way to obtain lower and upper bounds for the boundary of this set, what we call the threshold surface, given a particular code and constructions of logical gates. Our method uses only the logical failure probabilities after one concatenation, and moreover the running time of the algorithm scales linearly with respect to concatenation levels. We hope this will establish a reasonable goal for experiments to work towards a scalable quantum computer.

**T1.00340 Measurement of Diffraction Properties of Colloidal Crystals<sup>1</sup>**, NICHOLAS SELAN, MICHAEL BLADES, MIDHUN JOY, JAMES GILCHRIST, SLAVA ROTKIN, Lehigh University — Close-packed, self-assembled arrays of micrometer polystyrene or silica spheres are high quality artificial crystals that generate well-defined diffraction patterns in the visible range. Such crystals are explored as possible substrates for deposition of nanomaterials such as graphene. Quasi-monochromatic visible light diffraction microscopy is used to characterize effective refractive index and crystal structure, specifically grain size, orientation, and lattice parameters. These parameters can be used to monitor deformations of the colloidal crystal lattice during transfer of nanomaterials.

<sup>1</sup>NSF ECCS-1509786, N.S. acknowledges RET supplement to NSF ECCS-1202398

**T1.00341 Nonparametric estimation of quantum states, processes and measurements**, PAVEL LOUGOVSKI, RYAN BENNINK, Oak Ridge National Lab — Quantum state, process, and measurement estimation methods traditionally use parametric models, in which the number and role of relevant parameters is assumed to be known. When such an assumption cannot be justified, a common approach in many disciplines is to fit the experimental data to multiple models with different sets of parameters and utilize an information criterion to select the best fitting model. However, it is not always possible to assume a model with a finite (countable) number of parameters. This typically happens when there are unobserved variables that stem from hidden correlations that can only be unveiled after collecting experimental data. How does one perform quantum characterization in this situation? We present a novel nonparametric method of experimental quantum system characterization based on the Dirichlet Process (DP) that addresses this problem. Using DP as a prior in conjunction with Bayesian estimation methods allows us to increase model complexity (number of parameters) adaptively as the number of experimental observations grows. We illustrate our approach for the one-qubit case and show how a probability density function for an unknown quantum process can be estimated.

**T1.00342 Adsorption and Transport of Methane Molecules through One-Dimensional Channels in Dipeptide-Based Materials**, DANIELE PARADISO, Department of Chemistry, University of Tennessee, Knoxville, TN, United States, ENRICO PERELLI CIPPO, CNR - IFP, Milano, Italy, GIUSEPPE GORINI, Department of Physics, Milano-Bicocca University, Milano, Italy, GIORGIO ROSSI, Department of Physics, Universita' degli Studi di Milano, Milano, Italy, JOHN Z. LARESE, Department of Chemistry, University of Tennessee, Knoxville, TN, United States — The development of new materials for use in energy and environmental applications is of great interest, in particular in the areas of gas separation and carbon capture, where molecular transport plays a significant role. The dipeptides are organic molecules that offer an attractive possibility in such areas, because they form open hexagonal crystalline structures (space group P6<sub>1</sub>) with quasi one-dimensional channels of tunable pore diameters in the range 3-6 Å. These molecular crystals exhibit selective adsorption, as well as, water and gas transport properties: these are believed to result from collective vibrations of the crystal structure that are coupled to the motions of the guest molecules within the channels. Current studies focus on characterizing the system methane and L-Isoleucyl-L-Valine (IV): this was initially done with high-resolution adsorption isotherms; then, high-resolution Inelastic Neutron Scattering measurements at the Spallation Neutron Source (BASIS spectrometer) revealed clear rotational tunneling peaks, offering details to unravel the potential energy surface of the system, as well as, evidences that channels flexibility and dynamical motion of the molecules have influence on the dipeptides adsorption properties.

**T1.00343 Development of Cellulose/PVDF-HFP Composite Membranes for Advanced Battery Separators** , ALEJANDRO CASTILLO, VICTOR AGUBRA, MATAZ ALCOUTLABI, YUANBING MAO, University of Texas Rio Grande Valley — Improvements in battery technology are necessary as Li-ion batteries transition from consumer electronic to vehicular and industrial uses. An important bottleneck in battery efficiency and safety is the quality of the separators, which prevent electric short-circuits between cathode and anode, while allowing an easy flow of ions between them. In this study, cellulose acetate was dissolved in a mixed solvent with poly(vinylpyrrolidone) (PVP), and the mixture was forcespun in a pseudo paper making process to yield nanofibrillated nonwoven mats. The mats were soaked in NaOH/Ethanol to strip PVP and regenerate cellulose from its acetate precursor. The cellulose mats were then dipped in poly(vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP) to yield the cellulose/PVDF-HFP composite membranes. These membranes were characterized chemically through FTIR spectroscopy and solvent-stability tests, thermally through DSC, physically by stress/strain measurements along with weight-based electrolyte uptake, and electrically by AC-impedance spectroscopy combined with capacitive cycling.

**T1.00344 An Automated, High-Throughput System for GISAXS and GIWAXS measurements of thin films<sup>1</sup>** , ERIC SCHAIBLE, Lawrence Berkeley National Laboratory, JESSICA JIMENEZ, Lawrence Livermore Natl Lab, MATTHEW CHURCH, Matthew Church Engineering and Design, EUNHEE LIM, University of California Santa Barbara, POLITE STEWART, Lawrence Berkeley National Laboratory, ALEXANDER HEXEMER, Lawrence Berkeley National Laboratory — Grazing incidence small-angle X-ray scattering (GISAXS) and grazing incidence wide-angle X-ray scattering (GIWAXS) are important techniques for characterizing thin films. In order to meet rapidly increasing demand, the SAXSWAXS beamline at the Advanced Light Source (beamline 7.3.3) has implemented a fully automated, high-throughput system to conduct SAXS, GISAXS and GIWAXS measurements. An automated robot arm transfers samples from a holding tray to a measurement stage. Intelligent software aligns each sample in turn, and measures each according to user-defined specifications. Users mail in trays of samples on individually barcoded pucks, and can download and view their data remotely. Data will be pipelined to the NERSC supercomputing facility, and will be available to users via a web portal that facilitates highly parallelized analysis.

<sup>1</sup>Support provided by the Joint Center for Artificial Photosynthesis (JCAP)

**T1.00345 Energy storage by droplet/bubble capillary force** , ZHIFENG ZHANG, The Pennsylvania State University, XIAOLONG ZHANG, Washington State University, TONY JUN HUANG, The Pennsylvania State University, XIAOLIN CHEN, Washington State University — In present research, a capillary energy storage device is designed by a channel-expansion chamber structure. In the proposed model, the energy is stored in the form of compressed droplet/ bubble in a smaller channel with the release of energy in the form of capillary driven flow. The power output curve for this device is provided by numerical studies. Trials are also engaged to design a continuous output supply by considering the power output and the viscous loss. This device can potentially be used in both micro- and nano- scale energy storage.

**T1.00346 Imaging ballistic carrier trajectories in graphene using scanning gate microscopy<sup>1</sup>** , ZIWEI DOU, University of Cambridge, SEI MORIKAWA, University of Tokyo, SHU-WEI WANG, CHARLES SMITH, University of Cambridge, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute of Materials Science, SATORU MASUBUCHI, TOMOKI MACHIDA, University of Tokyo, MALCOLM CONNOLLY, University of Cambridge — Graphene layers encapsulated by hexagon boron-nitride enable charge carriers to travel ballistically over several microns and provide an opportunity to realise electron optics with Dirac fermions. Scanning gate microscopy is a valuable tool for directly imaging such effects and has recently been applied to investigate coherent scattering in graphene *pnp* junctions [1]. In this work we use SGM to image magnetic focusing of ballistic carriers in a graphene device [2]. By locally varying the carrier concentration and electrostatic potential with the tip we are able to image electrons bouncing from the graphene edges. Moreover, by refocusing misaligned electrons back to collector, our results show how scanning probe tips can be used as mobile lenses for manipulating Dirac fermions in novel device concepts. [1] E.D. Herbschleb, et al., Phys. Rev. B 92, 125414 (2015) [2] S. Morikawa, et al., Appl. Phys. Lett. 107, 243102 (2015); S. Bhandari, et al., arXiv:1510.05197 (2015).

<sup>1</sup>Supported by EPSRC

**T1.00347 NEXT GENERATION GAMMA RAY DIAGNOSTICS FOR THE NATIONAL IGNITION FACILITY** , HANS HERRMANN, Y.H. KIM, A.M. MCEVOY, A.B. ZYLSTRA, C. S. YOUNG, F. E. LOPEZ, J.R. GRIEGO, V. E. FATHERLEY, J. A. OERTEL, H. J. JORGENSON, D. B. BARLOW, Los Alamos National Laboratory, W. STOEFFL, J. A. CHURCH, J.E. HERNANDEZ, A. CARPENTER, Lawrence Livermore National Laboratory, M. S. RUBERY, C. J. HORSFIELD, S. GALES, A. LEATHERLAND, Atomic Weapons Establishment, T. HILSABECK, J.D. KILKENNY, General Atomics, R. M. MALONE, K. MOY, National Security Technologies, J.D. HARES, Kentech Instruments Ltd., J. MILNES, Photek Ltd. — Fusion reaction history and ablator areal density measurements based on gamma ray detection are an essential part of Inertial Confinement Fusion (ICF) experiments on the National Ignition Facility (NIF). Capability improvements are being implemented in sensitivity, temporal and spectral response relative to the existing Gamma Reaction History diagnostic (GRH-6m). The “Super” Gas Cherenkov Detector (GCD) [1] will provide 200x more sensitivity, reduce the effective temporal resolution from 100 to 10 ps, and lower the energy threshold from 2.9 to 1.8 MeV, relative to GRH-6m. The Gamma-to-Electron Magnetic Spectrometer (GEMS) [2] - a Compton spectrometer intended to provide true gamma energy resolution ( $\leq 5\%$ ) for isolation of specific lines such as  $t(d,\gamma)$ ,  $D(n,\gamma)$ ,  $^{12}C(n,\gamma)$  and energetic charged particle nuclear reactions indicative of ablator/fuel mix. [1] H.W. Herrmann, et al., Rev. Sci. Instrum. 85, 11E124 (2014) [2] Y. Kim, et al., Rev. Sci. Instrum. 85, 11E122 (2014)

**T1.00348 Thermodynamic, Modeling and Neutron Investigations of Cycloalkanes Adsorbed on MgO (100) and Graphite Basal Plane** , FATEMA WAHIDA, NICHOLAS STRANGE, JOHN Z. LARESE, Department of Chemistry, University of Tennessee, Knoxville, TN — Understanding the adsorption of molecules on solid surfaces is central to many scientific and technological challenges. Solid surfaces such as metal oxides, carbonaceous archetypes, porous silica, and metal organic frameworks currently represent significant components of nanomaterial research because of their widespread use in optoelectronics, separation chemistry, and catalysis. Understanding the interaction between adsorbed molecules and surfaces is a necessity for developing synthetic methods to produce materials with specific functional properties. An investigation of the effects of molecular and adsorbate symmetry is proposed in this study. The principal aim of this work is to identify the role of surface and molecular symmetry on the physicochemical properties of 2D layers of cyclic molecules adsorbed on metal oxide and semiconductor substrates. Initially our characterization will focus on the thermodynamic and microscopic structure and dynamics of cyclopentane and cyclohexane on the MgO (100) surface and graphite basal plane. In order to realize this goal adsorption isotherms, inelastic neutron scattering (INS) and molecular dynamics (MD) simulation studies will be performed to investigate the structure, dynamics and wetting properties.

**T1.00349 Resistance-Strain Relation On Vanadium Dioxide Thin Films** , ALI AMIRI, PATRICK LECLAIR, University of Alabama, Department of Physics, ARUN GUPTA, University of Alabama, MINT Center — Vanadium dioxide is a strongly correlated material with a sharp metal to insulator transition at  $\sim 341$  K. It is well known that the strain along c-axis can change the transition temperature, but the other effects of the strain have not been drawing much attention. In this work we have studied the effects of the strain on resistance changes in the polycrystalline and epitaxial films. Polycrystalline films of  $VO_2$  are deposited on the  $Pb(Mg_{1/3}Nb_{2/3})_2O_7$  (PMN-PT) using a  $SiO_2$  buffer layer. The strain on film is tuned by applying a bias electric field through the piezoelectric substrate, and the resistance is measured using four-probe method. The epitaxial films of  $VO_2$  are grown on  $TiO_2$  (001) and have been glued to PMN-PT substrate to transfer strain. The change in the resistance of the epitaxial films is measured to be only about 30% more than polycrystalline films for the same amount of strain. We have studied the strain-induced resistance changes as a function of temperature. we have shown that the resistance is more sensitive to strain in the metallic phase.

**T1.00350 Nonlinear Dynamic Model Explains The Solar Dynamic**, MARIA KUMAN, Holistic Research Institute, 1414 Barcelona Dr., Knoxville, TN 37923 — Nonlinear mathematical model in torus representation describes the solar dynamic. Its graphic presentation shows that without perturbing force the orbits of the planets would be circles; only perturbing force could elongate the circular orbits into ellipses. Since the Hubble telescope found that the planetary orbits of other stars in the Milky Way are also ellipses, powerful perturbing force must be present in our galaxy. Such perturbing force is the Sagittarius Dwarf Galaxy with its heavy Black Hole and leftover stars, which we see orbiting around the center of our galaxy. Since observations of NASAs SDO found that magnetic fields rule the solar activity, we can expect when the planets align and their magnetic moments sum up, the already perturbed stars to reverse their magnetic parity (represented graphically as periodic looping through the hole of the torus). We predict that planets aligned on both sides of the Sun, when their magnetic moments sum-up, would induce more flares in the turbulent equatorial zone, which would bulge. When planets align only on one side of the Sun, the strong magnetic gradient of their asymmetric pull would flip the magnetic poles of the Sun. The Sun would elongate pole-to-pole, emit some energy through the poles, and the solar activity would cease. Similar reshaping and emission was observed in stars called magnetars and experimentally observed in super-liquid fast-spinning Helium nanodroplets. We are certain that NASAs SDO will confirm our predictions.

**T1.00351 Reconstructing quantum states from local data**, MILAN HOLZAEPEL, Institut fuer Theoretische Physik, Universitaet Ulm, Germany, MARCUS CRAMER, Institut fuer Theoretische Physik, Leibniz Universitaet Hannover, Germany, NILANJANA DATTA, Statistical Laboratory, Centre for Mathematical Sciences, University of Cambridge, UK, MARTIN PLENIO, Institut fuer Theoretische Physik, Universitaet Ulm, Germany — Quantum spin chains are systems of extreme complexity, in the sense that the number of parameters that fully characterize the state of a quantum spin chain grows exponentially with the number of spins. Yet, physically relevant subsets of all quantum states can be well-approximated by a small number of parameters using well-known methods such as Matrix Product States (MPS). The structure of such states can guarantee reconstruction of the state from the measurement of a small number of simple observables, merely growing linearly with the number of spins. We compare two classes of quantum states which admit efficient reconstruction from incomplete, local information: States which have vanishing conditional mutual information, and the recently introduced class of states with non-decreasing operator Schmidt rank under partial traces which includes generic Matrix Product Operators (MPO). It is well-known that Rényi entropies can be used to characterize the bond dimension of a pure MPS, i.e. the number of parameters required to describe the state. For mixed MPOs, no similar relation is known. Our comparison provides a first relation between the mutual information and the bond dimension of an MPO representation of a mixed state.

**T1.00352 Validation of Capillarity Theory at the Nanometer Scale by Atomistic Computer Simulations of Water Droplets and Bridges in Contact with Hydrophobic and Hydrophilic Surfaces**, NICOLAS GIOVAMBATTISTA, CUNY-Brooklyn Coll, ALEXANDRE ALMEIDA, ADRIANO ALENKAR, Instituto de Física, Universidade de São Paulo, 05508-090, São Paulo, SP, Brazil, SERGEY BULDYREV, Department of Physics, Yeshiva University, 500 West 185th Street, New York, New York 10033, United States — Capillarity is the study of interfaces between two immiscible liquids or between a liquid and a vapor. Capillarity theory (CT) was created in the early 1800s and it is applicable to macroscopic ( $>1\ \mu\text{m}$ ) systems. In general, macroscopic theories are expected to fail at  $<10\ \text{nm}$  scales where molecular details may become relevant. We show that, surprisingly, CT provides satisfactory predictions at  $210\ \text{nm}$  scales. Specifically, we perform atomistic molecular dynamics (MD) simulations of water droplets and capillary bridges of different symmetry in contact with various surfaces. The surfaces correspond to hydroxylated silica, modified to cover a wide range of hydrophobicity/hydrophilicity. In agreement with CT, it is found that (i) water contact angle is independent of the droplet/bridge geometry and depends only on the surface employed; (ii) CT provides the correct droplet/bridge profile for all hydrophobic/hydrophilic surfaces considered; and, remarkably, (iii) CT works even for the very small droplets/bridges studied, for which the smallest dimension is  $\approx 2\ \text{nm}$ . We confirm the self-consistency of CT at  $210\ \text{nm}$  scales by calculating the *capillary forces* between different surfaces induced by capillary bridges; the agreement between MD simulations and CT theory is remarkable.

**T1.00353 A novel cell penetrating peptide carrier for the delivery of nematocidal proteins drug**, JEA HYUN KIM, Korea Minjok Leadership Academy (KMLA) — Nematodes have recently become a primary source of harmful diseases to the environment that inflict harsh damages to pine trees and marine species. However, nematodes cannot be killed by normal pesticides or chemicals due to their thick outer protective layer mainly composed of collagen and cuticles. Thus, a novel approach to trigger intracellular delivery of chemicals through the layers of nematodes is required. In this study, the selection of the novel CPP was carefully progressed through protein database and serial digested fragmentation, internalization of each amino sequence was analyzed through flow cytometry and confocal microscope. As one of the most effective CPP material, JH 1.6 was compared with other major CPPs and its cellular toxicity was investigated. Furthermore, JH 1.6 was attached to various RNA, DNA, and proteins and internalization efficiency was evaluated for mammalian cells. To examine its effects on nematodes in vivo, JH 1.6 was conjugated with nematocidal protein - botulinum neurotoxin (BnT) and treated in *C.elegans* as a model animal. The results showed that JH 1.6 had high relative internalization rate and low cellular toxicity compared to other major CPP such as TAT and GV1001 peptides.

**T1.00354 The Role of Ligand in the Mechanical Properties of Self-Assembled Nanoparticle Films**, SEAN GRIESEMER, James Franck Institute, The University of Chicago, SEAN YOU, Department of Chemistry & Chemical Biology, Harvard University, PONGSAKORN KANJANABOOS, Materials Science and Engineering, Mahidol University, EDWARD BARRY, Center for Nanoscale Materials, Argonne National Laboratory, WEI BU, Center for Advanced Radiation Sources, The University of Chicago, STUART RICE, James Franck Institute, The University of Chicago and Department of Chemistry, The University of Chicago, BINHUA LIN, James Franck Institute, The University of Chicago and Center for Advanced Radiation Sources, The University of Chicago — Self-assembled films of nanoparticles (NP) capped with ligands at the air/water interface exhibit rich mechanical responses to compression including hashing, wrinkling, and folding, which are the combined result of particle- and ligand-based interactions. Previous studies have shown that a high concentration of ligands inhibits wrinkling and folding, but the mechanism remains elusive. By using inductively coupled plasma optical emission spectrometry (ICP-OES) to measure the ligand concentration of our NP solutions and then back-adding excess ligands at controlled amounts, we precisely control ligand-based interactions, enabling an investigation of how these interactions guide self-assembly and correspondingly on mechanical properties. Our experiments reveal that increasing the ligand concentration of the films causes the formation of free-ligand islands in addition to an increase in the interparticle separation. These effects are correlated with the previously observed inhibition of wrinkling and folding, as well as a decrease in the dilatational and shear moduli. This work was supported by the University of Chicago Materials Research Science and Engineering Center, NSF-DMR-1420709.

**T1.00355 Interleukin 18 secretion and its effect in improving Chimeric Antigen Receptors efficiency<sup>1</sup>**, JAE-KUN KIM, Fort Lee HS, New Jersey — Clinical trials have shown that chimeric antigen receptor T cells modified to target cancer cells expressing a surface antigen found on immature B-cells. The purpose of this experiment is to take a pro-inflammatory cytokine, and analyze its effect in improving the efficiency of the T cells. IL-18 has been previously shown to recruit T cells to the tumor site and improve their secretion of cytotoxic cytokines. A human model of the proposed armored T cell has been created and has shown success in combating cancer cells in vitro. The next step is to design and produce a murine model to test in vivo in immunocompetent mice. This research project aimed to create two models: one utilizing 2A peptides and another utilizing IRES elements as a multicistronic vector. Both models would require the insertion of the desired genes into SFG backbones. IRES, a DNA element which acts as a binding site for the transcriptional machinery to recognize which part of the DNA to transcribe, commonly found in bicistronic vectors, is large with 500-600 base pairs, and has a lower transgene expression rate. P2A is smaller, only consisting of about 20 amino acids, and typically has a higher transgene expression rate, which may or may not result in higher effectiveness of the model.

<sup>1</sup>I would like to thank Dr. Renier Brentjens for being a mentor who cared about giving his interns as much educational value as possible.

**T1.00356 Towards Producing Black Nobel Laureates Affiliated with "African Universities"** , JUDE KENNETH, African Univ — While Africa has produced a handful Nobel laureate in literature and peace, it has continued to shy away from producing any in the other categories. The reason is not farfetched; our university system is not up to standard. It is saddening that in this century, African countries place emphasis on certificates and not on knowledge. This has made the continent produce students that lack the intellectual capability, experimental ability, fundamental training, creativity, and motivation to excel except they get a foreign training. It is this backdrop that precipitated the research into the methods of teaching and research in universities across Africa. The study is designed to identify the problems and proffer solution to them. Two important questions immediately come to mind. (1) What factors account for the difficulty in producing Nobel laureates affiliated with African universities? (2) What strategies could be adopted to improve teaching and research in African universities? Several factors were investigated which revolve around funding, the competence of the lecturers, quality of students admitted, attitude of the students, parents and government. Nigerian universities were investigated and important deductions were made. During the study an inquiry was made on the method of instruction at various universities, from result obtained, the study therefore concluded that adequate funding, the presence of erudite scholars and brilliant minds will produce future Nobel laureate affiliated with the continent. The study therefore recommended admission and employment of only students and lecturers who have got a thing for academics into the universities and adequate funding of universities and research centres.

**T1.00357 Applied research for quantitative analysis of fluorescent whitening agent in emulsion paint** , LIN ZHANG, Hohai University — Fluorescent whitening agents (FWAS) are widely used in the emulsion paint for brightening effect. In spite of extensive use of FWAS, there are no reports about the measurement method of FWAS in emulsion paint. In this work, a very simple quantitative approach is proposed. Based on the digital grayscale images of three-dimensional fluorescence spectra and two-dimensional fluorescence images, several wavelet moment invariants are calculated and used to establish the standard models for the quantitative analysis. The influence factors of storage time and exposure time are also studied here. Measurement results indicated the feasibility and precision of using this method for quantitative analysis of FWAS. The research results also provides a reliable basis for the application of FWAS in emulsion paint. Keywords: fluorescent whitening agents, three-dimensional fluorescence spectra, fluorescence image, wavelet moment invariants

**T1.00358 Weyl semimetal generated from Dirac semimetal using off-resonance light** , JIE CAO, Hohai University — We propose a simple realization of a three-dimensional (3D) Weyl semimetal phase using off-resonance circularly polarized light in a 3D Dirac semimetal with mirror symmetry. We show that a fourfold degeneracy Dirac node can be further evolved into two Weyl nodes in the context of our simplified model using both analytical and numerical methods. Observable properties of Weyl semimetal such as surface Fermi arc can be realized since the distance of the two Weyl points in momentum space is proportional to the Fermi velocity. We also use the axionic field theory to discuss the realistic case and find similar conclusion.

**T1.00359 Investigation of Local Structure and Cation Ordering in Dielectric Oxide Microwave Ceramics with stoichiometry  $A(Li_x(Nb,Ta)_y)O_3$  Using  $^7Li$  and  $^{93}Nb$  solid-state NMR spectroscopy.** , RONY KALFARISI, NMR Spectroscopy Group, Physics Department, College of William and Mary — The local structure and cation ordering in dielectric oxide microwave ceramics with stoichiometry  $A(Li_x(Nb,Ta)_y)O_3$  are investigated using  $^7Li$  and  $^{93}Nb$  solid-state NMR spectroscopy. For all samples,  $^7Li$  MAS NMR spectra show one strong and sharp resonance peak indicating one unique environment which corresponds to local lithium environment of nearest B-site neighbor (nBn) surrounded by 4  $LiO_6$  octahedra and 2  $NbO_6$  octahedra ( $TaO_6$  in some samples). In addition to this,  $^7Li$  MAS NMR spectrum of  $(Ca_{2/3}La_{1/3})(Li_{1/3}Nb_{2/3})O_3$  show one additional weak and broad resonance peak which can be assigned to nBn of 3  $LiO_6$  octahedra and 3  $NbO_6$  octahedra.  $^{93}Nb$  MAS NMR spectra of samples with niobium content, show a resonance peak with tail toward the low frequency limit, an evidence to the existence of chemical shifts and quadrupole couplings distributions. Both  $(Sr_{2/3}La_{1/3})(Li_{1/3}Nb_{2/3})O_3$  and  $Ca(Li_{1/4}Nb_{3/4})O_3$  spectra show one broad resonance peak, which can be interpreted as one  $NbO_6$  octahedron nBn with many slight variations through out the sample. While  $(Ca_{2/3}La_{1/3})(Li_{1/3}Nb_{2/3})O_3$  spectra show four peaks correspond to four distinct  $NbO_6$  octahedra local nBn environments with the nBn configuration as: (i) 3  $LiO_6$  and 3  $NbO_6$ ; (ii) 2  $LiO_6$  and 4  $NbO_6$ ; (iii) 1  $LiO_6$  and 5  $NbO_6$ ; (iv) all 6  $NbO_6$

**T1.00360 3D cancer cell migration in a confined matrix** , AMANI ALOBAIDI<sup>1</sup>, BO SUN<sup>2</sup>, Oregon State Univ — Cancer cell migration is widely studied in 2D motion, which does not mimic the invasion processes in vivo. More recently, 3D cell migration studies have been performed. The ability of cancer cells to migrate within the extracellular matrix depends on the physical and biochemical features of the extracellular matrix. We present a model of cell motility in confined matrix geometry. The aim of the study is to study cancer migration in collagen matrix, as a soft tissue, to investigate their motility within the confined and surrounding collagen environment. Different collagen concentrations have been used to show the ability of these cancer cells to move through such a complex structure by measuring Cancer cell migration velocity as well as the displacement.

<sup>1</sup>graduate student physics department

<sup>2</sup>Assistant Professor, physics department, Oregon state university

**T1.00361 Blackhole formula and example relativity** , PHILIP SHIN<sup>1</sup>, None — Black hole formula 1) Second dimension (x,y)  $f(x)=y$  Energy  $E=m*c^2$  2) Thirddimension(x,y,z) really  $x = y = z$  Blackhole formula  $Root(c^2) = c = Root(E/m)$  As mass go the velocity of light, mass become black holes so there are energy as multiply by mass. Example relativity When  $E = m * c^2$  1)  $Root(c^2) = c = Root(E/m)$  2)  $3*c*Root(c^2) = 3*c*Root(E/m) = 3*c^2$  From 1) to 2) as an example, As velocity is faster, mass increased. It means when velocity is increased, sec(t)

<sup>1</sup>The number is good to study physics.

**T1.00362 ABSTRACT WITHDRAWN —**

**T1.00363 Epitaxial growth of Cu films on Ag(111) characterized on monitoring the evolution of their surface states** , DAH-AN LUH, CHIH-HAO HUANG, Department of Physics, National Central University, CHENG-MAW CHENG, KU-DING TSUEI, National Synchrotron Radiation Research Center — The growth of Cu on Ag(111) attracts interest because of its unusual growth behavior. Previous STM work indicated that, when Cu was deposited on Ag(111) at room temperature, Cu islands formed with a Cu coverage as small as 0.02 ML. However, a (99) reconstruction was observed on the surface of these Cu islands, suggesting that the surface of the Cu islands on Ag(111) might be covered with one atomic layer of Ag. The suggestion was not verified because the STM lacked the capability to discern various chemical species. To address the issue, we characterized the growth of Cu films on Ag(111) with a novel approach based on ARPES. On monitoring the evolution of the surface states, we showed that the surface of the Cu islands on Ag(111) with the (99) reconstruction was indeed covered with Ag. Our results also showed that the mobility of Ag on Cu(111) greatly depends on temperature. Ag does not migrate on the surface of the Cu islands at a low temperature, but does at 300 K and significantly at 380 K. In addition, the migration of Ag on Cu is associated with the existence of the Ag(111) surface; Ag atoms migrate to the Cu(111) surface not through the Cu film but along the walls of the holes in the Cu films that penetrate deeply into the Ag substrate.

**T1.00364 Studying the Enhanced Ductility of Bimodal Nanocrystalline Copper Using a Coarse-Grained Model** , GUO-JIE JASON GAO, Natl Taiwan Univ, YUN-JIANG WANG, Chinese Academy of Sciences, SHIGENOBU OGATA, Osaka University — Viewing a bimodal configuration of nanocrystalline copper as composed of soft grains containing stiff cores, we proposed a coarse-grained model with systematically tunable stiffness of grains to study the enhanced ductility of bimodal nanocrystalline copper [Y. Wang, M. Chen, F. Zhou, and E. Ma, Nature 419 (2002) 912]. Using molecular dynamics simulations, we shear our model quasistatically. Our results not only qualitatively confirms that a bimodal configuration could behave more ductile than a monomodal one but also predicts there exists a range of ratio of soft/stiff domains that best minimizes shear localization. Moreover, our model indicates that a bimodal configuration could sometimes exacerbate shear localization and therefore jeopardize ductility if the ratio of soft/stiff domains is not properly chosen. This may explain why some experimental results are hard to be reproduced.

**T1.00365 Biocompatible Ferromagnetic Cr-Trihalide Monolayers** , QIANG SUN, Peking University — Cr with an electronic configuration of  $3d^5 4s^1$  possesses the largest atomic magnetic moment ( $6\mu_B$ ) of all elements in the 3d transition metal series. Furthermore, the trivalent chromium ( $Cr^{3+}$ ) is biocompatible and is widely found in food and supplements. Here using first principles calculations combined with Monte Carlo simulations based on Ising model, we systematically study a class of 2D ferromagnetic monolayers  $CrX_3$  ( $X = Cl, Br, I$ ). The feasibility of exfoliation from their layered bulk phase is confirmed by the small cleavage energy and high in-plane stiffness. Spin-polarized calculations, combined with self-consistently determined Hubbard  $U$  that accounts for strong correlation energy, demonstrate that  $CrX_3$  ( $X=Cl, Br, I$ ) monolayers are ferromagnetic and Cr is trivalent and carries a magnetic moment of  $3\mu_B$ , the resulting  $Cr^{3+}$  ions are biocompatible. The corresponding Curie temperatures for  $CrCl_3$ ,  $CrBr_3$ ,  $CrI_3$  are found to be 66, 86, and 107 K, respectively, which can be increased to 323, 314, 293 K by hole doping. The biocompatibility and ferromagnetism render these Cr-containing trichalcogenide monolayers unique for applications.

**T1.00366 Spectral Gauss quadrature method with subspace interpolation for Kohn-Sham Density functional theory** , XIN WANG, US Army Rsch Lab - Aberdeen — Algorithms with linear-scaling ( $\mathcal{O}(N)$ ) computational complexity for Kohn-Sham density functional theory (K-S DFT) is crucial for studying molecular systems beyond thousands of atoms. Of the  $\mathcal{O}(N)$  methods that use a polynomial-based approximation of the density matrix, the linear-scaling spectral Gauss quadrature (LSSGQ) method (Suryanarayana *et al.*, JPMPS, 2013) has been shown to exhibit the fastest convergence. The LSSGQ method requires a Lanczos procedure at every node in a real-space mesh, leading to a large computational pre-factor. We propose a new interpolation scheme specific to the LSSGQ method that lift the need to perform a Lanczos procedure at every node in the real-mesh. This interpolation will be referred to as subspace interpolation. The key idea behind subspace interpolation is that there is a large overlap in the Krylov-subspaces produced by the Lanczos procedures of nodes that are close in real-space. The subspace interpolation scheme takes advantage of the block-Lanczos procedure to group the Krylov-subspaces from a few representative nodes to approximate the density matrix over a large collection of nodes. Subspace interpolation outperforms cubic-spline interpolation by several orders of magnitude.

**T1.00367 Quantum Monte Carlo with known sign structures** , JOHAN NILSSON, Uppsala University — We investigate the merits of different Hubbard-Stratonovich transformations (including fermionic ones) for the description of interacting fermion systems, focusing on the single band Hubbard model as a model system. In particular we revisit an old proposal of Batrouni and Forcrand (PRB 48, 589 1993) for determinant quantum Monte Carlo simulations, in which the signs of all configurations is known beforehand. We will discuss different ways that this knowledge can be used to make more accurate predictions and simulations.

I have another submission in the same category:

MAR16-2015-004583

**T1.00368 High-temperature transport properties of a two-dimensional material** Santa Cruz, EDWARD PEREPELITSKY, University, JERNEJ MRAVLJE, Jozsef Attila University, Hungary — We study the frequency and momentum dependence of the single-particle scattering rate and its consequence of this is a resistivity with a non-monotonic temperature dependence. We are able to calculate the first few moments of the scattering rate in arbitrary dimensions. Further in the case of two dimensions we find a relation between these moments and those of the optical conductivity  $\sigma(\omega) = \lim_{k \rightarrow 0} \text{Im} \chi(k, \omega)$ .

<sup>1</sup>The work at UCSC was supported by the National Science Foundation Grant DMR-06ER46319.

I request that these be sequentially placed in the same session.

**T1.00369 Anharmonicity alters the stability of  $Fe_7C_3$  at the conditions of the Earth's core** , ZAMAAN RAZA, NINA SHULUMBA, OLLE HELLMAN, Linköping Univ - Linköping, LEONID DUBROVINSKY, Universitat Bayreuth - Bayreuth, IGOR ABRIKOSOV, Linköping Univ - Linköping — Recently, a new orthorhombic phase of iron carbide ( $Fe_7C_3$ ) with an unusually high Poisson's ratio was discovered experimentally, raising the possibility that it may be important at the Earth's core. However, calculations of the Gibbs free energy in the quasiharmonic approximation suggested that it would be metastable with respect to the well known hexagonal phase at the pressure and temperature of the Earth's core. We present new anharmonic calculations of the Gibbs free energy using the temperature-dependent effective potential (TDEP) method, which suggest that the orthorhombic phase is more stable at the conditions of the Earth's core. Anharmonicity is shown to be important at relatively low temperatures, and has a decisive effect on the phase diagram. Moreover, we show that  $Fe_7C_3$  decomposes to form  $Fe_2C$  and  $Fe_3C$  over a narrow region of the phase diagram between the orthorhombic and hexagonal phases.

**T1.00370 Role of Nanostructure Coating Quality in Delay of Surface Flooding during Jumping Droplet Condensation**, DANIEL J PRESTON, DION ANTAO, MIT, NENAD MILJKOVIC, UIUC, BANAFSHEH BARABADI, JOHN QUEENEY, EVELYN WANG, MIT — Vapor condensation is commonly observed in everyday life and routinely used in industry as an effective means of transferring heat. In industrial systems, condensed vapor typically forms a thin liquid film which is not desired due to the large thermal resistance to heat transfer; however, if the condensing surface is functionalized with a hydrophobic coating, the condensate forms discrete liquid droplets which shed at sizes approaching the capillary length and refresh the surface for re-nucleation, resulting in a 5–7x heat transfer improvement. Furthermore, when a micro- or nanostructured surface is functionalized, a superhydrophobic surface can be created on which small ( $\approx 10$ – $100$   $\mu\text{m}$ ) droplets coalesce and can spontaneously jump away from the surface due to release of excess surface energy; this jumping droplet mode of condensation has been shown to increase heat transfer by an additional 30 – 40%. However, at elevated supersaturations, nanostructured superhydrophobic surfaces can become flooded with condensate and form pinned droplets which cannot jump, thereby eliminating the desired heat transfer improvement. In this work, we experimentally demonstrated a delay in the supersaturation at which surface flooding occurs by reducing the hydrophobic coating defect density. This resulted in a lower proportion of structure unit cells occupied by condensate, which allowed higher droplet mobility and jumping at elevated supersaturation.

**T1.00371 Analysis of Adsorbed Natural Gas Tank Technology**, ERNEST KNIGHT, CONRAD SCHULTZ, TYLER RASH, ELMAR DOHNKE, DAVID STALLA, ANDREW GILLESPIE, MARK SWEANY, FLORIAN SEYDEL, PETER PFEIFER, Univ of Missouri - Columbia — With gasoline being an ever decreasing finite resource and with the desire to reduce humanity's carbon footprint, there has been an increasing focus on innovation of alternative fuel sources. Natural gas burns cleaner, is more abundant, and conforms to modern engines. However, storing compressed natural gas (CNG) requires large, heavy gas cylinders, which limits space and fuel efficiency. Adsorbed natural gas (ANG) technology allows for much greater fuel storage capacity and the ability to store the gas at a much lower pressure. Thus, ANG tanks are much more flexible in terms of their size, shape, and weight. Our ANG tank employs monolithic nanoporous activated carbon as its adsorbent material. Several different configurations of this Flat Panel Tank Assembly (FPTA) along with a Fuel Extraction System (FES) were examined to compare with the mass flow rate demands of an engine.

**T1.00372 Development of facile property calculation model for adsorption chillers based on equilibrium adsorption cycle.**, MASATO YANO, KENJI HIROSE, MINORU YOSHIKAWA, NEC smart energy lablatory, THERMAL MANAGEMENT TECHNOLOGY TEAM — Facile property calculation model for adsorption chillers was developed based on equilibrium adsorption cycles. Adsorption chillers are one of promising systems that can use heat energy efficiently because adsorption chillers can generate cooling energy using relatively low temperature heat energy. Properties of adsorption chillers are determined by heat source temperatures, adsorption/desorption properties of adsorbent, and kinetics such as heat transfer rate and adsorption/desorption rate etc. In our model, dependence of adsorption chiller properties on heat source temperatures was represented using approximated equilibrium adsorption cycles instead of solving conventional time-dependent differential equations for temperature changes. In addition to equilibrium cycle calculations, we calculated time constants for temperature changes as functions of heat source temperatures, which represent differences between equilibrium cycles and real cycles that stemmed from kinetic adsorption processes. We found that the present approximated equilibrium model could calculate properties of adsorption chillers (driving energies, cooling energies, and COP etc.) under various driving conditions quickly and accurately within average errors of 6% compared to experimental data.

**T1.00373 A learner's multiple views of the connection between mathematics and quantum mechanics**, VESAL DINI, DAVID HAMMER, Tufts Univ — Students' physical intuitions and prior knowledge are critical to making sense of and solving problems in classical mechanics. In quantum mechanics (qm), coordinating concepts connected to such everyday thinking becomes more difficult. How then can students develop coherence in their knowledge of qm? Consider how experts do it: they build meaning in, around, and through the mathematics of the theory. This view on the role of mathematics, which is one of among many possible to take, seems most productive for qm. In our work to characterize student views of knowledge that emerge in the context of qm coursework, we came to analyze one student who mostly adopted such a view until a shift in context moved him to express an alternative. We present his case and discuss important implications for instruction.

**Thursday, March 17, 2016 2:30PM - 5:30PM –**  
**Session V1 DCMP DMP: Non-Equilibrium Aspects of Electron-Boson Coupling in High Temperature Superconductors** Ballroom I - Zhi-Xun Shen, Stanford University

**2:30PM V1.00001 Understanding electron-boson coupling in high temperature superconductors using time-resolved photoemission.**, SHUOLONG YANG, Stanford University — Time- and angle-resolved photoelectron spectroscopy (trARPES) is a powerful technique for studying non-equilibrium properties of high temperature superconductors. The access to electronic band structure upon optical excitation enables a detailed investigation of the temporal evolution of photo-excited carriers. With strong optical excitations changing electronic properties non-adiabatically, coherent phonon modes can also be launched and detected. We employed trARPES to study both the copper- and iron-based high temperature superconductors. In optimally doped Bi<sub>2</sub>212, we find that the trARPES-derived population lifetimes deviate from the ARPES-derived single-particle lifetimes by one to two orders of magnitude [1]. This disparity can only be understood if processes beyond electron-phonon interactions play a significant role in the electron dynamics. In FeSe/SrTiO<sub>3</sub> systems, we observe an abrupt phonon frequency renormalization in the monolayer FeSe as compared to thicker films [2]. This result sets the basis to quantitatively understand the interfacial lattice strain. Combining the collective response of the electronic bands with information about the underlying coherent lattice motion measured by time-resolved X-ray diffraction, we develop a fundamental understanding of the electron-phonon coupling in FeSe [3]. These examples demonstrate some remarkable microscopic insights on electronic and phononic properties which can only be accessed by trARPES. [1] S.-L. Yang et al. Phys. Rev. Lett. 114, 247001 (2015) [2] S.-L. Yang et al. Nano Lett. 15, 4150 (2015) [3] S. Gerber et al. in preparation (2015)

**3:06PM V1.00002 Femtosecond snapshots of the electron-boson coupling in copper oxides and other correlated materials**, CLAUDIO GIANNETTI, Università Cattolica del Sacro Cuore — One of the pivotal questions in the physics of unconventional superconductors is whether the low-energy dynamics of the charge carriers is mediated by bosons with a characteristic timescale. This issue has remained elusive as electronic correlations are expected to greatly accelerate the electron–boson scattering processes, confining them to the very femtosecond timescale. Recent advances in ultrafast spectroscopy allowed us to simultaneously push the time resolution and frequency range of transient reflectivity measurements, up to the point of direct observing the effective electron–boson interaction in doped copper oxides. The extremely fast timescale ( $\sim 15$  fs) is in agreement with numerical calculations based on the  $t - J$  model and the repulsive Hubbard model, in which the relaxation of the photo-excited charges is achieved via inelastic scattering with short-range antiferromagnetic excitations with an energy spectrum extending up to  $\sim 300$  meV. Our results support a scenario in which the strong local magnetic correlations provide a dissipative channel that is effective on the 10 fs timescale. Secondly, we will present very recent results on the model system Na<sub>2</sub>IrO<sub>3</sub>, in which the interplay of the spin-orbit coupling, the onsite Coulomb repulsion and the hopping within the Ir hexagons gives rise to a complex magnetic ground state, characterized by strong antiferromagnetic correlations below 100 K and the emergence of a zig-zag magnetic phase at T=12 K. The energy exchange between the photoexcited charge carriers and the antiferromagnetic background is observed by monitoring a specific high-energy quasi-molecular orbital, which turns out to be sensitive to the magnetization of the system.

### 3:42PM V1.00003 Signatures of electron-boson coupling in the time domain: beyond the equilibrium interpretation

ALEXANDER KEMPER, North Carolina State University — A powerful method to study the interactions between electrons and bosons in high- $T_c$  superconductors is the measurement of the single-particle spectral function. The recent development of time-resolved ARPES (tr-ARPES) has allowed this measurement to be performed out of equilibrium, where the material is driven by an ultrafast laser pump pulse. We have developed a theoretical framework to complement to these experiments, and here we report on several aspects of electron-boson coupling out of equilibrium. First, we will illustrate how time-resolved spectroscopy can be used to study the coupling between electrons and phonons observing the decay rate of the transient signals as a function of energy, momentum, and time. A sufficiently strongly coupled phonon will exhibit a signature in the tr-ARPES spectra as both a kink in the dispersion as well as a sharp change of the decay rates, and we will discuss how these effects appear out of equilibrium. [1][2] Second, we will focus on the return to equilibrium in systems with multiple interaction types, and show that there are two distinct types of scattering processes: those types of interactions that conserve the energy within a subsystem, and those that do not. While in equilibrium these two contribute equally to the linewidth, we will show that out of equilibrium they behave differently – the first type are mainly responsible for thermalization within the electronic subsystem, whereas the second type drain the energy out. As a result, the scattering rates out of equilibrium can be vastly different from the linewidth, and the features of the second type of interactions can be clearly observed.[3][4]

1. M. Sentef et al., Phys. Rev. X 3, 041033 (2013)
2. A.F. Kemper et al., Phys. Rev. B 90, 075126 (2014)
3. S.L. Yang et al., Phys. Rev. Lett. 114, 247001 (2015)
4. J. Rameau et al., arXiv:1505.07055

### 4:18PM V1.00004 Time-resolved study of Higgs mode in superconductors<sup>1</sup>

RYO SHIMANO, Cryogenic Research Center and Department of Physics, The University of Tokyo — The behavior of superconductors far from equilibrium has been intensively studied over decades. Goals of these studies are the elucidation of bosonic fluctuations essential for the pairing mechanisms, the manifestation of competing orders or hidden phases, and the optical manipulation of superconductivity. The study of collective modes is crucially important for these perspectives as it provides the information on the dynamics of order parameters in non-equilibrium states. Generally, collective modes in ordered phases associated with spontaneous symmetry breaking are classified into 1) gapless phase modes and 2) gapped amplitude modes. In superconductors, the phase mode is eaten by gauge field, according to the Anderson-Higgs mechanism. The remaining amplitude mode is recently termed as Higgs mode from its analogy to the Higgs boson in particle physics. Despite its long history of investigation, unambiguous observation of Higgs mode has remained elusive. This is because the Higgs mode does not have a charge nor electric dipole and therefore it does not couple directly to the electromagnetic field. Here we report on our recent observation of Higgs mode in s-wave superconductors by using THz-pump and THz-probe spectroscopy technique. After nonadiabatic excitation near the superconducting gap energy with monocycle THz pulses, Higgs mode was observed as oscillations in the transmission of THz probe pulse. The resonant nonlinear coupling between the Higgs mode and coherent radiation field was also discovered, resulting in an efficient third order harmonic generation of the incident THz radiation. The extension of experiments to multiband superconductors and unconventional superconductors will be discussed.

<sup>1</sup>Time-resolved study of Higgs mode in superconductors

### 4:54PM V1.00005 Optical probes of symmetry breaking in magnetic and superconducting

$\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ <sup>1</sup>, JOSEPH ORENSTEIN, UC Berkeley/LBNL — The discovery of iron pnictide superconductors has opened promising new directions in the effort to fully understand the phenomenon of high- $T_c$ , with a focus on the connections between superconductivity, magnetism, and electronic nematicity. The  $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$  (P:Ba122) system in particular has received attention because isovalent substitution of As for P generates less disorder than doping on the Fe site. The phase diagram of P:Ba122 is characterized by a line of simultaneous antiferromagnetic (AF) and tetragonal-to-orthorhombic transitions,  $T_s(x)$ , that penetrates the superconducting dome at  $x=0.28$ , just below optimal doping ( $x_{opt}=0.30$ ). In this work, we use spatially-resolved optical polarimetry and photomodulated reflectance to detect linear birefringence and therefore breaking of 4-fold rotational ( $C_4$ ) symmetry. In underdoped ( $x<0.28$ ) samples, birefringence appears at  $T>T_s$  and grows continuously with decreasing  $T$ . The birefringence is unidirectional in a large ( $300\text{ }\mu\text{m} \times 300\text{ }\mu\text{m}$ ) field of view, suggesting that  $C_4$  breaking in this range of  $T$  is caused by residual strain that couples to a diverging nematic susceptibility. Birefringence maps just below  $T_s(x)$  show the appearance of domains, indicating the onset of spontaneous symmetry breaking to an AF ground state. Surprisingly, in samples with  $x>0.28$ , in which the low  $T$  phase is superconducting/ tetragonal rather than AF/orthorhombic,  $C_4$  breaking is observed as well, with an abrupt onset and domain formation at 55 K. We tentatively associate these features with a transition to an AF phase induced by residual strain, as previously proposed [H.-H. Kuo et al. Phys. Rev. B86, 134507 (2012)] to account for structure in resistivity vs.  $T$ . Time-resolved photomodulation allow us to follow the amplitude of the AF order with time following pulsed photoexcitation. Below  $T_c$  the AF order at first weakens, but then strengthens in response to the photoinduced weakening of superconductivity. This complex time evolution is accounted for quantitatively by a model based on the coexistence and competition of AF and superconducting order.

<sup>1</sup>We gratefully acknowledge support by the U.S. Department of Energy, Office of Science, Materials Sciences and Engineering Division, and the Gordon and Betty Moore Foundations EPIQS Initiative through Grant GBMF4537.

## Thursday, March 17, 2016 2:30PM - 5:30PM –

Session V2 DCMP GSOFT: Liquid Droplets: From Surface Topology to Active Motion Ballroom II - Paul Chakin, New York University

### 2:30PM V2.00001 Vapour-mediated sensing and active motion in two-component droplets

MANU PRAKASH, Department of Bioengineering, Stanford University, USA — No abstract available.

### 3:06PM V2.00002 Toroidal Nematics

ALBERTO FERNANDEZ-NIEVES, Physics. Georgia Tech — We will discuss how nematic liquid crystals organize inside toroidal droplets. When the director is parallel to the bounding surface, we find spontaneous reflection symmetry breaking, which we attribute to the role played by saddle-splay contributions to the Frank free energy. When the director is perpendicular to the bounding surface, we find that the structure is reminiscent of the escape radial configuration seen in cylinders, but with a central doubly-twisted organization, which we attribute to the geometry of the torus. We will end by presenting recent experiments with active nematics on the toroidal surface. In this case, topology and activity both affect the structure and dynamics of the material.

**3:42PM V2.00003 Active Mesogenic Droplets: Impact of Liquid Crystallinity and Collective Behavior<sup>1</sup>**, CHRISTIAN BAHR<sup>2</sup>, Max Planck Institute for Dynamics and Self-Organization (MPIDS), Göttingen, Germany — Droplets of common mesogenic compounds show a self-propelled motion when immersed in aqueous solutions containing ionic surfactants at concentrations well above the critical micelle concentration. After introducing some general properties of this type of artificial microswimmer, we focus on two topics: the influence of liquid crystallinity on the swimming behavior and the collective behavior of ensembles of a larger number of droplets. The mesogenic properties are not essential for the basic mechanism of self-propulsion, nevertheless they considerably influence the swimming behavior of the droplets. For instance, the shape of the trajectories strongly depends on whether the droplets are in the nematic or isotropic state. The droplet swimmers are also ideally suited for the study of collective behavior: Microfluidics enables the generation of large numbers of identical swimmers and we can tune their buoyancy. We report on the collective behavior in three-dimensional environments.

<sup>1</sup>Supported by the Deutsche Forschungsgemeinschaft (SPP 1726 "Microswimmers")

<sup>2</sup>In collaboration with Carsten Krüger, Gunnar Klös, Chenyu Jin, Corinna C. Maass, and Stephan Herminghaus

**4:18PM V2.00004 Dynamically Reconfigurable Complex Emulsions via Tunable Interfacial Tensions**, TIMOTHY SWAGER, Department of Chemistry, Massachusetts Institute of Technology — This lecture will focus on the design of systems wherein a reconfiguration of the materials can be triggered chemically or mechanically. The utility of these methods is to generate transduction mechanisms by which chemical and biological sensors can be developed. Three different types of systems will be discussed. (1) Particles wherein a protease enzyme releases strain in the particle by breaking crosslinks. (2) Assemblies of polymers at air water interfaces and the demonstration of a luminescence strain response upon compression. (3) Dynamic colloids produced from immiscible fluorocarbon/hydrocarbon mixtures and ability to convert the core and shell layers of the particles as well as the conversion to Janus particles. The latter systems morphology changes can be triggered chemically or optically.

**4:54PM V2.00005 How faceted liquid droplets grow tails: from surface topology to active motion<sup>1</sup>**, ELI SLOUTSKIN, Physics Department and Institute of Nanotechnology & Advanced Materials, Bar-Ilan University — Among all possible shapes of a volume  $V$ , a sphere has the smallest surface area  $A$ . Therefore, liquid droplets are spherical, minimizing their interfacial energy  $\gamma A$  for a given interfacial tension  $\gamma > 0$ . This talk will demonstrate that liquid oil (alkane) droplets in water, stabilized by a common surfactant can be temperature-tuned to adopt icosahedral and other faceted shapes, above the bulk melting temperature of the oil. Although emulsions have been studied for centuries no faceted liquid droplets have ever been reported. The formation of an icosahedral shape is attributed to the interplay between  $\gamma$  and the elastic properties of the interfacial monomolecular layer, which crystallizes here 10-15K above bulk melting, leaving the droplet's bulk liquid. The icosahedral symmetry is dictated by twelve five-fold topological defects, forming within the hexagonally-packed interfacial crystalline monolayer. Moreover, we demonstrate that upon further cooling this 'interfacial freezing effect makes  $\gamma$  transiently switch its sign, leading to a spontaneous splitting of droplets and an active growth of their surface area, reminiscent of the classical spontaneous emulsification, yet driven by completely different physics. The observed phenomena allow deeper insights to be gained into the fundamentals of molecular elasticity and open new vistas for a wide range of novel nanotechnological applications, from self-assembly of complex shapes to new delivery strategies in bio-medicine.

<sup>1</sup>Acknowledgment is made to the Donors of the American Chemical Society Petroleum Research Fund for support of this research and to the Kahn Foundation for the purchase of equipment.

## Thursday, March 17, 2016 2:30PM - 5:30PM —

Session V3 GSNP: Complex Network Dynamics Ballroom III - Adilson Motter, Northwestern University

**2:30PM V3.00001 Cascading Failures and Recovery in Networks of Networks<sup>1</sup>**, SHLOMO HAVLIN, Bar Ilan University — Network science have been focused on the properties of a single isolated network that does not interact or depends on other networks. In reality, many real-networks, such as power grids, transportation and communication infrastructures interact and depend on other networks. I will present a framework for studying the vulnerability and the recovery of networks of interdependent networks. In interdependent networks, when nodes in one network fail, they cause dependent nodes in other networks to also fail. This is also the case when some nodes like certain locations play a role in two networks—multiplex. This may happen recursively and can lead to a cascade of failures and to a sudden fragmentation of the system. I will present analytical solutions for the critical threshold and the giant component of a network of  $n$  interdependent networks. I will show, that the general theory has many novel features that are not present in the classical network theory. When recovery of components is possible global spontaneous recovery of the networks and hysteresis phenomena occur and the theory suggests an optimal repairing strategy of system of systems. I will also show that interdependent networks embedded in space are significantly more vulnerable compared to non embedded networks. In particular, small localized attacks may lead to cascading failures and catastrophic consequences. Thus, analyzing data of real network of networks is highly required to understand the system vulnerability. References: [1] S. Buldyrev, R. Parshani, G. Paul, H.E. Stanley, S. Havlin, Nature, 465, 0893 (2010) [2] R. Parshani, S. Buldyrev, S. Havlin, PRL, 105, 048701 (2010) [3] R. Parshani, S.V. Buldyrev, S. Havlin, PNAS 108, 1007 (2011) [4] J. Gao, S. Buldyrev, H. E. Stanley, S. Havlin, Nature Physics, 8, 40 (2012). [5] A. Bashan et al, Nature Communications 3, 702 (2012) [6] A. Bashan et al, Nature Physics, 9, 667 (2013) [7] A Majdandzic et al, Nature Physics 10 (1), 34 (2014)

<sup>1</sup>DTRA, ONR, Israel Science Foundation

**3:06PM V3.00002 The Life-Changing Magic of Nonlinearity in Network Control**, SEAN CORNELIUS, Northeastern University, Center for Complex Network Research — The proper functioning and reliability of many man-made and natural systems is fundamentally tied to our ability to control them. Indeed, applications as diverse as ecosystem management, emergency response and cell reprogramming all, at their heart, require us to drive a system to—or keep it in—a desired state. This process is complicated by the nonlinear dynamics inherent to most real systems, which has traditionally been viewed as the principle obstacle to their control. In this talk, I will discuss two ways in which nonlinearity turns this view on its head, in fact representing an asset to the control of complex systems. First, I will show how nonlinearity in the form of multistability allows one to systematically design control interventions that can deliberately induce “reverse cascading failures”, in which a network spontaneously evolves to a desirable (rather than a failed) state. Second, I will show that nonlinearity in the form of time-varying dynamics unexpectedly makes temporal networks easier to control than their static counterparts, with the former enjoying dramatic and simultaneous reductions in all costs of control. This is true despite the fact that temporality tends to fragment a network's structure, disrupting the paths that allow the directly-controlled or “driver” nodes to communicate with the rest of the network. Taken together, these studies shed new light on the crucial role of nonlinearity in network control, and provide support to the idea we can control nonlinearity, rather than letting nonlinearity control us.

**3:42PM V3.00003 Novel percolation transitions and coupled catastrophes**, RAISSA D'SOUZA, University of California, Davis — Collections of interdependent networks are at the core of modern society, spanning physical, biological and social systems. Simple mathematical models of the structure and function of networks can provide important insights into real-world systems, enhancing our ability to steer and control them. Here our focus is on abrupt changes in networks, due both to phase transitions and to jumping between bi-stable equilibria. We begin with an overview of novel classes of percolation phase transitions that result from repeated, small interventions intended to delay the transition. These new phenomena allow us to extend percolation approaches to modular networks, Brownian motion, and cluster growth dynamics. We then focus on abrupt transitions due to a system jumping between bi-stable equilibria, modeled as a cusp catastrophe in nonlinear dynamics. We show that when systems that each undergo a cusp catastrophe interact, we can observe a new phenomena of catastrophe-hopping leading to non-local cascading failures. Here an intermediate system facilitates the propagation of a sudden change or collapse, and we show that catastrophe hopping is consistent with the outbreak of protests observed during the Arab Spring of 2011.

**4:18PM V3.00004 Interdisciplinary applications of network dynamics: From microscopic to Macroscopic**<sup>1</sup>, HAWOONG JEONG, KAIST, Korea — Everything touches everything. We are living in a connected world, which has been modeled successfully by complex networks. Ever since, network science becomes new paradigm for understanding our connected yet complex world. After investigating network structure itself, our focus naturally moved to dynamics of/on the network because our connected world is not static but dynamic. In this presentation, we will briefly review the historical development of network science and show some applications of network dynamics ranging from microscopic (metabolic engineering, PNAS, 104 13638) to macroscopic scale (price of anarchy in transportation network, Phys.Rev.Lett. 101 128701).

<sup>1</sup>Supported by National Research Foundation of Korea through Grant No. 2011-0028908

**4:54PM V3.00005 Rank Dynamics**, CARLOS GERSHENSON, Universidad Nacional Autonoma de Mexico — Studies of rank distributions have been popular for decades, especially since the work of Zipf. For example, if we rank words of a given language by use frequency (most used word in English is the, rank 1; second most common word is of, rank 2), the distribution can be approximated roughly with a power law. The same applies for cities (most populated city in a country ranks first), earthquakes, metabolism, the Internet, and dozens of other phenomena. We recently proposed rank diversity to measure how ranks change in time [1], using the Google Books Ngram dataset. Studying six languages between 1800 and 2009, we found that the rank diversity curves of languages are universal, adjusted with a sigmoid on log-normal scale. We are studying several other datasets (sports, economies, social systems, urban systems, earthquakes, artificial life). Rank diversity seems to be universal, independently of the shape of the rank distribution. I will present our work in progress towards a general description of the features of rank change in time, along with simple models which reproduce it. [1]Cocho G, Flores J, Gershenson C, Pineda C, Sanchez S (2015) Rank Diversity of Languages: Generic Behavior in Computational Linguistics. PLoS ONE 10(4): e0121898. <http://dx.doi.org/10.1371/journal.pone.0121898>

**Thursday, March 17, 2016 2:30PM - 5:30PM –**  
**Session V4 DPOLY: Where Morphology Meets Functionality: Light and Electron Transporting Polymeric Complexes** Ballroom IV - Enrique Gomez, Pennsylvania State University

**2:30PM V4.00001 From Morphology to Interfaces to Tandem Geometries: Enhancing the Performance of Perovskite/Polymer Solar Cells**<sup>1</sup>, THOMAS RUSSELL, University of Massachusetts — We have taken a new approach to develop mesoporous lead iodide scaffolds, using the nucleation and growth of lead iodide crystallites in a wet film. A simple time-dependent growth control enabled the manipulation of the mesoporous lead iodide layer quality in a continuous manner. The morphology of lead iodide is shown to influence the subsequent crystallization of methyammoniumleadiodide film by using angle-dependent grazing incidence x-ray scattering. The morphology of lead iodide film can be fine-tuned, and thus the methyammoniumleadiodide film quality can be effectively controlled, leading to an optimization of the perovskite active layer. Using this strategy, perovskite solar cells with inverted PHJ structure showed a *PCE* of 15.7 per cent with little hysteresis. Interface engineering is critical for achieving efficient solar cells, yet a comprehensive understanding of the interface between metal electrode and electron transport layer (ETL) is lacking. A significant power conversion efficiency (PCE) improvement of fullerene/perovskite planar heterojunction solar cells was achieved by inserting a fulleropyrrolidine interlayer between the silver electrode and electron transport layer. The interlayer was found to enhance recombination resistance, increases electron extraction rate and prolongs free carrier lifetime. We also uncovered a facile solution-based fabrication of high performance tandem perovskite/polymer solar cells where the front sub-cell consists of perovskite and the back sub-cell is a polymer-based layer. A record maximum PCE of 15.96 per cent was achieved, demonstrating the synergy between the perovskite and semiconducting polymers. This design balances the absorption of the perovskite and the polymer, eliminates the adverse impact of thermal annealing during perovskite fabrication, and affords devices with no hysteresis.

<sup>1</sup>This work was performed in collaboration with Y. Liu, Z. Page, D. Venkataraman and T. Emrick (UMASS), F. Liu (LBNL) and Q. Hu and R. Zhu (Peking University) and was supported by the Office of Naval Research under contract N00014-15-1-2244xx.

**3:06PM V4.00002 Microwave absorption of free carriers in doped conjugated polymer films**, GARRY RUMBLES, National Renewable Energy Laboratory — Flash photolysis time-resolved microwave conductivity (*fp*-TRMC) is a powerful spectroscopic tool for the detection of mobile charges in organic systems, such as conjugated polymers. We will report on a study of charge carrier generation in a number of polymer systems where the solid-state microstructure (SSM) of the thin films can be controlled using both molecular structure and processing conditions. By incorporating a low concentration of molecular acceptors, such as metallo-phthalocyanines, as well as substituted fullerenes and perylenes, the driving force for photoinduced electron transfer can be controlled through the excited state energy and the reduction potential. Our results indicate the importance of the crystalline phase of the polymer to stabilise and reduce the rate of recombination of the holes with the electrons that remain trapped on the acceptor. In addition, the role that the SSM plays on the stabilization of bound electron-hole pairs, or charge-transfer (CT) states will be examined.

**3:42PM V4.00003 Making Glasses Conduct: Electrochemical Doping of Redox-Active Polymer Thin Films**, BRYAN BOUDOURIS, Purdue University — Optoelectronically-active macromolecules have been established as promising materials in myriad organic electronic applications (e.g., organic field-effect transistors (OFETs) and organic photovoltaic (OPV) devices). To date, however, the majority of the work surrounding these materials has focused on materials with a great deal of conjugation along their macromolecular backbones and with varying degrees of crystalline structure. Here, we describe an emerging class of macromolecular charge conductors, radical polymers, that: (1) do not contain conjugation and (2) are completely amorphous glasses. Radical polymers contain non-conjugated macromolecular backbones and stable radical sites along the side chains of the electronically-active materials. In contrast to conjugated polymer systems, these materials conduct charge in the solid state through oxidation-reduction (redox) reactions along these pendant groups. Specifically, we demonstrate that controlling the chemical functionality of the pendant groups and the molecular mobility of the macromolecular backbones significantly impacts the charge transport ability of the pristine (i.e., not doped) radical polymers species. Through proper control of these crucial parameters, we show that radical polymers can have electrical conductivity and charge mobility values on par with commonly-used conjugated polymers. Importantly, we also highlight the ability to dope radical polymers with redox-active small molecule species. This doping, in turn, increases the electrical conductivity of the glassy radical polymer thin films in a manner akin to what is observed in traditional conjugated polymer systems. In this way, we establish a means by which to fabricate optically-transparent and colorless thin film glasses capable of conducting charge in a rather rapid manner. We anticipate that these fundamental insights will prove crucial in developing new transparent conducting layers for future electronic applications.

**4:18PM V4.00004 Reversible Optical Control of polymer doping: Mechanism and applications**, ADAM MOULE, University of California, Davis — No abstract available.

**4:54PM V4.00005 Nanoparticle Polymer Hybrids for Solar Cells<sup>1</sup>**, MICHAEL MACKAY, Univ of Delaware — Polymer-based solar cells are unique since their processing is extremely cost effective compared to silicon-based solar cells. They are also much less energy intensive to manufacture. However, their power conversion efficiency is low. Discussion of what affects this property in the context of the morphology characterized through thermal analysis as well as x-ray and neutron scattering will be given.

<sup>1</sup>Support is gratefully acknowledged from the Department of Materials Science and NIST Award 70NANB10H256 through the Center for Neutron Science at the University of Delaware

**Thursday, March 17, 2016 2:30PM - 5:30PM —**  
**Session V5 GMAG DMP: Frustrated Magnetism: Low Dimensional Magnets II** 301 - Alexander Chernyshev, University of California, Irvine

**2:30PM V5.00001 Chiral spin liquids in arrays of spin chains**, RODRIGO PEREIRA, University of Sao Paulo — The chiral spin liquid proposed by Kalmeyer and Laughlin is a spin analogue of the fractional quantum Hall effect: it has gapped bulk quasiparticles, charge-neutral chiral edge modes and topological order in the ground state. Recently there has been unambiguous numerical evidence that the chiral spin liquid can be stabilized as the ground state of extended Heisenberg models on the kagome lattice. I will talk about an analytical approach to investigate the emergence and the properties of the chiral spin liquid phase in spatially anisotropic 2D lattices. The approach is inspired by coupled-wire constructions of quantum Hall states: starting from a quasi-1D system, we build towards the 2D limit by coupling Heisenberg chains with three-spin interactions that drive the chiral spin order. Using a renormalization group analysis, we show that the chiral spin liquid is more easily stabilized in the kagome lattice than in the triangular lattice. Moreover, using the conformal field theory that describes single chains, we explicitly construct the operators that create bulk quasiparticles and those that account for the topological degeneracy on the torus. I will also discuss possible extensions of this approach to construct more exotic quantum spin liquids.

**3:06PM V5.00002 Entanglement Entropy and Topological Order in Resonating Valence-Bond Quantum Spin Liquids**, JULIA WILDEBOER, National High Magnetic Field Laboratory, ALEXANDER SEIDEL, Washington University in St. Louis, ROGER MELKO, University of Waterloo, PI — On the triangular and kagome lattices, short-ranged resonating valence bond (RVB) wave functions can be sampled without the sign problem using a recently-developed Pfaffian Monte Carlo scheme [1]. In this talk [2], we present a study of the Renyi entanglement entropy in these wave functions using a replica-trick method [3]. Using various spatial bipartitions, including the Levin-Wen construction, our finite-size scaled Renyi entropy gives a topological contribution consistent with  $\gamma = \ln(2)$ , as expected for a gapped  $Z_2$  quantum spin liquid. We prove that the mutual statistics are consistent with the toric code anyon model and rule out any other quasiparticle statistics such as the double semion model.

[1] J. Wildeboer and A. Seidel, PRL **109**, 147208 (2012).

[2] J. Wildeboer, A. Seidel, and R. G. Melko, submitted to PRL.

[3] M. B. Hastings, I. Gonzalez, A. B. Kallin, and R. G. Melko, PRL **104**, 157201 (2010).

**3:18PM V5.00003 A numerical study of the energy gap of the quantum dimer-pentamer model**, OWEN MYERS, University of Vermont, CHRIS HERDMAN, University of Waterloo — We present a study of the energy gap in the quantum dimer-pentamer model (QDPM) on the square lattice. This model is a generalization of the square lattice quantum dimer model (QDM), with a configuration space comprising fully-packed hard-core dimer coverings of the lattice, as well as configurations containing pentamers, where four dimers touch a vertex. Thus in the QDPM, the fully-packed, hard-core constraint of the QDM is relaxed such that the local dimer number at each vertex is fixed modulo 3; correspondingly, the local  $U(1)$  gauge symmetry of the QDM Hilbert space is reduced to a local  $Z_3$  gauge symmetry in the QDPM. Previous work has demonstrated the disordered quantum liquid nature of the ground state of the QDPM at the Rokhsar-Kivelson point. Here we present a study of the energy gap above the ground state at the RK point, as computed via Monte Carlo from imaginary time correlations. To investigate the possibility of  $Z_3$  topological order in this system, we study both the dimer density correlations as well as a  $Z_3$  generalization of  $Z_2$  vison correlations. Such vison correlations have previously been shown to display the nature of the low lying excitations in  $Z_2$  topologically ordered QDMs.

**3:30PM V5.00004 A quantum spin liquid with a large topological degeneracy<sup>1</sup>**, OLEG TCHERNYSHYOV, HAOYU WANG, Johns Hopkins University, YUAN WAN, Perimeter Institute — We present a model of a quantum spin liquid in two dimensions with a large topological degeneracy. The model has spins of length  $S = 1/2$  on sites of a triangular lattice interacting via a 6-spin term. As in models of Kitaev and Wen [1-3], elementary building blocks in our model are strings of several distinct types. Ends of these strings are elementary particles: 4 bosons and 3 fermions. Particles of different types are mutual semions. The degeneracy of the ground state on a torus is  $2^{7-1} = 64$ . Elementary excitations of the model are boson-fermion pairs, which come in  $3 \times 4 = 12$  distinct types. [1] A. Kitaev, Ann. Phys. **303**, 2 (2003). [2] X.-G. Wen, Phys.Rev.Lett. **90**, 016803 (2003). [3] A. Kitaev, Ann. Phys. **321**, 2 (2006).

<sup>1</sup>Research funding comes from the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02-08ER46544.

**3:42PM V5.00005 Magnetic Frustration from Nonuniform  $g$ -factors<sup>1</sup>**, WEIGUO YIN, Brookhaven National Laboratory — Frustrated magnets are commonly known as materials in which localized magnetic moments, or spins, interact through competing exchange interactions that cannot be simultaneously satisfied. Here we show that even when the exchange interactions are fully cooperative, magnetic frustration can be induced by nonuniform Landé  $g$  factors, leading to a mutual interplay of typical ferromagnetic (FM) and antiferromagnetic (AF) features. This novel physics—exactly demonstrated in the one-dimensional Ising model with alternating  $g$  factors [1]—provides new insight into the puzzling phenomenon that the magnetic susceptibility of many AF or FM materials is FM-like at low temperature but AF-like at high temperature. Furthermore, we found a unique magnetic-field-driven quantum critical point at which one half of the spins are frozen into a complete order and the other half are fully disordered. The present theory joins the recent intensive search for frustrated magnets beyond the “standard model” of condensed matter physics. It could broaden our understanding and design of exotic magnetic behaviors such as spin ice, spin glass, and spin liquid that are essential to quantum computing, spintronics, and high-temperature superconductivity. [1] W.-G. Yin and C. R. Roth, arXiv:1510.00030.

<sup>1</sup>Work supported by U.S. Department of Energy, Office of Basic Energy Science, under Contract No. DE-AC02-98CH10886.

**3:54PM V5.00006 Quantum Spin Fluctuations and magnons in antiferromagnetically coupled bilayers with tuneable intra-bilayer exchange - the case of  $\text{Cr}_2\text{W}(\text{Te})\text{O}_6$ <sup>1</sup>**, KINGSHUK MAJUMDAR, Grand Valley State Univ, S. D. MAHANTI, Michigan State University, East Lansing — Recent neutron diffraction studies have shown that in  $\text{Cr}_2(\text{W},\text{Te})\text{O}_6$  systems, which consist of bilayers with strong antiferromagnetic inter-bilayer coupling between Cr moments, the intra-bilayer coupling between the Cr moments can be tuned from ferro (for W) to antiferro (for Te). Ab initio density functional calculations provide a microscopic understanding of the magnetic structure but cannot explain the magnitude of the ordered  $\text{Cr}^{3+}$  moments. In order to understand the reduction of the ordered moment (ROM) caused by quantum spin fluctuations we have studied the magnon dispersion and ROM using a two parameter quantum Heisenberg spin Hamiltonian with tuneable intra- ( $j$ ) and antiferromagnetic inter- ( $J$ ) bilayer couplings. The magnon dispersion and sublattice magnetization have been calculated using non-linear spin wave theory up to second-order corrections in spin  $S$ .

<sup>1</sup>We acknowledge the use of HPC cluster at GVSU, supported by the National Science Foundation Grant No. CNS-1228291.

**4:06PM V5.00007 Complex field-induced states in Linarite  $\text{PbCuSO}_4(\text{OH})_2$  with a variety of high-order exotic  $\text{SDW}_p$  states<sup>1</sup>**, STEFAN SÜLLOW, TU Braunschweig, Braunschweig, Germany — Low-temperature neutron diffraction and NMR studies of field-induced phases in linarite are presented for magnetic fields  $H\parallel b$  axis. This way, we establish the magnetic phase diagram up to saturation. A two-step spin-flop transition is observed as well as a transition transforming a helical magnetic ground state into an unusual magnetic phase with sine-wave modulated moments  $\parallel H$  enclosing all other magnetic phases in the  $T-H$  phase diagram. An effective  $\tilde{J}_1 - \tilde{J}_2$  single-chain model with a magnetization-dependent frustration ratio  $\alpha_{eff} = -\tilde{J}_1/\tilde{J}_2$  is proposed. The latter is governed by skew interchain couplings and shifted to the vicinity of the ferromagnetic critical point. It explains qualitatively the observation of a rich variety of exotic (for strongly correlated cuprate spin-1/2 Heisenberg systems) longitudinal collinear spin-density wave  $\text{SDW}_p$  states ( $9 \geq p \geq 2$ ).

<sup>1</sup>Work supported by the DFG under contracts WO 1532/3-1 and SU 229/9-1

**4:42PM V5.00008 Large-scale simulations of spin-density-wave order in frustrated lattices**, KIPTON BARROS, CRISTIAN BATISTA, Los Alamos National Laboratory, GIA-WEI CHERN, University of Virginia — We investigate spin-density-wave (SDW) phases within a generalized mean-field approximation. This approach incorporates the thermal fluctuations of SDW order and the development of short-range order above magnetic ordering temperatures  $T_c$ . Using a new Langevin dynamics method, we study mesoscale structures associated with triple-Q SDW states that are induced by Fermi surface nesting in triangular and kagome lattice Hubbard models. The core of our linear-scaling Langevin dynamics simulations is an efficient stochastic kernel polynomial method for computing the electron density matrix. We also investigate exotic phases above  $T_c$  arising from preformed magnetic moments.

**4:54PM V5.00009 Electronic route to stabilize nanoscale spin textures in itinerant frustrated magnets**, SANJEEV KUMAR, IISER Mohali, SAHINUR REJA, JEROEN VAN DEN BRINK, IFW Dresden, Germany — We unveil novel spin textures in an itinerant fermion model on a frustrated triangular lattice in the limit of low electronic density. Using hybrid Monte Carlo simulations on finite clusters we identify two type of nanoscale spin textures in the background of  $120^\circ$  order: (i) a planar ferromagnetic cluster, and (ii) a non-coplanar cluster with spins oriented perpendicular to the  $120^\circ$  plane. Both these textures lead to localization of the electronic wavefunctions and are in-turn stabilized by the concomitant charge modulations. The non-coplanar spin texture is accompanied by an unusual scalar chirality pattern. A well defined electric charge and magnetic moment associated with these textures allow for their easy manipulation by external electric and magnetic fields – a desirable feature for data storage. We identify a localization-delocalization behavior for electronic wavefunctions which is unique to frustrated magnets, and propose a general framework for stabilizing similar spin textures in spin-charge coupled systems.

**5:06PM V5.00010 Stability and magnetization curve of spin-nematic phase slightly below saturation field**, HIROAKI UEDA, Toyama Prefectural University, KEISUKE TOTSUKA, Yukawa Institute for Theoretical Physics — We discuss the magnetization process slightly below the saturation field in frustrated magnets. A condensation of bound magnons on the spin-polarized state induces either a spin nematic phase or a state with phase separation. The (effective) interaction between the bound magnon pairs not only is crucial to the stability of the nematic phase, but also determines the slope of the magnetization curve near saturation. We generally derive the expression of this interaction by using the perturbative scattering theory. By applying the method to coupled zigzag chains  $\text{LiCuVO}_4$ , we find the positive pair-pair interaction implying the stability of the spin nematic phase. We also point out that the magnetization curve of  $\text{LiCuVO}_4$  is almost vertical (i.e. very large  $dM/dH$ ) near the saturation exhibiting one-dimensional feature despite non-negligible interchain couplings.

**5:18PM V5.00011 Density-matrix renormalization group study of triangular and square Hubbard models**, SHIGETOSHI SOTA, RIKEN AICS, TAKAMI TOHYAMA, Tokyo University of Science, TOMONORI SHIRAKAWA, SEIJI YUNOKI, RIKEN — We perform large-scale density-matrix renormalization group calculations for two-dimensional Hubbard models with a triangular lattice and a square lattice [T. Tohyama, K. Tsutsui, M. Mori, S. Sota, and S. Yunoki, Phys. Rev. B **92**, 014515 (2015)]. In the triangular Hubbard model, we determined a boundary between metal and insulator and a boundary between spin-liquid and antiferromagnetic phases. The presence of spin-liquid phase is confirmed by spin-spin correlation function. In the square Hubbard model, we introduce a second-neighbor hopping interaction and calculate the dynamical spin correlation function to clarify the doping dependence of magnon excitations. We find a shift of a peak position toward higher energy in the electron-doped side, being consistent with recent resonant-inelastic x-ray scattering.

**Thursday, March 17, 2016 2:30PM - 5:30PM —**

**Session V6 GMAG DMP: Bulk Multiferroics** 302 - Srinivasa Singamaneni, North Carolina State University

**2:30PM V6.00001 Electric field control of magnetization dynamics in multiferroics**, VETLE RIS-INGGARD, IRYNA KULAGINA, JACOB LINDER, Department of Physics, Norwegian University of Science and Technology — Multiferroics with a strong magnetoelectric coupling hold great promise in spintronics because they enable magnetic control of the electric polarization as well as electric control of the magnetization. We take an analytical approach, using the Landau-Lifshitz-Gilbert equation to describe the dynamic state of the magnetization. In particular, we show that in insulating multiferroics which exhibit the inhomogeneous magnetoelectric effect there exists an electrically controlled magnon-induced torque that acts even on a homogeneous magnetization. Unlike the magnon-induced torques that arise from Dzyaloshinskii-Moriya interactions or in the proximity of a topological insulator, the strength and direction of this torque is tunable by the externally applied electric field.

**2:42PM V6.00002 Understanding the spin-driven polarizations in  $\text{BiMO}_3$  ( $M = 3d$  transition metals) multiferroics.**<sup>1</sup>, SANTOSH KC, JUN HEE LEE, VALENTINO R. COOPER, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA — Bismuth ferrite ( $\text{BiFeO}_3$ ), a promising multiferroic, stabilizes in a perovskite type rhombohedral crystal structure (space group  $R3c$ ) at room temperature. Recently, it has been reported that in its ground state it possess a huge spin-driven polarization [1]. To probe the underlying mechanism of this large spin-phonon response, we examine these couplings within other Bi based  $3d$  transition metal oxides  $\text{BiMO}_3$  ( $M = \text{Ti, V, Cr, Mn, Fe, Co, Ni}$ ) using density functional theory. Our results demonstrate that this large spin-driven polarization is a consequence of symmetry breaking due to competition between ferroelectric distortions and anti-ferrodistortive octahedral rotations. Furthermore, we find a strong dependence of these enhanced spin-driven polarizations on the crystal structure; with the rhombohedral phase having the largest spin-induced atomic distortions along [111]. These results give us significant insights into the magneto-electric coupling in these materials which is essential to the magnetic and electric field control of electric polarization and magnetization in multiferroic based devices. [1] J. H. Lee, and R. S. Fishman, <http://arxiv.org/abs/1504.07106>

<sup>1</sup>Research is supported by the US Department of Energy, Office of Science, Basic Energy Sciences, Materials Science and Engineering Division and the Office of Science Early Career Research Program (V.R.C) and used computational resources at NERSC.

**2:54PM V6.00003 Spin Excitations and Phonon Anomaly in Quasi-1D Spiral Magnet  $\text{CuBr}_2$** , YUAN LI, CHONG WANG, DAIWEI YU, LICHEN WANG, FA WANG, Peking University, China, KAZUKI IIDA, KAZUYA KAMAZAWA, CROSS, Japan, SHUICHI WAKIMOTO, Japan Atomic Energy Agency —  $\text{CuBr}_2$  can be considered as a model quasi-one-dimensional (quasi-1D) spin-1/2 magnet, in which the frustrating ferromagnetic nearest-neighbor and antiferromagnetic next-nearest-neighbor exchange interactions give rise to a cycloidal magnetic order below  $T_N = 73$  K. The removal of inversion symmetry by the magnetic order also makes the material a type-II multiferroic system with a remarkably simple crystal structure. Using time-of-flight inelastic neutron scattering spectroscopy, we have determined the spin-wave as well as phonon spectra throughout the entire Brillouin zone. The spin-wave spectrum exhibits pronounced anisotropy and magnon damping, consistent with the materials quasi-1D nature and the non-collinear spin structure. The phonon spectrum exhibits dramatic discontinuities in the dispersion across the quasi-1D magnetic wave vector, indicative of strong magnetoelastic coupling and possibly of a spin-orbital texture that comes along with the spin correlations.

**3:06PM V6.00004 Magnetic and Magnetoelastic Excitations in the Multiferroic  $\text{CuBr}_2$  determined by Raman, Infrared and Neutron Spectroscopy**, CHONG WANG, DAIWEI YU, RONGYAN CHEN, XINYU DU, LICHEN WANG, XIAOQIANG LIU, ICQM, Peking University, KAZUKI IIDA, KAZUYA KAMAZAWA, Comprehensive Research Organization for Science and Society, Japan, SHUICHI WAKIMOTO, Japan Atomic Energy Agency, JI FENG, NANLIN WANG, YUAN LI, ICQM, Peking University, YUAN LI GROUP AT ICQM PEKING UNIVERSITY TEAM, NANLIN WANG GROUP AT ICQM PEKING UNIVERSITY TEAM, JI FENG GROUP AT ICQM PEKING UNIVERSITY TEAM, COMPREHENSIVE RESEARCH ORGANIZATION FOR SCIENCE AND SOCIETY (CROSS) TEAM, SHUICHI WAKIMOTO COLLABORATION — Multiferroicity was recently discovered in anhydrous copper (II) bromide  $\text{CuBr}_2$  with a rather high transition temperature ( $T_N = 73.5$  K). By the combination of the Raman, Infrared (IR) and inelastic neutron scattering (INS) experiments, evidences for strong magneto-elastic coupling and magneto-elastic excitations are found in  $\text{CuBr}_2$ . In the Raman spectra, a range of broad peaks were observed with the indications of magnetic and phonon origin at the same time. The inelastic neutron scattering experiment reveals that those nontrivial broad peaks originate from the sites of the phonons at incommensurate Q vectors that correspond to the spiral magnetic order. These results strongly suggest the existence of hybrid excitations that involve both the spin and lattice degrees of freedom, and render  $\text{CuBr}_2$  a promising platform for studying dynamic magneto-elastic coupling.

**3:18PM V6.00005 Pressure effect on ferroelectric properties of multiferroics  $\text{RMn}_2\text{O}_5$ , ( $R = \text{Gd, Tm}$ )**, NARAYAN POUDEL, MELISSA GOOCH, BERND LORENZ, TcSUH and Department of Physics, University of Houston, CHING-WU CHU, TcSUH and Department of Physics, University of Houston and Lawrence Berkeley National Laboratory, JAEWOOK KIM, SANG-WOOK CHEONG, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University — The pressure effect on the ferroelectric properties of the multiferroics  $\text{GdMn}_2\text{O}_5$  and  $\text{TmMn}_2\text{O}_5$  is studied up to 18.2 kbar. Unlike in  $\text{RMn}_2\text{O}_5$  ( $R = \text{Tb, Ho, Y}$ ), no significant change in polarization is observed in  $\text{TmMn}_2\text{O}_5$  up to 16.6 kbar. However, a new ferroelectric phase is observed in  $\text{GdMn}_2\text{O}_5$  above a critical pressure,  $P_c = 10$  kbar at higher temperature. Our result indicates that pressure decouples the Gd moment from the Mn spin system and splits the ferroelectric phase. Thermal expansion data shows a large increase of the  $c$  axis at the ambient-pressure ferroelectric transition. The pressure-induced contraction of the  $c$  lattice parameter is found to be the cause for splitting of ferroelectric phase by decoupling of two spin systems above  $P_c$ . The pressure-temperature phase diagram is derived based on dielectric and ferroelectric properties.

**3:30PM V6.00006 Doping-Tunable Ferrimagnetic Phase with Large Linear Magnetoelectric Effect in a Polar Magnet  $\text{Fe}_2\text{Mo}_3\text{O}_8$** <sup>1</sup>, TAKASHI KURUMAJI, RIKEN, CEMS, SHINTARO ISHIWATA, Univ. Tokyo, YOSHINORI TOKURA, RIKEN, CEMS, STRONG CORRELATION PHYSICS RESEARCH GROUP TEAM, ISHIWATA LABORATORY TEAM — The magnetoelectric (ME) effect, i.e., cross control of magnetization (electric polarization) by an external electric (magnetic) field, may introduce a new design principle for novel spin devices. To enhance the ME signal, control of a phase competition has recently been revealed as a promising approach. Here, we report the successful chemical-doping control of the distinct ME phases in a polar magnet  $\text{Fe}_2\text{Mo}_3\text{O}_8$ , in which an antiferromagnetic state is competing with a ferrimagnetic state. We demonstrate that Zn doping stabilizes the metamagnetic state to realize the spontaneous ferrimagnetic state and varies the ME coefficients from large negative to large positive values; for instance, the diagonal component of the ME coefficients under the magnetic field perpendicular to the polar axis varies from  $-142 \mu\text{Vs/m}$  to  $107 \mu\text{Vs/m}$  by doping Zn from 12.5% to 50%. This remarkable doping control of the ME property originates from coexisting distinct ME mechanisms, which are selectively tunable by substituting one of the two distinct magnetic sites in the unit cell with nonmagnetic Zn.

<sup>1</sup>This work was partly supported by Grants-In-Aid for Scientific Research (Grant No. 24224009) from the MEXT of Japan and the FIRST Program by JSPS

**3:42PM V6.00007 Field evolution of magnetism in multiferroic  $(\text{ND}_4)_2[\text{FeCl}_5(\text{D}_2\text{O})]$** <sup>1</sup>, WEI TIAN, HUIBO CAO, JIAQIANG YAN, BRIAN SALES, JAIME FERNANDEZ-BACA, Oak Ridge National Laboratory —  $(\text{NH}_4)_2[\text{FeCl}_5(\text{H}_2\text{O})]$  is a new organic multiferroic material that exhibits a very rich magnetic field versus temperature ( $B$  vs.  $T$ ) phase diagram. The material undergoes two successive magnetic transitions at 7.3K and 6.8K, with the onset of ferroelectricity at 6.8K at  $B=0\text{T}$ . Applying magnetic field with  $B//a$ -axis or  $B//c$ -axis induces transitions to different ferroelectric phases, and the electric polarization direction rotates from  $P//a$ -axis at  $B=0\text{T}$  to  $P//c$ -axis at  $B=5\text{T}$ . Here we report single crystal neutron diffraction results studied with  $B//a$ -axis that elucidate the field evolution of magnetism associated with different ferroelectric phases in  $(\text{NH}_4)_2[\text{FeCl}_5(\text{H}_2\text{O})]$ .

<sup>1</sup>Research conducted at ORNL's High Flux Isotope Reactor was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U. S. Department of Energy.

**3:54PM V6.00008 Mueller matrix ellipsometry studies of the optical phonons and crystal field excitations in multiferroic orthoferrites  $\text{RFeO}_3$  ( $\text{R}=\text{Tb}, \text{Dy}$ )**<sup>1</sup>, V.A. MARTINEZ, T.N. STANISLAVCHUK, A.A. SIRENKO, Department of Physics, New Jersey Institute of Technology, Newark, New Jersey 07102, USA, A.P. LITVINCHUK, Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, Texas 77204, USA, YAZHONG WANG, S.W. CHEONG, Rutgers Center for Emergent Materials and Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA — Optical properties of multiferroic orthoferrites  $\text{RFeO}_3$  ( $\text{R}=\text{Tb}, \text{Dy}$ ) bulk crystals have been studied in the far-infrared range from 50 to 1000  $\text{cm}^{-1}$  and temperatures from 7 K to 300 K. Mueller matrix and rotating analyzer ellipsometry measurements were carried out at the U4IR beamline of the National Synchrotron Light Source at Brookhaven National Lab. Optical phonon spectra and crystal field excitations were measured for all three orthorhombic axes of  $\text{RFeO}_3$ . In the experimental temperature dependencies of the phonon frequencies we found non-Grüneisen behavior caused by the electron-phonon and spin-phonon interactions. We determined the symmetries and selection rules for the crystal field transitions in  $\text{Tb}^{3+}$  and  $\text{Dy}^{3+}$  ions. Magnetic field dependencies of the optical spectra allowed us to determine anisotropy of the crystal field g-factors for  $\text{Tb}^{3+}$  and  $\text{Dy}^{3+}$  ions.

<sup>1</sup>This Project is supported by collaborative DOE Grant DE-FG02-07ER46382 between Rutgers U. and NJIT. Use of NSLS-BNL was supported by DOE DE-AC02-98CH10886. V.A. Martinez was supported by NEU NSF-1343716.

**4:06PM V6.00009 Unusual ferroelectricity induced by the Jahn-Teller effect: A case study on lacunar spinel compounds**, KE XU, HONGJUN XIANG, Fudan Univ — The Jahn-Teller effect refers to the symmetry-lowering geometrical distortion in a crystal (or nonlinear molecule) due to the presence of a degenerate electronic state. Usually, the Jahn-Teller distortion is not polar. Recently,  $\text{GaV}_4\text{S}_8$  with a lacunar spinel structure was found to undergo a Jahn-Teller distortion from a cubic to ferroelectric rhombohedral structure at  $T_{\text{JT}} = 38\text{ K}$ . Here, we carry out a general group theory analysis to show how and when the Jahn-Teller effect gives rise to ferroelectricity. On the basis of this theory, we find that the ferroelectric Jahn-Teller distortion in  $\text{GaV}_4\text{S}_8$  is due to the noncentrosymmetric nature of the parent phase and a strong electron-phonon interaction related to two low-energy  $T_2$  phonon modes. Interestingly,  $\text{GaV}_4\text{S}_8$  is not only ferroelectric, but also ferromagnetic with a magnetic easy axis along the ferroelectric direction. This suggests that  $\text{GaV}_4\text{S}_8$  is a multiferroic material in which an external electric field may control its magnetization direction. Our study not only explains the Jahn-Teller physics in  $\text{GaV}_4\text{S}_8$ , but also paves a way for searching and designing different ferroelectrics and multiferroics.

**4:18PM V6.00010 Interplay between magnetism and octahedra distortion in the hybrid improper multiferroic  $\text{Ca}_3\text{Mn}_{1.9}\text{Ti}_{0.1}\text{O}_7$** <sup>1</sup>, FENG YE, Oak Ridge National Lab, JINCHEN WANG, Renmin University of China, JAIME FERNANDEZ-BACA, ANTONIO DOS SANTOS, Oak Ridge National Lab, BIN GAO, SANG-WOOK CHEONG, Rutgers University — A novel microscopic mechanism has been proposed to search for ferroelectric material for realistic application. The instability of the polar phonon mode is driven by the simultaneous condensation of two nonpolar lattice modes associated with oxygen octahedron rotation and tilt modes, and is responsible for the polar symmetry observed in the Ruddlesden-Popper compounds. We have used single crystal neutron diffraction to investigate the temperature and pressure dependence of these oxygen octahedron distortions in  $\text{Ca}_3\text{Mn}_{1.9}\text{Ti}_{0.1}\text{O}_7$  which has a structural transition at 365 K and antiferromagnetic order at 120 K. We observed a strong interplay between magnetism and the local oxygen distortion near the magnetic transition. The control of the magnetism through octahedron rotation is also discussed.

<sup>1</sup>Research at ORNL was sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

**4:30PM V6.00011 Dynamics of the  $\text{Ho}^{+3}$  magnetism in the multiferroic compound  $\text{HoMnO}_3$  investigated via time domain terahertz spectroscopy**, N.P. ARMITAGE, N.J. LAURITA, Johns Hopkins University, RONGWEI HU, S-W CHEONG, Rutgers University — The multiferroic insulator  $\text{HoMnO}_3$  possesses a diverse array of magnetism due to both magnetically active  $\text{Mn}^{+3}$  and  $\text{Ho}^{+3}$  moments, the latter of which sit at two distinct sites within its non-inversion symmetric hexagonal crystal structure. While previous studies have focused on the ordering of the  $\text{Mn}^{+3}$  moments, little is known about the magnetic structure below 5K where it is believed that there is at least partial ordering of the  $\text{Ho}^{+3}$  ions. In principle, magnetic exchange interactions exist between both distinct  $\text{Ho}^{+3}$  and  $\text{Mn}^{+3}$  ions, resulting in a complex phase diagram with as many as five distinct phases found below  $T = 5\text{ K}$  and  $H = 3\text{ T}$ . While previous infrared studies have focused on the  $\text{Ho}^{+3}$  crystal field levels, the spin excitations in the low frequency end of the far infrared remain unknown. We report the finding of new infrared absorptions via time domain terahertz spectroscopy which we attribute to the  $\text{Ho}^{+3}$  moments. The corresponding field dependence is studied.

**4:42PM V6.00012 Electric Field Effect on the Magnetic Order in Multiferroic  $\text{LuMnO}_3$** , CHUNRUO DUAN, JUNJIE YANG, Univ of Virginia, LELAND HARRIGER, NIST Center for Neutron Research, DESPINA LOUCA, Univ of Virginia —  $\text{LuMnO}_3$  belongs to the family of hexagonal multiferroics in which ferroelectric and magnetic orders coexist and compete. The  $\text{Mn}^{3+}$  ions reside on a triangular lattice that is geometrically frustrated but undergoes a Neel transition at  $T_N \sim 90\text{ K}$ . Neutron experiments under electric field were carried out on a single crystal of  $\text{LuMnO}_3$  at SPINS to investigate the coupling of the electric field to the magnetic order. The elastic and inelastic scattering around the commensurate (101) magnetic peak and the Mn trimerization induced (100) peak with and without electric field were investigated. When applying an E-field of 13.3 kV/cm along the (001) direction on an unpoled sample, an increase in (101) peak as well as a shift of the inelastic excitation near (100) to higher  $\Delta E$  have been observed. Once the sample is polarized, these effects exist without the field. On the other hand, an E-field along (110) direction shows almost no effect. The spin arrangement of the magnetic order is within the ab-plane, thus the Dzyaloshinskii-Moriya interaction explains why a polarization perpendicular to the magnetic moment gives a larger effect. The implication will be discussed.

**4:54PM V6.00013 First-principles studies of magnetoelectric coupling in hexagonal LuFeO<sub>3</sub> under applied electric fields**, YUBO ZHANG, HONGWEI WANG, PRATIKKUMAR DHUVAD, Temple Univ, XIAOSHAN XU, University of Nebraska, MASSIMILIANO STENGEL, Institut de Ciència de Materials de Barcelona, XIFAN WU, Temple Univ — The recently stabilized hexagonal LuFeO<sub>3</sub> thin-film provides an opportunity in realizing the magnetoelectric coupling in multiferroic materials, in which the weak ferromagnetism due to Dzyaloshinskii-Moriya interaction was found to be closely associated with the trimerization (K<sub>3</sub>) mode. Here, we performed first-principles calculations in hexagonal LuFeO<sub>3</sub> and studied the variations of weak ferromagnetic moment under applied electric fields. It is found that the weak ferromagnetism is a property that can be directly tuned by the external electric fields. As an improper ferroelectric material, such a magnetoelectric coupling is realized by the strong interaction between the trimerization mode and ferroelectric mode. Under the electric field poling, ferroelectric mode will respond. A change in ferroelectric distortion will in turn affect the amplitude of trimerization mode, and therefore, the weak ferromagnetism. Interestingly, the magnetoelectric coupling in LuFeO<sub>3</sub> shows a strong nonlinear behavior originating again from the coupling between the trimerization and ferroelectric modes due to its improper nature.

**5:06PM V6.00014 Energetics of Intrinsic Defects in hexagonal LuFeO<sub>3</sub>**, TULA R. PAUDEL, EVGENY Y. TSYMBAL, Department of Physics and Astronomy & Nebraska Center for Materials and Nanoscience, University of Nebraska — The hexagonal Lutetium Ferrite (*h*-LuFeO<sub>3</sub>) is one of the few multiferroic materials where the spontaneous ferroelectric and magnetic ordering are simultaneously present at room temperature. Here, we investigate energetics of the intrinsic defects *h*-LuFeO<sub>3</sub> using the first-principles supercell approach in the dilute limit. We find the possibility of intermixing, i.e., Lu replacing Fe when *h*-LuFeO<sub>3</sub> is grown at the Lu rich conditions, and Fe replacing Lu when this compound is grown at the Fe rich conditions. In addition, our calculations predict the formation of a large number of oxygen vacancies when *h*-LuFeO<sub>3</sub> is grown in the reducing conditions. We find that even when the concentration of oxygen vacancies is large, they do not create as much free charge as they form relatively deep localized defect states. Cation vacancies are predicted to have shallow transition levels and the large formation energy, which makes them unlikely in this compound. The electronic structure of all these defects and their effect on the magnetic and polarization properties of *h*-LuFeO<sub>3</sub> are discussed.

**5:18PM V6.00015 Magneto-electric control of toroidic moments in multiferroic LiCoPO<sub>4</sub>**, JUDIT ROMHNYI, Max Planck Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart, Germany, VILMOS KOCSIS, ISTVN KZSMRKI, Department of Physics, Budapest University of Technology and Economics, 1111 Budapest, Hungary, KARLO PENC, Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungarian Academy of Sciences, P.O.B. 49, H-1525 Budapest, Hungary — In addition to the three widely known forms of ordering, elastic, electric and magnetic orders, a new so called ferrotoroidic phase has been recently observed.[1] The toroidic moment is asymmetric under both time reversal and space inversion symmetries allowing ferrotoroidic materials to exhibit intrinsic magneto-electric effect. Possibility to control magnetic properties using electric field makes such materials desirable for applications. We discuss the magneto-electric control of toroidic moments in the multiferroic material, LiCoPO<sub>4</sub>. Based on symmetry arguments we derive microscopic model for induced polarization and 'toroidization'. Using multiboson approach we investigate the experimentally observed magnon absorption spectrum following different magneto-electric poling processes. We reproduce the mono-domain ferrotoroidic state established by magneto-electric poling, as well as unconventional optical properties, such as the unidirectional light transmission, emerging in magnon spectrum of LiCoPO<sub>4</sub>. [1] Bas B. Van Aken et al, Nature 449, 702-705 (11 October 2007), Anne S. Zimmermann et al, Nature Communications 5, Article number: 4796

## Thursday, March 17, 2016 2:30PM - 5:06PM –

Session V7 DMP FIAP: Dopants and Defects in Semiconductors: Silicon and Germanium 303

- Leonard Feldman, Rutgers University

**2:30PM V7.00001 Scanning Tunneling Spectroscopy Study of Single Layer Step Edges on Si (100) Surfaces.**, XIQIAO WANG, University of Maryland-College Park, PRADEEP NAMBOODIRI, KAI LI, XIAO DENG, RICHARD SILVER, National Institute of Standard and Technology — Advanced Hydrogen lithography enables the fabrication of atomically precise donor-based quantum devices on Si(100) surfaces. Understanding the defect and step edge interaction with local electronic and geometric structures is needed to properly interpret device measurement results. Low temperature Si epitaxy, used to encapsulate devices, introduces island growth and step edges near/above buried donor nanostructures, presenting a real challenge in relocating and characterizing buried donor devices using Scanning Tunneling Microscopy/Spectroscopy (STM/STS). We present spatially resolved STS results across single layer steps on Si(100) surfaces. While the electronic properties across SA steps were found to be very similar to that on flat terraces, we observed an edge induced gap state on rebonded SB step edges, which was assigned to the unpaired dangling bond state at the lower edge atom of the rebonded SB steps. In addition, we used computational simulation within Bardeen's formalism to probe the influence of subsurface doping density profiles on the observed STS features over step edges and other defects. This study will help to elucidate the role played by surface step edges and subsurface doping densities in characterizing surface and subsurface nanostructures using STS/STM.

**2:42PM V7.00002 Structural and electrical properties of silicon hyperdoped with gold**, JAY MATH-EWS, Department of Physics, University of Dayton, YINING LIU, Electro-Optics Program, University of Dayton, GIRISH MALLADI, HARRY EFSTATHIADIS, SUNY Polytechnic Institute, JEFFREY WARRENDER, US Army ARDEC-Bent Labs — Recent advances in the field of laser hyperdoping have produced a new class of materials that could lead the way to silicon-based, CMOS-compatible infrared detectors. Using the method of ion implantation followed by pulsed laser melting (II-PLM), silicon films with impurities at concentrations well above the solid solubility limit can be fabricated. Recent work has centered around Si:Au, from which prototype IR detectors have been successfully fabricated, but there are still many questions about the structural, electrical, and optical properties of this material. In order to enhance the infrared absorption and achieve high-efficiency devices, a thorough understanding of these properties is necessary, and the processes for device fabrication must be optimized. In this work, we explore the structural and electrical properties of Si:Au hyperdoped films. Si:Au films were annealed at various temperatures, and RBS channeling was used to measure the fraction of Au atoms sitting at substitutional sites. Additionally, transmission line method (TLM) and van der Pauw (VDP) test structures were fabricated in order to investigate formation of Ohmic contacts on the hyperdoped films and to study the electrical properties of Si:Au.

**2:54PM V7.00003 Intersubband scattering in modulation-doped Si two-dimensional electron gases**, YI-HSIN SU, JIUN-YUN LI, Graduate Institute of Electronic Engineering, National Taiwan University, Taipei, Taiwan, LEONID ROKHINSON, Department of Physics, Purdue University, West Lafayette, IN, USA, JAMES STURM, Department of Electrical Engineering, Princeton University, Princeton, NJ, USA — A bilayer of modulation doped two-dimensional electron gas (2DEG) is of great interest to probe Coulomb drag. For bottom-doped Si 2DEGs, impurity scattering due to poor phosphorus (P) turn-off results in low carrier mobility. Here we demonstrate a record-high electron mobility of 470,000 cm<sup>2</sup>/V-s at 0.3 K in a bottom-doped 2DEG, comparable to that in top-doped structures. The power-law exponent of mobility vs. density was also evaluated for different P turn-off slopes. With fast turn-off, the power is 1.5, indicative of dominant remote doping scattering. The power decreases with slower P turn-off due to the enhanced scattering from the segregated P atoms. Further, for the first time, we report the second subband occupancy and intersubband scattering in a single Si quantum well, supported by the Shubnikov-de Haas oscillation data.

**3:06PM V7.00004 Extending silicon's infrared response through laser hyperdoping with gold**, JEFFREY WARRENDER, QUENTIN HUDSPETH, US Army ARDEC-Benet Laboratories, HARRY EFSTATHIADIS, SUNY-Polytechnic Institute, ELIF ERTEKIN, University of Illinois at Urbana-Champaign, JAY MATHEWS, University of Dayton — Pulsed laser melting of silicon ion-implanted with gold has recently been shown to form a highly crystalline layer with a significantly greater-than-equilibrium gold concentration.[1] Rudimentary devices made with such a laser-doped layer exhibit device response at room temperature under illumination by infrared photons with wavelengths out to 2200 nm.[2] The external quantum efficiency in the infrared is approximately  $10^{-4}$ . In this presentation, we will describe efforts to increase the quantum efficiency and avert the high cost and time of ion implantation. We study the effect of varying the gold implantation dose on the resultant gold concentration in the layer and the optoelectronic properties of the layer. Additionally, we show that an alternative approach to incorporating the gold, through deposition of a thin gold layer onto the silicon surface prior to laser melting, achieves gold concentrations comparable to those achievable by ion implantation, approximately  $2 \times 10^{19}$  atoms per cubic centimeter. We perform optoelectronic measurements on layers fabricated in this way and compare to the results obtained when using the preparation method detailed in [1] and [2]. [1] Recht *et al.*, *J. Appl. Phys.* **114**, 124903 (2013) [2]Mailoa *et al.*, *Nature Communications* **5**, 3011 (2014)

**3:18PM V7.00005 Theoretical interpretation of donor wavefunctions STM images in silicon<sup>1</sup>**, BELITA KOILLER, A. L. SARAIVA, RODRIGO B. CAPAZ, Instituto de Física, Universidade Federal do Rio de Janeiro, Brazil, M.J. CALDERÓN, ICMM-CSIC, Madrid, Spain, J. SALFI, B. VOISIN, J. BOCQUEL, S. ROGGE, Centre for Quantum Computation and Communication Technology, Sydney, Australia — Single dopant wavefunctions in Si have recently been probed by scanning tunneling spectroscopy, revealing localized patterns of resonantly enhanced tunneling currents. We show that the shapes of the conducting splotches resemble cuts through Kohn-Luttinger (KL) hydrogenic envelopes, which modulate the interfering Bloch states of conduction electrons. All the non-monotonic features of the current profile are consistent with the charge density fluctuations observed between successive {001} atomic planes, including a counter-intuitive reduction of the symmetry – a heritage of the lowered point group symmetry at these planes. A model-independent analysis of the diffraction figure constrains the value of the electron wavevector to  $k_0 = (0.82 \pm 0.03)(2\pi/a_{\text{Si}})$ . Unlike prior measurements, averaged over a sizeable density of electrons, this estimate is obtained directly from isolated electrons. We further investigate the model-specific anisotropy of the wave function envelope, related to the effective mass anisotropy. This anisotropy appears in the KL variational wave function envelope as the ratio between Bohr radii  $b/a$ .

<sup>1</sup> Authors thank partial support by CNPq, FAPERJ in Brazil, by FIS2012-33521, MINECO in Spain and by ARC CE110001027 and ARO W911NF-08-1-0527 in Australia.

**3:30PM V7.00006 Interstitial Functionalization in elemental Si**, BORIS KIEFER, EDWIN FOHTUNG, New Mexico State University — Societies in the 21<sup>st</sup> century will face many challenges. Materials science and materials design will be essential to address and master some if not all of these challenges. Semiconductors are among the most important technological material classes. Properties such as electrical transport are strongly affected by defects and a central goal continues to be the reduction of defect densities as much as possible in these compounds. Here we present results of interstitial Fe doping in elemental Si using first-principles DFT calculations. The preliminary results show that Fe will only occupy octahedral interstitial sites. The analysis of the electronic structure shows that the compounds are ferromagnetic and that a bandgap opens as interstitial Fe concentrations decrease, with a possible intermittent semi-metallic phase. The formation energy for interstitial Fe is unfavorable, as expected, by ~1.5 eV but becomes favorable as the chemical potential of Fe increases. Therefore, we expect that biasing the system with an external electrical field will lead to the formation of these materials. Thus, our results show that interstitial defects can be beneficial for the design of functionalities that differ significantly from those of the host material.

**3:42PM V7.00007 Isolation of dangling bond states on Si(100) surfaces for quantum information applications**, PETER SCHERPELZ, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago — Hydrogen resist lithography allows dangling bonds to be created and manipulated on Si(100) surfaces, both for use as a controlled quantum system, and as a step in the deterministic placement of dopants at the single-atom level. However, previous experiments and computations [1] have shown conflicting results on the location of dangling bond energy levels, which can impact their utility as qubits. Here we use large-scale density functional theory and many-body perturbation theory (GW) calculations to show that in clean, H-passivated Si(100)-(2x1) surfaces a singly-occupied dangling bond does not give rise to an electronic state isolated from the valence bands. However, very thin (1-3 nm) samples terminated by a (100) surface should provide isolated singly-occupied and doubly-occupied dangling bond states. We also explore the effect of strain, and consider novel uses of boron dopants. [1] See e.g. Bellec *et al.* *Phys. Rev. B* (2013), Ye *et al.* *Surf. Sci.* (2013), Schofield *et al.* *Nat. Commun.* (2013), Wieferink *et al.* *Phys. Rev. B* (2010).

**3:54PM V7.00008 Hybrid functional calculations of Copper impurities and related complexes in Silicon**, ABHISHEK SHARAN, Department of Physics and Astronomy, University of Delaware, Newark DE 19716, ZHIGANG GUI, ANDERSON JANOTTI, Materials Science and Engineering, University of Delaware, Newark DE 19716 — Copper impurities affect electronic and optical properties of semiconductors. Cu is an ubiquitous impurity and can be introduced unintentionally during various processing step. In silicon, the fast-diffusing interstitial Cu donor often passivates shallow-acceptor dopants, affecting the electronic characteristics of devices, while deep levels associated with other forms of the Cu impurity degrade device performance. Here we revisit the problem of the Cu impurity in Si using first principles calculation based on a hybrid functional. We discuss the relative stability of the substitutional and interstitial forms, as well as the formation of complexes with hydrogen and oxygen impurities. The results of our calculations will be compared with recent experiments on the electrical activity of Cu impurities in Si.

**4:06PM V7.00009 Impurity distribution in high purity germanium crystal and its impact on the detector performance.**, GUOJIAN WANG, Department of Physics, University of South Dakota, MARK AMMAN, Ernest Orlando Lawrence Berkeley National Laboratory, University of California, HAO MEI, DONGMING MEI, Department of Physics, University of South Dakota, KLAUS IRMSCHER, Leibniz Institute for Crystal Growth, YUTONG GUAN, GANG YANG, Department of Physics, University of South Dakota — High-purity germanium crystals were grown in a hydrogen atmosphere using the Czochralski method. The axial and radial distributions of impurities in the crystals were measured by Hall effect and Photo-thermal ionization spectroscopy (PTIS). Amorphous semiconductor contacts were deposited on the germanium crystals to make detectors. Three planar detectors were fabricated from three crystals with different net carrier concentrations (1.7, 7.9 and  $10 \times 10^{10} \text{ cm}^{-3}$ ). We evaluated the electrical and spectral performance of three detectors. Measurements of gamma-ray spectra from <sup>137</sup>Cs, <sup>241</sup>Am and <sup>60</sup>Co sources demonstrate that the detectors have excellent energy resolution. The relationship between the impurities and detector's energy resolution was analyzed. Keywords: High-purity germanium crystal, High-purity germanium detector This work is supported by DOE grant DE-FG02-10ER46709 and the state of South Dakota..

**4:18PM V7.00010 Interface effects on acceptor silicon qubits<sup>1</sup>**, JOSE CARLOS ABADILLO-URIEL, MARIA JOSE CALDERON, CSIC - Madrid — Recently, proposals of acceptor-based qubits have drawn considerable attention due to the long range strong dipolar inter-qubit coupling and the possibility of exploiting the spin-orbit interaction to couple spins to phonons or oscillating electric fields. Dopant-based quantum computing implementations often require the dopants to be situated close to an interface to facilitate qubit manipulation with local gates. Interfaces not only modify the energies of the bound states but also affect their symmetry. Making use of the successful effective mass theory we study the energy spectra of acceptors in Si or Ge taking into account the quantum confinement, the dielectric mismatch and the central cell effects. The presence of an interface puts constraints to the allowed symmetries and leads to the splitting of the bulk four-fold degenerate ground state in two Kramers doublets. We show that, as the acceptor gets closer to the interface, the entire spectrum is compressed. Inversion symmetry breaking also implies parity mixing which affects the allowed optical transitions. Consequences for acceptor qubits are discussed.

<sup>1</sup>The authors acknowledge support from MINECO-Spain through Grants FIS2012-33521 and BES-2013-065888.

**4:30PM V7.00011 Quantum states of interacting point defects in silicon**, STEVEN SCHOFIELD, HOLLY HEDGELAND, MANUEL SIEGL, DAVID BOWLER, University College London — We investigate point defect induced quantum states on silicon surfaces using low temperature scanning tunneling microscopy and spectroscopy (STM/STS). We compare defect states produced at missing H atom sites on the Si(001):H monohydride surface and those formed at boron deficient sites of the B-saturated Si(111):B- $\sqrt{3} \times \sqrt{3}R30^\circ$  surface. We find good agreement between measured differential conductance and first principles calculations of the states. Furthermore we explore the interaction of pairs of defects in a range of varying close proximity arrangements and find non-linear interference between the laterally extended excited states of the point defects. The results support the interpretation of interacting excited states as we have presented previously [Nature Communications 4 (2013) 1649].

**4:42PM V7.00012 Quantum Point Contacts and Valley Filters on a 6-fold Degenerate Hydrogen-terminated Si(111) Surface**, LUKE D. ROBERTSON, U. of Maryland, BINHUI HU, NIST Gaithersburg, B. E. KANE, U. of Maryland — Hydrogen-terminated Si(111) surfaces preserve the 6-fold valley degeneracy and anisotropic electron mass predicted in bulk Si, providing a unique environment for 2-D electron systems (2DESs). Our group has demonstrated high mobility as well as the fractional quantum Hall effect for electrons confined on the Si(111) surfaces, establishing evidence that they are ideal platforms for 2DESs and lower dimensional systems. Recently, we have succeeded in fabricating high mobility ambipolar devices and have found that heavily p-doped regions can be used as lateral depletion gates for confinement of 2DESs induced by a top gate [1]. Here, we describe our efforts to extend this technology to the nanoscale and in particular towards the fabrication of quantum point contacts (QPCs). QPCs realized in materials with anisotropic electron mass may exhibit valley filter phenomena [2] leading to extreme sensitivity to single donor occupancy, and thus are of interest to measurement schemes for donor-based quantum information processing. Preliminary measurements and fabrication techniques will be discussed. [1] B. Hu, et al, arXiv, 1509.03849 (2015) [2] Gunawan et al, Phys. Rev. B, 74, 155436 (2006)

**4:54PM V7.00013 Electron spin resonance and relaxation of defects and donors in Silicon Nanowires**, MARCO FANCIULLI, University of Milano Bicocca, Department of Materials Science, MATTEO BELLI, Laboratorio MDM, IMM-CNR, STEFANO PALEARI, ANTONIO PIZIO, University of Milano Bicocca, Department of Materials Science — The current status of the investigation of defects in silicon nanowires and at the interface between the group IV semiconductor and its oxide in 1D nanostructures is reviewed and discussed. The paper concentrates on nanowires produced by metal assisted chemical etching. Donors (such as P and As) and defects at the interface between the semiconductor and its oxide (namely, the Pb centers) are investigated by continuous wave (CW) and pulsed Electron Paramagnetic Resonance (pEPR). The role in the de-activation mechanism of donors played by hydrogen and Pb centers is discussed. The characteristic times, the spin-lattice T1 and spin-spin T2, of the Pb centers are also reported in this study. Their behavior as a function of the temperature is addressed in the framework of Two-Level-Systems. TLS are usually invoked wherever there is a disordered system, which in the case of Pb centers is represented by the amorphous oxide side. The model includes a low- and a high-temperature regime. It is worth noticing that bulk techniques such as CW and pEPR are applied to surface defects thanks to the enhanced surface-to-volume ratio. The results of the present investigation highlight a possible issue for the exploitation of nanostructures in fields like spin-based quantum computing, i.e. the spin-lattice relaxation and the decoherence induced by the TLS in the Pb centers.

## Thursday, March 17, 2016 2:30PM - 4:54PM – Session V8 DCMP: Superconductivity: Proximity Effects and SN Junctions II 304 -

**2:30PM V8.00001 Evidence for a  $\pi$ -junction in Nb/F/Nb' trilayers from superfluid density measurements<sup>1</sup>**, THOMAS LEMBERGER, MICHAEL HINTON, STANLEY STEERS, BRYAN PETERS, FENGYUAN YANG, The Ohio State University — Two-coil measurements of the sheet superfluid density of Nb/NiV/Nb' trilayers reveal the transition temperatures and volume superfluid densities of both Nb layers, as functions of the thickness,  $d_F$ , of the intervening ferromagnetic (F) Ni<sub>0.96</sub>V<sub>0.04</sub> layer. The upper transition occurs when the thicker Nb layer goes superconducting and superfluid first appears. Fitting the high-temperature superfluid density to an appropriate functional form reveals the presence of a lower "transition" where additional superfluid appears. This event is really a crossover, but the difference is irrelevant here. There is a surprising minimum in superfluid densities of both Nb layers at  $d_F \approx 30$  Å, followed by a slow rise. This behavior suggests that a  $\pi$  phase difference between the Nb layers develops at  $d_F \approx 30$  Å and continues to larger F thickness.

<sup>1</sup>Supported in part by NSF grant DMR-0805227.

**2:42PM V8.00002 Checking for odd-triplet pairing using novel superconducting spin valves<sup>1</sup>**, PAVEL N. LAPA, Argonne National Laboratory, Texas A&M University, TRUPTI KHAIRE, JUNJIA DING, JOHN E. PEARSON, VALENTYN NOVOSAD, AXEL HOFFMANN, J.S. JIANG, Argonne National Laboratory — An excitation of odd-triplet pairing in a superconducting spin valve can be revealed by measuring the dependence of the superconducting critical temperature  $T_c$  with increasing non-collinearity of the magnetizations in adjacent ferromagnetic layers. A standard approach to create such a non-collinear magnetization configuration is to pin one ferromagnetic layer and control the magnetization in another layer by rotating the multilayer in a small magnetic field. Unfortunately, the rotation can modify the vortex current which also strongly affects the critical temperature. To exclude such spurious effects, we designed and fabricated a novel superconducting spin valve which allows us to create non-collinear magnetization configurations without using a sample rotator. The valve's operational principle is based on pinning of a synthetic antiferromagnet (SAF) by exchange coupling it to FeMn layer. The ability to imprint non-collinear magnetization configurations in the spin valve was confirmed using giant magnetoresistance (GMR) measurements. The response of the magnetizations on an external magnetic field was simulated based on a coherent rotation model. The dependence of the Nb layer  $T_c$  on imprinted magnetization configuration will be presented.

<sup>1</sup>Work was supported by The Department of Energy Office of Science, Material Science and Engineering Division.

**2:54PM V8.00003 Colossal Triplet Spin-Valve Effect in Heterostructures containing 100% Spin Polarised  $\text{Fe}_{0.8}\text{Co}_{0.2}\text{Si}^1$** , GAVIN BURNELL, NATHAN SATCHELL, BENJAMIN STEELE, PRIYASMITA SINHA, CHRISTOPHER MARROWS, School of Physics and Astronomy, University of Leeds, SEAN LANGRIDGE, ISIS Neutron and Muon Source, STFC Rutherford Appleton Laboratory, UK EPSRC SUPERCONDUCTING FERROMAGNETIC METAMATERIAL CONSORTIUM COLLABORATION — At the interface between a superconductor (S) and ferromagnet (F), an inhomogeneity can convert singlet Cooper pairs into the (spin aligned) long ranged triplet component (LRTC). Manipulation of the LRTC forms the basis of the emerging field of super-spintronics. The prototypical device in this field is the superconducting spin valve (SSV), where LRTC generation can be controlled by the relative orientation of two F layers in a heterostructure. This generation is accompanied by an observed suppression in the superconductors critical temperature ( $T_c$ ). Motivated by a recent report of colossal proximity effects in a  $F_1/F_2/S$  SSV containing 100% spin polarized  $\text{CrO}_2$  as the bottom drainage layer<sup>2</sup>, we explore the possibility of using highly spin polarized,  $\text{Fe}_{0.8}\text{Co}_{0.2}\text{Si}$  as  $F_1$ . The observed  $T_c$  suppression of 830 mK is nearly an order of magnitude larger than previous studies using standard F layers with Nb, and is consistent with that seen in  $\text{CrO}_2$ . Our results confirm the special importance of high spin polarization in the formation of the LRTC, and we offer the field a new material as a fundamental building block for incorporation into future super-spintronic devices.

<sup>1</sup>UK EPSRC Grants EP/J010634/1, EP/I000933/1

<sup>2</sup>A. Singh, *et al.*, **Phy. Rev. X** 5, 021019

**3:06PM V8.00004 Remote Induced Magnetism in a Normal Metal coupled to a Superconductor/Ferromagnet Heterostructure**, NATHAN SATCHELL, University of Leeds, MACHIEL G. FLOKSTRA, University of St Andrews, JANGYONG KIM, GAVIN BURNELL, University of Leeds, PETER J. CURRAN, SIMON J. BENDING, University of Bath, JOSHANIEL F. K. COOPER, CHRISTY J. KINANE, SEAN LANGRIDGE, ISIS Neutron and Muon Source, ALDO ISIDORI, MATTHIAS ESCHRIG, NATALIA PUGACH, Royal Holloway, HUBERTUS LUETKENS, ANDREAS SUTER, THOMAS PROKSCHA, Paul Scherrer Institut, STEPHEN L. LEE, University of St Andrews, SFM CONSORTIUM COLLABORATION — Integrating superconductors (S) into ferromagnetic (F) heterostructures has revealed a rich area of novel physics and led to the development of superconducting spintronics. Of particular interest is the prototypical device, the S spin valve. In this work we use neutron and muon techniques to study the local magnetic profile in such a device, looking for an induced magnetism expected at the S/F interface. Instead we observe an additional unexpected moment arising neither in the S nor F layers, but in the normal metal cap<sup>1</sup>. The magnetisation is always antiparallel to the direction of an applied field (to align the F layers) and appears at the onset of superconductivity, increasing in strength with decreasing temperature. The profile of this induced moment is inconsistent with any known or predicted phenomena. What is particularly remarkable is that there is no applied current or temperature gradients meaning the effect manifests in equilibrium.

<sup>1</sup>M. G. Flokstra, *et al.*, **Nat. Phys.** doi:10.1038/nphys3486 (2015)

**3:18PM V8.00005 Controlling superconducting spin flow with a single homogeneous ferromagnet: interference, torque and spin-flip immunity<sup>1</sup>**, SOL JACOBSEN, IRYNA KULAGINA, JACOB LINDER, Norwegian University of Science and Technology (NTNU) — Superconducting spintronics has the potential to overcome the Joule heating and short decay lengths of electron transport by harnessing the dissipationless spin currents of superconductors in thin-film devices. Using conventional singlet superconductive sources, such dissipationless currents have only been demonstrated experimentally using intricate magnetically inhomogeneous multilayers, which can be difficult to construct, control and measure. Here we present analytic and numerical results proving the possibility of both generating and controlling a long-ranged spin supercurrent using only one single homogeneous magnetic element (arXiv:1510.02488). The spin supercurrent generated in this way does not decay spatially, in stark contrast to normal spin currents that remain polarized only up to the spin relaxation length. Through a novel interference term between long-ranged and short-ranged Cooper pairs, we expose the existence of a superconductivity-mediated torque even without magnetic inhomogeneities, showing that the different components of the spin supercurrent polarization respond fundamentally differently to a change in the superconducting phase difference. This establishes a mechanism for tuning dissipationless spin and charge flow separately via superconductors.

<sup>1</sup>Supported by COST Action MP-1201 and RCN Grant numbers 205591, 216700 and 24806

**3:30PM V8.00006 Field-History Dependence of the Superconducting Transition Temperature in Erbium/Niobium Bilayers**, JAMES WITT, NATHAN SATCHELL, University of Leeds, SEAN LANGRIDGE, STFC, GAVIN BURNELL, University of Leeds — Recently, there has been much interest in a new class of superconducting (S) spintronic devices based upon hybrid S/F (ferromagnet) heterostructures. The prototypical super-spintronic device is the superconducting spin valve (SSV), within which the critical temperature ( $T_c$ ) of an S layer can be controlled by the relative orientation of two or more F layers. Such manipulation of the F layers requires careful engineering of the heterostructure and the rotation of the structure with respect to an applied magnetic field. Here, we show that such control over  $T_c$  is also possible in a simple S/F bilayer. By manipulating the remanent magnetic state of a thin Er layer — which is proximity coupled to a Nb S layer — we are able to demonstrate a high level of control over the  $T_c$  of the Nb (which is measured in zero field). The shifts in  $T_c$  are comparable in size to the largest seen in the SSV and are manipulated using solely the field history. The system can be reset by warming the sample through the Er Curie temperature (approximately 20 K). Our results are of particular interest due to the simplicity of both the bilayer and the measurement geometry in comparison to the SSV.

**3:42PM V8.00007 Conductance spectroscopy of topological superconductor wire junctions<sup>1</sup>**, F. SETIAWAN, Condensed Matter Theory Center and Joint Quantum Institute, University of Maryland, College Park, PHILIP BRYDON, University of Maryland College Park and University of Otago, JAY SAU, Condensed Matter Theory Center and Joint Quantum Institute, University of Maryland, College Park — We study the zero-temperature transport properties of one-dimensional normal metal-superconductor (NS) junctions with topological superconductors across their topological transitions. Working within the Blonder-Tinkham-Klapwijk (BTK) formalism generalized for topological NS junctions, we analytically calculate the differential conductance for tunneling into two models of a topological superconductor: a spinless intrinsic  $p$ -wave superconductor and a spin-orbit-coupled  $s$ -wave superconductor in a Zeeman field. The zero-bias conductance takes nonuniversal values in the nontopological phase while it is robustly quantized at  $2e^2/h$  in the topological regime. Despite this quantization at zero voltage, the zero-bias conductance only develops a peak (or a local maximum) as a function of voltage for sufficiently large interfacial barrier strength, or certain parameter regimes of spin-orbit coupling strength. Our calculated BTK conductance also shows that the conductance is finite inside the superconducting gap region because of the finite barrier transparency, providing a possible mechanism for the observed soft gap feature in the experimental studies.

<sup>1</sup>Work is done in collaboration with Sankar Das Sarma and supported by Microsoft Q, LPS-CMTC, and JQI-NSF-PFC.

**3:54PM V8.00008 Detecting a quantum critical point in topological SN junctions<sup>1</sup>**, YASHAR KOMIJANI, Rutgers University, IAN AFFLECK, University of British Columbia — A spin-orbit coupled quantum wire, with one end proximate to an s-wave superconductor, can become a topological superconductor, with a Majorana mode localized at each end of the superconducting region. It was recently shown that coupling one end of such a topological superconductor to two normal channels of interacting electrons leads to a novel type of frustration and a quantum critical point when both channels couple with equal strength. We propose an experimental method to access this critical point in a single quantum wire and show its resilience to disorder.

<sup>1</sup>This research was supported in part by NSERC, CIFAR and the Swiss National Science Foundation.

**4:06PM V8.00009 On correlation between zero bias conductance peaks and topological invariants in semiconductor Rashba nanowires<sup>1</sup>**, AMIT NAG, Condensed Matter Theory Center, Department of Physics, Univ of Maryland-College Park, JAY SAU, Condensed Matter Theory Center and Joint Quantum Institute, Department of Physics, Univ of Maryland-College Park — The observed zero bias peak in tunneling conductance experiments on semiconductor Rashba nanowire is a signature of presence of Majorana zero modes. Characteristics of zero bias conductance peak (ZBCP) namely, height, width and peak splitting, are a function of microscopic parameters. Zero modes have finite splitting as a result of finiteness of the nanowire rendering the ground state only approximately topological i.e. zero modes are only approximately Majoranas. We calculate the scattering matrix topological invariant to quantify the quality of approximate Majorana modes and study its relation to observed characteristics of ZBCP. Furthermore we study the effect of dephasing on the topological invariant. Finally, we draw connection between the characteristics of the ZBCP and probability of observing non-Abelian statistics in proposed future experiments involving braiding of Majorana modes.

<sup>1</sup>Work is done in collaboration with Sankar Das Sarma and supported by LPS-MPO-CMTC, Microsoft Q, Univ. of Maryland startup grants and JQI-NSF-PFC

**4:18PM V8.00010 ABSTRACT WITHDRAWN —**

**4:30PM V8.00011 SPT 2-Channel Kondo Model in the Structure of Normal Metal/Quantum Dot/**DIII**-class Topological Superconductor**, WEI-JIANG GONG, university of texas at dallas, ZHEN GAO, north-eastern university, China — We investigate the Kondo effect in a structure which is constructed by embedding one quantum dot between a normal metal and a **DIII**-class topological superconductor supporting Majorana doublets at its ends. It is observed that Kondo correlation occurs between the localized state in the dot and two continuum states simultaneously, i.e., the continuum state in the metal and the continuum Andreev reflection state between the metal and topological superconductor. As a result, the Kondo model Hamiltonian is topologically protected by the  $SU(2) \times Z_2 T$  symmetry. More interestingly, two new Kondo temperatures appear in this system, in comparison with the normal Kondo model. This phenomenon exactly reflects the special role of Majorana doublet in tuning the Kondo effect.

**4:42PM V8.00012 Controlling the critical temperature of superconducting hybrid structures with spin-orbit coupling**, JABIR ALI OUASSOU, SOL JACOBSEN, JACOB LINDER, NTNU — Based on our recent publication Phys. Rev. B **92** 024510 (2015), we present theoretical predictions for the effect of spin-orbit coupling on the critical temperature of superconductor/ferromagnet bilayers. More specifically, we consider mesoscopic diffusive bilayers where the ferromagnet has (i) pure Rashba coupling and (ii) Rashba–Dresselhaus coupling, and show that one can achieve a superconducting spin-valve effect in both of these structures. Furthermore, it is shown that if the Rashba and Dresselhaus coupling have similar magnitudes, the critical temperature of the bilayer can change with over 35 percent as the in-plane magnetization is rotated by 90 degrees. In contrast to existing designs for superconducting spin-valves which require inhomogeneous magnetization, such as having multiple layers with noncollinear magnetizations, the critical temperature in our proposed setup is tunable with one single homogeneous ferromagnet. Thus, these results highlight a new way to exert control over superconductivity in proximity structures, which may prove easier to manufacture and control than the existing designs.

**Thursday, March 17, 2016 2:30PM - 5:30PM —**

**Session V11 DMP GERA FIAP: Thermoelectrics: McGroddy Prize and Novel Materials** 307 - Eric Toberer, Colorado School of Mines

**2:30PM V11.00001 James C. McGroddy Prize for New Materials Talk: From discovery to design of new materials**, MERCOURI G. KANATZIDIS, Northwestern Univ — The design and discovery of new materials and their crystal growth is critical for continued scientific and technological progress far into the future. It is also a fundamental goal of condensed matter science. We have been developing the chemistry of novel chalcogenide and intermetallic materials which define a remarkably broad set of structurally diverse compounds, associated with a wide range of physical properties and impacting a variety of physics and materials science issues. In contrast to solid-state methods, materials syntheses in liquid fluxes permit crystallization at lower temperatures due to facile diffusion and possible chemical reactions with the flux itself. These reactions can produce a wide range of materials, often metastable such as oxides, chalcogenides and intermetallics, but typically the formation paths are obscure or poorly understood. In this talk I will describe how we observe, understand, and engineer the formation of compounds from inorganic melts and an approach we call panoramic synthesis. I will also highlight some of our recent results on the discovery of remarkable materials and crystal structures and how they can be leveraged for achieving unusual or enhanced properties of interest in a variety of fields such as thermoelectrics,  $\gamma$  ray detection, superconductivity, topological properties, nonlinear optics, etc.

**3:06PM V11.00002 Thermoelectric Properties of Cd Based Zintl Phase Compounds**, ABHISHEK SINGH, TRIBHUWAN PANDEY, Indian Institute of Science — Zintl phase compounds can be described as covalently-bonded anion substructures surrounded by highly electro-positive cations exhibiting essential features for thermoelectric applications. By combining first principles electronic structure and Boltzmann transport theory, here we report excellent thermoelectric properties of CdSb and  $ACd_2Sb_2$  (where, A = Ca, Ba, Sr). The electronic structure shows heavy and light bands near the band edges, which lead to large power factor resulting in good thermoelectric performance. We also calculate lattice thermal conductivity by solving Boltzmann Transport equation using an iterative method. The large Grüneisen parameters and low phonon group velocity indicate strong anharmonicity in these compounds, which results in low lattice thermal conductivity. The low thermal conductivity and the excellent transport properties lead to a high ZT value of 1.9 in  $CaCd_2Sb_2$  and  $BaCd_2Sb_2$  at moderate p and n-type doping. These results indicate that well optimized Cd based Zintl phase compounds have a potential to match the performance of conventional thermoelectric materials.

**3:18PM V11.00003 Impact of electron doping on structure and dynamics of synthetic tetrahedrite<sup>1</sup>**, JENNIFER L. NIEDZIELA, ANDREW F. MAY, MICHAEL A. MCGUIRE, Oak Ridge National Laboratory, Materials Science Division, DOUGLAS L. ABERNATHY, Oak Ridge National Laboratory, Quantum Condensed Matter Division, MELANIE J. KIRKHAM, Oak Ridge National Laboratory, Instrument and Source Division, EDGAR LARA-CURZIO, OLIVIER DELAIRE, Oak Ridge National Laboratory, Materials Science Division — Microscopic control of lattice thermal conductivity is critical to the development of thermoelectric materials. One route to this control is manipulation of anharmonic lattice dynamics with chemical doping. Tetrahedrite compounds, which display an intrinsic lattice anharmonicity, are promising candidates for thermoelectric application, and here we present results of neutron scattering studies on synthetic  $\text{Cu}_{12-x}\text{Zn}_x\text{Sb}_4\text{S}_{13}$ , ( $x = 0, 2$ ). The undoped compound exhibits a structural phase transition associated with a metal-insulator transition near 88 K. Doping with Zn results in the stabilization of the structure, and enhancement of a low energy vibrational mode associated with incoherent oscillations of Cu. The low energy mode is localized, and exhibits pronounced softening with temperature. The ability to tune the location of this low-energy mode with doping may provide a means to enhance the phonon-phonon scattering that leads to low thermal conductivity in these materials, and a corresponding enhancement of the thermoelectric properties.

<sup>1</sup>This work was supported by the United States Department of Energy

**3:30PM V11.00004 Spectroscopic evidence for temperature dependent relative movement of light and heavy hole valence bands of PbQ (Q=Te,Se,S)**, UTPAL CHATTERJEE, JUNJING ZHAO, University of Virginia, MERCOURI KANATZIDIS, CHRISTOS MALLIAKAS, Northwestern University — We have conducted temperature dependent Angle Resolved Photoemission Spectroscopy (ARPES) studies of the electronic structures of PbTe, PbSe and PbS. Our ARPES measurements provide direct evidences for the light hole upper valence bands (UVBs) and the so-called heavy hole lower valence bands (LVBs), and an unusual temperature dependent relative movement between their band maxima leading to a monotonic decrease in the energy separation between LVBs and UVBs with increase in temperature. This enables convergence of these valence bands and consequently an effective increase in the valley degeneracy in PbQ at higher temperatures, which has long been believed to be the driving factor behind their extraordinary thermoelectric performance.

**3:42PM V11.00005  $p \times n$ -Transverse Thermoelectrics: Single leg thermoelectrics with scalable integration and cryogenic promise<sup>1</sup>**, M. GRAYSON, Northwestern University — Under the  $p \times n$  type transverse thermoelectric paradigm electrons dominate conduction in one direction and holes dominate perpendicularly, allowing electrical current to drive transverse heat flow [1]. Bulk anisotropic crystals, superlattices, and nanowire arrays have all been previously proposed as viable  $p \times n$  materials. This talk will describe the general philosophy behind  $p \times n$ -type transverse thermoelectrics as well as the tensor equations that define their anisotropic Seebeck effect. The advantages of single-leg thermoelectric devices – available only to transverse thermoelectrics – are detailed. Various device geometries are discussed which take advantage of the single-leg nature, in particular to provide advantages for cryogenic thermoelectric cooling and integrated thermal management. [1] Chuanle Zhou, S. Birner, Yang Tang, K. Heinselman, and M. Grayson, Phys. Rev. Lett. 110, 227701 (2013).

<sup>1</sup>Supported by AFOSR FA9550-15-1-0377

**4:18PM V11.00006 Copper Selenide Nanocrystals as a High Performance, Solution Processed Thermoelectric Material**, JASON FORSTER, Lawrence Berkeley National Lab, JARED LYNCH, Nanosys, NELSON COATES, California Maritime Academy, AYASKANTA SAHU, Lawrence Berkeley National Lab, JUN LIU, North Carolina State University, DAVID CAHILL, University of Illinois at Urbana Champaign, JEFF URBAN, Lawrence Berkeley National Lab — Nano-structuring a thermoelectric material often results in enhanced performance due to a decrease in the materials thermal conductivity. Traditional nano-structuring techniques involve ball milling a bulk material followed by spark plasma sintering, a very energy intensive process. In this talk, we will describe the development of a self-assembled, high-performing, nano-structured thin film based on copper selenide nanocrystals. Mild thermal annealing of these films results in concurrent increases in the Seebeck coefficient and electrical conductivity. We are able to achieve power factors at room temperature that are as high as the best spark plasma sintered materials. These solution-processed films have potential applications as conformal, flexible materials for thermoelectric power generation.

**4:30PM V11.00007 NMR and specific heat study of atomic dynamics and spin-orbit behavior in  $\text{Cu}_{2-x}\text{Ag}_x\text{Te}$** , ALI A. SIRUSI, Texas AM University, SEDAT BALLIKAYA, University of Istanbul, JING-HAN CHEN, Texas AM University, CTIRAD UHER, University of Michigan, JOSEPH H. ROSS, JR., Texas AM University — We report studies of  $\text{Cu}_2\text{Te}$  and  $\text{Cu}_{2-x}\text{Ag}_x\text{Te}$ , promising candidates for thermoelectric and photovoltaic applications. Cu and Te NMR show that above a well-defined 200 K onset,  $\text{Cu}_2\text{Te}$  exhibits Cu-ion hopping, leading to the higher-temperature superionic motion. In  $\text{Cu}_{1.98}\text{Ag}_{0.2}\text{Te}$  the onset increases to 250 K. In the low-temperature static phase the properties are nearly identical. Aside from Korringa terms there are large diamagnetic contributions for all nuclei, comparable to those for other systems with very large spin-orbit and/or inverted band configurations. Thus the system may be a topologically interesting system like the similar phase  $\text{Ag}_2\text{Te}$ . Results will be compared to DFT calculations of NMR shifts. The low-temperature spectra also indicate two distinct local environments for Cu sites, one corresponding to high symmetry such as characterizes the high-temperature cubic phase, and one with much more asymmetry. In addition, specific heat results are consistent with about 50% of the Cu ions being weakly bound on Einstein-oscillator sites. We tentatively connect these results to reported local inhomogeneity due to vacancy condensation in similar systems.

**4:42PM V11.00008 Thermoelectric Properties of CuAgSe doped with Co, Cr.<sup>1</sup>**, PETER CZAJKA, MENGJIANG YAO, CYRIL OPEIL, Department of Physics, Boston College — Thermoelectric materials represent one way that reliable cooling below the boiling point of nitrogen can be realized. Current materials do not exhibit sufficiently high efficiencies at cryogenic temperatures, but significant progress is being made. One material that has generated significant interest recently is CuAgSe. It has been demonstrated (Ishiwata et al., Nature Mater. 2013) that doping CuAgSe with 10% Ni at the Cu sites increases the material's thermoelectric figure of merit (ZT) at 100 K from 0.02 to 0.10. This is intriguing not just because of the dramatic effect that the Ni doping produces, but also because CuAgSe is a semimetal and semimetals are not usually able to exhibit the kind of asymmetric carrier activation necessary for strong thermoelectric performance. In order to further investigate the unusual nature of thermoelectricity in CuAgSe and its strong dependence on chemical composition, we have synthesized and measured the thermoelectric properties of a series of CuAgSe samples doped with Co and Cr. Temperature-dependent magnetic and thermoelectric transport properties of CuAgSe as a function of Co and Cr doping will be discussed.

<sup>1</sup>This work is supported by the Department of Defense, AFOSR, MURI Program Contract FA9550-10-1-0533 and the Trustees of Boston College.

**4:54PM V11.00009 Low Temperature Thermoelectric Characterization of Ag<sub>2</sub>Se.<sup>1</sup>** , FIVOS DRYMIOTIS, DAVID NEFF, MICHAEL CONEY, SABAH BUX, JEAN-PIERRE FLEURIAL, NASA/Jet Prop Lab — Previous work on Ag<sub>2</sub>Se showed that this n-type material could have a dimensionless thermoelectric figure of merit (zT) ~1 at room temperature, due to its high mobility and low thermal conductivity. However, the results from the initial reports have not yet been reproduced. In this talk, I will summarize our efforts to replicate the aforementioned thermoelectric performance, and also discuss the experimental setup that we utilized in order to perform the low-temperature thermoelectric characterization of this material.

<sup>1</sup>This work was performed at the California Institute of Technology/Jet Propulsion Laboratory under contract with the National Aeronautics and Space Administration. This work was supported by JPLs Research and Technology Development Program.

**5:06PM V11.00010 Molecular-Dynamics (MD) Simulations of Copper Diffusion in Copper Chalcogenides** , JING WANG, None — It was recently discovered that copper chalcogenides Cu<sub>2</sub>S and Cu<sub>2</sub>Se are viable candidates for thermoelectric materials with high figure of merit (ZT) values at temperatures around 1,000 K [1,2]. And the possible reason for the high ZT is the low thermal conductivity arising from liquid-like Cu atoms in those phases. In this work, we perform first-principles molecular dynamics simulations to study the motion of Cu atoms in the high-temperature phases of Cu<sub>2</sub>S and Cu<sub>2</sub>Se and confirm the liquid nature of Cu atoms. To get a better understanding of the diffusion patterns of the systems, we have examined all the three phases of Cu<sub>2</sub>S (monoclinic, hexagonal and cubic phases with increasing temperature). Starting from the hexagonal phase the Cu atoms show a disordered/liquid-like feature with a jump diffusion pattern. We find that the diffusion is faster in x-y directions than in the z direction. A more isotropic diffusion pattern is found for high-temperature cubic phase with a much larger diffusion coefficient.1] Y. He et al. Adv. Mater. 26, 3974 (2014) 2] H. L. Liu et al. Nat. Mater. 11, 422 (2012)

**5:18PM V11.00011 Impact of Lone-Pair Electrons on Thermal Conductivity in CuSbS<sub>2</sub> Compound<sup>1</sup>** , BAOLI DU, RUIZHI ZHANG, KAN CHEN, MICHAEL REECE, Queen Mary University of London, MATERIAL RESEARCH INSTITUTE TEAM — Compounds with intrinsically low lattice thermal conductivity are of practical importance for thermoelectric energy conversion. Recent studies suggest that s<sub>2</sub> lone pair orbital electrons are a key contributing factor to the anomalously low lattice thermal conductivity of chalcogenide compounds that contain a nominally trivalent group VA element. CuSbS<sub>2</sub> has an orthorhombic structure with space group Pnma. The pyramidal SbS<sub>5</sub> units are separated by CuS<sub>4</sub> tetrahedron so that the base of the square pyramidal units are aligned to face one another, thus directing the Sb lone pair electron density into the void separating the SbS<sub>5</sub> units. Different from tetrahedrite, all the Cu atoms are bonded in the CuS<sub>4</sub> tetrahedron. So, it has a perfect structure to study the influence of electron lone pair on thermal conductivity without the impact from trigonal coordinated Cu. In this work, the trivalent transition metal atom Fe and IIIA atom Ga without lone-pair electrons were chosen to substitute Sb in CuSbS<sub>2</sub>. The changes in the bonding environment by foreign atoms and their influences on the thermal properties have been studied and correlated.

<sup>1</sup>Marie Curie International Incoming Fellowship of the European Community Human Potential Program under Contract no. PIIF-GA-2013-622847

**Thursday, March 17, 2016 2:30PM - 3:42PM —**  
**Session V12 FIAP: FIAP Prize Session** 308 - Barbara Jones, IBM

**2:30PM V12.00001 George E. Pake Prize: A Few Challenges in the Evolution of Semiconductor Device/Manufacturing Technology** , ROBERT DOERING, Texas Instruments, Inc. — In the early 1980s, the semiconductor industry faced the related challenges of “scaling through the one-micron barrier” and converting single-level-metal NMOS integrated circuits to multi-level-metal CMOS. Multiple advances in lithography technology and device materials/process integration led the way toward the deep-sub-micron transistors and interconnects that characterize today’s electronic chips. In the 1990s, CMOS scaling advanced at an accelerated pace enabled by rapid advances in many aspects of optical lithography. However, the industry also needed to continue the progress in manufacturing on ever-larger silicon wafers to maintain economy-of-scale trends. Simultaneously, the increasing complexity and absolute-precision requirements of manufacturing compounded the necessity for new processes, tools, and control methodologies. This talk presents a personal perspective on some of the approaches that addressed the aforementioned challenges. In particular, early work on integrating silicides, lightly-doped-drain FETs, shallow recessed isolation, and double-level metal will be discussed. In addition, some pioneering efforts in deep-UV lithography and single-wafer processing will be covered. The latter will be mainly based on results from the MMST Program – a \$100M+, 5-year R&D effort, funded by DARPA, the U.S. Air Force, and Texas Instruments, that developed a wide range of new technologies for advanced semiconductor manufacturing. The major highlight of the program was the demonstration of sub-3-day cycle time for manufacturing 350-nm CMOS integrated circuits in 1993. This was principally enabled by the development of: (1) 100% single-wafer processing, including rapid-thermal processing (RTP), and (2) computer-integrated-manufacturing (CIM), including real-time, in-situ process control.

**3:06PM V12.00002 The ”Music” of Light: Optical Resonances for Fun and Profit** , RAYMOND BEAUSOLEIL, Hewlett Packard Labs, 1501 Page Mill Rd., Palo Alto, CA 94304 — Moore’s Law has set great expectations that the performance/price ratio of commercially available semiconductor devices will continue to improve exponentially at least until the end of this decade. But the physics of the metal wires that connect the transistors on a silicon chip already places stringent limits on the performance of integrated circuits, making their continued dramatic improvement highly unlikely. In this talk, I will introduce the basic concept of an optical resonance in a microscopic dielectric cavity in the context of the same type of spatial boundary conditions that give each musical instrument its unique sound. Then I will illustrate applications of these resonances to information technology in a variety of forms and functions using examples from my own laboratory at HP, such as chip-scale optical networks, quantum bits based on spins in diamond, and ultrafast optical switches that could become the foundation for a new generation of optical computers. Our goal is to conduct advanced research that could precipitate an “optical Moore’s Law” and allow exponential performance gains to continue through the end of the next decade.

**Thursday, March 17, 2016 2:30PM - 5:30PM —**  
**Session V13 GMAG DMP: Heat Current Effects on Magnetization Dynamics** 309 - Jean-Philippe Ansermet, Ecole Polytechnique Federale de Lausanne, Switzerland

**2:30PM V13.00001 Giant thermal spin torque assisted magnetic tunnel junction switching** , AAKASH PUSHP, IBM Almaden Res Ctr — Spin-polarized charge-currents induce magnetic tunnel junction (MTJ) switching by virtue of spin-transfer-torque (STT). Recently, by taking advantage of the spin-dependent thermoelectric properties of magnetic materials, novel means of generating spin-currents from temperature gradients, and their associated thermal-spin-torques (TSTs) have been proposed, but so far these TSTs have not been large enough to influence MTJ switching. Here we demonstrate significant TSTs in MTJs by generating large temperature gradients across ultrathin MgO tunnel barriers that considerably affect the switching fields of the MTJ. We attribute the origin of the TST to an asymmetry of the tunneling conductance across the zero-bias voltage of the MTJ. Remarkably, we estimate through magneto-Seebeck voltage measurements that the charge-currents that would be generated due to the temperature gradient would give rise to STT that is a thousand times too small to account for the changes in switching fields that we observe. Reference: A. Pushp\*, T. Phung\*, C. Rettner, B. P. Hughes, S.-H. Yang, S. S. P. Parkin, 112, 6585-6590 (2015).

**3:06PM V13.00002 Picosecond Spin Caloritronics**, DAVID G. CAHILL, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign — The coupling of spin and heat, i.e., spin caloritronics, gives rise to new physical phenomena in nanoscale spin devices and new ways to manipulate local magnetization. Our work in this field takes advantage of recent advances in the measurement and understanding of heat transport at the nanoscale using ultrafast lasers. We use a picosecond duration pump laser pulses as a source of heat and picosecond duration probe laser pulses to detect changes in temperature, spin accumulation, and spin transfer torque using a combination of time-domain thermoreflectance and time-resolved magneto-optic Kerr effect. Our pump-probe optical methods enable us to change the temperature of ferromagnetic layers on a picosecond time-scale and generate enormous heat fluxes on the order of  $100 \text{ GW m}^{-2}$  that persist for  $\sim 30 \text{ ps}$ . Thermally-driven ultrafast demagnetization of a perpendicular ferromagnet leads to spin accumulation in a normal metal and spin transfer torque in an in-plane ferromagnet. The data are well described by models of spin generation and transport based on differences and gradients of thermodynamic parameters. The spin-dependent Seebeck effect of a perpendicular ferromagnetic layer converts a heat current into spin current, which in turn can be used to exert a spin transfer torque (STT) on a second ferromagnetic layer with in-plane magnetization. Using a [Co,Ni] multilayer as the source of spin, an energy fluence of  $\approx 4 \text{ J m}^{-2}$  creates thermal STT sufficient to induce  $\approx 1 \%$  tilting of the magnetization of a 2 nm-thick CoFeB layer.

**3:42PM V13.00003 Ultrafast spin-transfer torque driven by femtosecond pulsed-laser excitation.**, BERT KOOPMANS, Eindhoven Univ of Tech — A hot topic in the field of ultrafast laser-induced manipulation of the magnetic state is that of the role and exploitation of laser-induced spin currents. Intense debate has been triggered by claims that such a spin-transfer, e.g. in the form of super-diffusive spin currents over tens of nanometers, might be a main contributor to the demagnetization process in ferromagnetic thin films after femtosecond laser excitation. In this presentation the underlying concepts will be introduced and recent developments reviewed. Particularly we demonstrate the possibility to apply a laser-induced *spin transfer torque* on a free magnetic layer, using a non-collinear multilayer configuration consisting of a free in-plane layer on top of a perpendicularly magnetized injection layer, as separated by a nonmagnetic spacer. Interestingly, this approach allows for a quantitative measurement of the amount of spin transfer. Moreover, it might provide access to novel device architectures in which the magnetic state is controlled by fs laser pulses. Careful analysis of the resulting precession of the free layer allows us to quantify the applied torque, and distinguish between driving mechanisms based on laser-induced transfer of hot electrons versus a spin Seebeck effect due to the large thermal gradients. Further engineering of the layered structures in order to gain fundamental understanding and optimize efficiencies will be reported. A simple model that treats local non-equilibrium magnetization dynamics to spin transport effects via a spin-dependent chemical potential will be introduced.

**4:18PM V13.00004 Magnetization dynamics under heat current in metallic spin valves and in insulators**, HAIMING YU, Beihang University — Spin caloritronics, an emerging branch of spintronics, studying the addition of thermal effects to the electrical and magnetic properties of nanostructures, has recently seen a rapid development. It has been predicted by Hatami et al. that a heat current can exert a spin torque on the magnetization in a nanostructure, analogous to the well-known spin-transfer torque induced by an electrical current. We provided the experimental evidence for the thermal spin-transfer torque effect in spin valves, showing the switching field change with heat current. I will present measurements of the second harmonic voltage response of Co-Cu-Co pseudo-spinvalves deposited in the middle of Cu nanowires. Both the magnitude of the second harmonic response of the spin valve and the field value of the maximum response are found to be dependent on the heat current. Both effects show that the magnetization dynamics of the pseudo-spinvalves is influenced by the heat current. Thus, the data provide a quantitative estimate of the thermal spin torque exerted on the magnetization of the Co layers. In addition, I will present recent study on the magnetization dynamics in a magnetic insulator YIG film under in-plane heat current. The ferromagnetic resonance linewidth is found to be tuned by the applied temperature gradient, i.e. narrowing and broadening. This suggests that the Gilbert damping parameter is compensated or reinforced by the applied temperature gradient in respective direction. These observations can be understood as a heat-driven spin torque in magnetic insulators.

**4:54PM V13.00005 Magnetic equivalent of the Seebeck effect.**, SYLVAIN BRECHET, EPFL — Spin caloritronics seeks to investigate the effect of a thermal gradient on the electronic charge and spin degrees of freedom. In a conductor, a thermal gradient leads a transport of the conduction electrons that in turn generate an electric field along the temperature gradient, which is the well-known Seebeck effect. In an insulator, there are no conduction electrons. Thus no electronic charge transport takes place. However, the electronic spins can reorient themselves in the presence of a temperature gradient as they precess around an external field oriented along the temperature gradient. In fact, the temperature gradient generates a magnetic induction field in the plane orthogonal to the temperature gradient. The effect is the magnetic analog of the Seebeck effect and is thus referred to as the magnetic Seebeck effect. It has been observed for the propagation of spin waves along and against a temperature gradient in a YIG slab. The propagation of spin waves against the temperature gradient lead to a positive thermal damping and the propagation along the temperature gradient leads to the opposite effect, namely a negative thermal damping. Thus, the magnetic Seebeck effect generate of heat driven spin torque that can generate a positive or a negative thermal damping. The magnetic Seebeck effect has been recently established using a fundamental variational approach. In many experimental situations, the system can be treated as a classical continuum with magnetisation on the scale of interest where the quantum fluctuations average out and the underlying microscopic structure is smoothed out. For the propagation of magnetisation waves in a stationary state, the system is slightly out of equilibrium but the magnetic kinetic energy is constant. In such a case, the action of the system is a functional of the magnetisation and the magnetisation current. Since the magnetisation is a function of the temperature, the action variation yields an explicit expression for the magnetic induction field generated by the temperature gradient. This field lead to a heat driven spin torque that has the same geometry in an insulator than the spin transfer torque proposed by Berger and Slonczewski in a conductor.

**Thursday, March 17, 2016 2:30PM - 4:54PM —**

**Session V14 FEd: TA Professional Development: Excellent TA's Making Excellent Researchers**

310 -

**2:30PM V14.00001 Using the TA to Prepare Graduate Students for Research and Employment**, KENNETH HELLER, School of Physics & Astronomy, University of Minnesota — One of the most underused components of the physics graduate program is the time spent being a teaching assistant (TA). Often the TA duties consist of grading and trying to help undergraduates survive a physics course. How those duties are accomplished is left to each TA. The most common TA preparation, if it exists, has a narrow focus on the class being taught. Preparation consists of describing, or perhaps practicing, specific teaching skills and gaining familiarity with the equipment used in the laboratory portion of the class. Instead TAs can be integrated into the entire course in which they function so that they learn the course as a system. This means treating a course in the same way one approaches a research project with the TAs as members of the research team headed by a faculty advisor. TA preparation is broadened and support includes the management, teamwork, and communication skills necessary. This makes the TAs more efficient and effective teachers while explicitly connecting the TA experience to the "soft" skills they need in their own research careers whether in industry, national laboratories, or academia. This talk describes such a program, functioning for over 20 years at the University of Minnesota, that takes no more time than the usual TA but results in graduate students that are more satisfied with their TA experience, are better prepared to function in research groups, and provide a better classroom experience for their undergraduate students.

**3:06PM V14.00002 Mobilizing the Forgotten Army: Improving Undergraduate Math and Science Education through Professional Development of Graduate Teaching Assistants<sup>1</sup>** , JORDAN GERTON, University of Utah — Evidence-based best practices for improving undergraduate STEM education abound. Unfortunately, these practices have not been widely adopted, in part because typical dissemination efforts are mediated in a top-down fashion and fail to obtain critical buy-in from key local stakeholders. Here, we present a novel framework to increase nationwide uptake of STEM-education best practices through grassroots propagation of Professional Development programs for Graduate Teaching Assistants (GTA-PD). Our model pays special attention to overcoming resistance to change by soliciting, from the very start, critical buy-in from departmental chairs, faculty, and GTAs who have direct control over and responsibility for instruction. A key component of our approach involves an annual National GTA Workshop where faculty-GTA leadership teams from many different Physics and Chemistry departments come together to develop best-practices-based GTA-PD improvement plans for their own departments while guided by a core group of nationally recognized expert practitioners in GTA-PD and STEM education. As a pre-condition for participation, each department chair must pledge to facilitate implementation of their leadership teams plan; additional and ongoing support is provided by the core group of experts, together with other teams from the workshop cohort. Our initial pilot efforts point to success via enthusiastic buy-in within each STEM department due to the potential for immediate positive impacts on both undergraduate instruction and the long term research productivity of GTAs. In the future, longitudinal data on the progress of the GTA-PD programs will be gathered and analyzed to provide guidance for improving the success of future GTA-PD programs.

<sup>1</sup>Financial support provided by the Research Corporation for Science Advancement and the American Chemical Society

**3:42PM V14.00003 TA Professional Development: A Graduate Student's Perspective** , EMILY ALICEA-MUNOZ, Georgia Inst of Tech — Graduate Teaching Assistants (GTAs) are essential for teaching large introductory physics classes. In such courses, undergraduates spend approximately half of their in-class contact time in instructional environments (e.g., labs and recitations) supervised by GTAs, which means GTAs can have a large impact on student learning. Therefore it is crucial to adequately prepare GTAs before they first enter the classroom, and to offer them continued support throughout. Since many of the skills required to become effective teachers will also be relevant to their future research careers, it is useful for a GTA preparation program to also include professional development strategies. But what exactly do GTAs get out of these programs? The School of Physics at Georgia Tech runs a preparation and mentoring program for GTAs that focuses on pedagogical knowledge, physics content, and professional development, as well as their intersections. Nearly seventy graduate students have gone through this program in the three years since it was established. Here we discuss the impact this program has had on our GTAs, from their own point of view: the program's effect on their teaching abilities, how it has influenced their attitudes towards teaching, what elements they have found useful, and what changes they have suggested to its curriculum. We find that, in general, GTAs are more receptive when the curriculum is more hands-on and they are presented with frequent opportunities for practice and feedback.

**4:18PM V14.00004 A Joint Pedagogy Course for Learning Assistants and Teaching Assistants** , JOSHUA VON KORFF, Georgia State University — No abstract available.

**Thursday, March 17, 2016 2:30PM - 5:30PM —**

**Session V15 DMP: 2D Materials: Charge Density Waves** 314 - Ken Burch, Boston College

**2:30PM V15.00001 Weakly Bound and Strongly Interacting: NbSe<sub>2</sub> and 1T-TaS<sub>2</sub> in the 2D Limit** , ADAM TSEN, University of Waterloo and Columbia University — The layered metallic dichalcogenides are known to exhibit rich collective electron phases such as charge density waves, spin density waves, and superconductivity. In the past, studies on graphene and various semiconducting dichalcogenides have shown that taking layered materials to their physical two-dimensional (2D) limit leads to fundamental changes in band structure, allowing for a powerful experimental knob to tune for electronic functionality. In contrast, due to their instability in the ambient environment, the effect of thickness control over such collective electron phases has been largely unexplored in metallic systems. We have recently demonstrated a new experimental platform for the isolation and assembly of environmentally sensitive 2D materials in inert atmosphere. I will discuss our recent studies of the charge density wave material 1T-TaS<sub>2</sub> and superconducting NbSe<sub>2</sub> in the atomically thin limit, made possible using this technique. For 1T-TaS<sub>2</sub>, we find that the lock-in transition to commensurate charge ordering becomes increasingly metastable for reduced thickness, allowing for all-electrical control over this phase transition in the 2D state. In NbSe<sub>2</sub>, a small magnetic field induces a transition to a quantum metallic phase, the resistivity of which obeys a unique field-scaling property. These methods and experiments open new doors for the study of other correlated 2D materials in the immediate future.

**3:06PM V15.00002 Nanostructure of the charge density wave domains in 1T-TaS<sub>2</sub>** , SOHAM BANERJEE, Columbia University, YUE CAO, Brookhaven National Lab, DENNIS WANG, Columbia University , STEPHAN HRUSZKEWYCZ, MARTIN HOLT, Argonne National Lab, SIMON BILLINGE , Columbia University — The connection between structural and electronic phase separation is thought to play an important role in strongly correlated systems, where ordering at the nanoscale modifies exotic macroscopic properties. 1T-TaS<sub>2</sub> offers us a rare example of a layered material exhibiting both the Mott state and a diversity of charge density wave (CDW) phases, in close analogy to a number of high temperature superconductors with pseudogap behavior. While local scanning probes have identified electronic nanoscale phase separation in low dimensional CDW systems, an explanation of the lattice response to electronic instabilities remains unsettled. Of the 1T-TaS<sub>2</sub> CDW phases, a nearly commensurate (NC) phase is segregated, with nanoscale commensurate CDW domains, separated by metallic incommensurate regions (domain walls). Here, we demonstrate the use of scanning probe X-ray nanodiffraction to analyze structural perturbations in NC 1T-TaS<sub>2</sub> that arise due to an incommensurability of the CDW wavevector and the underlying lattice.

**3:18PM V15.00003 Magnetic Field Studies Near Superconducting Transition in MBE Grown Monolayer NbSe<sub>2</sub> on Bilayer Graphene** , SEITA ONISHI, UC Berkeley/Lawrence Berkeley National Lab. (LBNL), MIGUEL M. UGEDA, UC Berkeley/CIC nanoGUNE, YI ZHANG, LBNL/SLAC National Accelerator Lab., YI CHEN, CLAUDIA OJEDA-ARISTIZABAL, UC Berkeley, HYEJIN RYU, SUNG-KWAN MO, ZAHID HUSSAIN, Lawrence Berkeley National Lab., ZHI-XUN SHEN, SLAC National Accelerator Lab./Stanford University, MICHAEL F. CROMMIE, ALEX ZETTL, UC Berkeley/Kavli ENSI/LBNL — Following the work by Frindt [1] on the superconductivity of NbSe<sub>2</sub> at reduced thicknesses, recent breakthroughs have enabled the study of bilayers and monolayers. Staley et. al. [2], Tsen et. al. [3], Cao et. al. [4] and Xi et. al. [5] have studied superconductivity in bilayers and monolayers of NbSe<sub>2</sub> after mechanical exfoliation and encapsulation with another layered material to protect from air. In this work, we have investigated the superconductivity in monolayer NbSe<sub>2</sub> prepared by molecular beam epitaxy growth (MBE) on bilayer graphene (BLG) [6]. The superconducting transition has an onset temperature of 1.9K, midpoint temperature of 0.65K and reaches zero resistance at 0.46K. The upper critical field perpendicular to the NbSe<sub>2</sub> monolayer is 0.5T at 100mK. We will show the effect of magnetic fields near the superconducting transition and compare with existing theories. [1] R. Frindt, Phys. Rev. Lett. 28, 299 (1972). [2] N. E. Staley, et. al., Phys. Rev. B 80, 184505 (2009). [3] A. W. Tsen, et. al., arXiv:1507.08639 [cond-Mat.supr-Con] 1 (2015). [4] Y. Cao, et. al., Nano Lett. 15, 4914 (2015). [5] X. Xi, et. al., arXiv:1507.08731 [cond-Mat.supr-Con] 1 (2015). [6] M. M. Ugeda, et al., Nat. Phys. 10.1038/nphys3527 (2015).

**3:30PM V15.00004 The Upper Critical Field of Bilayer NbSe<sub>2</sub>**, BENJAMIN HUNT, Carnegie Mellon University, ADAM W. TSEN, Y. D. KIM, Columbia University, Z. J. YUAN, S. JIA, Peking University, R. J. CAVA, Princeton University, J. HONE, Columbia University, P. KIM, Harvard University, ABHAY PASUPATHY, CORY DEAN, Columbia University — We report on the fate of the superconducting state of bilayer NbSe<sub>2</sub> in a large parallel magnetic field. Due to strong spin-orbit coupling, the system exhibits an out-of-plane polarization of electron spins in each valley, which leads to an enhanced upper critical field  $H_{c2}^{\parallel}$  as compared to that expected from the Pauli limit  $H_p$  [1]. We explore the behavior of  $H_{c2}^{\parallel}(T)$  in the low temperature limit, down to  $T = 0.3\text{K}$  (approximately  $0.06T_c$ ), and we find a maximum upper critical field of 28 T which is  $\sim 3$  times the Pauli limit. We find that the measured  $H_{c2}^{\parallel}(T)$  deviates significantly from the standard pair-breaking theory as  $T \rightarrow 0$ , and we compare our results to recent observations of Ising superconductivity in NbSe<sub>2</sub> [1] and in ionic-liquid-gated MoS<sub>2</sub> [2], as well as to calculations of  $H_{c2}$  based on realistic band structure of NbSe<sub>2</sub>. References: [1] Xi et al. arXiv:1507.08731 (2015) [2] Saito et al. arXiv:1506.04146 (2015)

**3:42PM V15.00005 Superconductivity and charge density waves in atomically thin NbSe<sub>2</sub>**, XIAOXIANG XI, Pennsylvania State University — Atomically thin van der Waals materials have emerged as a frontier for both fundamental physics and device applications. Although novel single-particle and excitonic properties have been extensively studied, the collective electron phenomena in these materials remain less well understood. In this talk, we will discuss superconductivity and charge-density-wave (CDW) order in atomically thin group-V transition metal dichalcogenide NbSe<sub>2</sub> down to the monolayer limit. Electrical transport measurements show that the superconducting transition temperature decreases monotonically with reducing the layer thickness. The temperature dependent Raman scattering, on the other hand, shows enhanced CDW order as the sample thickness reduces. While the former can be understood mainly as the result of reduced interlayer Cooper pairing, the latter arises from the enhanced electron-phonon coupling in atomically thin samples. Magnetotransport measurements further reveal the effect of spin-momentum locking, a consequence of broken inversion symmetry and strong spin-orbit coupling in monolayer NbSe<sub>2</sub>, on Cooper pairing and the in-plane upper critical fields. These results set the stage for the exploration and control of collective electronic phases in 2D NbSe<sub>2</sub> and related systems.

**4:18PM V15.00006 Charge Density Waves in the bulk and mono-layer VSe<sub>2</sub>**, YANG-HAO CHAN, CHING-MING WEI, Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan, MEI-YIN CHOU, School of Physics, Georgia Institute of Technology, USA — Charge density waves (CDWs) are widely observed in the layered transition-metal dichalcogenides (TMDs). With the capability of preparing atomically thin samples in the experiment, the underlying mechanism of the formation of CDWs and the role played by dimensionality in TMDs can now be studied in great detail. We present the first-principles calculations on bulk and mono-layer VSe<sub>2</sub>. Our results agree with the experimental findings that the dominant CDW phase has a  $4\times 4\times 3$  supercell structure in the bulk system. Electronic structure calculations suggest Fermi-surface nesting is a relevant mechanism. On the other hand, we find a new  $3\sqrt{3}\times 3\sqrt{3}$  CDW phase as the lowest energy structure in the mono-layer case induced by strong electron-phonon interaction. We also find that substantial hole doping leads to a CDW-superconducting (SC) phase transition. The SC transition temperature is predicted to be higher than that of the bulk from our first-principles calculations.

**4:30PM V15.00007 Scanning Tunneling Microscopy and Spectroscopy of Graphene on NbSe<sub>2</sub>**, SHENGQIANG HUANG, ZHIMING ZHANG, MATTHEW YANKOWITZ, BRIAN J. LÉROY, Univ of Arizona — A wide range of phenomena can be induced in graphene by creating vertical heterostructures with other two-dimensional materials. NbSe<sub>2</sub> is a layered transition metal dichalcogenide that exhibits a charge density wave transition below  $T_{cdw} = 33\text{ K}$  and then becomes superconducting below  $T_c = 7.2\text{ K}$ . By placing monolayer graphene on NbSe<sub>2</sub> the interplay between charge density waves, superconductivity and Dirac fermions can be explored. We use low temperature scanning tunneling microscopy and spectroscopy to study the electronic properties of this van der Waals heterostructure. We observe the coexistence of a moiré pattern and charge density wave in the graphene on NbSe<sub>2</sub> heterostructure.

**4:42PM V15.00008 Scanning Tunneling Microscopy Study of Atomic and Electronic Structures of PbTaSe<sub>2</sub>**, TIEN-MING CHUANG, Institute of Physics, Academia Sinica, Taipei 11529, Taiwan, SYU-YOU GUAN, Institute of Physics, National Taiwan University, Taipei 10617, Taiwan, PENG-JEN CHEN, Department of Physics, National Tsing Hua University, Hsinchu 30013, Taiwan, TAY-RONG CHANG, Department of Physics, Princeton University, Princeton, NJ 08544, USA, RAMAN SANKAR, FANG-CHENG CHOU, Center for Condensed Matter Sciences, National Taiwan University, Taipei 10617, Taiwan, HORNG-TAY JENG, Department of Physics, National Tsing Hua University, Hsinchu 30013, Taiwan, CHIA-SENG CHANG, Institute of Physics, Academia Sinica, Taipei 11529, Taiwan — The non-centrosymmetric PbTaSe<sub>2</sub> becomes superconducting at  $T_c = 3.7\text{K}$  and is proposed to have a 3D massive Dirac fermions by large spin orbital coupling. The observation of topological nodal line states has been reported by recent ARPES measurements, making this material a great candidate to investigate the coupling between topological states and superconductivity. Here we conduct detail studies on cleaved PbTaSe<sub>2</sub> surfaces by spectroscopic imaging-scanning tunneling microscope. Our results reveal several types of cleaved surfaces, within which each exhibits distinct different LDOS from scanning tunneling spectroscopy measurements. We identify different surface terminations from their atomic structures and their corresponding electronic properties both above and below  $T_c$ . We will report the impact on superconducting properties of different surfaces, and also discuss the relation between the surface state and superconductivity.

**4:54PM V15.00009 Zone-center phonons of bulk, few-layer, and monolayer 1T-TaS<sub>2</sub>: Application to Raman scattering<sup>1</sup>**, OLIVER R ALBERTINI, Georgetown University, RUI ZHAO, Pennsylvania State University, REBECCA L MCCANN, Georgetown University, SIMIN FENG, MAURICIO TERRONES, Pennsylvania State University, JAMES K FREERICKS, Georgetown University, JOSHUA A ROBINSON, Pennsylvania State University, AMY Y LIU, Georgetown University — The transition metal dichalcogenide 1T-TaS<sub>2</sub> has attracted attention for decades due to its multiple charge density wave phases. More recently it is being considered as a 2D device material, due to the wide range of electrical conductivities in these phases. The metal-insulator transition that occurs when the commensurate charge density wave forms is particularly attractive. We present first-principles calculations of the vibrational properties of 1T-TaS<sub>2</sub> for various thicknesses in the high-temperature (undistorted) phase and the low-temperature commensurate charge density wave phase. We also present measurements of the Raman frequencies for bulk and few-layer samples in the low-T phase. We find strong evidence for the low-T commensurate charge density wave state remaining stable as the crystal is thinned, even down to one layer. We explore the effects of substrate-induced strain on the vibrational spectrum and propose polarized Raman spectroscopy as a method for quickly identifying the c-axis orbital texture in the low-T phase. This orbital texture has recently been identified as playing a role in the metal-insulator transition.

<sup>1</sup>NSF Grants DMR-1358978 & EFRI-143307

**5:06PM V15.00010 Structural, electronic and vibrational properties of few-layer 2H- and 1T-TaSe<sub>2</sub><sup>1</sup>**, JIA-AN YAN, MACK DELA CRUZ, Department of Physics, Astronomy and Geosciences, Towson University, BRANDON COOK, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN, 37831 USA, KALMAN VARGA, Department of Physics and Astronomy, Vanderbilt University, Nashville, Tennessee 37235, USA — Two-dimensional metallic transition metal dichalcogenides (TMDs) are of interest for studying phenomena such as charge-density wave (CDW) and superconductivity. Few-layer tantalum diselenides (TaSe<sub>2</sub>) are typical metallic TMDs exhibiting rich CDW phase transitions. However, a description of the structural, electronic and vibrational properties for different crystal phases and stacking configurations, essential for interpretation of experiments, is lacking. We present first-principles calculations of structural phase energetics, band dispersion near the Fermi level, phonon properties and vibrational modes at the Brillouin zone center for different layer numbers, crystal phases and stacking geometries. Evolution of the Fermi surfaces as well as the phonon dispersions as a function of layer number reveals dramatic dimensionality effects in this CDW material. Our results indicate strong electronic interlayer coupling, detail energetically possible stacking geometries, and provide a basis for interpretation of Raman spectra.

<sup>1</sup>This work is supported by the FCSM Undergraduate Research Committee, the Faculty Development and Research Committee grant (OSPR No. 140269) and the FCSM Fisher General Endowment at the Towson University.

**5:18PM V15.00011 Memristive phase switching in two-dimensional 1T-TaS<sub>2</sub> crystals**, MASARO YOSHIDA, TAKASHI GOKUDEN, RYUJI SUZUKI, YIJIN ZHANG, MASAKI NAKANO, YOSHIHIRO IWASA, Department of Applied Physics, The University of Tokyo — Among 2D materials with correlated electrons, 1T-TaS<sub>2</sub> is one of the most attracting systems with charge density wave (CDW) phases [1]. In this presentation, we report an electrical switching between various non-volatile metastable electronic phases in 1T-TaS<sub>2</sub> thin flakes. By applying a high lateral electric field, we realized multiple metastable states, where the system shows truly metallic behavior. The emergence of novel ground states, possibly stabilized by the slow kinetics due to the reduced dimensionality [2], reflects the electronic complexity in 2D materials with nanometer thickness. [1] M. Yoshida et al. Sci. Rep. 4, 7302 (2014); [2] M. Yoshida et al. Sci. Adv. 1, e1500606 (2015).

## **Thursday, March 17, 2016 2:30PM - 5:30PM – Session V16 DCMP DMP: Optical Studies of Transition Metal Dichalcogenides 315 -**

**2:30PM V16.00001 All-Optical Materials Design of Dissipationless Chiral Edge Modes in Transition-Metal Dichalcogenides**, MARTIN CLAASSEN, Department of Applied Physics, Stanford University, CHUNJING JIA, BRIAN MORITZ, THOMAS DEVEREAUX, Stanford Institute for Materials and Energy Sciences, SLAC & Stanford University — Spurred by the recent progress in transient melting, enhancement and induction of electronic order, a particularly tantalizing prospect concerns the possibility to instead access dynamical steady states with distinct non-equilibrium phase transitions, to affect electronic transport. Here, we show that the interplay of crystal symmetry and optical pumping of monolayer transition-metal dichalcogenides (TMDCs) provides a novel avenue to engineer topologically-protected chiral edge modes, facilitating optically-switchable conduction channels that are insensitive to disorder. Intriguingly, while TMDCs are canonically described as condensed-matter realizations of massive relativistic fermions, here we predict from first principles that circularly-polarized pumping instead accesses the intrinsic three-band nature near the band edges to selectively photo-induce topological band inversions at low pump intensities, while simultaneously limiting absorption for sub-gap pump frequencies. The results presented provide a new strategy to predict and design topological materials out of equilibrium, and should be readily applicable to other classes of semiconductors.

**2:42PM V16.00002 Magnetic brightening of dark excitons in transitional metal dichalcogenides**, XIAO-XIAO ZHANG, Columbia University, ZHENG GUANG LU, National High Magnetic Field Laboratory, TING CAO, University of California, Berkeley, FAN ZHANG, JAMES HONE, Columbia University, STEVEN G. LOUIE, University of California, Berkeley, ZHIQIANG LI, DMITRY SMIRNOV, National High Magnetic Field Laboratory, TONY HEINZ, Stanford University — Transitional metal dichalcogenides (TMDC) in the MX<sub>2</sub> (M = Mo, W, X = S, Se) family represent an excellent platform to study of excitonic effects. At monolayer thickness, these materials exhibit both direct band-gap character and enhanced excitonic interactions. Theoretical studies suggest that both the valence and conduction bands are split and exhibit spin polarized character at the K/K' valleys. The lowest energy band-edge excitons are predicted to have different spin configurations for different materials in this family. When the lowest lying exciton has parallel electron and hole spin, radiative decay is forbidden and the state is dark. Here we demonstrate that by applying an in-plane magnetic field we can perturb the exciton spin configuration and brighten this state, allowing it to undergo radiative decay. We identify such a brightened dark state by the emergence of a new emission peak lying below the absorption peak, with a strength growing with applied in-plane magnetic field. On the other hand, for monolayer MoSe<sub>2</sub>, where no low-lying dark state is expected, we do not see the growth of a new emission feature under application of an in-plane magnetic field. Our experimental findings are in agreement with the calculated properties of dark excitons based on GW plus Bethe-Salpeter equation approach

**2:54PM V16.00003 Studies of low temperature photoluminescence spectra and excitonic valley polarization in monolayer MoTe<sub>2</sub>**, SANDHAYA KOIRALA, SHINICHIRO MOURI, YUHEI MIYAUCHI, KAZUNARI MATSUDA, Kyoto Univ - Uji Campus, KYOTO UNIVERSITY TEAM — Recently, atomically thin layered transition-metal dichalcogenide (TMDs) in the form MX<sub>2</sub> (M = Mo, W, X = S, Se, Te) have attracted much interest from the viewpoints of their fundamental physics and potential applications [1, 2]. The characteristic optical features of semiconducting TMDs arise from excitons confined in their atomically thin layers. Molybdenum ditelluride MoTe<sub>2</sub> has attracted emerging research interest because of optical gap energy (lowest exciton transition) of 1.09 eV, and large spin-orbit coupling of 250 meV. Temperature-dependent photoluminescence (PL) and polarization-resolved PL measurement were performed for mechanically exfoliated monolayer MoTe<sub>2</sub> from 4.4 to 300 K. At a low temperature, the PL spectra from MoTe<sub>2</sub> show two sharp peaks for excitons and charged excitons (trions). The systematic temperature-dependent PL measurements reveal that the homogeneous linewidth of the exciton peak broadens linearly as the temperature increased due to exciton-acoustic-phonon interactions [3]. From polarization-resolved PL measurements, the valley polarization of above 40 % in the exciton state has been observed at low temperatures. In this meeting, we will discuss about exciton dephasing and valley polarization in monolayer MoTe<sub>2</sub>. [1] D. Kozawa, K. Matsuda, G. Eda et al., Nat. Commun. 5, 4543 (2014). [2] S. Mouri, Y. Miyauchi and K. Matsuda, Nano Lett. 15, 2336 (2015). [3] S. Koirala, K. Matsuda et al., submitted for publication.

**3:06PM V16.00004 Observation and Characterization of Biexciton States in high-quality Monolayer WS<sub>2</sub>**<sup>1</sup>, MITSUHIRO OKADA, Nagoya Univ, YUHEI MIYAUCHI, Kyoto Univ, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, KAZUNARI MATSUDA, Kyoto Univ, HISANORI SHINOHARA, RYO KITaura, Nagoya Univ — Group-VI transition metal dichalcogenides (TMDCs) have attracted a great deal of attention due to the optical properties dominated by excitonic effects, where emissions in PL arise from excitons and trions are seen even in room temperature (RT). In recent studies on PL emissions from WS<sub>2</sub>, one of TMDCs has shown that even biexcitons can be observed at 4 K with high-power excitation of 50,000 W/cm<sup>2</sup>. In this work, we report the observation of biexciton states at temperature higher than 80 K with excitation power lower than 25 W/cm<sup>2</sup>, by using a high-quality monolayer WS<sub>2</sub> grown directly onto the hBN. PL spectra of the WS<sub>2</sub>/hBN measured at RT show a very sharp excitonic PL emission with a FWHM of 21.5 meV, and at 82.7 K the PL spectra show three additional peaks at the lower energy site. The excitation power dependence and the lifetime measurement of PL peak at 2.00 eV clearly show that this PL peak can be attributed to biexcitons, which has been observed with a low excitation power down to 24 W/cm<sup>2</sup>. We think that the minimal amount of trapping sites in high-quality WS<sub>2</sub>/hBN used is a key factor in the observation of biexcitons at over 80 K and a low excitation power.

<sup>1</sup>This work was supported by Scientific Research on Innovative Areas (No. 25107002) from MEXT, Japan and Leading Graduate School Program, Nagoya University.

**3:18PM V16.00005 High field magneto-spectroscopy of excitons in monolayer WSe<sub>2</sub>**, ZHENG GUANG LU, National High Magnetic Field Laboratory and Florida State University, XIAOXIAO ZHANG, Columbia University, JONATHAN LUDWIG, National High Magnetic Field Laboratory and Florida State University, FAN ZHANG, Columbia University, KOMALAVALLI THIRUNAVUKKUARASU, National High Magnetic Field Laboratory, SEONGPHILL MOON, National High Magnetic Field Laboratory and Florida State University, JAMES HONE, Columbia University, TONY HEINZ, Stanford University, DMITRY SMIRNOV, National High Magnetic Field Laboratory — We have performed circularly polarized photoluminescence (PL) experiments on monolayer WSe<sub>2</sub> in magnetic fields up to 31T and at temperatures between 2K and 45K, focusing on the emission from the neutral (X<sup>0</sup>) and negatively charged (X<sup>-</sup>) excitons. A parallel magnetic field does not affect the exciton energy. At 45K, a perpendicular magnetic field (Faraday geometry) induces linear shift of about 0.12 meV/T ≈ 2μB for both X<sup>0</sup> and X<sup>-</sup> peaks indicating lifting of the valley degeneracy. The magnitude of this valley Zeeman shift agrees with the valence band edge lifting due to atomic orbital contribution. The change of the X<sup>-</sup> PL intensity with the magnetic field suggests that the intravalley configuration is the lower energy state of the trion in WSe<sub>2</sub>. At lower temperatures, the X<sup>0</sup> exhibits the same shift with the magnetic field as at 45K, while the X<sup>-</sup> shows a more pronounced and non-linear shift with respect to magnetic field.

**3:30PM V16.00006 Strong Circularly Polarized Photoluminescence From Multilayer MoS<sub>2</sub> Through Plasma Driven Direct-Gap Transition**, ROHAN DHALL, University of Southern California, KYLE SEYLER, University of Washington, ZHEN LI, University of Southern California, DARSHANA WICKRAMARATNE, MAHESH NEUPANE, UC Riverside, IOANNIS CHATZAKIS, University of Southern California, EWA KOSMOWSKA, XEI Scientific, ROGER LAKE, UC Riverside, XIAODONG XU, University of Washington, STEPHEN CRONIN, University of Southern California — We report circularly polarized photoluminescence spectra taken from few layer MoS<sub>2</sub> after treatment with a remotely generated oxygen plasma. Here, the oxygen plasma decouples the individual layers in MoS<sub>2</sub> by perturbing the weak interlayer van der Waals forces without damaging the lattice structure. This decoupling causes a transition from an indirect to a direct band gap material, which causes a strong enhancement of the photoluminescence intensity. Furthermore, up to 80% circularly polarized photoluminescence is observed after plasma treatment of few layer MoS<sub>2</sub> flakes, consistent with high spin polarization of the optically excited carriers. A strong degree of polarization continues up to room temperature, further indicating that the quality of the crystal does not suffer degradation due to the oxygen plasma exposure. Our results show that the oxygen plasma treatment not only engineers the van der Waals separation in these TMDCs multilayer for enhanced PL quantum yields, but also produces high quality multilayer samples for strong circularly polarized emission, which offers the benefit of layer index as an additional degree of freedom, absent in monolayer MoS<sub>2</sub>.

**3:42PM V16.00007 Nanosecond Valley Polarization in Suspended Monolayer Tungsten Sulfide**, ANDY BARRETTE, CHAO XU, YIFEI YU, YILING YU, LINYOU CAO, KENAN GUNDOGDU, North Carolina State Univ, GUNDOGDU GROUP TEAM, NANOSCALE PHOTOPHYSICS AND PHOTOCHEMISTRY GROUP TEAM — Monolayer transition metal dichalcogenides (TMD) have a vast range of interesting electronic and optical characteristics due to symmetry properties and selection rules. For carriers, these properties result in coupled spin and valley degrees of freedom and coupling between valley polarization circular polarization of excitation source. Because of these unique properties, TMDs are thought to have potential valleytronic applications, however to the detriment of these potential applications, recent optical studies have shown that carriers undergo valley relaxation very quickly, within tens of picoseconds. Using circularly polarized ultrafast transient absorption spectroscopy, we find that valley relaxation in suspended tungsten sulfide (WS<sub>2</sub>) decays on the order of a nanosecond - two orders of magnitude slower than in supported samples. We discuss our results in the context of recent theoretical work which suggests that the predominant valley relaxation mechanism in monolayer TMDs is the electron-hole exchange interaction. Finally, we use valley relaxation measurements at several temperatures to conclude that the remaining nanosecond valley relaxation results from the flexural phonon mechanism.

**3:54PM V16.00008 Imaging Spin Dynamics in Monolayer WS<sub>2</sub> by Time-Resolved Kerr Rotation Microscopy**, ELIZABETH BUSHONG, KELLY (YUNQIU) LUO, The Ohio State University, KATHLEEN MCCREARY, Naval Research Laboratories, MICHAEL NEWBURGER, SIMRANJEET SINGH, The Ohio State University, BEREND JONKER, Naval Research Laboratories, ROLAND KAWAKAMI, The Ohio State University — Monolayer transition metal dichalcogenides (TMDs) such as WS<sub>2</sub> offer a unique platform to probe spin and valley degrees of freedom in two-dimensional condensed matter systems. TMDs are of great interest because they have a direct band gap and optical selection rules that permit the excitation of both valley and spin-polarized electrons. Strong spin-orbit coupling leads to valley-dependent spin-splitting in both the conduction and valence bands, which may suppress spin relaxation and inhibit intervalley scattering, thereby increasing both the spin and valley lifetimes. To measure spin and valley dynamics of CVD grown WS<sub>2</sub>, we developed time-resolved Kerr rotation microscopy with spatial resolution of ~1 micron and temporal resolution of 150 fs. We observe a long spin lifetime of 5.1 ns in WS<sub>2</sub> at T = 6.5 K. We spatially map the spin populations at a given time delay, and observe a complex spatial dependence of the spin lifetimes with regions of spin lifetime less than 100 ps and regions of spin lifetime greater than 5 ns separated by only a few microns. To understand the origin of the long-lived spin states, we investigate the relationship between spin lifetime and the photoluminescence intensity. Application of in-plane magnetic fields shows an oscillatory and non-oscillatory component, indicating two spin populations that experience different effective fields.

**4:06PM V16.00009 Infrared and visible magneto-optical studies of centimeter-scale monolayer MoS<sub>2</sub>**, MUMTAZ MURAT ARIK, ALOK MUKHERJEE, JUNGRYEOL SEO, CHUAN ZHAO, PAYAM TAHERI, BRETT BLIZZARD, HAO ZENG, JOHN CERNE, State Univ of NY - Buffalo — We report extensive magneto-optical measurements on monolayer MoS<sub>2</sub> at temperatures down to 10K and magnetic fields up to 7T. The centimeter-scale monolayer MoS<sub>2</sub> films are grown by the vapor transport method, where a 5 Å-thick pre-deposited MoO<sub>3</sub> film is sulfurized. We measure polarization-sensitive transmission, reflection, photoluminescence, and Kerr response in the infrared and visible range (0.100 – 2.75 eV). We explore the dependence of the optical and electronic properties on the substrate. This work is supported by NSF-DMR1410599 and NSF CBET-1510121.

**4:18PM V16.00010 Exciton and Trion Valley dynamics in WSe<sub>2</sub> measured by two-color pump-probe<sup>1</sup>**, AKSHAY SINGH, KHA TRAN, JOE SEIFERT, YIPING WANG, Univ of Texas, Austin, MARIE SCOTT, university of washington, seattle, DENNIS PLESKOT, NATHANIEL GABOR, University of California, Riverside, JIAQIANG YAN, DAVID MANDRUS, University of Tennessee, Knoxville, XIAODONG XU, university of washington, seattle, XIAOQIN LI, Univ of Texas, Austin — Monolayer transition metal dichalcogenides are semiconducting materials demonstrating spin-valley coupling as well as quasiparticles with large binding energies. These quasiparticles, excitons and trions (charged excitons), have quite different spin polarization properties, with the trion having larger spin lifetimes than excitons. Photoluminescence and time resolved Kerr rotation techniques have been used earlier to measure spin lifetimes. However, most of these early optical measurements have relied on non-resonant excitation conditions which tend to mask the intrinsic valley (spin) scattering properties. Here, we use circularly polarized two-color pump probe spectroscopy to measure valley (spin) polarization in monolayer WSe<sub>2</sub> at low temperatures. We utilize quasi-resonant excitation with pump 1 meV (0.5 nm) spectrally separated from the probe, thus resulting in very efficient valley initialization. We present polarization resolved measurements on resonantly excited excitons and trions, which suggest that trions have larger spin lifetimes. Further, we probe spin polarization of trions when pumping at exciton energies, and vice-versa. We discuss the relative importance of different scattering mechanism at play.

<sup>1</sup>We acknowledge support from ARO and AFOSR

**4:30PM V16.00011 Band edge identification and carrier dynamics of CVD MoS<sub>2</sub> monolayer measured by broadband Femtosecond Transient Absorption Spectroscopy**, SHROUQ ALEITHAN, MAKSYM LIVSHITS, Ohio Univ, JEFFREY RACK, University of New Mexico, MARTIN KORDESCH, ERIC STINAFF, Ohio Univ — Two-dimensional atomic crystals of transition metal dichalcogenides are considered promising candidates for optoelectronics, valleytronics, and energy harvesting devices. These materials exhibit excitonic features with high binding energy as a result of confinement effect and reduced screening when the material is thinned to monolayer. However, previous theoretical and experimental studies report different binding energy results. This work further examines the electronic structure and binding energy in this material using broadband Femtosecond Transient Absorption Spectroscopy. Samples of MoS<sub>2</sub> were grown by chemical vapor deposition, pumped with femtosecond laser, and probed by femtosecond white light resulting in broadband differential absorption spectra with three distinct features related to the three dominant absorption peaks in the material: A, B, and C. The dependence of the transient absorption spectra on excitation wavelength and layer number provides evidence of a band gap located at C (2.9 eV) and therefore an excitonic binding energy of 1 eV. Additional features in the spectra identified as a broadening of the absorption features caused by carrier scattering, surface defects and trap states.

**4:42PM V16.00012 Ultrafast spectroscopy of exciton and exciton dynamics in mono and few layers of WS<sub>2</sub>**, SUDIKSHA KHADKA, SHROUQ ALEITHAN, MAX LIVSHITS, JEFFREY J. RACK, MARTIN KORDESCH, ERIC STINAFF, Ohio University — Single layer of Transitional metal dichalcogenides (MX<sub>2</sub>) are 2D semiconductors that have a direct band gap in visible spectrum and fill the gap in between 2D metallic and insulating materials. They have possible application in optoelectronic devices, photovoltaics and photodetection, molecular sensing, 'valleytronics', and flexible transparent electronics. Tungsten Disulphide (WS<sub>2</sub>), one of the member of MX<sub>2</sub> family, has a direct band gap of 2.2 eV and a large valley splitting of about 0.4 eV. Here, we present a detailed study of exciton states and their decay mechanisms in mono and few layer WS<sub>2</sub> using femto-second transient absorption spectroscopy. We report a new peak at 3.010.1 eV whose origin in k space is believed to be at or around K point and further investigation is underway. The exponential fitting of decay curve of the exciton A reveals three time components as 1.70.3 ps, 33.510 ps and 67015 ps, most likely corresponding to carrier-carrier scattering, carrier-phonon scattering, and radiative relaxation respectively.

**4:54PM V16.00013 Tunable second harmonic generation of monolayer MoS<sub>2</sub> by Se doping<sup>1</sup>**, C. T. LE, Univ of Ulsan, D. J. CLARK, Binghamton University, V. SENTHILKUMAR, Univ of Ulsan, J. I. JANG, Binghamton University, H.-Y. CHO, Y. S. KIM, Univ of Ulsan, BINGHAMTON UNIVERSITY COLLABORATION — As a transition metal dichalcogenides whose bandgap becomes direct with inversion symmetry breaking in the monolayer limit, MoS<sub>2</sub> has been getting ample attention as next-generation nonlinear optic material for its strong optical nonlinear properties. In this study, we demonstrate the wavelength second harmonic generation tunability of monolayer Mo(S, Se)<sub>2</sub>. Employing the two-zone furnaces system, we selenized as-grown monolayer MoS<sub>2</sub> at different temperature. X-ray photoluminescence spectroscopy was used to confirm the chemical composition of selenized film. Photoluminescence spectra shows the red shift in optical bandgap from 1.83 to 1.53 eV as a function of concentration Se replacing S. Second harmonic generation characteristics were measured in reflection geometry using ps pulse from Nd:YAG laser. Applying the previous bulk model, we calculated that the maximum value of  $\chi^{(2)}$  varied from ~40 pm/V for pure MoS<sub>2</sub> to ~100 pm/V for pure MoSe<sub>2</sub>. We believe that our findings along with the ability to stack different 2D materials will create stacked 2D heterostructure with high  $\chi^{(2)}$  over a wide range of wavelength from visible to NIR.

<sup>1</sup>This research was supported by Priority Research Centers Program (2009-0093818), the Basic Science Research Program (2015-019609), and Basic Research Lab Program (2014-071686) through the National Research Foundation of Korea (NRF), funded by the Korean g

**5:06PM V16.00014 Optical coherence in atomic monolayer transition metal dichalcogenides limited by electron-phonon interactions<sup>1</sup>**, PRASENJIT DEY, JAGANNATH PAUL, University of South Florida, ZEFANG WANG, Pennsylvania State University, CHRISTOPHER STEVENS, CUNMING LIU, University of South Florida, ALDO ROMERO, West Virginia University, JIE SHAN, Pennsylvania State University, DAVID HILTON, University of Alabama Birmingham, DENIS KARAIKAJ, University of South Florida, ALDO ROMERO COLLABORATION, ZEFANG WANG, JIE SHAN COLLABORATION, DAVID HILTON COLLABORATION — We systematically investigate the excitonic dephasing of three representative transition metal dichalcogenides, namely MoS<sub>2</sub>, MoSe<sub>2</sub> and WSe<sub>2</sub> atomic monolayer thick and bulk crystals, in order to gain proper understanding of the factors that determine the optical coherence in these materials. Coherent nonlinear optical spectroscopy, temperature dependent absorption combined with 'ab initio' theoretical calculations of the phonon spectra, indicate electron-phonon interactions to be the limiting factor.

<sup>1</sup>The research at USF, Penn. State, and UAB is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-SC0012635.

**5:18PM V16.00015 The Eigenstate Thermalization Hypothesis in 1D Anyon Chains**, FIONA BURNELL, University of Minnesota, ANUSHYA CHANDRAN, Perimeter Institute, MARC SCHULZ, University of Minnesota — For ergodic systems with Hilbert spaces satisfying a local product structure, the eigenstate thermalization hypothesis (ETH) is relatively well-established. Using exact diagonalization studies, we investigate whether quantum spin chains based on SU(2)<sub>k</sub> anyon theories, which do not admit a Hilbert space with an exactly local product structure, also satisfy ETH, and which observables exhibit this behaviour.

**Thursday, March 17, 2016 2:30PM - 5:30PM –**  
**Session V17 DMP: 2D Devices: Spin Transport, Spin Orbit Coupling** 316 - Xia Hong, University of Nebraska-Lincoln

**2:30PM V17.00001 Optimizing Spin Generation in 2D Materials: Topological Insulators and Graphene**, CHING-TZU CHEN, IBM Thomas J Watson Research Center — Novel two-dimensional electronic systems with Dirac-like dispersion present unique opportunities for spintronic applications. In this seminar I will discuss two specific examples. First we examine the potential of topological insulators as spin-source materials. Using a new spin-polarized tunneling method [1], giant charge-spin conversion efficiency in topological insulators is revealed, well exceeding that in conventional magnetic tunnel junctions.[2] Through a comparative study between Bi<sub>2</sub>Se<sub>3</sub> and (Bi,Sb)<sub>2</sub>Te<sub>3</sub>, we verify the topological-surface-state origin of the observed giant spin signals and further extract the energy dependence of the effective spin polarization in Bi<sub>2</sub>Se<sub>3</sub>. [2] Next we explore the potential of interfacial exchange interaction in 2D materials for spin control and spin generation. Using graphene as a prototype, we demonstrate that its coupling to a model magnetic insulator (EuS) produces a substantial magnetic exchange field ( $>14$  T), which yields orders-of-magnitude enhancement in the spin signal originated from the Zeeman spin-Hall effect.[3] Furthermore, the strong exchange field lifts the spin degeneracy of graphene in the quantum Hall regime, which may lead to interesting spin-polarized edge transport and thus open up new application space for classical and quantum information processing. [1] Luqiao Liu, Ching-Tzu Chen, J. Z. Sun, Nature Physics 10, 561–566 (2014). [2] Luqiao Liu, A. Richardella, Ion Garate, Yu Zhu, N. Samarth, and Ching-Tzu Chen, Physical Review B 91, 235437 (2015). [3] Peng Wei, Sunwoo Lee, Florian Lemaire, Lucas Pinel, Davide Cutaia, Wujoon Cha, Donald Heiman, James Hone, Jagadeesh S. Moodera, Ching-Tzu Chen, Giant Interfacial Exchange Field in a 2D Material/Magnetic-Insulator Heterostructure: Graphene/EuS, arXiv:1510.05920.

**3:06PM V17.00002 A theoretical design of graphene-based spin field-effect transistors**, LIXUE LIU, University of Science and Technology of China, SHUDUN LIU, University of Louisville, WENGUANG ZHU, University of Science and Technology of China — The search for a feasible design of graphene-based materials for spintronics applications has been intensified in recent years. Encouraged by recent experimental achievements, here we propose a new scheme to realize graphene-based spin field-effect transistors. The new design is constituted of a half-hydrogenated graphene nanoroad embedded in a fully-hydrogenated graphene. Using first-principles density function theory calculations, we demonstrate that such a design can convert non-magnetic pristine graphene into a bipolar ferromagnetic semiconductor. More importantly, the magnetism of such a nanoroad is very robust: independent of its width and orientation. We also discuss the stability of such nanoroads, as well as a simple design of an all-electric controlled device for generation and detection of a fully spin-polarized electric current.

**3:18PM V17.00003 Giant Rashba spin splitting in Bi bilayer induced by a 2D ferroelectric substrate**, JIANBAO ZHU, University of Science and Technology of China, DI XIAO, Carnegie Mellon University, WENGUANG ZHU, University of Science and Technology of China — Based on density functional theory calculations, we discover that a Bi layer when placed on the top of a recently predicted 2D ferroelectric material with spontaneous out-of-plane electric polarization can exhibit giant Rashba-type spin splitting of over 200 meV, while the whole system still remains semiconducting. In addition, the magnitude of the Rashba spin splitting can be tuned by switching the dipole orientation of the 2D ferroelectric substrate. This finding provides a promising 2D material system for spintronics.

**3:30PM V17.00004 Spin-orbit interactions in two-dimensional holes in quasi-triangular wells: variational calculations**, ELIZABETH MARCELLINA, ALEX HAMILTON, The University of New South Wales, ROLAND WINKLER, Northern Illinois University, DIMITRIE CULCER, The University of New South Wales, UNSW COLLABORATION, NIU COLLABORATION — Spin-orbit (SO) interactions in semiconductors are key to the realization of semiconductor spintronic devices and quantum information processing. Low-dimensional holes are strongly SO-coupled systems, as such, they offer the promise of all-electrical spin control which can lead to more efficient electronic devices. However the spin properties of holes are highly complex, and heavily influenced by the nature of the confining potential. So far, calculations on two-dimensional holes in semiconductor heterojunctions have mostly been numerical and material-specific. In this work, we develop variational-based methods, which are easy to use and applicable to various materials, to quantify SO interactions in two-dimensional holes confined in self-consistent quasi-triangular wells. In particular, we calculate the SO hole spin-splittings and effective masses in common semiconductor materials such as GaAs, Ge, InSb, InAs, and Si. Our results show that the strength of SO interactions is very sensitive to the material type and that in zincblende materials with a bulk inversion asymmetry (BIA), the dominant contribution to the SO interaction is still the structure inversion asymmetry (SIA) term corresponding to the confinement potential.

**3:42PM V17.00005 Kondo physics in the presence of Rashba spin-orbit interactions**, ARTURO WONG, CNYN, UNAM, Mexico, SERGIO ULLOA, NANCY SANDLER, Ohio University, KEVIN INGERSANT, University of Florida — Recent theoretical studies have shown that Rashba spin-orbit interactions in a two-dimensional electron gas (2DEG) affect the thermodynamics of the impurity Kondo effect only through changes in the host density of states [1]. These changes are generally modest [1], but yield exponential enhancement of the Kondo temperature  $T_K$  [2] if the 2DEG can be tuned to a helical regime in which all electrons at the Fermi surface have the same relation between the directions of their spin and momentum. It has been proposed to access the helical regime using irradiation with circularly polarized light, giving rise to an effective Zeeman splitting of the conduction band without any direct splitting of the impurity level. We show that under this scenario, the impurity contribution to the system's net angular momentum is a universal function of the Zeeman energy divided by a temperature scale that (surprisingly at first sight) is not  $T_K$ , but rather is proportional to  $T_K$  divided by the impurity hybridization width. This universal scaling can be understood via a perturbative treatment of irradiation-induced changes in the electron densities of states. [1] R. Zitko and J. Bonca, Phys. Rev. B 84, 193411 (2011). [2] A. Wong, S. E. Ulloa, N. Sandler, and K. Ingersent, arXiv:1509.08433.

**3:54PM V17.00006 Measurement of Spin Torques in WTe<sub>2</sub>/Ferromagnet Bilayers**, DAVID MACNEILL, GREGORY M. STIEHL, MARCOS H. D. GUIMARÃES, JIWOONG PARK, DANIEL C. RALPH, Cornell University — WTe<sub>2</sub> is a semimetallic transition metal dichalcogenide (TMD) stable in the  $T_d$  crystal structure. The strong spin-orbit coupling, metallic conduction, and crystalline layered structure of the material make it interesting for both fundamental and applied spintronics research, but measurements of the spin transport properties (e.g., the spin Hall conductivity) are lacking. Here we report measurements of current induced spin torques in WTe<sub>2</sub>/Ferromagnet bilayers, detected using spin torque ferromagnetic resonance. We will attempt to distinguish whether these torques arise from interfacial spin-orbit coupling or the spin Hall effect in the TMD. We study these torques as a function of TMD layer number, from bulk to few-layer, and correlate our results with layer-number dependent charge transport measurements.

**4:06PM V17.00007 Spin relaxation in hole-doped transition metal dichalcogenides with the crystal defects**, TETSURO HABE, MIKITO KOSHINO, Tohoku University — We theoretically investigate the electronic spin relaxation effect in the hole-doped monolayer and bilayer transition-metal dichalcogenides in the presence of the crystal defects. We simulate lattice vacancies in the multi-orbital tight-binding model obtained by the first-principle method and actually estimate the spin relaxation rate by using the tight-binding model. In the monolayer, the spin-relaxation time is found to be much longer than the momentum relaxation time, and this is attributed to the fact that the spin hybridization in the band structure is suppressed by the mirror reflection symmetry. The bilayer TMD has a much shorter spin relaxation time in contrast because of the stronger spin hybridization due to the absence of the mirror symmetry.

**4:18PM V17.00008 Induced spin orbit coupling in graphene by proximity to transition metal dichalcogenides monolayer<sup>1</sup>**, ABDULRHMAN ALSHARARI, SERGIO ULLOA, Ohio Univ, MAHMOUD ASMAR, Louisiana State University — Proximity effects resulting from depositing a graphene layer on a substrate may induce spin depend interactions that change the topological properties of graphene. A suitable candidate to study this effect is a transition metal dichalcogenides substrate. A 2D layer of these materials has a large SOC that in turn induces a sizable effect near the graphene Dirac points. Graphene and 2D TMDs are nearly commensurate lattices, producing an interesting moiré pattern when adhered to one another. We study theoretically the electronic structure of graphene-TMD systems using a tight binding formalism. We find that graphene exhibits a strong proximity SOC, in addition to other perturbations that strongly affect the states; the linear dispersion near the neutrality point becomes gapped. Based on symmetries allowed by the heterostructure, we find the effective Hamiltonian to describe the low energy states. We find that diagonal SOC and staggered potential terms characterize the wave functions, akin to the structure in TMDs. A relative voltage between the layers enhances the proximity SOC in graphene, providing a tunable effect that may impact the optoelectronic properties of the system.

<sup>1</sup>This work supported by NSF and SACM

**4:30PM V17.00009 Electronic transport in the quantum spin Hall state due to the presence of adatoms in graphene<sup>1</sup>**, LEANDRO LIMA, CAIO LEWENKOPF, Federal Fluminense University — Heavy adatoms, even at low concentrations, are predicted to turn a graphene sheet into a topological insulator with substantial gap. The adatoms mediate the spin-orbit coupling that is fundamental to the quantum spin Hall effect. The adatoms act as local spin-orbit scatterer inducing hopping processes between distant carbon atoms giving origin to transverse spin currents. Although there are effective models that describe spectral properties of such systems with great detail, quantitative theoretical work for the transport counterpart is still lacking. We developed a multiprobe recursive Green's function technique with spin resolution to analyze the transport properties for large geometries. We use an effective tight-binding Hamiltonian to describe the problem of adatoms randomly placed at the center of the honeycomb hexagons, which is the case for most transition metals. Our choice of current and voltage probes is favorable to experiments since it filters the contribution of only one spin orientation, leading to a quantized spin Hall conductance of  $e^2/h$ . We also discuss the electronic propagation in the system by imaging the local density of states and the electronic current densities.

<sup>1</sup>The authors acknowledge the Brazilian agencies CNPq, CAPES, FAPERJ and INCT de Nanoestruturas de Carbono for financial support

**4:42PM V17.00010 Current-Controlled Spin Flip in Magnetically-Substituted Graphene Nanoribbons: Toward the Realization of Graphene-Based Spintronic Devices<sup>1</sup>**, J.T. HARALDSEN, Department of Physics, University of North Florida, G. HOUCINS, C.B. CROOK, Department of Physics and Astronomy, James Madison University, JIAN-XIN ZHU, Theoretical Division and Center for Integrated Nanotechnologies, Los Alamos National Laboratory, A.V. BALATSKY, Institute for Materials Science, Los Alamos National Laboratory — We examine the possibility of using graphene nanoribbons with directly substituted chromium atoms as spintronic device. Using density functional theory, we simulate a voltage bias across a constructed graphene nanoribbon in a device setup, where a magnetic dimer has been substituted into the lattice. Using a first principles approach, we calculate the electronic and magnetic properties as a function of Hubbard U, voltage, and magnetic configuration. Through a calculation of the energy of each magnetic configuration, we can determine that initial antiferromagnetic ground state flips to a ferromagnetic state with applied bias. Mapping this transition point to the calculated conductance for the system reveals that there is a distinct change in conductance through the graphene nanoribbon, which indicates the possibility of a spin valve. We also show that this corresponds to a distinct change in the induced magnetization within the graphene. Our goal is to show that graphene, while already being used in electronic, may also have spintronic capabilities as well.

<sup>1</sup>JTH, CBC, GH, and AVB acknowledge support from the Institute for Materials Science via the United States Basic Energy Sciences (E304)

**4:54PM V17.00011 The spin orbit coupling and magnetization in graphene/YIG and WTe<sub>2</sub>/graphene/YIG<sup>1</sup>**, MASATOSHI ONOUE, RUQIAN WU, Univ of California - Irvine, BOWEN YANG, JING SHI, Univ of California - Riverside — Quantum anomalous Hall effect (QAHE) may occur in graphene if there are both exchange field and Rashba spin-orbit coupling (SOC). Since pristine graphene is not magnetic and has extremely weak SOC, these two ingredients need to be induced externally through the proximity effect or electric field. Recently experiment found the anomalous Hall effect in graphene when it is supported on yttrium-iron-garnet (YIG), indicating the proximity-induced spin polarization in graphene. However QAHE has not been observed due to small Rashba SOC. In this work, we explore the means that may lead to strong enhancement of Rashba SOC, through first-principles calculations for graphene/YIG and WTe<sub>2</sub>/graphene/YIG. We find that the Rashba SOC strength is only 1.1 meV for graphene on YIG, whereas the exchange splitting is sizeable, 15 meV. The coverage of a WTe<sub>2</sub> layer on graphene/YIG enhances the Rashba SOC but lowers the magnetization. The presence of electric field may offer a balance between these two quantities and the physical origins will be discussed.

<sup>1</sup>The work was supported by DOE-BES (UCI: Grant No. DE-FG02-05ER46237; UCR: DE-FG02-07ER4635) and by NERSC for computing time.

**5:06PM V17.00012 ABSTRACT WITHDRAWN —**

**5:18PM V17.00013 Measurement of current-generated torques in transition metal dichalcogenide / ferromagnet bilayers**, GREGORY M. STIEHL, DAVID MACNEILL, MARCOS H. D. GUIMARÃES, HUI GAO, JIWOONG PARK, DANIEL C. RALPH, Cornell University — We present measurements of current-generated torques in ferromagnet / transition metal dichalcogenide (TMD) bilayers for a wide range of semi-conducting TMDs, including MoS<sub>2</sub>, MoSe<sub>2</sub>, WS<sub>2</sub> and WSe<sub>2</sub>. TMDs present a unique opportunity to study interfacial spin-orbit torques at the two dimensional limit due to a wide range in material properties and large spin-orbit coupling. Thin TMD films are either grown by chemical vapor deposition or exfoliated from readily available TMD crystals and are incorporated into ferromagnet / TMD bilayers by either evaporation or off-axis sputtering of the ferromagnet to avoid damage to the TMD surface. Measurements of the current-generated torque are made by spin transfer ferromagnetic resonance and the magneto-optical Kerr effect. Dependence on layer number, spin-orbit coupling strength, mobility and gate dependence will be explored.

**Thursday, March 17, 2016 2:30PM - 5:30PM —**

**Session V18 GMAG DMP: Skyrmion Dynamics and Motion** 317 - Vincent Cros, Unite Mixte de Physique CNRS/Thales

**2:30PM V18.00001 Room-temperature creation and spin-orbit torque-induced manipulation of skyrmions in thin film**, GUOQIANG YU, PRAMEY UPADHYAYA, XIANG LI, WENYUAN LI, Electrical Engineering, UCLA, SE KWON K IM, Physics and Astronomy, UCLA, YABIN FAN, KIN L. WONG, Electrical Engineering, UCLA, YAROSLAV TSEKOVNYAK, Physics and Astronomy, UCLA, PEDRAM KHALILI AMIRI, KANG L. WANG, Electrical Engineering, UCLA — Magnetic skyrmions, which are topologically protected spin texture, are promising candidates for ultra-low energy and ultra-high density magnetic data storage and computing applications<sup>1, 2</sup>. To date, most experiments on skyrmions have been carried out at low temperatures. The choice of materials available is limited and there is a lack of electrical means to control of skyrmions. Here, we experimentally demonstrate a method for creating skyrmion bubbles phase in the ferromagnetic thin film at room temperature. We further demonstrate that the created skyrmion bubbles can be manipulated by electric current. This room-temperature creation and manipulation of skyrmion in thin film is of particular interest for applications, being suitable for room-temperature operation and compatible with existing semiconductor manufacturing tools. 1. Nagaosa, N., Tokura, Y. *Nature Nanotechnology* 8, 899-911 (2013). 2. Fert, A., *et al.*, *Nature Nanotechnology* 8, 152-156 (2013).

**2:42PM V18.00002 Spin Torque induced anti-vortex excitations**, KANAN OZBOZDUMAN, VEDAT KARAKAS, SEVDENUR ARPACI, ALI TAHA HABIBIOGLU, AISHA GOKCE, Bogazici Univ, ANNA GIORDANO, University of Messina, FEDERICA CELEGATO, Institute of Materials for Electronics and Magnetism, PAULA TIBERTO, Istituto Nazionale di Ricerca Metrologica, GIOVANNI FINOCCHIO, University of Messina, GULEN AKTAS, OZHAN OZATAY, Bogazici Univ — Nanodevices that are designed to stimulate the formation of unique magnetic configurations (vortex, anti-vortex, skyrmion etc.) are applicable to spin based technologies, namely, microwave oscillators and magnetic sensors. In this talk, we report the observed dynamic behavior of an anti-vortex, which had not been thoroughly studied due to the complexity in stabilization of the structure, by analyzing its interaction with magnetic field and DC current. Permalloy (Ni<sub>81</sub>Fe<sub>19</sub>) based 2x2μm<sup>2</sup> asteroid geometry devices, consisting of four tangent circles of equal radii, facilitate the nucleation of an anti-vortex pair at the center with the application of an in-plane AC demagnetizing field and an out of plane magnetic saturation field. Magnetic force microscopy (MFM) data shows that an external magnetic field can rearrange the positions of diagonally located anti-vortex pair. Spin torque effect induces an anti-vortex pair circular motion, known as gyration. The resulting RF signal is measured using the anisotropic magneto-resistance effect (AMR) which indicates a ~250-300 mΩ change in the resistance of our samples. This study will help develop our understanding of the anti-vortex, current and magnetic field interactions for practical on-chip microwave oscillator applications.

**2:54PM V18.00003 Observation of spin transfer torques in the transverse magnetic susceptibility of the Skyrmion lattice phase of MnSi**, FELIX RUCKER, CHRISTOPH SCHNARR, ANDREAS BAUER, CHRISTIAN PFLEIDERER, Lehrstuhl für Topologie Korrelierter Systeme, Technische Universität München, Garching, Germany — In the Skyrmion lattice phase of MnSi the observation of sizeable spin transfer torques [1-3] promises easy experimental access to the precise qualitative and quantitative form of the Landau Lifshitz Gilbert equation. We report measurements of the transverse magnetic susceptibility,  $\chi_{\perp}$ , in the skyrmion lattice phase of MnSi. Our measurements show a distinct increase of  $\chi_{\perp}$  with increasing current density around the critical current density  $j_c$ . We further find a sizable dissipative part of  $\chi_{\perp}$  evolving above  $j_c$ . We discuss the broader implications of our experimental findings, which provide, for the first time, a direct link between a thermodynamic property and the effects of spin transfer torques in skyrmion lattices.

[1] F. Jonietz *et al.*, *Science* **330**, 1648 (2010)

[2] T. Schulz *et al.*, *Nat. Phys.* **8**, 301 (2012)

[2] K. Everschor *et al.*, *Phys. Rev. B* **86**, 054432 (2012)

**3:06PM V18.00004 Chiral Skyrmion Hall effect in Antiferromagnets**, MATTHEW DANIELS, RAN CHENG, Carnegie Mellon University, JIANG XIAO, Fudan University, DI XIAO, Carnegie Mellon University — We study the interaction between magnetic skyrmions and spin wave currents in antiferromagnetic (AFM) insulators. Micromagnetic simulations reveal that magnon-skyrmion scattering in AFMs is dependent on the chirality of the spin wave, a degree of freedom unique to easy-axis AFMs. We also find nontrivial dynamical differences between circularly and linearly polarized waves incident upon AFM skyrmions in simulation. We characterize the resulting chiral magnon Hall effect using the O(3) nonlinear sigma model, and we elucidate the corresponding chiral skyrmion Hall effect as arising from certain magnon spin currents.

**3:18PM V18.00005 Ratchet Effects, Negative Mobility, and Phase Locking for Skyrmions on Periodic Substrates**, CHARLES REICHHARDT, DIPANJAN RAY, CYNTHIA OLSON REICHHARDT, Los Alamos National Laboratory — We examine the dynamics of skyrmions interacting with 1D and 2D periodic substrates in the presence of dc and ac drives. We find that the Magnus term strongly affects the skyrmion dynamics and that new kinds of phenomena can occur which are absent for overdamped ac and dc driven particles interacting with similar substrates. We show that it is possible to realize a Magnus induced ratchet for skyrmions interacting with an asymmetric potential, where the application of an ac drive can produce quantized dc motion of the skyrmions even when the ac force is perpendicular to the substrate asymmetry direction. For symmetric substrates it is also possible to achieve a negative mobility effect where the net skyrmion motion runs counter to an applied dc drive. Here, as a function of increasing dc drive, the velocity-force curves show a series of locking phases that have different features from the classic Shapiro steps found in overdamped systems. In the phase locking and ratcheting states, the skyrmions undergo intricate 2D orbits induced by the Magnus term.

**3:30PM V18.00006 FMR study of thin film FeGe skyrmionic material<sup>1</sup>**, VIDYA P. BHALLAMUDI, MICHAEL R. PAGE, JAMES GALLAGHER, CAROLA PURSER, JOSEPH SCHULZE, FENGYUAN YANG, P. CHRIS HAMMEL, Ohio State Univ - Columbus — Magnetic Skyrmions have attracted intense interest due to their novel topological properties and the potential for energy efficient computing. Magnetic dynamics play an important part in enabling some of these functionalities. Understanding these dynamics can shed light on the interplay of the various magnetic interactions that exist in these materials and lead to a rich magnetic phase diagram, including the Skyrmion phase. We have grown phase-pure FeGe epitaxial films on Si (111) and studied them using ferromagnetic resonance (FMR). FeGe has one of the highest recorded skyrmion transition temperatures, close to room temperature, and thin films are known to further stabilize the Skyrmion phase in the magnetic field-temperature space. We have performed cavity-based single frequency FMR from liquid nitrogen to room temperature on 120 nm thick films in both in-plane and out-of-plane geometries. The resulting complex spectra are consistent with those reported in literature for the bulk material and can be understood in terms of a conical model for the magnetism. Variable temperature broadband spectroscopy and measurements on thinner films, to better identify the various magnetic phases and their dynamic behavior, are ongoing and their progress will be discussed.

<sup>1</sup>Funding for this research was provided by the Center for Emergent Materials: an NSF MRSEC under award number DMR-1420451.

**3:42PM V18.00007 Magnetic excitations of the skyrmion host  $\text{Cu}_2\text{OSeO}_3$** , G S TUCKER, Laboratory for Quantum Magnetism, École polytechnique fédérale de Lausanne & Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, J S WHITE, Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, J ROMHÁNYI, Institute for Theoretical Solid State Physics, IFW Dresden, D SZALLER, I KÉZSMÁRKI, Department of Physics, Budapest University of Technology and Economics, B ROESSLI, U STUHR, Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, A MAGREZ, Laboratory for Crystal Growth, École polytechnique fédérale de Lausanne, F GROITL, Laboratory for Quantum Magnetism, École polytechnique fédérale de Lausanne & Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, P BABKEVICH, P HUANG, I ŽIVKOVIĆ, H M RØNNOW, Laboratory for Quantum Magnetism, École polytechnique fédérale de Lausanne — Inelastic neutron scattering (INS) has been used to measure the magnetic excitation spectrum along high-symmetry directions of the first Brillouin zone of the magnetic skyrmion hosting compound  $\text{Cu}_2\text{OSeO}_3$ . The INS data are mostly consistent with the predictions of a recently proposed model for the magnetic excitations in  $\text{Cu}_2\text{OSeO}_3$ , for which best-fit parameters will be reported. As will be shown, differences exist between the model predictions and the experimental findings in the form of two energy scales that likely arise due to neglected anisotropic interactions. Thus highlighting the need for the inclusion of anisotropy in future theoretical works aimed at a full microscopic understanding of the emergence of the skyrmion state in this material.

**3:54PM V18.00008 Staggered magnetization and low-energy magnon dispersion in the multi-ferroic skyrmion host  $\text{Cu}_2\text{OSeO}_3$** <sup>1</sup>, GUY G. MARCUS, BENJAMIN A. TRUMP, JONAS KINDERVATER, Institute for Quantum Matter and Johns Hopkins University, LACY L. JONES, MATTHEW B. STONE, Quantum Condensed Matter Division, Oak Ridge National Laboratories, TYREL M. MCQUEEN, Institute for Quantum Matter and Johns Hopkins University, COLLIN L. BROHOLM, Institute for Quantum Matter, Johns Hopkins University, and Quantum Condensed Matter Division, Oak Ridge National Laboratories — We present neutron diffraction and inelastic scattering of the insulating helimagnet,  $\text{Cu}_2\text{OSeO}_3$  which provide evidence for staggered magnetization and elucidate the associated low-energy magnon spectrum. The modulation wavelength of approximately  $\lambda \approx 50$  nm detected at antiferromagnetic Bragg points is of the same length scale as previously reported for the skyrmion lattice. This superstructure evidences the composite nature of the spin-1 tetrahedra that form the topological magnetic structure of the material. To understand the interplay of ferrimagnetism and long wavelength modulated magnetism, we have performed inelastic neutron scattering on a co-aligned sample of chemical vapor transport grown single crystals. We shall present the low-energy magnon dispersion and infer an effective spin Hamiltonian to account for the long-wavelength, low-energy magnetism of  $\text{Cu}_2\text{OSeO}_3$ .

<sup>1</sup>The work at IQM was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Material Sciences and Engineering, under Grant No. DEFG02-08ER46544. GGM also acknowledges support from the NSF-GRFP Grant No. DGE-1232825.

**4:06PM V18.00009 Neutron scattering study of the field-induced tricritical point in  $\text{MnSi}$** <sup>1</sup>, J. KINDERVATER<sup>2</sup>, A. BAUER, Physik-Department, Technische Universität München, Garching, Germany, M. GARST, Institute for Theoretical Physics, Universität zu Köln, Köln, Germany, M. JANOSCHEK, Los Alamos National Laboratory, Los Alamos, USA, N. MARTIN, S. MÜHLBAUER, W. HÄUSSLER, Heinz Maier-Leibnitz Zentrum, Technische Universität München, Garching Germany, P. BÖNI, C. PFLEIDERER, Physik-Department, Technische Universität München, Garching, Germany — The intermetallic compound  $\text{MnSi}$  attracts great scientific interest due to two unusual phase transitions, namely the transition from the conical phase to a skyrmion lattice in small fields and the transition from the helical to the paramagnetic phase without external magnetic field that was recently identified to be a fluctuation induced first-order transition, i.e. a so called Brazovskii-transition. Recent measurements of the specific heat provide striking evidence for a tricritical point (TCP), were the first order transition alters to second order. We report neutron spin echo measurements using the MIEZE technique. The recorded quasi elastic linewidth shows a change of the characteristic spin fluctuations at the TCP. The combination with additional SANS measurements and a generalized Brazovskii theory establishes a consistent picture of the statics and dynamics of the transition.

<sup>1</sup>Financial support by ERC-AdG (291079 TOPFIT) and through DFG TRR80 is greatly acknowledged.

<sup>2</sup>Institute for Quantum Matter and Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, USA

**4:18PM V18.00010 Controlling and imaging chiral spin textures**, GONG CHEN, Lawrence Berkeley National Laboratory — Chirality in magnetic materials is fundamentally interesting and holds potential for logic and memory applications [1,2,3]. Using spin-polarized low-energy electron microscopy at National Center for Electron Microscopy, we recently observed chiral domain walls in thin films [4,5]. We developed ways to tailor the Dzyaloshinskii-Moriya interaction, which drives the chirality, by interface engineering [6] and by forming ternary superlattices [7]. We find that spin-textures can be switched between left-handed, right-handed, cycloidal, helical and mixed domain wall structures by controlling uniaxial strain in magnetic films [8]. We also demonstrate an experimental approach to stabilize skyrmions in magnetic multilayers without external magnetic field [9]. These results exemplify the rich physics of chirality associated with interfaces of magnetic materials. [1] A. Fert et al. *Nat. Nanotechnol.* **8**, 152 (2013). [2] N. Nagaosa et al. *Nat. Nanotechnol.* **8**, 899 (2013). [3] W. Jiang et al. *Science* **349**, 283 (2015). [4] G. Chen, et al. *Phys. Rev. Lett.* **110**, 177204 (2013). [5] G. Chen, et al. *Adv. Mater.* **27**, 5738 (2015). [6] G. Chen, et al. *Nat. Commun.* **4**, 2671 (2013). [7] G. Chen, et al. *Appl. Phys. Lett.* **106**, 062404 (2015). [8] G. Chen, et al. *Nat. Commun.* **6**, 6598 (2015). [9] G. Chen, et al. *Appl. Phys. Lett.* **106**, 242404 (2015).

**4:54PM V18.00011 Observation of room-temperature skyrmion Hall effect.**, W. JIANG, Argonne National Laboratory, X. ZHANG, University of Hong Kong, P. UPADHYAYA, UCLA, W. ZHANG, Argonne National Laboratory, G. YU, UCLA, M. JUNGFLAISCH, F. FRADIN, J. PEARSON, Argonne National Laboratory, Y. TSERKOVNYYAK, K. WANG, UCLA, O. HEINONEN, Argonne National Laboratory, Y. ZHOU, University of Hong Kong, SUZANNE TE VELTHUIS, A. HOFFMANN, Argonne National Laboratory — The realization of room-temperature magnetic skyrmions is key to enabling the implementation of skyrmion-based spintronics. In this work, we present the efficient conversion of chiral stripe domains into Néel skyrmions through a geometrical constriction patterned in a  $\text{Ta}/\text{CoFeB}/\text{TaO}_x$  trilayer film at room temperature. This is enabled by an interfacial Dzyaloshinskii-Moriya interaction, and laterally divergent current-induced spin-orbit torques [1]. We further show the generation of magnetic skyrmions solely by the divergent spin-orbit torques through a nonmagnetic point contact. By increasing the current density, we observe the skyrmion Hall effect – that is the accumulation of skyrmions at one side of the device. The related Hall angle for skyrmion motion is also revealed under an *ac* driving current. Financial support for the work at Argonne came from Department of Energy, Office of Science, Basic Energy Science, Materials Sciences and Engineering Division, work at UCLA was supported by TANMS. Reference: [1] W. Jiang, et al., *Science*, 349, 283 (2015).

**5:06PM V18.00012 Controlling skyrmion helicity via engineered Dzyaloshinskii-Moriya interactions**, SEBASTIAN DIAZ, Department of Physics, University of California, San Diego, ROBERTO TRONCOSO, Departamento de Física, Universidad Técnica Federico Santa María, Chile — Single magnetic skyrmion dynamics in chiral magnets with a spatially inhomogeneous Dzyaloshinskii-Moriya interaction (DMI) is considered. Based on the relation between DMI coupling and skyrmion helicity, it is argued that the latter must be included as an extra degree of freedom in the dynamics of skyrmions. An effective description of the skyrmion dynamics for an arbitrary inhomogeneous DMI coupling is obtained through the collective coordinates method. The resulting generalized Thiele's equation<sup>1</sup> is a dynamical system for the center of mass position and helicity of the skyrmion. It is found that the dissipative tensor and hence the Hall angle become helicity dependent. The skyrmion position and helicity dynamics are fully characterized by our model in two particular examples of engineered DMI coupling: half-planes with opposite-sign DMI and linearly varying DMI. In light of a recent experiment<sup>2</sup> on the magnitude and sign of the DMI, our results constitute the first step toward a more complete understanding of the skyrmion helicity as a new degree of freedom that could be harnessed in future high-density magnetic storage and logic devices.

<sup>1</sup>Tretiakov et al., Phys. Rev. Lett. **100**, 127204 (2008).

<sup>2</sup>Shibata et al., Nature Nanotech. **8**, 723 (2013).

**5:18PM V18.00013 Quantum Anomalous Hall effect in a Topological Insulator coupled to a Skyrmion Lattice.**<sup>1</sup>, TONMOY BHOWMICK, YAFIS BARLAS, GEN YIN, ROGER LAKE, Univ of California - Riverside — A Skyrmion is a topologically protected spin texture characterized by a topological charge that has been experimentally observed in both bulk B20 compounds and thin films. In a quantum anomalous Hall phase, a material develops a topologically nontrivial electronic structure giving rise to quantized hall conductivity without any external magnetic field. We predict that a conventional bulk topological insulating material (e.g. Bi<sub>2</sub>Se<sub>3</sub>, Bi<sub>2</sub>Te<sub>3</sub>, Sb<sub>2</sub>Te<sub>3</sub>) in proximity with a Skyrmion crystal, with a weak exchange coupling, will be driven into an anomalous Hall insulating phase characterized by a nonzero integer chern number in the gap. We have calculated band structure, identified the gaps, and calculated the chern number at those gaps. The calculations show that the non trivial topological properties of the Skyrmion spin texture can be imprinted on the Dirac electrons of the topological insulator.

<sup>1</sup>Electronic structure calculations were supported by the NSF (ECCS-1408168). Micromagnetic simulations were supported by SHINES Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award DE-SC0012670

**Thursday, March 17, 2016 2:30PM - 5:30PM —**  
**Session V19 GMAG DMP: Magnetic Oxide Thin Films and Heterostructures: Spin Seebeck Effects** 318 - Jobu Matsuno, RIKEN

**2:30PM V19.00001 Paramagnetic and Antiferromagnetic Spin Seebeck Effect**, STEPHEN WU, Argonne National Laboratory — We report on the observation of the longitudinal spin Seebeck effect in both antiferromagnetic and paramagnetic insulators. By using a microscale on-chip local heater, it is possible to generate a large thermal gradient confined to the chip surface without a large increase in the total sample temperature. This technique allows us to easily access low temperatures (200 mK) and high magnetic fields (14 T) through conventional dilution refrigeration and superconducting magnet setups. By exploring this regime, we detect the spin Seebeck effect through the spin-flop transition in antiferromagnetic MnF<sub>2</sub> when a large magnetic field (>9 T) is applied along the easy axis direction. Using the same technique, we are also able to resolve a spin Seebeck effect from the paramagnetic phase of geometrically frustrated antiferromagnet Gd<sub>3</sub>Ga<sub>5</sub>O<sub>12</sub> (gadolinium gallium garnet) and antiferromagnetic DyScO<sub>3</sub> (DSO). Since these measurements occur above the ordering temperatures of these two materials, short-range magnetic order is implicated as the cause of the spin Seebeck effect in these systems. The discovery of the spin Seebeck effect in these two materials classes suggest that both antiferromagnetic spin waves and spin excitations from short range magnetic order may be used to generate spin current from insulators and that the spin wave spectra of individual materials are highly important to the specifics of the longitudinal spin Seebeck effect. Since insulating antiferromagnets and paramagnets are far more common than the typical insulating ferromagnetic materials used in spin Seebeck experiments, this discovery opens up a large new class of materials for use in spin caloritronic devices. All authors acknowledge support of the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES), Materials Sciences and Engineering Division. The use of facilities at the Center for Nanoscale Materials, was supported by the U.S. DOE, BES under contract No. DE-AC02-06CH11357.

**3:06PM V19.00002 Spin Seebeck measurements of current-induced switching in YIG**<sup>1</sup>, JASON BARTELL, COLIN JERMAIN, SRIHARSHA ARADHYA, Cornell University, HAILONG WANG, The Ohio State University, ROBERT BUHRMAN, Cornell University, FENGYUAN YANG, The Ohio State University, DANIEL RALPH, GREGORY FUCHS, Cornell University — Quantifying spin torques generated at the interface between a normal metal (NM) and a ferromagnetic insulator (FI) is an important step in understanding the spin hall effect without charge transport. Measuring magnetization in NM/FI devices is challenging, however, because both magnetoresistive and magneto-optical signals are tiny in thin-film bilayers. We show that a promising alternative measurement approach is the use of picosecond thermal gradients to study spin torques in Pt/Yttrium Iron Garnet (YIG) bilayers. Recently, we demonstrated the application of heat to stroboscopically transduce a local magnetic moment into an electrical signal via the time resolved anomalous Nernst effect (TRANE) in ferromagnetic metals [1]. Using a similar geometry the spin Seebeck effect of YIG combined with the inverse spin Hall effect of Pt enables measurement of local magnetization [2]. Here we describe our study using this technique to study current-induced switching in Pt/YIG with sub-10 nm thick YIG films. [1] Bartell et al., Nat. Commun. **6**, 8460 (2015). [2] Weiler et al., Phys. Rev. Lett. **108**, 106602 (2012).

<sup>1</sup>We acknowledge support from AFOSR

**3:18PM V19.00003 Irreversible Thermodynamics of Uniform Ferromagnets with Spin Accumulation: Bulk and Interface Phenomena**, WAYNE SASLOW, Texas A&M Univ, FUXIANG LI, Los Alamos National Laboratory, TOMOHIRO TANIGUCHI, National Institute of Advanced Industrial Science and Technology (AIST), Spintronics Research Center — We extend the irreversible thermodynamics of uniform ferromagnets to include the non-equilibrium phenomenon of spin accumulation, both for conductors and for insulators. The dynamics of the quantization axis  $\hat{M}$  is governed by the Landau-Lifshitz equation. The spin accumulation, whose longitudinal and transverse parts we label  $\delta M$  and  $\vec{m}$ , is due to a non-equilibrium distribution of magnetic excitations. Its dynamics is governed by a Bloch equation that includes spin diffusion. We also consider transport across surfaces, including boundary conditions for  $\hat{M}$ ,  $\delta M$ , and  $\vec{m}$ , and apply the results to the nature of the reciprocity between spin transfer torque and spin pumping.

**3:30PM V19.00004 Temperature dependences of magnetic anisotropy and longitudinal spin Seebeck effect in  $\text{Y}_3\text{Fe}_5\text{O}_{12}$** <sup>1</sup>, VIJAYSANKAR KALAPPATTIL, RAJA DAS, MANH-HUONG PHAN, HARIHARAN SRIKANTH, Department of Physics, University of South Florida, Tampa FL 33620 — Spin caloritronics is an emerging, exciting research area in condensed matter owing to its potential use in advanced spintronics devices. Pure spin current without having charge current has been achieved through spin Seebeck effect (SSE). Over the last 7 years SSE has been observed in ferromagnetic metals, insulators, and semiconductors using longitudinal and transverse SSE measurement configurations. In this work, we have carried out an experimental study to understand the effect of magnetic anisotropy on the temperature evolution of longitudinal spin Seebeck effect (LSSE) in a single crystalline yttrium iron garnet (YIG). The effective anisotropy field ( $H_K$ ) and inverse spin Hall (ISH) voltage ( $V_{ISH}$ ) were measured using the radio-frequency transverse susceptibility (TS) and LSSE configuration, respectively. The  $V_{ISH}$  of a 15 nm Pt strip on (6\*2\*1 mm) YIG slab with a temperature gradient of 3 K was measured in the temperature range of 120 to 300 K. The observed values of  $V_{ISH}$  vary from 1 microV for 120 K to 0.5 microV for 300 K. These values fall into the previously reported theoretical and experimental results. The temperature evolution of  $H_K$  has been compared with that of  $V_{ISH}$  to gain better fundamental understanding.

<sup>1</sup>Work is supported by ARO through Grant No. W911NF-15-1-0626

**3:42PM V19.00005 Investigation of the timescale of the spin-Seebeck effect in yttrium iron garnet from pico to nanoseconds**<sup>1</sup>, JOHN JAMISON, ZIHAO YANG, ROBERTO MYERS, Ohio State Univ - Columbus — We investigate the timescale of the spin-Seebeck effect (SSE) in yttrium iron garnet (YIG) by exciting transient thermal gradients with 150-fs laser heating pulses. The transient thermal gradient generates a spin current which is measured by a Pt top contact via the inverse spin Hall-effect (ISHE). A pulse selection system is used to lower the repetition rate of the laser to low frequencies (e.g. 10 kHz) such that the transient thermal gradient decays completely before the arrival of the next pulse. Lock-in detection, referenced at the laser repetition rate, is used to measure ISHE as a function of magnetic field, verifying that SSE is generated from the individual ultrafast laser pulses. Next, utilizing an optical delay line we vary the time delay between two equal fluence pulses. The correlated ISHE signal is measured with lock-in detection as a function of delay time with 0.1 ps resolution out to 1 ns to examine the characteristic decay times of the ultrafast laser pulse induced spin-Seebeck effect.

<sup>1</sup>Work supported by ARO MURI W911NF-14-1-0016.

**3:54PM V19.00006 Heat Transport between Antiferromagnetic Insulators and Normal Metals**, EIRIK LOHAUGEN FJAERBU, HANS SKARVAAG, ERLAND G. TVETEN, ARNE BRATAAS, Norwegian University of Science and Technology (NTNU) — Antiferromagnetic insulators can become active spintronics components by controlling and detecting their dynamics via spin currents in adjacent metals. This cross-talk occurs via spin-transfer and spin-pumping, phenomena that have been predicted to be as strong in antiferromagnets as in ferromagnets. In a recent article,<sup>1</sup> we demonstrate that a temperature gradient drives a significant heat flow from magnons in antiferromagnetic insulators to electrons in adjacent normal metals. The same coefficients as in the spin-transfer and spin-pumping processes also determine the thermal conductance. However, in contrast to ferromagnets, the heat is not transferred via a spin Seebeck effect which is absent in antiferromagnetic insulator-normal metal systems. Instead, the heat is proportional to a large staggered spin Seebeck effect.

<sup>1</sup>A. Brataas, H. Skarsvåg, E. G. Tveten and E. L. Fjærbu, arXiv:1506.06705 (2015)

**4:06PM V19.00007 Spin Nernst and torque effects in Dzyaloshinskii-Moriya ferromagnets.**<sup>1</sup>, ALEXEY A. KOVALEV, VLADIMIR ZYUZIN, University of Nebraska-Lincoln — We predict that a temperature gradient can induce a magnon-mediated intrinsic torque and a transverse spin current in ferromagnets with non-trivial magnon Berry curvature. With the help of a microscopic linear response theory of nonequilibrium magnon-mediated torques and spin currents we identify the interband and intraband components that manifest in ferromagnets with Dzyaloshinskii-Moriya interactions and magnetic textures. In addition to the torque and spin current, we also identify the mechanical torque effect in accordance with the conservation of angular momentum. To illustrate and assess the importance of such effects, we apply our theory to the magnon-mediated spin Nernst and torque responses in a kagome lattice ferromagnet.

<sup>1</sup>DOE Early Career Award DE-SC0014189, NSF under Grants Nos. Phy1415600, PHY11-25915, DMR-1420645

**4:18PM V19.00008 Spin-Hall magnetoresistance and spin Seebeck effect in Pt/CoCr<sub>2</sub>O<sub>4</sub> bilayer system**, AISHA AQEEL, NYNKE VLIETSTRA, JEROEN A. HEUVER, Zernike Institute for Advanced Materials, University of Groningen, The Netherlands, GERRIT E. W. BAUER, Institute for Materials Research and WPI-AIMR, Tohoku University, Sendai, Miyagi 980-8577, Japan, BEATRIZ NOHEDA, BART J. VAN WEES, THOMAS T. M. PALSTRA, Zernike Institute for Advanced Materials, University of Groningen, The Netherlands — Recently, the spin-Hall Magnetoresistance (SMR) and the spin Seebeck effect (SSE) have attracted much interest in the field of spintronics. However, these effects have been studied only for collinear magnetic systems. The nature and sensitivity of these effects in non-collinear magnets is still unknown. Here, we investigate the SMR and the SSE in the Pt/CoCr<sub>2</sub>O<sub>4</sub> heterostructure, by using a lock-in detection technique[1]. CoCr<sub>2</sub>O<sub>4</sub> (CCO) is a spinel with a collinear ferrimagnetic state below  $T_c = 94$  K and non collinear magnetic phases at lower temperatures. We investigated the SMR and the SSE at different temperatures (5K-300K). We observe a large enhancement in SMR and SSE in the non-collinear phase of the CCO. Moreover, finite SMR and SSE signals are also observed above  $T_c$ , where CCO is in the paramagnetic state. Our results show that SMR and SSE are very sensitive to the different magnetic phases of the CCO. [1] N. Vlietstra et al., Phys. Rev. B **90**, 174436 (2014)

**4:30PM V19.00009 Spin Seebeck Effect Signals from Antiferromagnets**<sup>1</sup>, ARATI PRAKASH, JACK BRANGHAM, FENGYUAN YANG, JOSEPH HEREMANS, The Ohio State University — The Longitudinal Spin Seebeck Effect (LSSE), in which a heat current stimulates spin propagation across an interface between a magnetic material and a normal metal, is well established and observed in ferromagnetic systems [1]. Data have been presented indicating that antiferromagnetic systems could also give rise to LSSE signals [2]. We report here on LSSE signal measured on the Pt/NiO/YIG structure, where NiO is an antiferromagnet. This system is reported to exhibit antiferromagnonic transport [3]. We explore the dependence of the signal on the thickness of the NiO and YIG layers. We also report its temperature dependence, which was not explored before [3]. The results are interpreted in terms of the temperature dependence of the magnon density of states. It appears that magnon modes with energies below about 40 K are most involved in the process, as was the case to the LSSE on YIG itself [4]. Preliminary results using other antiferromagnets and other inverse spin-Hall layers look promising and will also be reported. [1] S. R. Boona et al., Energy Environ. Sci. **7** 885-910 (2014) [2] Y. Ohnuma et al. Phys. Rev. B **87** 014423 (2012) [3] H. Wang, Phys. Rev. Lett. **113**, 097202 (2014) [4] Y. Jin et al., Phys. Rev. B **92**, 054436 (2015)

<sup>1</sup>Work supported by ARO- MURI W911NF-14-1-0016

**4:42PM V19.00010 Effects of thermal magnetic fluctuations on spin transport in Pt.**<sup>1</sup>, RYAN FREEMAN, ANDREI ZHOLUD, RONGXING CAO, SERGEI URAZHIDIN, Emory University — Despite extensive studies and applications of Pt as a spin Hall material in spintronic devices, its spin-dependent transport properties are still debated. We present a comprehensive experimental study of spin transport in Pt, utilizing measurements of giant magnetoresistance (GMR) in nanoscale Permalloy (Py)-based spin valves with Pt inserted in the nonmagnetic spacer. The spin diffusion length and the interfacial spin flipping coefficients are extracted from the dependence of MR on the Pt thickness. For samples with Pt separated from Py by Cu spacers, the spin diffusion length is 6 nm at 7K, and decreases to 3 nm at room temperature. The interfacial spin flipping decreases with increasing temperature, resulting in nonmonotonic temperature dependence of MR in samples with thin Pt. In contrast, in samples with Pt in direct contact with Py, we do not observe such a nonmonotonic dependence, and the spin diffusion length is significantly larger than in samples with Pt surrounded by Cu spacers. Our results indicate a large effect of the giant paramagnetic fluctuations in the nearly ferromagnetic Pt. These fluctuations are suppressed due to the proximity magnetism when Pt is in contact with Py, resulting in enhanced spin diffusion length and reduced spin flipping at the Pt interfaces. These observations indicate the need for a critical revision of spin transport and spin Hall-related properties of Pt-based structures.

<sup>1</sup>supported by NSF ECCS-1305586

**4:54PM V19.00011 Magnon-drag contribution to the Nernst effect of single-crystal iron**, SARAH WATZMAN, The Ohio State University, HYUNGYU JIN, Stanford University, JOSEPH HEREMANS, The Ohio State University — The thermopower of single-crystal iron has recently been proven to be dominated by magnon-drag [1]. Experimental results align with hydrodynamic and microscopic theories [2] that underline the similarity between the magnon-drag charge Seebeck effect and the spin-Seebeck effect. Here, the results are expanded to the Nernst effect. The Nernst coefficient of iron is shown to be quite large and is expected to contain a contribution similar to the spin-Seebeck effect. In this case, it is present in the absence of a ferromagnet-normal metal interface or spin-orbit interactions. This talk will present a new model based on ambipolar transport. Spin-up and spin-down electrons are considered as charge carriers with separate magnon-drag Seebeck coefficients. The difference between these partial Seebeck coefficients leads to a large magnon-drag Nernst coefficient in the absence of a skew force. Furthermore, methods to increase the thermopower of iron while maintaining its magnon-drag effects will be presented with preliminary results. 1. S. J. Watzman et al., San Antonio APS March Meeting talk (2015) 2. M. E. Lucassen et al., Appl. Phys. Lett. **99** 262506 (2011)

**5:06PM V19.00012 Time-domain measurement of spin-Seebeck effect as a function of temperature: interface magnon effect**, ZIHAO YANG, Department of Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, USA, JOHN JAMISON, Department of Material Science and Engineering, The Ohio State University, Columbus, Ohio, USA, ROBERTO MYERS, Department of Electrical and Computer Engineering, The Ohio State University, Columbus, Ohio, USA — Time-resolved longitudinal spin Seebeck effect (LSSE) measurements allow a means to separate the influence of thermally excited electrons, phonons and magnons on the detected spin current. In this study, we measured the time dependence of the LSSE signal in Pt/YIG structures using a high bandwidth oscilloscope and a modulated CW laser from 20 K to 300 K. The rise of the LSSE signal is sharp and not truncated indicating that the measurement is not limited by the bandwidth of the setup. The temporal profile of the LSSE signal consists of two distinct components, a fast rise (200 ns) and a slow rise. The fast component is temperature independent and roughly on par with the rise time of the modulated laser intensity, while the slow component does not saturate upto 50  $\mu$ s. We model the temporal evolution of the LSSE signal by carrying out three-temperature 3D time domain heat diffusion finite element modeling of the magnon temperature gradient profile in YIG to determine the electron, magnon, and phonon temperature profile versus time. It is found that the magnon temperature gradient near the YIG interface exhibits the same fast rise time that is measured in the LSSE signal. We discuss implications for this measurement on the existing models of LSSE.

**5:18PM V19.00013 Non-local thermal spin injection to study spin diffusion in yttrium iron garnet**<sup>1</sup>, BRANDON GILES, Dept. of Materials Science and Engineering, The Ohio State University, ZIHAO YANG, JOHN JAMISON, Dept. of Electrical and Computer Engineering, The Ohio State University, ROBERTO MYERS, Dept. of Materials Science and Engineering, The Ohio State University — Understanding the generation, detection, and manipulation of spin current is critical for the development of devices that depend on spin transport for information processing and storage. Recent studies have shown that spin transport over long distances is possible in the magnetic insulator yttrium iron garnet (YIG) through the diffusion of non-equilibrium magnons. Electrically excited magnons have been shown to diffuse up to 40 $\mu$ m at room temperature [1], while thermally injected magnons were detected at ranges greater than 125 $\mu$ m at 23K [2]. However, much work is still required to fully understand the processes responsible for magnon diffusion. Here, we present an in-depth study of the diffusion of magnons in YIG. By using the non-local thermal spin detection method [2], we analyze spin transport as a function of temperature. Spin diffusion maps, which can be used to experimentally determine the spin diffusion length in YIG as a function of temperature, are presented. [1] L. J. Cornelissen, *et al.* Nat Phys (2015). [2] B. L. Giles, *et al.* arXiv:1504.02808 [cond-Mat] (2015).

<sup>1</sup>Work supported by the Army Research Office MURI W911NF-14-1-0016

**Thursday, March 17, 2016 2:30PM - 5:30PM –**

**Session V20 DMP DCOMP: Explicitly Correlated Methods and Quantum Few-Body Systems**

319 - Sergiy Bubin, Nazarbayev University

**2:30PM V20.00001 Possibilities of the free-complement methodology for solving the Schrödinger equation of atoms and molecules**, HIROSHI NAKATSUJI, Quantum Chemistry Research Institute — Chemistry is a science of complex subjects that occupy this universe and biological world and that are composed of atoms and molecules. Its essence is diversity. However, surprisingly, whole of this science is governed by simple quantum principles like the Schrödinger and the Dirac equations. Therefore, if we can find a useful general method of solving these quantum principles under the fermionic and/or bosonic constraints accurately in a reasonable speed, we can replace somewhat empirical methodologies of this science with purely quantum theoretical and computational logics. This is the purpose of our series of studies – called exact theory in our laboratory. Some of our documents are cited below [1-8]. The key idea was expressed as the free complement (FC) theory (originally called ICI theory [3]) that was introduced to solve the Schrödinger and Dirac equations analytically. For extending this methodology to larger systems, order N methodologies are essential, but actually the antisymmetry constraints for electronic wave functions become big constraints. Recently [8], we have shown that the antisymmetry rule or 'dogma' can be very much relaxed when our subjects are large molecular systems. In this talk, I want to present our recent progress in our FC methodology. The purpose is to construct predictive quantum chemistry that is useful in chemical and physical researches and developments in institutes and industries. [1] H. Nakatsuji, Acc. Chem. Res. **45**, 1480 (2012). [2] H. Nakatsuji and H. Nakashima, TSUBAME e-Science J. **11**, 8, 24 (2014). [3] H. Nakatsuji, Phys. Rev. Lett. **93**, 030403 (2004). [4] H. Nakatsuji and H. Nakashima, Phys. Rev. Lett. **95**, 050407 (2005). [5] H. Nakatsuji, *et al.*, Phys. Rev. Lett. **99**, 240402 (2007). [6] H. Nakatsuji and H. Nakashima, J. Chem. Phys. **142**, 084117 (2015). [7] H. Nakashima and H. Nakatsuji, J. Chem. Phys. **139**, 044112 (2013). [8] H. Nakatsuji and H. Nakashima, J. Chem. Phys. **142**, 194101 (2015).

### 3:06PM V20.00002 Natural generalization of Slater determinants to more than one dimension

, DENIS SUNKO, Department of Physics, Faculty of Science, University of Zagreb — The calculation of realistic  $N$ -body wave functions for identical fermions is still an open problem in physics, chemistry, and materials science, even for  $N$  as small as two. Here a fundamental algebraic structure of many-body Hilbert space is described, enabling theoretically well-founded systematic investigation of wave-function space. The structure allows an arbitrary many-fermion wave function to be written in terms of a finite number of antisymmetric functions called shapes, which cannot be constructed by combining one-dimensional wave functions. Shapes naturally generalize the single-Slater-determinant form for the ground state to more than one dimension. Their number is exactly  $N!^{d-1}$  in  $d$  dimensions. A general algorithm is given to list them all in terms of standard Slater determinants. Conversely, excitations which can be induced from the one-dimensional case are bosonised into a system of distinguishable bosons, called Euler bosons, much like the electromagnetic field is quantized in terms of photons distinguishable by their wave numbers. Their wave functions are given explicitly in terms of elementary symmetric functions, reflecting the fact that the fermion sign problem is trivial in one dimension. The shapes are all possible vacua for the Euler bosons.

### 3:18PM V20.00003 Configuration space method for calculating binding energies of exciton complexes in quasi-1D/2D semiconductors.<sup>1</sup>

, IGOR BONDAREV, North Carolina Central University — A configuration space method, pioneered by Landau and Herring in studies of molecular binding and magnetism[1], is developed to obtain universal asymptotic relations for lowest energy exciton complexes (trion, biexciton) in confined semiconductor nanostructures such as nanowires and nanotubes[2], as well as coupled quantum wells. Trions are shown to be more stable (have greater binding energy) than biexcitons in strongly confined quasi-1D structures with small reduced electron-hole masses. Biexcitons are more stable in less confined quasi-1D structures with large reduced electron-hole masses. The theory predicts a crossover behavior, whereby trions become less stable than biexcitons as the transverse size of the quasi-1D nanostructure increases, which might be observed on semiconducting carbon nanotubes of increasing diameters. This method is also efficient in calculating binding energies for trion-type electron-hole complexes formed by indirect excitons in double coupled quantum wells, quasi-2D nanostructures that show new interesting electroabsorption/refraction phenomena. — [1]Landau & Lifshitz, Quantum Mechanics; C.Herring, RMP 34, 631 (1962). [2]I.V.Bondarev, PRB 90, 245430 (2014); PRB 83, 153409 (2011).

<sup>1</sup>Supported by DOE-DE-SC0007117

### 3:30PM V20.00004 Tests for Wavelets as a Basis Set<sup>1</sup>

, THOMAS BAKER, Department of Physics & Astronomy, University of California, Irvine, CA 92697, GLEN EVENBLY, Institute for Quantum Information and Matter, California Institute of Technology, Pasadena CA 91125, USA, STEVEN WHITE, Department of Physics & Astronomy, University of California, Irvine, CA 92697 — A wavelet transformation is a special type of filter usually reserved for image processing and other applications. We develop metrics to evaluate wavelets for general problems on test one-dimensional systems. The goal is to eventually use a wavelet basis in electronic structure calculations. We compare a variety of orthogonal wavelets such as coiflets, symlets, and daubechies wavelets. We also evaluate a new type of orthogonal wavelet with dilation factor three which is both symmetric and compact in real space.

<sup>1</sup>This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award DE-SC008696.

### 3:42PM V20.00005 How competitive are expansions in orbital products with explicitly correlated expansions

, KRZYSZTOF SZALEWICZ, University of Delaware — Helium dimer potential is of great importance for metrology since several future measurement standards will be based on helium gas. Such potential can be used to predict all thermodynamic properties of diffuse helium gas (nonadditive three-body potential is needed for higher densities). The accuracy required by these standards is so high, that in the past work of our group we had to include nonadiabatic, relativistic, and quantum electrodynamics effects. The current state is that the largest contribution to the uncertainty of the helium dimer potential is due to the Born-Oppenheimer (BO) part of this potential. This uncertainty was reduced and became comparable to other uncertainties in the new calculations that will be presented. These calculations used explicitly correlated Gaussian (ECG) basis sets and represent nearly exact solutions of the Schrödinger equation in the BO approximation. Similar calculations were also performed in orbital basis sets using a multilevel approach up to the full configuration interactions level. Largest existing basis sets were used at each level so that our calculations represent the best results that can currently be obtained using orbitals. These results will be critically compared with those obtained using ECG bases.

### 4:18PM V20.00006 New Types of Explicitly Correlated Gaussian Functions for Non-Born-Oppenheimer Molecular? Calculations.

, MARTIN FORMANEK, KEITH JONES, University of Arizona, SERGIY BUBIN, Nazarbayev University, LUDWIK ADAMOWICZ, University of Arizona — In this work we explore the possibility of using a new functional form of Explicitly Correlated Gaussian-type functions (ECGs) for performing non-Born-Oppenheimer calculations of diatomic molecular systems. Namely we focus our attention on ECGs with pre-exponential factors in the form of sin/cos functions of the square of the internuclear distance (sin/cos-ECGs). These ECGs can be generated as linear combinations of ECGs with complex exponential parameters (complex-ECGs) The complex-ECGs were previously used to calculate energy levels of He atom [1] and with the sin/cos-ECGs the vibrational energy levels for the H<sub>2</sub> molecule described by an effective Morse potential were calculated [2]. The focus of this study is ab-initio description of a real diatomic molecule, namely HD<sup>+</sup>, within the framework where the BO approximation is not assumed using these basis sets. The aim is to compare their accuracy and efficiency with ECGs with pre-exponential factors in the form of even powers of the internuclear distance and to assess their potential usefulness in non-BO calculations of molecules with more than two nuclei. [1] S. Bubín and L. Adamowicz, J. Chem. Phys. 124, 224317 (2006) [2] M. Formanek, K.L. Sharkey, N. Kirnosov and L. Adamowicz, J. Chem. Phys. 141, 154103 (2014)

### 4:30PM V20.00007 Complex explicitly correlated Gaussians for non-Born–Oppenheimer calculations of small molecules<sup>1</sup>

, SERGIY BUBIN, Nazarbayev University, LUDWIK ADAMOWICZ, University of Arizona — Non-Born–Oppenheimer calculations of molecular systems, where all particles are properly treated on an equal footing, represents a big challenge for the theory. Due to the huge difference in the masses of the electrons and nuclei the latter move more slowly and their correlation functions have distinct localization around the equilibrium internuclear separations. This feature is hard to implement in explicitly correlated variational approaches with Gaussian type basis functions while maintaining an analytic integrability of all necessary matrix elements. In this work we demonstrate that the difficulties can be overcome by using complex Gaussians. In our benchmark calculations on HD<sup>+</sup> molecular ion we have achieved excellent performance of this simple complex basis set that is on par or better than what was seen in previous Non-BO calculations of small diatomic molecules.

<sup>1</sup>This work has been supported by the Ministry of Education and Science of Kazakhstan

#### 4:42PM V20.00008 How Large are Nonadiabatic Effects in Atomic and Diatomic Systems?<sup>1</sup>

YUBO YANG, University of Illinois Urbana Champaign, ILKKA KYLANPAA, Tampere University of Technology, NORM TUBMAN, University of California, Berkeley, JARON KROGEL, Oak Ridge National Laboratory, SHARON HAMMES-SCHIFFER, DAVID CEPERLEY, University of Illinois Urbana Champaign — We have developed a fixed-node quantum Monte Carlo method to simulate atoms and molecules without the Born-Oppenheimer approximation with sub milli-Hartree accuracy [1]. For this purpose, we construct trial wave functions with nodes that depend on both the electronic and ionic positions. We report ground-state energies and the ionization energies for the first-row atoms and atomization energies for the first-row hydrides. The latter show effects of the nonadiabatic coupling between electrons and nuclei. We discuss how the method scales to larger systems. [1] Y. Yang, I. Kylänpää, N. M. Tubman, J. T. Krogel, S. Hammes-Schiffer, D. M. Ceperley, J. Chem. Phys. **143**(12), 2015.

<sup>1</sup>DOE DE-FG02-12ER46875, DOE DE-NA0001789, NSF CHE-13-61293, NSF OCI-1053575, DOE DE-AC05-00OR22725

#### 4:54PM V20.00009 The structure of the second-order non-Born-Oppenheimer density matrix

**D2:**<sup>1</sup> EDUARDO LUDENA, CIDNA-ESPOL, Guayaquil, Ecuador, PETER IZA, Department of Physics, ESPOL, Guayaquil, Ecuador, YOSSLEN ARAY, MAURICIO CORNEJO, CIDNA-ESPOL, Guayaquil, Ecuador, DIK ZAMBRANO, Department of Physics, ESPOL, Guayaquil, Ecuador — Properties of the non-Born-Oppenheimer 2-matrix are examined. Using a coordinate system formed by internal translationally invariant plus the total center-of-mass coordinates it is shown that regardless of the point of reference selected, the operator for the reduced second order density matrix, 2-RDM, solely depends upon the translationally invariant internal coordinates. We apply this result to examine the nature of the 2-RDM extracted from the exact analytical solutions for model non-Born-Oppenheimer four-particle systems of the Coulomb-Hooke and Moshinsky types. We obtain for both these models explicit closed-form analytic expressions for the electron and nuclear 2-RDM. An explicit expression is also obtained for the electron-nuclear 2-RDM in the Moshinsky case, which shows coupling between the electron and nuclear coordinates.

<sup>1</sup>EVL and YA acknowledge support of SENESCYT's Prometheus Program

#### 5:06PM V20.00010 Extracting g tensor values from experimental data with Markov Chain

**Monte Carlo methods**, ANAGHA KULKARNI, Department of Electrical and Computer Engineering, University of Delaware, WEIWEN LIU, Department of Material Sciences and Engineering, University of Delaware, RYAN ZURAKOWSKI, Department of Biomedical Engineering, University of Delaware, MATTHEW DOTY, Department of Material Sciences and Engineering, University of Delaware — Quantum Dot Molecules (QDMs) have emerged as a new platform for optoelectronic and spintronic devices. QDMs consist of multiple Quantum Dots (QDs) arranged in close proximity such that interactions between them can tailor their optical and spin properties. These properties can be tuned during growth and in-situ by applying electric fields that vary the coupling between QDs, which controls the formation of delocalized molecular-like states. Engineering the formation of molecular states in QDMs can be used to achieve new functionalities unavailable with individual QDs. Using molecular engineering approaches to tailor QDMs require precise knowledge of parameters such as binding energies of charge complexes, magnitude of many body interactions or components of the g tensor. Precise values of these parameters are difficult to extract from either experimental measurements or theoretical calculations. We develop and demonstrate a Markov Chain Monte Carlo method for extracting elements of the g tensor for a single hole confined in a QDM from photoluminescence data obtained as a function of electric and magnetic fields. This method can be applied to extract precise quantitative values of other physical parameters from sparse experimental data on a variety of systems.

#### 5:18PM V20.00011 QUANTUM MONTE CARLO METHOD FOR HEAVY ATOMIC AND MOLECULAR SYSTEMS WITH SPIN-ORBIT INTERACTIONS<sup>1</sup>

**CODY MELTON, LUBOS MITAS, North Carolina State Univ** — We present a new quantum Monte Carlo (QMC) method that can treat spin-orbit and other types of spin-dependent interactions explicitly. It is based on generalization of the fixed-phase and projection of the nonlocal operators with spinor trial wave functions. For testing the method we calculate several atomic and molecular systems such as Bi, W, Pb, PbH and PbO, some of them with both large- and small-core pseudopotentials. We validate the quality of the results against other correlated methods such as configuration interaction in two-component formalism. We find excellent agreement with extrapolated values for the total energies and we are able to reliably reproduce experimental values of excitation energies, electron affinity and molecular binding. We show that in order to obtain the agreement with experimental values the explicit inclusion of the spin-orbit interactions is crucial.

<sup>1</sup>U.S. D.O.E. grant de-sc0012314 and NERSC Contract No. DE-AC02-05CH11231

## Thursday, March 17, 2016 2:30PM - 5:30PM –

Session V21 GSCCM DCOMP DMP: Materials at Extremes: Warm Dense Matter 320 - Arianna Gleason, Los Alamos National Laboratory

#### 2:30PM V21.00001 Study of the Warm Dense Matter with XANES spectroscopy - Applications to planetary interiors

ADRIEN DENOEUDE, CEA — With the recent discovery of many exoplanets, modelling the interior of these celestial bodies is becoming a fascinating scientific challenge. In this context, it is crucial to accurately know the equations of state and the macroscopic and microscopic physical properties of their constituent materials in the Warm Dense Matter regime (WDM). Moreover, planetary models rely almost exclusively on physical properties obtained using first principles simulations based on density functional theory (DFT) predictions. It is thus of paramount importance to validate the basic underlying mechanisms occurring for key planetary constituents (metallization, dissociation, structural modifications, phase transitions, etc....) as pressure and temperature both increase<sup>1,2</sup>.

In this work, we were interested in two materials that can be mainly found in the Earth-like planets: silica, or SiO<sub>2</sub>, as a model compound of the silicates that constitute the major part of their mantles, and iron, which is found in abundance in their cores. These two materials were compressed and brought to the WDM regime by using strong shock created by laser pulses during various experiments performed on the LULI2000 (Palaiseau, France) and the JLF (Livermore, US) laser facilities and on the LCLS XFEL (Stanford, US). In order to penetrate this dense matter and to have access to its both ionic and electronic structures, we have probed silica and iron with time-resolved X-ray Absorption Near Edge Structure (XANES)<sup>3</sup>. In parallel with these experiments, we performed quantum molecular dynamics simulations based on DFT at conditions representative of the region investigated experimentally so as to extract the interesting physical processes and comprehend the limits of the implemented models<sup>4</sup>. In particular, these works allowed us to highlight the metallization processes of silica in temperature<sup>5</sup> and the structural changes of its liquid in density, as well as to more constrain the melting curve of iron at very high pressures.

<sup>1</sup>K. Umemoto et al., Science 311, 983 (2006)

<sup>2</sup>D. Hicks et al., Phys. Rev. Lett, 97, 025502 (2006)

<sup>3</sup>A. Benuzzi-Mounaix et al., Phys. Rev. Lett, 107, 165006 (2011)

<sup>4</sup>V. Recoules et al., Phys. Rev. B, 80, 064110 (2009)

<sup>5</sup>A. Denoeud et al., Phys. Rev. Lett, 113, 116404 (2014)

**3:06PM V21.00002 Free-electron x-ray laser measurements in isochorically heated warm dense matter** , PHILIPP SPERLING, SLAC National Accelerator Laboratory, HYUN CHUNG, International Atomic Energy Agency, LUKE FLETCHER, ERIC GALTIER, ELISEO GAMBOA, HAE JA LEE, SLAC National Accelerator Laboratory, YULTUZ OMARBAKIYEVA, HEIDI REINHOLZ, GERD RPKE, Rostock University, ULF ZASTRAU, European XFEL GmbH, SIEGFRIED GLENZER, SLAC National Accelerator Laboratory — We present the highly-resolved measurements of inelastic x-ray scattering spectra in an ultrafast heated solid. The obtained spectra from the isochorically heated foils permit a direct temperature dependent determination of plasma properties, e.g. transport coefficient. X-ray pulses from the seeded Linac Coherent Light Source delivering an average of 0.3 mJ of 8 keV x-ray photons in a 0.005% bandwidth pulse, have been focused to micrometer diameter focal spots isochorically heating solid materials to temperatures up to several eV. The inelastic forward scattering spectra resolve electronic plasma oscillations that directly allow an accurate determination of the electron temperature and density indicating a warm dense matter state. This accuracy enable us to extract plasma properties, e.g. the electrical conductivity, and enables the validation of existing theories.

**3:18PM V21.00003 Hot-dense hydrogen study up to 300 GPa** , CHANG-SHENG ZHA, Carnegie Institution of Washington — Hydrogen study under extreme pressure-temperature conditions has fundamental importance for the development of condensed physics. The prediction of insulator to metallic state transition at sufficient high pressure has been a long-standing open question for the high pressure physics community. Recently, more experimental and theoretical interests were focused on the hot-dense state of hydrogen. A numerous investigations indicated a turnover melting line with a maximum point around ~100 GPa. First-principle theoretical models indicate that the metallization could be a liquid-liquid transition just above the melting line. Experiments for these studies were mostly conducted in shock compression or pulsed laser heating in static compression resulted in large controversy observations. Hydrogen study also has been one of the engines driving the advance of static pressure-temperature technologies. New developments in hydrogen study have brought static pressure generation and signal probing technique into 300 ~400 GPa range, leading to more new phases found. New experimental results using static pressure-temperature DAC techniques demonstrate that hydrogen has much more complicated phase behaviors at multiple megabar pressure range than that expected previously.

**3:30PM V21.00004 Hydrogen Deuteride to 3.4 Megabar Mixed Isotopes and New Phases<sup>1</sup>** , RANGA DIAS, ORI NOKED, ISAAC SILVERA, Lyman Laboratory of Physics, Harvard University, Cambridge, MA 02138 — We present infrared absorption studies of solid hydrogen deuteride to pressures as high as 3.4 megabar in a diamond anvil cell and temperatures in the range 5 to 295 K. Above 198 GPa the sample transforms to a mixture of , and, interpreted as a process of dissociation and recombination. Three new phases-lines are observed, two of which differ remarkably from those of the high-pressure homonuclear species, but none are metallic. The time-dependent spectral changes are analyzed to determine the molecular concentrations as a function of time.y.

<sup>1</sup>The NSF, grant DMR-1308641 and the DOE Stockpile Stewardship Academic Alliance Program, grant DE-FG52-10NA29656 supported this research.

**3:42PM V21.00005 A Transition to Metallic Hydrogen: Evidence of the Plasma Phase Transition<sup>1</sup>** , ISAAC SILVERA, MOHAMED ZAGHOO, Lyman Laboratory of Physics, Harvard University, Cambridge, MA 02138, ASHKAN SALAMAT, Department of Physics, Univ. of Nevada at Las Vegas — The insulator-metal transition in hydrogen is one of the most outstanding problems in condensed matter physics. The high-pressure metallic phase is now predicted to be liquid atomic from T=0 K to very high temperatures. We have conducted measurements of optical properties of hot dense hydrogen in the region of 1.1-1.7 Mbar and up to 2200 K in a diamond anvil cell using pulsed laser heating of the sample. We present evidence in two forms: a plateau in the heating curves (average laser power vs temperature) characteristic of a first-order phase transition with latent heat, and changes in transmittance and reflectance characteristic of a metal for temperatures above the plateau temperature. For thick films the reflectance saturates at ~0.5. The phase line of this transition has a negative slope in agreement with theories of the so-called plasma phase transition.

<sup>1</sup>The NSF, grant DMR-1308641, the DOE Stockpile Stewardship Academic Alliance Program, grant DE-FG52-10NA29656, and NASA Earth and Space Science Fellowship Program, Award NNX14AP17H supported this research.

**3:54PM V21.00006 High pressure hydrogen stabilised by quantum nuclear motion<sup>1</sup>** , RICHARD NEEDS, BARTOMEU MONSERRAT, CHRIS PICKARD, University of Cambridge — Hydrogen under extreme pressures is of fundamental interest, as it might exhibit exotic physical phenomena, and of practical interest, as it is a major component of many astrophysical objects. Structure searches have been successful at identifying promising candidates for the known phases of high pressure hydrogen. However, these searches have so far been restricted to the location of minima of the potential energy landscape. In this talk, we will describe a new structure searching method, “saddle-point ab initio random structure searching” (sp-AIRSS), that allows us to identify structures associated with saddle points of the potential energy landscape. Using sp-AIRSS, we find two new high-pressure hydrogen structures that exhibit a harmonic dynamical instability, but quantum and thermal anharmonic motion render them dynamically stable. These structures are formed by mixed layers of strongly and softly bound hydrogen molecules, and become thermodynamically competitive at the highest pressures reached in experiment. The experimental implications of these new structures will also be discussed.

<sup>1</sup>BM is supported by Robinson College, Cambridge, and the Cambridge Philosophical Society. RJN and CJP are supported by the Engineering and Physical Sciences Research Council (EPSRC) of the UK.

**4:06PM V21.00007 Warm dense iron equation of state from quantum molecular dynamics** , TRAVIS SJOSTROM, SCOTT CROCKETT, Los Alamos National Laboratory — Through quantum molecular dynamics (QMD), utilizing both Kohn-Sham (orbital-based) and orbital-free density functional theory, we calculate the equation of state of warm dense iron in the density range 7-30 g/cm<sup>3</sup> and temperatures from 1 to 100 eV. A critical examination of the iron pseudopotential is made, from which we find the previous QMD calculations of Wang *et al.* [Phys. Rev. E 89, 023101 (2014)] to be in error. Our results also significantly extend the ranges of density and temperature which are attempted in that prior work. We calculate the shock Hugoniot and find very good agreement with experimental results to pressures over 20 TPa. Additionally we have utilized the QMD results to generate a new SESAME tabular equation of state for fluid iron, accurate in the warm dense matter region, and also extending to much broader regions of density and temperature than can be accessed by the QMD alone.

**4:18PM V21.00008 Overview of Warm Dense Matter Experiments at LCLS** , ERIC GALTIER, SLAC - Natl Accelerator Lab, ANNA LEVY, Sorbonne Universits, UPMC, CNRS, INSP, GARETH WILLIAMS, GoLP/IPFN-Laboratorio Associado, IST, LUKE FLETCHER, SLAC - Natl Accelerator Lab, FABIEN DORCHIES, JRME GAUDIN, Universit de Bordeaux, CNRS, CEA, CELIA, PHILIPP SPERLING, SLAC - Natl Accelerator Lab — Warm Dense Matter (WDM) is found in numerous astrophysical systems, from giant planets to brown dwarves or cool dense stars. Being this intermediate regime where condensed matter or plasma theories do not apply, it can be produced in all laser-induced plasma experiments on Earth. As a consequence, understanding its properties is fundamental and the whole community is investigating this extreme state of matter. With the advent of the 4th generation of light sources, namely the Free Electron Lasers (FELs), a new way of producing and diagnosing WDM becomes available. In 2009, the Linac Coherent Light Source (LCLS) at SLAC was the first FEL to produce X-ray photons to be used by the user community. Since then, various experiments took place at LCLS to produce and measure specific physical properties of WDM. In this talk, we will present an overview of key experiments performed at LCLS to study WDM. The LCLS has been used in a variety of configuration: as the main heating mechanism, as a probe or both at the same time. When used as a probe, high power lasers have been used to shock matter and excite it into the WDM regime. Finally, we will describe exciting perspectives on the WDM research, as the LCLS-II will become available in about 5 years.

**4:30PM V21.00009 First-principles equation of state and electronic properties of warm dense oxygen**, SHUAI ZHANG, KEVIN DRIVER, FRANÇOIS SOUBIRAN, BURKHARD MILITZER, University of California, Berkeley — We perform all-electron path integral Monte Carlo (PIMC) and density functional theory molecular dynamics (DFT-MD) calculations to explore warm dense matter states of oxygen. Our simulations cover a wide density-temperature range of  $1\text{--}100\text{ g cm}^{-3}$  and  $10^4\text{--}10^9\text{ K}$ . By combining results from PIMC and DFT-MD, we are able to compute pressures and internal energies from first-principles at all temperatures and provide a coherent equation of state. We compare our first-principles calculations with analytic equations of state, which tend to agree for temperatures above  $8 \times 10^6\text{ K}$ . Pair-correlation functions and the electronic density of states reveal an evolving plasma structure and ionization process that is driven by temperature and density. As we increase the density at constant temperature, we find that the ionization fraction of the  $1s$  state decreases while the other electronic states move towards the continuum. Finally, the computed shock Hugoniot curves show an increase in compression as the first and second shells are ionized. This work is funded by the DOE (DE-SC0010517).

**4:42PM V21.00010 Nuclear quantum effects in high-pressure ice**, Yael Bronstein, Philippe Depondt, Fabio Finocchi, Université Pierre et Marie Curie — Because of their mass, hydrogen nuclei are subjected to nuclear quantum effects (NQE), mainly tunneling and zero-point energy. They can be crucial to describe correctly the properties of H-containing systems, even at room temperature. A prototypical example of the importance of NQE is the transition from asymmetric H-bonds in phase VII to symmetric bonds in phase X of high-pressure ice, in which NQE drastically reduce the transition pressure<sup>1</sup>. However, natural ice is rarely pure and even small concentrations of salt (LiCl or NaCl) in ice have a strong effect on the phase diagram: the VII to X transition is shifted to higher pressures, questioning the resilience of NQE in the presence of ionic impurities<sup>2</sup>. We investigate these questions using the Quantum Thermal Bath<sup>3</sup>, a semi-classical Langevin dynamics, taking into account both NQE and thermal effects in pure and salty ices. We show why NQE can be sensitive to the presence of impurities and that non-trivial phenomena could result, such as the spectacular upshift of the transition pressure and the peculiar motion of ions.

<sup>1</sup>Benoit et al, Nature 392, 258 (1999); Bronstein et al, Phys. Rev. B 89, 214101 (2014)

<sup>2</sup>Bove et al, PNAS 112, 8216 (2015)

<sup>3</sup>Dammak et al, Phys. Rev. Lett. 103, 190601 (2009)

**4:54PM V21.00011 Influence of exchange-correlation temperature effects on electric conductivity of aluminum in WDM regime**<sup>1</sup>, VALENTIN KARASIEV, LÁZARO CALDERÍN, SAM TRICKEY, Physics Dept., Univ. Florida — Calculation of transport properties in the warm dense matter (WDM) regime and comparison with experiment is an important development challenge. Computationally affordable, reliable theoretical methods are required. Current best practice is Kohn-Sham molecular dynamics (KS-MD) to sample ionic configurations and Kubo-Greenwood (KG) conductivity calculations at selected configurations. Relevant aspects are (i) the very high computational cost and unfavorable cost-scaling of the KS-MD at WDM temperatures, and (ii) neglect of explicit temperature effects in the ground state exchange-correlation (XC) functionals often used to approximate the XC free energy. We address both issues. We sample configurations of aluminum ions in the WDM regime with drastically lowered MD cost via finite-temperature orbital-free MD, including explicitly T-dependent XC [1]. Then we delineate the XC T-effects by comparing KG conductivities calculated with and without explicit XC T-dependence. The result is that explicitly T-dependent XC gives an unequivocal improvement with respect to experiment for aluminum at low material density and elevated temperatures. [1] V.V. Karasiev, T. Sjostrom, J. Dufty, and S.B. Trickey, Phys. Rev. Lett. 112, 076403 (2014)

<sup>1</sup>Supported by U.S. Dept. of Energy, grant DE-SC0002139

**5:06PM V21.00012 Orbital-free Molecular Dynamics Simulations to Characterize the Liquid-vapor Critical Point of Aluminum**<sup>1</sup>, DEBAJIT CHAKRABORTY, VALENTIN KARASIEV, QTP, Department of Physics, U. Florida, Gainesville, FL 32611, SAMUEL TRICKEY, QTP, Department of Physics and Chemistry, U. Florida, Gainesville, FL 32611 — Aluminum is frequently used in warm-dense matter (WDM) experiments. However, experimental diagnostic limitations make computational exploration of the Al liquid-vapor transition important[1]. The elevated temperature and low-density make ab initio molecular dynamics (AIMD) with Kohn-Sham (KS) density functional theory (DFT) searches for the divergent compressibility extremely time consuming. Orbital free DFT (OFDFT) in principle is a cost-effective alternative. Here we report on calculations utilizing the PROFESS@QuantumEspresso interface [2] to explore suitable pseudo-potentials [3], the limitations of our wholly constraint-based VT84F [4] non-interacting free-energy functional as exposed in the low-density regime, and possible extensions or extrapolations via tunable non-interacting free energy functionals [5]. [1] Atom. Proc. Plasmas CP-1161 K. B. Fournier ed. (2009); [2] Comput. Phys. Commun. **185**, 3240 (2014); [3] J. Phys.: Condens. Matter **2**, 351 (1990); [4] Phys. Rev. B **88**, 161108(R) (2013); [5] "Tunable non-interacting free-energy functionals", V.V. Karasiev {unpublished}

<sup>1</sup>Work supported by U.S. Dept. of Energy, grant DE-SC0002139

**5:18PM V21.00013 Accurate exchange-correlation energies for the warm dense electron gas**, FIONN MALONE, Imperial College London, NICHOLAS BLUNT, Cambridge University, JAMES SHEPHERD, Massachusetts Institute of Technology, DEREK LEE, JAMES SPENCER, MATTHEW FOULKES, Imperial College London — The accurate treatment of matter at high temperatures and densities is of increasing importance to many fields in physics and chemistry, with applications ranging from planetary physics to inertial confinement fusion and plasmonic catalysis. Faithfully including the effects of temperature in density functional theory simulations of warm dense matter requires accurate results for the uniform electron gas (UEG) across the whole temperature-density plane. While accurate ground state quantum Monte Carlo data have existed for over 30 years<sup>1</sup>, there remains significant disagreement between results obtained using different path integral Monte Carlo methods at finite temperature<sup>2,3</sup>. To resolve this disagreement, we use the systematically improvable density matrix quantum Monte Carlo method<sup>4,5</sup> to calculate the exchange-correlation energy of the UEG. We also demonstrate how the evaluation of free energies emerges naturally from our method.

<sup>1</sup>Phys. Rev. Lett. 45, 566 (1980)

<sup>2</sup>Phys. Rev. Lett. 110, 146405 (2013)

<sup>3</sup>Phys. Rev. Lett. 115, 130402 (2015)

<sup>4</sup>Phys. Rev. B 89, 245124 (2014)

<sup>5</sup>J. Chem. Phys. 143, 044116 (2015)

**Thursday, March 17, 2016 2:30PM - 4:30PM –**

**Session V22 DCOMP: Classical Monte Carlo and Molecular Dynamics** 321 - Paul Kent, Oak Ridge National Laboratory

**2:30PM V22.00001 Monte Carlo Simulation of a Novel Classical Spin Model with a Tricritical Point** , TYLER CARY, RICHARD SCALETTAR, RAJIV SINGH, University of California, Davis — Recent experimental findings along with motivation from the well known Blume-Capel model has led to the development of a novel two-dimensional classical spin model defined on a square lattice. This model consists of two Ising spin species per site with each species interacting with its own kind as perpendicular one dimensional Ising chains along with complex and frustrating interactions between species. Probing this model with Mean Field Theory, Metropolis Monte Carlo, and Wang Landau sampling has revealed a rich phase diagram which includes a tricritical point separating a first order magnetic phase transition from a continuous one, along with three ordered phases. Away from the tricritical point, the expected 2D Ising critical exponents have been recovered. Ongoing work focuses on finding the tricritical exponents and their connection to a supersymmetric critical point.

**2:42PM V22.00002 Molecular dynamics simulations of Leidenfrost droplets on a vibrating nano ratchet** , ABHISHEK KUMAR, NICKOLAY LAVRIK, MIGUEL FUENTES-CABRERA, Oak Ridge National Laboratory — Asymmetrically nanostructured surfaces can function as Brownian ratchets, that is, create a bias in mass or energy flows in response to thermal noise or in a more general case, isotropic excitations. Recently, experimental studies have shown that it is possible to induce directional movement of water droplets deposited on a vertically vibrating hydrophobic substrate made of inclined nanopillars. To investigate this issue, we have performed large-scale molecular dynamics (MD) simulations of a water droplet on a pillared graphitic substrate. We have found that our results not only reproduce the experimental behavior but also reveal new phenomena. In particular, it was found that at certain critical amplitude and frequency, the motion of the droplet transits from circular to linear-oscillatory along the substrate. The transition ultimately depends on the relative size of droplet and pillars, suggesting new ways of controlling the movement of water droplets on superhydrophobic substrates.

**2:54PM V22.00003 Observation of 2D Ising criticality of liquid-gas transition by the flowgram method<sup>1</sup>** , MAX YARMOLINSKY, ANATOLY KUKLOV, CSI and the Graduate Center, CUNY — We study the critical properties of the transition in 2D liquid-gas system with the square-well potential interaction by Monte Carlo simulations in the grand canonical ensemble. Due to lack of the underlying Ising symmetry, the analysis cannot be done reliably by the standard methods applicable to lattice systems. In contrast, the analysis based on the flowgram method<sup>2</sup> allowed us to find the critical point to significantly higher (and controllable) accuracy than in previous studies by other authors. Simulations were performed in a progression of sizes  $L$  up to size  $L = 84$ , with the particle numbers varying over 3 orders of magnitude and the subcritical behavior not extending beyond  $L = 10 - 15$ . The finite size scaling analysis of the critical exponents and their ratio,  $\mu$  and  $\gamma/\nu$ , gives values consistent with the 2D Ising universality class within 1-2% of errors. Our result essentially closes proposals that the nature of the liquid-gas transition might be different from the Ising model in systems with short-range interactions.

<sup>1</sup>This work was supported by the NSF grant PHY1314469

<sup>2</sup> A. B. Kuklov, N.V. Prokof'ev, B.V. Svistunov, and M. Troyer, Ann. of Phys., **321**, 1602 (2006).

**3:06PM V22.00004 Heat Transfer in Porous Crystals Containing Adsorbed Gases** , HASAN BABAEI, CHRISTOPHER WILMER, University of Pittsburgh — Using molecular modeling, we investigated heat transfer phenomena in a porous crystal containing gases. This study was motivated by the challenge of quickly dissipating heat generated in metal-organic frameworks (MOFs) during gas adsorption. Our study reveals that thermal conductance is dominated by lattice thermal conductivity in the crystal, and that conductance decreases as the density of gas in the pores increases. We show that the observed decreased conductivity is due to phonon scattering in the crystal due to interactions with gas molecules. We have also investigated the effect of pore size and shape on thermal transport in these structures. We show that thermal conductivity of pure nanoporous crystals decreases with pore size. For nanoporous crystals with small pores, gas adsorption reduces thermal conductivity due to more phonon scatterings, whereas for larger pores, the increase in gas loading does not affect lattice thermal conductivity. We show that the probability of gas-crystal collisions is smaller for larger pores, which explains why loaded gases do not significantly affect thermal conductivity of large pore structures.

**3:18PM V22.00005 Renormalized Multicanonical Sampling in Two-Dimensional Systems** , YONG HWAN LEE, DAVID YEVIK, Univ of Waterloo — This presentation considers the relative speed and accuracy of the recently introduced renormalized multicanonical sampling method [D. Yevick, Int. J. Mod. Phys. C, 1650033] in the context of the 2 dimensional Ising model. In particular, the technique is compared to a method in which the transition matrix is constructed during a multicanonical determination of the density of states. In the comparison, the simulation speed is significantly increased by the renormalized sampling and the calculations with the transition matrices obtained from the multicanonical refinement steps of the renormalized algorithm improves the simulation speed and accuracy further.

**3:30PM V22.00006 Dynamic Algorithms for Transition Matrix Generation<sup>1</sup>** , DAVID YEVIK, YONG HWAN LEE, University of Waterloo — The methods of [D. Yevick, Int. J. Mod. Phys. C, 1650041] for constructing transition matrices are applied to the two dimensional Ising model. Decreasing the system temperature during the acquisition of the matrix elements yields a reasonably precise specific heat curve for a 32x32 spin system for a limited number (50-100M) of realizations. If the system is instead evolved to first higher and then lower energies within a restricted interval that is steadily displaced in energy as the computation proceeds, a modification which permits backward displacements up to a certain lower bound for each forward step ensures acceptable accuracy. Additional constraints on the transition rule are also investigated.

<sup>1</sup>The Natural Sciences and Engineering Research Council of Canada (NSERC) and CIENA are acknowledged for financial support.

**3:42PM V22.00007 “Binless Wang-Landau sampling” - a multicanonical Monte Carlo algorithm without histograms<sup>1</sup>** , YING WAI LI, MARKUS EISENBACH, National Center for Computational Sciences, Oak Ridge National Laboratory — Inspired by the very successful Wang-Landau (WL) sampling<sup>2</sup>, we innovated a multicanonical Monte Carlo algorithm to obtain the density of states (DOS) for physical systems with continuous state variables. Unlike the original WL scheme where the DOS is obtained as a numerical array of finite resolution, our algorithm assumes an analytical form for the DOS using a well chosen basis set, with coefficients determined iteratively similar to the WL approach. To avoid undesirable artificial errors caused by the discretization of state variables, we get rid of the use of a histogram for keeping track of the number of visits to energy levels, but store the visited states directly for the fitting of coefficients. This new algorithm has the advantage of producing an analytical expression for the DOS, while the original WL sampling can be readily recovered.

<sup>1</sup>This research was supported by the Office of Science of the Department of Energy under contract DE-AC05-00OR22725.

<sup>2</sup>F. Wang and D. P. Landau, Phys. Rev. Lett. **86**, 2050 (2001).

**3:54PM V22.00008 Critical nonequilibrium relaxation in cluster algorithms in the BKT and weak first-order phase transitions**, YOSHIHIKO NONOMURA, Computational Materials Science Unit, National Institute for Materials Science (NIMS), Tsukuba, Ibaraki 305-0044, Japan, YUSUKE TOMITA, College of Engineering, Shibaura Institute of Technology, Saitama 337-8570, Japan — Recently we showed that the critical nonequilibrium relaxation in cluster algorithms is widely described by the stretched-exponential decay of physical quantities in the Ising [1] or Heisenberg [2] models. Here we make a similar analysis in the Berezinsky-Kosterlitz-Thouless (BKT) phase transition in the 2D XY model (simple exponential decay) and in the weak first-order phase transition in the 2D  $q = 5$  Potts model (power-law decay) [3], which means that these phase transitions can clearly be characterized by the present analysis. These relaxation behaviors are compared with those in the 3D and 4D XY models (second-order phase transition) and in the 2D  $q$ -state Potts models ( $2 \leq q \leq 4$  for second-order and  $q \geq 6$  for strong first-order phase transitions).

[1] Y. Nonomura, J. Phys. Soc. Jpn. **83**, 113001 (2014); [2] Y. Nonomura and Y. Tomita, arXiv:1508.05218; [3] Y. Nonomura and Y. Tomita, arXiv:1509.08352.

**4:06PM V22.00009 Real Space Alternatives to the Ewald: Shifted Electrostatics for Multipoles**, MADAN LAMICHHANE, THOMAS PARSONS, KATHIE NEWMAN, J. DANIEL GEZELTER, Univ of Notre Dame — We have developed three real-space methods for computing electrostatic interactions in Molecular Dynamics (MD): Gradient Shifted Force (GSF), Shifted Potential (SP), and Taylor Shifted Force (TSF) [1]. Electrostatic interaction energies, forces, and torques of the molecules obtained from these methods were tested against an analytical as well as a reference method in a variety of condensed phase environments. Tests show that electrostatic energies, forces, and torques evaluated from our real-space methods show excellent agreement with the computationally expensive Ewald method. Total energy is conserved in molecular systems interacting using GSF and TSF methods. Different structural and dynamical properties of the multipolar fluids have been investigated. Recently, we have developed methods for evaluating dielectric properties for dipolar and quadrupolar fluids. Results for the dielectric constant of dipolar and quadrupolar fluids evaluated using the fluctuation and perturbation method will also be discussed. [1] M. Lamichhane *et al.*, J. Chem. Phys **141**, 134109 (2014); **141**, 134110 (2014).

**4:18PM V22.00010 A robust high-order ideal magnetohydrodynamic solver**, DAVID SEAL, U.S. Naval Academy, ANDREW CHRISTLIEB, XIAO FENG, Michigan State University, QI TANG, Rensselaer Polytechnic Institute — In this work we present a robust high-order numerical method for the ideal magnetohydrodynamics (MHD) equations. Our method is single-stage and single-step, and hence amenable to adaptive mesh refinement (AMR) technology. The numerical robustness of the scheme is realized by accomplishing a total of two unrelated tasks: we retain positivity of the density and pressure by limiting fluxes similar to what happens in a flux corrected transport method, and we obtain divergence free magnetic fields by implementing an unstaggered transport method for the evolution of the magnetic potential. We present numerical results in two and three dimensions that indicate the utility of the scheme. These results include several classical test problems such as Orszag-Tang, cloud shock interactions and blast wave problems.

## Thursday, March 17, 2016 2:30PM - 5:30PM —

Session V23 DCMP: Superconductors: STM of Fe-based, Cuprates, and others 322 -

**2:30PM V23.00001 STM/S study on the role of Arsenic in Iron-based Superconductivity at Atomic Scale**, S. H. PAN, Inst. of Physics, CAS; TcSUH, Univ. of Houston, J. X. YIN, Institute of Physics, CAS, ZHENG WU, TcSUH, Univ. of Houston, ANG LI, TcSUH, Univ. of Houston, J. H. WANG, TcSUH, Univ. of Houston, X. J. LIANG, Institute of Physics, CAS, C. L. ZHANG, Rice Univ, P. C. DAI, Rice University, C. -S. TING, TcSUH, Univ of Houston, J. P. HU, Institute of Physics, CAS, Z. Q. WANG, Boston College, H. P. HOR, TcSUH, Univ. of Houston, G. F. CHEN, HONG DING, Institute of Physics, CAS — We use scanning tunneling microscopy /spectroscopy to investigate the role of Arsenic in superconducting Ba<sub>0.4</sub>K<sub>0.6</sub>Fe<sub>2</sub>As<sub>2</sub> by directly breaking and repairing the local Fe-As structure. After the up-As-layer peeled away, the tunneling spectrum of the exposed Fe surface reveals a shallow incoherent gap, indicating a severe suppression of superconductivity without As covering. When an As-dimer is placed on the same Fe surface, a localized topographic feature is formed due to p-d orbital hybridization and the superconducting coherent peaks recover locally with the superconducting gap size exactly the same as the Fe-layer with a complete As-coverage. These observations unravel the Fe-As interactions on an atomic scale and imply its essential roles in the Fe-based superconductivity.

**2:42PM V23.00002 Surface effect of epitaxially grown BaFe<sub>2</sub>As<sub>2</sub> surface – Scanning Tunneling Microscopy and Photoemission spectroscopy study**, SUNGMIN KIM, SUNWOUK YI, MINJUN LEE, HANHO LEE, HOYEON JEON, YONGCHAN YOO, INHAE ZOH, CHAO ZHANG, MYUNGCHUL OH, YOUNG KUK, Department of Physics and Astronomy, Seoul National University — The electronic properties of Co-doped BaFe<sub>2</sub>As<sub>2</sub> (BFCA) iron pnictide superconductors were studied using scanning tunneling microscopy and spectroscopy. BFCA samples with superconducting transition temperatures 22-27 K, were grown on SrTiO<sub>3</sub>(100) by pulsed laser deposition (PLD) growth under ultrahigh vacuum condition. As-grown surfaces revealed  $2 \times 2$  or  $2\sqrt{2} \times 2\sqrt{2}$  structures as a function of bias voltage at 4.3 K. Missing row structures were also observed on as-grown samples, suggesting many nucleation sites and resultant antiphase boundaries. The I-V and dI/dV spectra were deviated from the bulk spectrum obtained by contact conductance measurement. After removing surface layers by ion beam sputtering, different spectra were observed. The obtained spectra were explained with the surface state effect in BFCA samples as compared with DFT calculations.

**2:54PM V23.00003 Elasto-Scanning Tunneling Microscopy: Visualizing the Coupling of Strain to Electronic Nematicity in NaFeAs**, ERICK ANDRADE, AYELETE NOTIS, Columbia Univ, LINGYI XING, XIANCHENG WANG, CHANGQING JIN, Institute of Physics, Chinese Academy of Sciences, ABHAY PASUPATHY, Columbia Univ — Electronic nematicity is a widely observed phenomenon in the pnictide superconductors. In this phenomenon, the electronic structure breaks four-fold rotational symmetry and displays anisotropic behavior that can be observed in several transport and spectroscopic measurements. Understanding the driving force for the nematicity and its relationship to superconductivity remains a key goal in these materials. Motivated by transport measurements that indicate that the nematicity is strongly coupled to crystal strain, we developed a new experimental technique by which tunable uniaxial strain can be applied to a crystal while scanning tunneling microscopy is performed on the crystal surface. The technique allows us to track the same atomically resolved area of the sample as a function of strain. Using this new technique, we measure the response of the local density of states to strain in the tetragonal and orthorhombic phases of the crystal. In the orthorhombic phase, we find that strain can move structural domain walls but does not affect the magnitude of the electronic nematicity. On the other hand, in the tetragonal phase we find that strain controls the magnitude of the electronic nematicity, indicating that the material is in a paranematic state above the structural transition.

**3:06PM V23.00004 Quantum phase transition in Fe<sub>1+x</sub>(Te,Se) induced by Single-atomic Impurities studied by STM/S**, J. X. YIN, Institute of Physics, CAS, ZHENG WU, TcSUH University of Houston, XIONG HUANG, Z. Y. YE, RUI WU, X. J. LIANG, H. Q. MAO, JIAN LI, Institute of Physics, CAS, C. -S. TING, TcSUH University of Houston, J. P. HU, Institute of Physics, CAS, Z. Q. WANG, Boston College, P.-H. HOR, TcSUH University of Houston, HONG DING, S. H. PAN, Institute of Physics, CAS; Collaborative Innovation Center of Quantum Matter — Previously we discovered a robust zero-energy bound state at an interstitial Fe impurity (IFIs) in Fe<sub>1+x</sub>(Te,Se), which resembles the Majorana mode (Nature Physics **11**, 543, (2015)). Here we report our comprehensive study, using scanning tunneling microscopy/spectroscopy technique, of the global effect of IFIs on the ground state of Fe<sub>1+x</sub>(Te,Se) over a wide range of IFI concentration  $x$ . Our high resolution tunneling spectroscopy and quasi-particle interference data at very low temperature demonstrate that IFIs do not affect the electron pairing strength, while they cause significant dephasing effect, which eventually drives the ground state of the system from strong-coupling-superconductivity to diffusive-Bose-metal.

**3:18PM V23.00005 Reconciling STS and ARPES data for the correlated superconductor LiFeAs**, JONGBAE HONG, Center for Theoretical Physics of Complex Systems, Institute for Basic Science, DAVID ABERGEL, Nordita, KTH Royal Institute of Technology and Stockholm University, Roslagstullsbacken 23, SE-106 91 Stockholm, Sweden — The inconsistency between the density of states revealed by scanning tunneling spectroscopy (STS) and that given by angle-resolved photoemission spectroscopy (ARPES) is a substantial problem for understanding the nature of strongly correlated superconductors such as Fe-based LiFeAs and the cuprates. We reveal that the two side peaks commonly appearing in both pnictide and cuprate superconductors are the result of the non-equilibrium behavior associated with singlet cotunneling from the tip to the strongly correlated sample [1]. We accurately reproduce the STS line shape of the Fe-based LiFeAs using a sample density of states which coincides with ARPES data, thereby producing a unified description for these materials. [1] Jongbae Hong and D.S.L. Abergel, arXiv:1411.5532.

**3:30PM V23.00006 Anticorrelation between the parent charge transfer gap and maximum transition temperature in cuprates**, WEI RUAN, State Key Laboratory of Low Dimensional Quantum Physics, Department of Physics, Tsinghua University, CHENG HU, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, PENG CAI, State Key Laboratory of Low Dimensional Quantum Physics, Department of Physics, Tsinghua University, YINGYING PENG, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, XINTONG LI, ZHENQI HAO, State Key Laboratory of Low Dimensional Quantum Physics, Department of Physics, Tsinghua University, XINGJIANG ZHOU, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, ZHENG-YU WENG, Institute for Advanced Studies, Tsinghua University, YAYU WANG, State Key Laboratory of Low Dimensional Quantum Physics, Department of Physics, Tsinghua University — We use scanning tunneling spectroscopy to measure the electronic structure of the parent Mott insulator of three different types of cuprates. The charge transfer gap size exhibits pronounced variations, and more interestingly it shows an anticorrelation with the maximum superconducting transition temperature achieved at the optimal doping of each cuprate. This result suggests that the Mottness in parent cuprate plays a crucial role in determining the superconducting properties. In particular, reducing the electron correlation strength enhances superconductivity, which is consistent with the pairing mechanism based on the doped Mott insulator picture.

**3:42PM V23.00007 STM sub-gap structure in cuprates is a consequence of density waves, according to Mean-Field Theory and CDMFT<sup>1</sup>**, SIMON VERRET, Université de Sherbrooke, JYOTIRMOY ROY, TIFR Mumbai India, DAVID SÉNÉCHAL, A.-M. S. TREMBLAY, Université de Sherbrooke — Much work has been done to find how the pseudogap is related to charge density waves in cuprates. In scanning tunneling microscopy (STM) measurements, the superconducting gap and pseudogap of cuprates are sometimes accompanied by a small *sub-gap structure* at very low energy. This was documented early in vortex cores studies, and has now been reported at zero field for YBCO.(1) Here, we show that this can be caused by density waves, first through a standard mean-field approach, and then with Cellular Dynamical Mean-Field Theory for the Hubbard model using an exact diagonalization solver. We comment on the implication of these results for the relation between pseudogap and charge order. (1) Jens Bruér et al. arXiv:1507.06775

<sup>1</sup>Supported by NSERC, CIFAR and the Tier I Canada Research Chair Program

**3:54PM V23.00008 Theoretical visualization of charge order in cuprates**, PEAYUSH CHOUBEY, University of Florida, WEI-LIN TU, National Taiwan University, TING-KUO LEE, Institute of Physics, Academia Sinica, Taiwan., PETER HIRSCHFELD, University of Florida — The anti-phase charge density wave (AP-CDW) state obtained in [1] by solving the renormalized mean-field theory of the t-J model was shown to have a dominant d-form factor for the bond order. However, the local density of states (LDOS) is only defined at the Cu lattice site. In order to compare with scanning tunneling microscopy (STM) experiments [2] in detail, we compute the continuum LDOS in the AP-CDW state at typical STM tip heights using Bi<sub>2</sub>Sr<sub>2</sub>Ca<sub>2</sub>CuO<sub>2</sub> Wannier functions obtained from first principles [3]. The resulting spatial patterns compare very well with experimental results, and show the important role of the planar O2p states filtered through the BiO and SrO layers. In addition, we compute the Cu and O sublattice LDOS and Fourier transform it to obtain the amplitudes of s, s' and d-form factors actually reported in an STM experiment [4]. References:

1. Wei-Lin Tu and Ting-Kuo Lee, arXiv: 1505.07728.
2. Kazuhiro Fujita *et al.*, Proc. Natl. Acad. Sci. 111 30 (2014).
3. A. Kreisel *et al.*, Phys. Rev. Lett. 114, 217002 (2015).
4. M. H. Hamidian *et al.*, arXiv: 1507.07865.

**4:06PM V23.00009 Direct Local Measurement of the Superconducting Energy Gap of Nb doped SrTiO<sub>3</sub>**, JEONGHOON HA, Center for Nanoscale Science and Technology/NIST, Maryland NanoCenter/UMCP, Natl High Magnetic Field Lab/FSU, GURU KHALSA, FABIAN NATTERER, Center for Nanoscale Science and Technology/NIST, HONGWOO BAEK, Center for Nanoscale Science and Technology/NIST, Dept. of Phys. and Astro./SNU, Natl High Magnetic Field Lab/FSU, WILLIAM G. CULLEN, Center for Nanoscale Science and Technology/NIST, Maryland NanoCenter/UMCP, YOUNG KUK, Dept. of Phys. and Astro./ Seoul Natl Univ., JOSEPH A. STROSCIO, Center for Nanoscale Science and Technology/NIST — Strontium titanate (STO) is a perovskite metal oxide insulator that can be electron doped by substitution of Ti or Sr sites with Nb or La, respectively, or by oxygen vacancies. When doped to high electron densities with concentration in the range of  $5 \times 10^{19} \text{ cm}^{-3}$  to  $2 \times 10^{20} \text{ cm}^{-3}$ , STO becomes superconducting with a transition temperature below 400 mK, at a value highly dependent on the doping concentration. Previous observations were made on bulk crystals or films of doped STO by measuring the transitions in resistivity, magnetic susceptibility or thermal conductivity as a function of temperature or magnetic field. In this work, we use an ultra-low temperature scanning tunneling microscope (STM) to investigate the local electronic structure of the surface of Nb doped STO. The tunneling spectra taken at a sample temperature of  $\approx 10$  mK reveal a BCS energy gap of  $\Delta = 40$   $\mu\text{eV}$ . Temperature and magnetic field dependent tunneling measurements show a critical temperature of  $\approx 250$  mK and upper critical field of  $\approx 0.07$  T. This is the first report of direct measurement of superconducting STO using an STM.

#### 4:18PM V23.00010 Multiband superconductivity in $2H\text{-NbSe}_2$ probed by Doppler-modulated scanning tunneling spectroscopy<sup>1</sup>

, I. FRIDMAN, Quantum Applied Science and Research, Inc., C. KLOC, Nanyang Technological University, Singapore, C. PETROVIC, Brookhaven National Laboratory, J. Y. T. WEI, University of Toronto and Canadian Institute for Advanced Research — Cooper pairing in multiband superconductors can involve carriers from bands having different dimensionalities, and the interband coupling can provide for novel pairing interactions. In addition to  $\text{MgB}_2$ , recent experiments on  $2H\text{-NbSe}_2$  have studied the Fermi surface topology using angle- and temperature-dependent scanning tunneling spectroscopy.[1] We present another novel method for probing multiband pairing: using a field-induced diamagnetic supercurrent, applied along different crystal axes, to perturb the quasiparticle density-of-states spectrum. By measuring the evolution of the quasiparticle spectrum under finite superfluid momentum, we characterize the pairing gaps and gap anisotropies. This approach is demonstrated on  $2H\text{-NbSe}_2$  at 300 mK with a magnetic field of up to 9 T applied in the *ab*-plane.[2] The STM measurements revealed unambiguous evidence for multiband pairing, and evidence for a novel transition of the in-plane vortex lattice. We discuss the characteristics of this transition in light of data from other probes. [1] Y. Noat *et al.*, Phys. Rev. B 92, 134510 (2015). [2] I. Fridman *et al.*, Applied Physics Letters 99, 192505 (2011).

<sup>1</sup>Work supported by NSERC, CFI/OIT, CIFAR, U.S. DOE and Brookhaven Science Associates (No. DE-AC02-98CH10886).

#### 4:30PM V23.00011 Coherent long-range magnetic bound states in a superconductor

, GERBOLD MENARD, Univ Pierre et Marie Curie, SEBASTIEN GUISSART, Laboratoire de physique des solides, CHRISTOPHE BRUN, STEPHANE PONS, VASILY STOLYAROV, FRANCOIS DEBONTRIDDER, MATTHIEU LECLERC, Institut des nanosciences de Paris, ETIENNE JANOD, LAURENT CARIO, Institut des Materiaux Jean Rouxel, DIMITRI RODITCHEV, Institut des nanosciences de Paris, PASCAL SIMON, Laboratoire de physique des solides, TRISTAN CREN, Institut des nanosciences de Paris — Using low temperature scanning tunneling spectroscopy we accessed to localized states called Shiba states associated to magnetic impurities as well as their spatial dependence [1]. We studied samples of superconducting  $\text{NbSe}_2$  containing a really small concentration of native magnetic impurities. We observed the appearance of star-shaped structures around individual impurities with a size of the order of the coherence length of the superconductor ( $\approx 10$  nm). The fine study of our data revealed an oscillation of the density of states along the star branches. To further analyze our results, we performed tight-binding calculations which reproduced the observed spatial symmetry. A semi-analytical calculation also enabled us to establish a relation between the different spatial scales observed and the physical quantities associated to superconductivity, and to understand the role of dimensionality in such systems. [1] Nature Physics (2015), DOI:10.1038/NPHYS3508

#### 4:42PM V23.00012 Creating nanostructured superconductors on demand by local current annealing

, HONGWOO BAEK, Center for Nanoscale Science and Technology/NIST, Dept. of Phys. and Astro./SNU, JEONGHOON HA, DUMING ZHANG, BHARATH NATARAJAN, Center for Nanoscale Science and Technology/NIST, Maryland NanoCenter/UMCP, RONGWEI HU, KEFENG WANG, STEVEN ZIEMAK, JOHNPIERRE PAGLIONE, Dept. of Phys./UMCP, YOUNG KUK, Dept. of Phys. and Astro./SNU, JONATHAN P. WINTERSTEIN, RENU SHARMA, NIKOLAI B. ZHITENEV, JOSEPH A. STROSCIO, Center for Nanoscale Science and Technology/NIST — When the effective size of a superconductor becomes comparable to the characteristic length scales, dramatic changes can occur in the superconducting properties that allow various applications in quantum devices. However, challenges remain in controlling the shape and size of specific superconducting materials. Here, we report on a method to create nanostructured superconductors by partial crystallization of the half-Heusler material,  $\text{YPtBi}$  using scanning tunneling microscopy. Superconducting islands, with diameters in the range of 100 nm, were reproducibly created by local current annealing of disordered  $\text{YPtBi}$  in the tunneling junction. Tunneling spectra measured on the islands showed non-Bardeen-Cooper-Schreffer behavior with different energy gaps and critical values as a function of spatial position. With increasing magnetic field, conductance maps showed the sequential addition of single vortices in the nanostructure, which fused into a giant vortex ring at 1.25 T. These results demonstrate an interesting method of creating tailored superconductors with complex materials for future applications [1]. [1] H. Baek *et al.*, Phys. Rev. B 92, 094510 (2015).

#### 4:54PM V23.00013 Magnetic field dependence of the density of states and tilted vortex lattice in the superconductor $\beta\text{-Bi}_2\text{Pd}$

, EDWIN HERRERA-VASCO, ISABEL GUILLAMON, ANTON FENTE, Universidad Autonoma de Madrid, JOSE GALVIS, Universidad Central, ALEXANDRE CORREA, ROBERTO LUCCAS, FEDERICO MOMPEAN, MAR GARCIA HERNANDEZ, Instituto de Ciencia de Materiales, Consejo Superior de Investigaciones Cientificas, JEAN P. BRISON, Universite Grenoble Alpes, CEA, INAC-SPSMS, SEBASTIAN VIEIRA, HERMANN SUDEROW, Universidad Autonoma de Madrid — We present very low-temperature scanning tunneling microscopy (STM) experiments on the superconductor  $\beta\text{-Bi}_2\text{Pd}$ . We find a single superconducting gap from the zero-field tunneling conductance. We also find that the hexagonal vortex lattice is locked to the square atomic lattice. The magnetic field dependence of the intervortex tunneling conductance is higher than the one expected in a single-gap superconductor. Such an increase in the intervortex tunneling conductance has been found in superconductors with multiple superconducting gaps. We fit the upper critical field  $H_{c2}(T)$  and show that multiband Fermi surface is needed to explain the observed behavior. We propose that  $\beta\text{-Bi}_2\text{Pd}$  is a single-gap multiband superconductor. We have measured the tilted vortex lattice (TVL) using a three axis superconducting magnet. Our results give first real space imaging of the TVL in a nearly isotropic s-wave BCS superconductor. From a detailed study of the TVL varying polar and azimuthal angles, we find correlations between the square atomic lattice and the TVL.

#### 5:06PM V23.00014 Josephson STM at mK temperatures: Coupling to the electronic environment<sup>1</sup>

, MICHAEL DREYER, RAMI DANA, WAN-TING LIAO, CRIS LOBB, FRED WELLSTOOD, BOB ANDERSON, University of Maryland — Ultra-small Josephson junctions can couple to modes in the electronic environment. This leads to sub-gap peaks in the  $I(V)$  curve in addition to the phase diffuse supercurrent. The  $I(V)$  curve can - in principle - be explained by  $P(E)$  theory [1] which describes the probability of tunneling at energy  $E$ . A recent study [2] showed that antenna modes of the STM tips could be responsible for the observed sideband structures. In our case the explanation appears to be less simple. We employ a dual tip STM at a temperature of 30 mK [3]. The  $I(V)$  spectra of the two tips show distinct patterns with only one shared mode. While the supercurrent branch for the "inner" tip is visible, it is obscured by a resonance for the outer tip. Possible causes and applications to other systems will be discussed. [1] G.-L. Ingold, H. Grabert, U. Eberhardt, PRB 50(1), 395 (1994) [2] Berthold Jäck, *et. al.*, Appl. Phys. Lett. 106, 013109 (2015) [3] Anita Roychowdhury, *et. al.*, Rev. Sci. Inst., 85, 043706 (2014)

<sup>1</sup>Support from NSF (DMR- 0605763) and Laboratory for Physical Sciences

#### 5:18PM V23.00015 Friedel oscillations and quasiparticle interference: Complementary STM and REXS approach

, PEGOR AYNANIAN, Binghamton University, ANDRS GYENIS, Princeton University, EDUARDO DA SILVA NETO, University of British Columbia, FEIZHOU HE, RONNY SUTARTO, Canadian Light Source, ENRICO SCHIERLE, EUGEN WESCHKE, BESSY, MARIAM KAVAI, Binghamton University, RYAN BAUMBACH, Florida State University, JOE THOMPSON, ERIC BAUER, LANL, ZACHARY FISK, UC Irvine, ANDREA DAMASCELLI, University of British Columbia, ALI YAZDANI, Princeton University — The origin of a competing charge ordering in the high-temperature superconducting cuprates has recently been subject to intense experimental and theoretical debates. Dalla Torre *et al* theoretically proposed that Friedel oscillations can reproduce the experimentally observed scattering peak in the resonant elastic x-ray scattering (REXS) of cuprates [NJP, 17 022001 2015]. Using complementary spectroscopic imaging with the scanning tunneling microscope and REXS on the heavy fermion compound  $\text{CeMn}_5$  ( $M=\text{Co, Rh}$ ) we observe a scattering peak in REXS, similar, yet broader than that found in cuprates. Through temperature and doping dependent experiments, we demonstrate this enhanced peak to originate from the scattering of hybridized heavy *f*-electrons. We discuss the origin of this phenomenon and its relation to Friedel oscillations and charge ordering.

# Thursday, March 17, 2016 2:30PM - 5:18PM —

Session V24 DMP: Electron Transport at Nanoscale Interfaces 323 - Giacomo Lovat, Columbia University

## 2:30PM V24.00001 Ligand engineering of nanoparticle solar cells<sup>1</sup>, MARTON VOROS, Argonne Natl Lab —

Semiconductor nanoparticles (NP) are promising materials to build cheap and efficient solar cells. One of the key challenges in their utilization for solar energy conversion is the control of NP surfaces and ligand-NP interfaces. Recent experiments have shown that by carefully choosing the ligands terminating the NPs, one can tailor electronic and optical absorption properties of NP assemblies, along with their transport properties.[1] By using density functional theory based methods, we investigated how the opto-electronic properties of lead chalcogenide NPs may be tuned by using diverse organic and inorganic ligands. We interpreted experiments, and we showed that an essential prerequisite to avoid detrimental trap states is to ensure charge balance at the ligand-NP interface, possibly with the help of hydrogen treatment. [1] R. Crisp et al., Scientific Reports 5, 9945 (2015); C. Giansante et al., J. Am. Chem. Soc. 137, 1875 (2015).

<sup>1</sup>Work supported by the Center for Advanced Solar Photophysics, an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Office of Basic Energy Sciences.

## 3:06PM V24.00002 The effect of Ta "oxygen scavenger layer" on HfO<sub>2</sub>-based resistive switching behavior: thermodynamic stability, electronic structure, and low-bias transport, XIAOLIANG ZHONG,

Argonne Natl Lab, IVAN RUNGGER, Materials Division, National Physical Laboratory, TW11 0LW, UK, PETER ZAPOL, Argonne National Laboratory, HISAO NAKAMURA, YOSHIHIRO ASAI, National Institute of Advanced Industrial Science and Technology (AIST) Japan, OLLE HEINONEN, Argonne National Laboratory and Northwestern University — Metal-oxide-metal heterostructures are promising candidates for next-generation random access memories, which exhibit reversible resistive switching between high- and low-conductance states. Recent experimental work showed that inserting a metallic 'oxygen scavenger layer' between TiN electrode and HfO<sub>2</sub> significantly improves device switching performance. We show, using atomistic modeling within the GGA+U scheme of Density Functional Theory, that a Ta oxygen scavenger layer significantly enhances the thermodynamic stability of depleting oxygen from the oxide. Furthermore, the presence of a Ta layer reduces the dependence of the Schottky barrier heights on the location of the oxygen removed from the oxide matrix. Finally, the Schottky barrier height has a very small effect on the on-state low-bias conductance; this is more sensitive to the location of the depleted oxygen. We gratefully acknowledge the computing resources provided on Blues, a high-performance computing cluster operated by the Laboratory Computing Resource Center at Argonne National Laboratory. Work at Argonne was supported by U. S. DOE, Office of Science under Contract No. DE-AC02-06CH11357.

## 3:18PM V24.00003 Band alignment study on Al/SiO<sub>2</sub> and Cu/SiO<sub>2</sub> metal-oxide interface with the presence of point defect<sup>1</sup>, JIANQIU HUANG<sup>2</sup>, ERIC TEA<sup>3</sup>, CELINE HIN<sup>4</sup>, Virginia Tech —

Metal-Oxide interface has a wide use in electronic devices. Currently, technological development is aiming on the shrinkage of electronic devices' size. Based on the knowledge of electron tunneling effect, the reduction of dielectric thickness would cause an exponential increase on electron tunneling probability which contributes to current leakage. It might cause dielectric breakdown, which could make a severe and irreversible damage to the devices. Therefore, the main purpose of this study is to explore the possible factors that can lead to dielectric breakdown at metal-oxide interface. Density functional theory *ab initio* calculation has been applied to study the Al/SiO<sub>2</sub> and Cu/SiO<sub>2</sub> metal-oxide interface. Results on oxygen (di)vacancies at the interface will be presented and compared with the defect free model. The band alignment has been constructed to describe the variation of potential barrier height due to defect at interface. Results show the oxygen (di)vacancies at interface might trap electron and reduce potential barrier height. Moreover, the potential barrier height has a significant dependence on defects charge states.

<sup>1</sup>Supported by Air Force

<sup>2</sup>Ph.D student

<sup>3</sup>Pos Doctoral

<sup>4</sup>Advisor

## 3:30PM V24.00004 Voltage mediated metal to insulator transition in VO<sub>2</sub> and V<sub>2</sub>O<sub>3</sub> nanodevices<sup>1</sup>, ILYA VALMIANSKI, Physics Department, UC San Diego, J. GABRIEL RAMIREZ, Physics Department, Universidad de los Andes,

SIMING WANG, Livermore Berkeley National Laboratory, STEFAN GUENON, Physics Department, University of Tuebingen, IVAN K. SCHULLER, Physics Department, UC San Diego — We investigate the mechanism of the voltage mediated MIT in a series of vanadium oxides (VO<sub>2</sub> and V<sub>2</sub>O<sub>3</sub>) nano-scopc devices. All films presented ~4 orders of magnitude resistance change at the MIT. The devices consist of in-plane gold electrodes with 200 nm wide tip on top of lithographically defined vanadium oxide films. The gap size between electrodes was fixed at 140 nm. Unlike micron-scale devices, the current-voltage characteristics in nano-scale V<sub>2</sub>O<sub>3</sub> cannot be accounted solely by an inhomogeneous joule-heating model, suggesting additional mechanisms may be playing a role in the switching behavior. However, in the case of nano-scopc VO<sub>2</sub> devices, it may be possible to explain the results with only inhomogeneous heating. We perform detailed electrical and thermal Finite Element Method (FEM) calculations on both the VO<sub>2</sub> and V<sub>2</sub>O<sub>3</sub> devices. We couple the FEM analysis with a variety of theoretical models, which can shed light on the nanoscopic nature of the MIT in VO<sub>2</sub> and V<sub>2</sub>O<sub>3</sub>.

<sup>1</sup>Work supported by AFOSR.

## 3:42PM V24.00005 Ferroelectric Modulation of Two-dimensional Electron Gas Conductivity at Oxide Interfaces, WENXIONG ZHOU, JUN ZHOU, KUN HAN, SHENGWEI ZENG, ZHEN HUANG, THIRUMALAI VENKATESAN, ARIANDO

ARIANDO, Natl Univ of Singapore, NUSNNI-NANOCORE, NATIONAL UNIVERSITY OF SINGAPORE, SINGAPORE 117411 TEAM, DEPARTMENT OF PHYSICS, NATIONAL UNIVERSITY OF SINGAPORE, SINGAPORE 117542 TEAM, DEPARTMENT OF ELECTRICAL AND COMPUTER ENGINEERING, NATIONAL UNIVERSITY OF SINGAPORE, SINGAPORE 11757 TEAM — In this report, by inserting a ferroelectric Ba<sub>0.2</sub>Sr<sub>0.8</sub>TiO<sub>3</sub> layer between LaAlO<sub>3</sub>/SrTiO<sub>3</sub> heterostructure, a two-dimensional electron gas (2DEG) was found at LaAlO<sub>3</sub>/Ba<sub>0.2</sub>Sr<sub>0.8</sub>TiO<sub>3</sub> interface. With electrical, optical, piezoresponse force microscopic measurements and first-principle calculations, we studied the impact of this ferroelectric Ba<sub>0.2</sub>Sr<sub>0.8</sub>TiO<sub>3</sub> layer on the 2DEG. Both carrier density and mobility of the 2DEG can be modulated by changing the thickness of the ferroelectric layer. We also observed that Ba<sub>0.2</sub>Sr<sub>0.8</sub>TiO<sub>3</sub> layer can suppress oxygen vacancy formation, leading to observation of temperature-independent polarization-induced carrier density. These results indicate that the 2DEG at oxide interfaces can be ferroelectrically modulated.

## 3:54PM V24.00006 Energy Level Alignment at the Interface between Linear-Structured Benzenediamine Molecules and Au(111) Surface, GUO LI, TONATIUH RANGEL, ZHENFEI LIU, Lawrence Berkeley Natl Lab,

VALENTINO COOPER, Oak Ridge Natl Lab, JEFFREY NEATON, Lawrence Berkeley Natl Lab; UC-Berkeley; Kavli Energy NanoSciences Institute at Berkeley — Using density functional theory with model self-energy corrections, we calculate the adsorption energetics and geometry, and the energy level alignment of benzenediamine (BDA) molecules adsorbed on Au(111) surfaces. Our calculations show that linear structures of BDA, stabilized via hydrogen bonds between amine groups, are energetically more favorable than monomeric phases. Moreover, our self-energy-corrected calculations of energy level alignment show that the highest occupied molecular orbital energy of the BDA linear structure is deeper relative to the Fermi level relative to the isolated monomer and agrees well with the values measured with photoemission spectroscopy. This work supported by DOE.

**4:06PM V24.00007 Theory of work function tuning via mixed-monolayers on functional surfaces<sup>1</sup>**, MICHELE KOTIUGA, Physics Department, UC Berkeley & The Molecular Foundry, LBNL, PIERRE DARANCET, The Center for Nanoscale Materials, ANL, JEFFREY B. NEATON, Physics Department, UC Berkeley, The Molecular Foundry, LBNL & Kavli Energy NanoSciences Institute at Berkeley, Berkeley, CA — Self-assembled monolayers (SAMs) provide both stability and functionality of surfaces useful in optoelectronic nanoscale devices. The work function, level alignment and other electronic properties of functionalized surfaces can be tuned with the choice of molecule and an even finer control of the properties can be obtained with a SAM comprised of multiple types of molecules [1]. Modeling the effect on electronic properties of mixed-monolayers via ab initio calculations poses a challenge due to the large supercell required to capture a range of relative concentrations between the two types of molecules. Here, we present an implicit model - fit from density functional theory calculations - capturing local electrostatic interactions within the SAM primarily due to depolarization of the induced dipoles formed upon binding [2]. This quantitative model allows us to explore supercells with a large number of molecules and, thus, surface concentrations that are inhomogeneous in nature. We compare to experimental results of thiol terminated carboranes on gold [1]. [1] Kim et al., Nano Lett. 14, 2946 (2014) [2] Kotiuga et al., Nano Lett. 15, 4498 (2015)

<sup>1</sup>Supported by AFOSR MURI FA9550-12-1-0002 and U.S. DOE under Contract Nos. DE-AC02-06CH1135 & DE-AC02-06CH1231

**4:18PM V24.00008 Giant spatially-resolved self-assembled donor-acceptor molecular heterojunctions<sup>1</sup>**, JEFFREY R. GUEST, Center for Nanoscale Materials, Argonne National Laboratory, Argonne, IL, USA, JOSEPH A. SMERDON, Jeremiah Horrocks Institute of Mathematics, Physics and Astronomy, University of Central Lancashire, Preston, UK, NOEL C. GIEBINK, Department of Electrical Engineering, The Pennsylvania State University, University Park, PA, USA, NATHAN P. GUISENGER, PIERRE DARANCET, Center for Nanoscale Materials, Argonne National Laboratory, Argonne, IL, USA — Despite theoretical models predicting that rectification ratios (RR) >1000 should be achievable in molecular rectifiers, demonstrations of this have been rare. It has also been extremely challenging to unravel the structure-function relationships on the nanometer length scales that determine their behavior. Using scanning tunneling microscopy (STM) and spectroscopy (STS), we show that RRs >1000 at biases <500 mV are realized in the two-molecule limit for self-assembled donor-acceptor bilayers of pentacene on C<sub>60</sub> on Cu. We show that the system behaves as a molecular analog to a Schottky diode due to strong electronic coupling of C<sub>60</sub> to the metallic substrate, and electronic transport is dominated by sequential tunneling from semiconducting pentacene to metallic C<sub>60</sub>. Furthermore, we demonstrate the extreme sensitivity of the low-bias  $I(V)$  characteristics to the molecularly-resolved structure of the heterojunction (HJ), which leads to negative differential resistance and  $\sim 100\times$  variation in the rectification ratio within 2 nm of the edge of the molecular HJ.

<sup>1</sup>Support was provided by the Department of Energy Office of Basic Energy Sciences (SISGR Grant DE-FG02-09ER16109).

**4:30PM V24.00009 Transient magnetization of core excited organic molecules adsorbed on graphene<sup>1</sup>**, ABHILASH RAVIKUMAR, ANU BABY, HE LIN, GIAN PAOLO BRIVIO, Department of Materials Science, University of Milano-Bicocca, Milano, Italy, GUIDO FRATESI, Department of Physics, University of Milano, Milano, Italy — This work presents a density functional theory based computational investigation of electronic and magnetic properties of physisorbed and chemisorbed organic molecules on graphene in the ground state and core excited one at low molecular coverage. For physisorbed molecules, where the interaction with graphene is dominated by van der Waals forces and the system is non-magnetic in the ground state, it is found that the valence electrons relax towards a spin polarized configuration upon excitation of a core-level electron. The magnetism depends on efficient electron transfer from graphene on the femtosecond time scale. On the contrary, when graphene is covalently functionalized, the system is magnetic in the ground state presenting two spin dependent mid gap states localized around the adsorption site. At variance with the physisorbed case upon core-level excitation, the LUMO of the molecule and the mid gap states of graphene hybridize and the relaxed valence shell is not magnetic anymore.

<sup>1</sup>This project has received funding from the European Union Seventh Framework Programme under grant agreement n° 607232 [THINFACE]

**4:42PM V24.00010 Probing the molecular structure of doped sites within crystals by Pyroelectricity and Dispersion Corrected DFT modeling**, ELENA MEIRZADEH, IDO AZURI, DAVID EHRE, Weizmann Institute of Science, ANDREW M. RAPPE, University of Pennsylvania, MEIR LAHAV, LEEOR KRONIK, IGOR LUBOMIRSKY, Weizmann Institute of Science — We describe the analysis of polar architectures at the nanoscale by pyroelectric measurements and DFT. Controlled doping of crystals is a primary tool for modification of the properties of materials. Doping of non-polar molecular crystals with “tailor-made” auxiliaries often reduces their symmetry, and converts them into polar mixed crystals. Such crystals are pyroelectric, *i.e.* they display temporary surface charge if subjected to a temperature change. When the non-polar crystals of the amino-acids are doped with different amino acids of concentrations as low as <0.2%, they display measurable pyroelectric effect. Since such minute amount of guest creates measurable macroscopic polarization, implies a local polar dislocation of the neighboring host molecules. We demonstrate here, that the value and the temperature dependence of the pyroelectric coefficient, provides intimate information on the molecular packing arrangement of the doped sites. Different amino acids as dopants induce different pyroelectric effects: The pyroelectric coefficient is a) not temperature dependent; b) changes its sign upon heating. These differences were explained by the determination of the polar domains at the molecular level by the DFT.

**4:54PM V24.00011 ABSTRACT WITHDRAWN —**

**5:06PM V24.00012 Theory of Giant Rectification in Molecular Schottky Diodes<sup>1</sup>**, PIERRE DARANCET, Argonne Natl Lab — Following early theoretical models [1], efforts towards the synthesis and characterization of more efficient molecular diodes have consisted into attempts to increase the electron rich/poor characters of the donor/acceptor moieties, decrease their conjugation, and imbalance their coupling to the electrodes. The experimental poor performance of single-molecule diodes – with the notable exception of environment-induced diodes [2] – suggests that these physical parameters tend to be mutually exclusive in most molecular systems [3]. In this talk, inspired by recent observations of large rectification ratios at organic bilayers [4], we will show how molecules with a moiety strongly coupled to a metal electrode can, in principle, be used to optimize these different aspects simultaneously. Using first-principles calculations, we will show that this class of molecular systems –analog to macroscopic Schottky diodes, can display large rectification ratios at low operating voltages. [1] Taylor et al. Phys. Rev. Lett. 89, 138301 (2002); Andrews et al. JACS 130, 17309 (2008); [2] Capozzi et al. Nat. Nano 10, 522 (2015); [3] Mujica et al. Chem. Phys. 281, 147 (2002); Stokbro et al. JACS 125, 3674 (2003) ; [4] Smerdon et al., submitted.

<sup>1</sup>The submitted manuscript has been created by UChicago Argonne, LLC, Operator of Argonne National Laboratory (Argonne). Argonne, a U.S. Department of Energy Office of Science laboratory, is operated under Contract No. DE-AC02-06CH11357.

**Thursday, March 17, 2016 2:30PM - 5:18PM –**

**Session V25 DCMP: Superconductivity: Superconductor-Insulator Transitions** 324 - Eleanor Clements, University of South Florida

**2:30PM V25.00001 Negative magneto resistance and anisotropic transport in DC biased superconducting Ta films**, JUNGHYUN SHIN, SUNGYU PARK, EUNSEONG KIM, Center for Supersolid & Quantum Matter Research and Department of Physics, KAIST, Daejeon, 305-701, Republic of Korea — We investigated the field-tuned superconductor-insulator transition in DC biased Ta thin films. Differential resistance in direction parallel (x axis) and perpendicular (y axis) to DC bias (x axis) was measured simultaneously as functions of DC bias and magnetic field. The DC biased magneto-resistance,  $dV/dI$ , showed anisotropy; differential magneto-resistance exhibited peaks at high DC bias in the parallel measurements while monotonic increase in  $dV/dI$  was obtained in the perpendicular measurements. Besides, the critical fields determined by magneto-resistance isotherms cross-over reveal substantially different values depending on the measurement directions. Furthermore, the E-field scaling exponents show different values of 1.33 in perpendicular direction and of 0.82 in parallel direction which cannot be simply understood by the temperature scaling with electron heating.

**2:42PM V25.00002 Signature of Cooper pairs in the Metallic and Insulating Phases of Homogeneously Disordered Superconducting Ta Films<sup>1</sup>**, YIZE STEPHANIE LI, California State University, Bakersfield — With the increase of magnetic field or the decrease of sample thickness, homogeneously disordered superconducting Ta films undergo a superconductor-metal-insulator phase transition [1][2]. Each phase displays remarkably different nonlinear current-voltage (I-V) characteristics. The evolution of the nonlinear transport in the insulating phase exhibits a non-monotonic behavior as the magnetic field is increased, which could be evidence of the presence of localized Cooper pairs in the insulating phase [3]. As the metallic phase intervenes the superconducting and insulating states in Ta films, we further suggest that Cooper pairs also exist in the metallic ground state. References: [1] Y. Qin et al., Phys. Rev. B 73, 100505(R) (2006). [2] Y. Li et al., Phys. Rev. B 81, 020505 (R) (2010). [3] Y. S. Li, Supercond. Sci. Technol. 28, 025002 (2015).

<sup>1</sup>Data acquisition for this work was completed at the University of Virginia.

**2:54PM V25.00003 Superconductor-Insulator Transition and Fermi-Bose Crossovers<sup>1</sup>**, NANDINI TRIVEDI, The Ohio State University, YEN LEE LOH, University of North Dakota, MOHIT RANDEIRA, The Ohio State University, CHIA-CHEN CHANG, RICHARD SCALETTAR, University of California, Davis — The direct transition from an insulator to a superconductor (SC) in Fermi systems is a problem of long-standing interest, which necessarily goes beyond the standard BCS paradigm of superconductivity as a Fermi surface instability. We introduce here a simple, translationally-invariant lattice fermion model that undergoes a SC-insulator transition (SIT) and elucidate its properties using analytical methods and quantum Monte Carlo simulations. We show that there is a fermionic band insulator to bosonic insulator crossover in the insulating phase and a BCS-to-BEC crossover in the SC. The SIT is always found to be from a bosonic insulator to a BEC-like SC, with an energy gap for fermions that remains finite across the SIT. The energy scales that go critical at the SIT are the gap to pair excitations in the insulator and the superfluid stiffness in the SC. In addition to giving insights into important questions about the SIT in solid state systems, our model should be experimentally realizable using ultracold fermions in optical lattices. Ref: arXiv:1507.05641

<sup>1</sup>We gratefully acknowledge support from NSF DMR-1410364 (MR), DOE DE-FG02-07ER46423 (NT), and from the UC Office of the President (CC, RTS).

**3:06PM V25.00004 Critical Exponents of Dynamical Conductivity in 2D Percolative Superconductor-Insulator Transitions: Three Universality Classes**, PRAGALV KARKI, YEN LEE LOH, Univ of North Dakota — We simulate three types of random inductor-capacitor (LC) networks on 4000x4000 lattices. We calculate the dynamical conductivity using an equation-of-motion method in which timestep error is eliminated and windowing error is minimized [1]. We extract the critical exponent  $a$  such that  $\sigma(\omega) \propto \omega^{-a}$  at low frequencies. The results suggest that there are three different universality classes. The  $L_{ij}C_i$  model, with capacitances from each site to ground, has  $a = 0.32$ . The  $L_{ij}C_{ij}$  model, with capacitances along bonds, has  $a = 0$ . The  $L_{ij}C_iC_{ij}$  model, with both types of capacitances, has  $a = 0.30$ . This implies that classical percolative 2D superconductor-insulator transitions (SITs) generically have  $\sigma(\omega) \rightarrow \infty$  as  $\omega \rightarrow 0$ . Therefore, experiments that give a constant conductivity as  $\omega \rightarrow 0$  must be explained in terms of quantum effects. [1. Yen Lee Loh, Rajesh Dhakal, John F. Neis and Evan M. Moen, "Divergence of dynamical conductivity at certain percolative superconductor-insulator transitions", Journal of Physics: Condensed Matter 26, 50 (2014)]

**3:18PM V25.00005 The phase diagram and Bose metal in superconducting nanowires<sup>1</sup>**, TYLER MORGAN-WALL<sup>2</sup>, HANNAH HUGHES<sup>3</sup>, NIKOLAUS HARTMAN<sup>4</sup>, NINA MARKOVIC<sup>5</sup>, Johns Hopkins University — We experimentally investigated the transport properties of thin, narrow superconducting aluminum nanowires as a function of magnetic field and temperature. We characterized the full superconducting phase diagram with respect to magnetic field and temperature, and show the onset of a flux-flow phase for certain values of temperature and magnetic field. The flux-flow resistance follows the Bardeen-Stephen model and it is shown that the resistance increases linearly with respect to magnetic field in this region of the phase diagram. In addition, we show the saturation to a non-zero finite resistance state below the normal state resistance for certain magnetic fields as the temperature decreases to zero.

<sup>1</sup>This work is supported by NSF DMR-1507782.

<sup>2</sup>Current address: Institute for Defense Analyses

<sup>3</sup>Current address: University of Pennsylvania

<sup>4</sup>Current address: University of British Columbia

<sup>5</sup>Current address: Goucher College

**3:30PM V25.00006 Shrinking of the Cooper Pair Insulator Phase in Thin Films with Ultrasmall Superconducting Islands**, J.C. JOY, X. ZHANG, C. ZHAO<sup>1</sup>, J.M. VALLES, JR., Department of Physics- Brown University, G. FERNANDES, J.M. XU, Division of Engineering- Brown University — The ubiquity of the bosonic Cooper Pair Insulator (CPI) phase near the two-dimensional superconductor to insulator transition (SIT) is a long standing question. While a number of two dimensional materials exhibit bosonic insulating phases similar to the Mott Insulator in arrays of ultrasmall, Josephson coupled superconducting islands, others show behaviors consistent with a fermionic insulating phase. Utilizing specially prepared anodized aluminum oxide substrates, we are able to fabricate films reminiscent of arrays of superconducting islands whose properties are tunable by varying the substrate morphology. Our recent work has focused on arrays of islands which possess an energy level spacing comparable to the mean field superconducting gap, where one expects pair breaking followed by fermionic Anderson Localization as the dominant mechanism by which superconductivity is destroyed. Early results show that the paradigmatic bosonic insulator exists only very near the disorder tuned SIT, while films only marginally deeper in the insulating phase exhibit transport distinct from the CPIs reentrant, activated transport. We are grateful for the support of NSF Grant No. DMR-1307290, the AFOSR, and the AOARD.

<sup>1</sup>Currently at Northwestern Polytechnical University, Xian, China

**3:42PM V25.00007 Disorder induced superconductor-insulator transition in epitaxial  $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$  thin films**, HAN-BYUL JANG, CHAN-HO YANG, KAIST —  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$  is a well-known superconducting system showing various electronic properties as a function of Sr content. Especially, epitaxial thin layers of the compound show enormous increase of superconducting critical temperature ( $T_c$ ) by a compressive strain. It has been reported that  $T_c$  can be controlled by misfit strain, thickness, and oxygen annealing. In this study, we report structural and transport properties of high quality epitaxial  $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$  thin films. According to x-ray diffraction study, *c*-axis lattice parameter shows no significant change for various film thicknesses and the in-plane lattice parameters of the films are coherently matched with that of substrate. Electronic transport measurements show a clear superconductor-to-insulator transition (SIT), accompanying variation of  $T_c$  depending on film thickness. These results are analyzed by using the McMillan equation to find the relation between the  $T_c$  and a disorder correlating with film thickness. We have found the disorder exhibits an explicit power-law behavior with respect to film thickness in our  $\text{La}_{1.85}\text{Sr}_{0.15}\text{CuO}_4$  thin films.

**3:54PM V25.00008 Origin and consequences of the disorder-induced inhomogeneities in cuprate superconductors**, DEBMALYA CHAKRABORTY, Indian Institute of Science Education and Research Kolkata, Mohanpur Campus, India-741246, RAJDEEP SENSARMA, Department of Theoretical Physics, Tata Institute of Fundamental Research, Mumbai-400005, India, AMIT GHOSAL, Indian Institute of Science Education and Research Kolkata, Mohanpur Campus, India-741246 — The effect of potential impurities on cuprate superconductors are investigated within a formalism suitable for addressing the complex interplay of the bare repulsive electronic correlations and disorder, both being strong. We show that the mechanism governing the demise of superconductivity is rather subtle and differs from the conventional weak-coupling descriptions. While the superconductivity remains surprisingly robust for up to moderate disorder, it crashes down sharply at stronger disorders. The initial robustness is attributed to the strong repulsive correlations that smear out charge inhomogeneities by reorganizing the hopping on the bonds prohibiting formation of superconducting "islands". However, with increasing strength of disorder, the potential difference across some bonds reach the scale of the bandwidth and the overall energy of the system is reduced by prohibiting hopping on such links. Integrating this concept within our formalism, we show that the correlations fail to homogenize the system across these "cut-bonds". This produces Mott-insulating, Anderson-insulating, as well as locally superconducting regions interspersed among each other at strong disorder, eventually destroying the global superconductivity.

**4:06PM V25.00009 The half-filling paradox in  $\text{Pr}_2\text{CuO}_{4+\delta}$** , YOSHIHARU KROCKENBERGER, AI IKEDA, HIROSHI IRIE, HIDEKI YAMAMOTO, NTT Basic Research Labs — In a type-II superconductor, the onset of the superconducting state as a function of decreasing magnetic field  $H$  occurs at the upper critical magnetic field  $H_{c2}$ , dictated by the pairing gap  $\Delta$  through the coherence length  $\xi_0 \sim \nu_F/\Delta$ , via  $H_{c2} = \Phi_0/2\pi\xi_0^2$ . We show that the mean-free length  $\ell$  in superconducting  $\text{Pr}_2\text{CuO}_4$  can be as large as 85nm, or 200 unit cell lengths. Such large  $\ell$  values are directly related to residual resistivity ratios. While  $\text{Pr}_2\text{CuO}_{4+\delta}$  is commonly known as an antiferromagnetic insulator (AFI), we show that synthesis and annealing conditions govern  $\delta$ . For AFI  $\text{Pr}_2\text{CuO}_4$ , i.e.  $\ell \ll 2\text{nm}$ ,  $\delta$  is larger than 0.10 whereas  $\delta \ll 0.04$  in the superconducting state. In fact, this de-intercalation of apical oxygen is mandatory for the induction of superconductivity and is counter to early conclusions that all cuprate superconductors are AFI in their undoped state. It is not surprising that the AFI state found in cuprates with 5- and 6-fold coordinated copper is not established in cuprates with 4-fold coordinated copper, i.e.  $\delta < 0.04$ . Such coordination-driven phase transition is at the core of the long-term assumed half-filling paradox.

**4:18PM V25.00010 Investigating Links Between Enhanced Inhomogeneity and Robustness of the Superconducting State in Severely Underdoped, Ultrathin  $\text{CaYBCO}$** , STANLEY STEERS, THOMAS LEMBERGER, BRIAN BAKER, The Ohio State University — Multiple experiments in recent years have shown evidence for intrinsic inhomogeneity in the cuprate superconductors upon approach to the superconductor to insulator transition (SIT). We present experimental evidence of anomalous suppression of both the diamagnetic response and the resistivity in ultrathin Ca-doped YBCO over tens of Kelvin. We then present further experiments to investigate to what extent this suppression is related to increased inhomogeneity upon approach to the SIT. Finally, we compare these results in  $\text{CaYBCO}$  to experiments in other cuprate compounds from the literature.

**4:30PM V25.00011 Modulation of Superconductor-Insulator Transition in  $\text{NdBa}_2\text{Cu}_3\text{O}_{7-x}$  through Oxygen Migration by Electrolyte Gating**, LINGCHAO ZHANG, S.W. ZENG, D.Y. WAN, K. HAN, L.K. JIAN, A. ARIANDO, T. VENKATESAN, NATIONAL UNIVERSITY OF SINGAPORE, NUSNNI-NANOCORE TEAM — The technique of electric double layer transistor (EDLT) has been applied to several HTS, such as LSCO and YBCO. The interpretation of SIT in all these studies are attributed to electrostatically induced carriers. However, in several electrolyte gating experiments recently, the effect is mainly attributed to oxygen vacancy formation, with migration of oxygen from the film into ionic liquid. In this study, the modulation of SIT is performed in a 7uc NBCO EDLT. By applying positive  $V_g$ , the SC NBCO gradually transits to insulating. When  $V_g$  changes back to 0V, it remains insulating. If the mechanism is electrostatically induced carriers, it should recover SC. However, it is only when applying a reverse negative  $V_g$  that it can gradually recover SC. Meanwhile, after SIT and  $V_g$  back to 0V, another sample is taken out from PPMS. After careful remove of ionic liquid, it remains insulating. After annealing at  $\text{O}_2$  atmosphere, it recovers SC. These strongly support the underlying mechanism is oxygen migration, instead of electrostatically induced carriers. The  $R_c$  is extracted to be about 5320 $\Omega$ , suggestive of quantum phase fluctuation.

**4:42PM V25.00012 Phase Transitions in a Two-dimensional Electron System at Oxide Interface with Dual Gate Tuning**, ZHUOYU CHEN, HISASHI INOUE, HYEOK YOON, DI LU, TYLER MERZ, SEUNG SAE HONG, ADRIAN SWARTZ, YANWU XIE, Stanford University, HONGTAO YUAN, YASUYUKI HIKITA, SLAC National Accelerator Laboratory, HAROLD HWANG, Stanford University and SLAC National Accelerator Laboratory — The ground state of a two-dimensional (2D) electron system can be controlled by parameters including disorder, carrier density, and magnetic field. Using the conducting channel formed at the  $\text{LaAlO}_3/\text{SrTiO}_3$  (001) heterointerface, we performed magnetotransport measurements with simultaneous electric field effect gating from both the top epitaxial  $\text{LaAlO}_3$  layer and the back  $\text{SrTiO}_3$  (001) substrate. Besides conventional carrier density tuning, the structural asymmetry inherent to the dual-gate device also enables independent modulation of the disorder level in the conduction channel probed through carrier mobility. Under different top and back gate voltages and magnetic field combinations, the interface channel showed strikingly different conducting states including zero resistance (superconductor), saturating small finite resistance ("metal"), and increasing resistance (insulator), when approaching zero temperature. These results provide a unique opportunity for understanding the quantum phase transitions in 2D superconducting systems with continuously tunable parameters.

**4:54PM V25.00013 Behavior of an Amorphous Superconducting Thin Film in a Tunable Dissipative Environment<sup>1</sup>**, ILANA PERCHER, ALLEN GOLDMAN, University of Minnesota — It has been shown that a dissipative electrical environment supports superconductivity. This is particularly true for low-dimensional systems of disordered and granular superconductors close the insulating state, where Ohmic dissipation can damp the order parameter fluctuations that would otherwise destroy global phase coherence. We will present the latest results from experiments in which a homogeneously disordered indium oxide film is placed in very close proximity to a two dimensional electron gas (2DEG) within a gallium arsenide/aluminum gallium arsenide heterostructure. The dissipation provided by the 2DEG depends on its carrier concentration, which is varied electrostatically by means of a back gate. We are grateful to the groups of Prof. Rachel Goldman at University of Michigan and Prof. Aviad Frydman at Bar Ilan University for growing heterostructures and superconducting films (respectively) for this experiment.

<sup>1</sup>This work was supported by DOE Basic Energy Sciences Grant DE-FG02-02ER46004.

**5:06PM V25.00014 The role of disorder and electron-electron interactions in the superconductor-insulator transition of molybdenum disulfide**, JOSEPH PRESTIGIACOMO, NRC Postdoctoral Fellow: US Naval Research Laboratory, ANINDYA NATH, George Mason University, ANTHONY BOYD, ASEE Postdoctoral Fellow: US Naval Research Laboratory, QINGFENG LIU, JUDY WU, Kansas State University, THOMAS SUTTO, MICHAEL OSOFSKY, US Naval Research Laboratory — The 2D layered transition-metal dichalcogenide, MoS<sub>2</sub>, first garnered interest over 40 years ago when it was discovered that it becomes a superconductor (SC) after electrochemical intercalation with alkali- or alkali-earth metals. Recently, however, a superconductor-insulator (SI) transition was observed in MoS<sub>2</sub> by electric-field gating with ionic liquid (IL) dielectrics, substances that enable induced charge-carrier concentrations (n) much larger than are possible using conventional solid-state dielectric gate barriers. Despite this feat, detailed studies of gate-tuned metal-insulator transitions in MoS<sub>2</sub> have mainly focused on the understanding the various mobility-reducing scattering mechanisms thought to contribute to the smaller than predicted on/off ratios observed in MoS<sub>2</sub>-based FETs. In this presentation, we discuss the results of an investigation into the role of disorder and electron-electron interactions in the SI transition of mechanically-exfoliated multilayer and CVD-grown few-layer MoS<sub>2</sub> probed by carefully examining their low temperature magneto-transport properties as a function of charge carrier-concentration via IL-gating.

**Thursday, March 17, 2016 2:30PM - 5:30PM –**

**Session V26 DCMP DMP: Surface Studies of Beyond Graphene Materials (STM/ARPES)** 325

- Vinod Sangwan, Northwestern University

**2:30PM V26.00001 Variable Temperature Scanning Tunneling Microscopy of WTe<sub>2</sub>, MoTe<sub>2</sub> and alloyed MoWTe<sub>2</sub>**, DREW EDELBERG, DANIEL CHENET, LIOR EMBON, NATHAN ZHAO, AYELET NOTIS, ERICK ANDRADE, ABHAY PASUPATHY, Columbia Univ — The transition metal dichalcogenides MoTe<sub>2</sub> and WTe<sub>2</sub> grow in a Van der Waals layered structure and can be produced down to monolayer thickness. These materials exhibit multiple crystal structures with drastically differing electronic properties including semiconductor (2H) and metal (1T'). Nanoscale phase engineering has been proposed as a way to create a variety of device architectures. This phase engineering can be achieved by strain, chemical doping or alloying. Alloying in particular has been proposed as a facile technique to continuously tune the structural phase of the resultant material and thus lower the barrier for transitions between the insulating and metallic states. In this study we use variable temperature scanning tunneling microscopy to image both parent compounds MoTe<sub>2</sub>, WTe<sub>2</sub> and alloyed crystals MoWTe<sub>2</sub>. Using dI/dV spectroscopy we determine the nature of the insulating and metallic states of both the parent compounds as well as use this technique to characterize the properties of the alloyed material.

**2:42PM V26.00002 Local Spectroscopic Characterization of Spin and Layer Polarization in WSe<sub>2</sub>**, DEVIN MCKENZIE, MATTHEW YANKOWITZ, BRIAN LEROY, University of Arizona — Semiconducting transition metal dichalcogenides, such as WSe<sub>2</sub>, exhibit very strong spin-orbit coupling (SOC) at certain band extrema due to large in-plane dipole moments formed by their heavy constituent atoms. The strong SOC links the spin and valley degrees of freedom in monolayers. In bilayers, interlayer hopping is suppressed by this SOC, leading to a spontaneous layer polarization and a coupling of the layer pseudospin with the spin and valley degrees of freedom. We examine these effects by tracking allowed and forbidden electronic scattering pathways in monolayer and bilayer WSe<sub>2</sub> using scanning tunneling spectroscopy. Specifically, we observe a strong suppression of intervalley scattering in both monolayer and bilayer WSe<sub>2</sub> indicative of these band polarizations.

**2:54PM V26.00003 Resolving 2D Amorphous Materials with Scanning Probe Microscopy<sup>1</sup>**, KRISTEN M. BURSON, CHRISTIN BUECHNER, ADRIAN LEWANDOWSKI, MARKUS HEYDE, HANS-JOACHIM FREUND, Fritz-Haber Institute of the Max Planck Society — Novel two-dimensional (2D) materials have garnered significant scientific interest due to their potential technological applications. Alongside the emphasis on crystalline materials, such as graphene and hexagonal BN, a new class of 2D amorphous materials must be pursued. For amorphous materials, a detailed understanding of the complex structure is necessary. Here we present a structural study of 2D bilayer silica on Ru(0001), an insulating material which is weakly coupled to the substrate. Atomic structure has been determined with a dual mode atomic force microscopy (AFM) and scanning tunneling microscopy (STM) sensor in ultra-high vacuum (UHV) at low temperatures, revealing a network of different ring sizes. Liquid AFM measurements with sub-nanometer resolution bridge the gap between clean UHV conditions and the environments that many material applications demand. Samples are grown and characterized in vacuum and subsequently transferred to the liquid AFM. Notably, the key structural features observed, namely nanoscale ring networks and larger holes to the substrate, show strong quantitative agreement between the liquid and UHV microscopy measurements. This provides direct evidence for the structural stability of these silica films for nanoelectronics and other applications.

<sup>1</sup>KMB acknowledges support from the Alexander von Humboldt Foundation

**3:06PM V26.00004 Measurement of electrostatic potential variations between 2D materials using low-energy electron microscopy<sup>1</sup>**, SERGIO DE LA BARRERA, PATRICK MENDE, JUN LI, RANDALL FEENSTRA, Carnegie Mellon University, Department of Physics, YU-CHUAN LIN, JOSHUA ROBINSON, Pennsylvania State University, Materials Science and Engineering, SURESH VISHWANATH, HUILI XING, Cornell University, Electrical and Computer Engineering — Among the many properties that evolve as isolated 2D materials are brought together to form a heterostructure, rearrangement of charges between layers due to unintentional doping results in dipole fields at the interface, which critically affect the electronic properties of the structure. Here we report a method for directly measuring work function differences, and hence electrostatic potential variations, across the surface of 2D materials and heterostructures thereof using low energy electron microscopy (LEEM). Study of MoSe<sub>2</sub> grown by molecular beam epitaxy on epitaxial graphene on SiC with LEEM reveals a large work function difference between the MoSe<sub>2</sub> and the graphene, indicating charge transfer between the layers and a subsequent dipole layer. In addition to quantifying dipole effects between transition metal dichalcogenides and graphene, direct imaging of the surface, diffraction information, and the spectroscopic dependence of electron reflectivity will be discussed.

<sup>1</sup>This work was supported in part by the Center for Low Energy Systems Technology (LEAST), one of the six SRC STARnet Centers, sponsored by MARCO and DARPA.

**3:18PM V26.00005 Scanning tunneling spectroscopy of tungsten disulfide<sup>1</sup>**, MICHAEL LODGE, CAMERON GLASSCOCK, MASA ISHIGAMI, University of Central Florida — Atomically thin layers of tungsten disulfide possess interesting optoelectronic properties characterized by strong photoluminescence. Here we perform scanning tunneling microscopy and spectroscopy measurements of 2H WS<sub>2</sub> on silicon oxide substrates to understand how electronic properties are affected by defects and substrate-induced disorder. Specifically, the electronic property of tungsten disulfide is probed as a function of gate-induced carrier density.

<sup>1</sup>This work is based upon research supported by the National Science Foundation under Grant No. 0955625.

**3:30PM V26.00006 Structure and Electronic Properties of Single- to Few Layers Molybdenum Disulfide Films<sup>1</sup>**, D. TRAINER, A. PUTILOV, M. WOLAK, R. U. CHANDRASENA, Department of Physics, Temple University, Philadelphia, PA 19122, F. KRONAST, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, D-12489 Berlin, Germany, A. X. GRAY, X. X. XI, M. IAVARONE, Department of Physics, Temple University, Philadelphia, PA 19122 — Using high resolution scanning tunneling microscopy and spectroscopy (STM/STS) we have investigated the electronic properties of mono- to few layers molybdenum disulfide films grown on HOPG using ambient pressure chemical vapor deposition (APCVD). Atomic force microscopy and STM show that this growth technique produces crystalline triangular and hexagonal islands with varying thicknesses in 1 ML increments. The films exhibited a suppression of quasiparticle band-gap as a function of layer number as measured by local spectroscopy. Changes in the valence band edge were supported by photoemission electron microscopy (PEEM) measurements. We also report on a strain-induced contraction of the quasiparticle band-gap in proximity to grain boundaries and defects.

<sup>1</sup>This work was supported as part of the Center for the Computational Design of Functional Layered Materials, an Energy Frontier Research Center funded by the U.S. DOE, BES under Award DE-SC0012575

**3:42PM V26.00007 Scanning tunneling microscopy on CVD grown lateral graphene molybdenum disulfide heterostructures**, ALEXANDER KERELSKY, MINGHAO CHENG, XINJUE ZHONG, XIAODONG ZHAO, ALI DADGAR, DA WANG, Columbia Univ, HUI GAO, MARCOS GUIMARAES, KIBUM KANG, Cornell Univ, XIAOYANG ZHU, Columbia Univ, JIWOONG PARK, Cornell Univ, ABHAY N. PASUPATHY, Columbia Univ — We investigate the interface of single layer graphene, molybdenum disulfide lateral heterostructures using scanning tunneling microscopy (STM). Samples are fabricated using chemical vapor deposition to deposit graphene, photolithography to pattern graphene and metal-organic chemical vapor deposition to grow molybdenum disulfide in patterned areas. The lateral junction of the two materials allows investigation of structural and electronic properties at the interface of the two materials, an interface usually buried in conventional stacked heterostructures. STM is used to image the stitching of the two materials with nanoscale resolution. STM is also used to perform local spectroscopy, probing the local density of states on an atomic scale across the junction. Interesting phenomena such as the charge transfer and atomic bonding are investigated. The spatially changing chemical potential between the two materials is also examined at different gate voltages.

**3:54PM V26.00008 Monolayer MoS<sub>2</sub> on HOPG Studied by Scanning Tunneling Microscopy / Spectroscopy<sup>1</sup>**, CHUN-I LU, Department of Physics, National Taiwan University; National Synchrotron Radiation Research Center, C. BUTLER, Y.-H. CHU, H.-H. YANG, Department of Physics, National Taiwan University, C.-M. WEI, Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan, L.-J. LI, Physical Sciences and Engineering, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia., M.-T. LIN, Department of Physics, National Taiwan University; Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan, DEPARTMENT OF PHYSICS, NATIONAL TAIWAN UNIVERSITY TEAM, INSTITUTE OF ATOMIC AND MOLECULAR SCIENCES, ACADEMIA SINICA TEAM — Chemical Vapor Deposition (CVD) is a promising way to prepare 2D material such as graphene and MoS<sub>2</sub> for  $\mu\text{m}$ -scale. In this report, we deposit monolayer MoS<sub>2</sub> by CVD method on HOPG to create the heterojunction. We observe that, the alignment of triangle MoS<sub>2</sub> islands shows the tendency that they have some preferred directions from AFM morphology. From STM atomic resolution images, the moiré superstructures analysis could summarize that the MoS<sub>2</sub> lattice tends to have a small angle with graphite's lattice. On the other hand, we also take the tunneling spectra from the different moiré domains and the moiré hills, moiré valleys of the single moiré domain. The results reveal the extraordinary states, which appear in the band gap range of MoS<sub>2</sub>. We consider these states are the consequence of hybridized of two layers and be detected from the interlayer space.

<sup>1</sup>C.-I Lu et al, Appl. Phys. Lett. 106, 181904 (2015).

**4:06PM V26.00009 STM/STS Study of Surface Modification Effect on Bandgap Structure of Ti<sub>2</sub>C with -OH, -F, and -H.<sup>1</sup>**, SEONG JUN JUNG, SHEN LAI, TAEHWAN JEONG, SUNGJOO LEE, YOUNG JAE SONG, Sungkyunkwan Univ — In this presentation, we present Scanning Tunneling Microscopy (STM) and Spectroscopy (STS) study of bandgap structures of surface-modified Ti<sub>2</sub>C with -OH, -F, and -O in atomic scale. Since the discovery of new two dimensional (2D) materials like graphene, various 2D materials including transition metal dichalcogenide (TMD) have been intensively investigated. There are, however, still scientific issues to apply them to the device fabrications for controlling the appropriate bandgap structure with high field effect mobility. Recently another 2D materials of transition metal carbide (TMC), Ti<sub>2</sub>CT<sub>x</sub> with modifiable surface group T<sub>x</sub> (-OH, -F, and -O) was suggested. [S. Lai et. al, Nanoscale (2015), DOI: 10.1039/C5NR06513E]. This 2D material shows that the mobility at room temperature is less sensitive to the measured transport bandgap, which can imply that Ti<sub>2</sub>CT<sub>x</sub> can be a strong candidate of 2D TMC for application to the future electronic devices. Surface modification on the electronic structure of Ti<sub>2</sub>C by -OH, -F, and -O is, therefore, investigated by STM and STS in atomic scale. More scientific results will be further discussed in the presentation.

<sup>1</sup>This research was supported by Basic Science Research Program through the National Research Foundation of Korea funded by the Korean government (Grant Numbers: 2015R1A1A1A05027585, 20110030046, IBS- R011D1, 2014M3C1A3053024 and 2015M3A7B4050455)

**4:18PM V26.00010 An ARPES investigation of band evolution of MoS<sub>2</sub> in presence of high pressure hydrogen gas<sup>1</sup>**, SOOHYUN CHO, Yonsei University, BEOM SEO KIM, Seoul National University, BEOM YOUNG KIM, YEONGKWAN KIM, Lawrence Berkeley National Laboratory, BYUNG HOON KIM, Incheon National University, CHANGYONG KIM, Seoul National University, SEUNGRYONG PARK, Incheon National University, INCHEON NATIONAL UNIVERSITY COLLABORATION, LAWRENCE BERKELEY NATIONAL LABORATORY COLLABORATION — The monolayer MoS<sub>2</sub>, has a large direct band gap and spin band splitting in K-point which make it a good candidate for several applications such as solar cell, valley Hall transistor and so on. When it has more than two layers, turns into a semiconductor with indirect band gap. Theoretical predictions have revealed that the number of layers is directly related to number of bands. Also, it was recently reported that the resistivity of MoS<sub>2</sub> decreases when exposed to high pressure hydrogen gas for few hours. To investigate the evolution of energy bands as a function of high pressure hydrogen exposure, we performed angle resolved photoemission spectroscopy (ARPES) experiment on pristine and hydrogen treated bulk MoS<sub>2</sub>. Our result, is suggestive for quantum well state in the treated sample case, and impurity state induced by sulphur vacancy between valence and conduction band at K-point. We argue that the impurity state depending on momentum mediate decrease in resistivity.

<sup>1</sup>An ARPES investigation of band evolution of MoS<sub>2</sub> in presence of high pressure hydrogen gas

**4:30PM V26.00011 Investigation of the Spatially Resolved Electronic Structure of Single Layer WS<sub>2</sub> on Transition Metal Oxide Surfaces**, JYOTI KATOCH, THE OHIO STATE UNIVERSITY, SREN ULSTRUP, ROLAND KOCH, DANIEL SCHWARZ, Advanced Light Source, Lawrence Berkeley National Laboratory, SIMRANJEET SINGH, THE OHIO STATE UNIVERSITY, KATHY MCCREARY, Naval Research Laboratory, HYANG KEUN YOO, Advanced Light Source, Lawrence Berkeley National Laboratory, JINSONG XU, THE OHIO STATE UNIVERSITY, BERRY JONKER, Naval Research Laboratory, ROLAND KAWAKAMI, THE OHIO STATE UNIVERSITY, AARON BOSTWICK, ELI ROTENBERG, CHRIS JOZWIAK, Advanced Light Source, Lawrence Berkeley National Laboratory — The family of semiconducting single layer (SL) transition metal dichalcogenides (TMDs) have lately been intensely studied, owing to the strong coupling between spin and valley degrees of freedom as well as the presence of strongly bound excitons. The choice of supporting substrate is known to strongly influence these properties. We set out to investigate the electronic properties of CVD grown SL WS<sub>2</sub> transferred onto the dielectric oxide materials SrTiO<sub>3</sub> and TiO<sub>2</sub>. By using a combination of photoemission electron microscopy (PEEM) and angle-resolved photoemission (ARPES) with micrometer focus we obtain simultaneous spatial, momentum and energy-resolved information about SL WS<sub>2</sub> on a polar (SrTiO<sub>3</sub>) and a nonpolar (TiO<sub>2</sub>) surface for the first time.

**4:42PM V26.00012 Graphene protected surface state on Ir(111) with adsorbed lithium**, PREDRAG LAZIC, Institute Ruder Bokovic, PETAR PERVAN, MARIN PETROVIC, IVA SRUT-RAKIC, Institute of Physics, Zagreb, IVO PLETIKOSIC, Brookhaven National Laboratory, MARKO KRALJ, MILORAD MILUN, Institute of Physics, Zagreb, TONICA VALLA, Brookhaven National Laboratory — It is well known that electronic surface states (SS) get strongly perturbed upon the chemical adsorption of very small amount of adsorbates. Adsorption of lithium atoms on Ir(111) is no exception to that rule. Iridium SS gets strongly perturbed and is practically eradicated - it can not be seen as a sharp peak in the ARPES measurement. However, if the system is prepared with graphene on top of Ir/Li system, the iridium SS reappears. We present a combined experimental and theoretical study of the described system. Using the density functional theory calculations for large unit cells with disordered lithium atoms geometries on the (111) surface of iridium we were able to reproduce the results of the ARPES measurements - showing clearly that the SS signal is strongly suppressed when lithium is adsorbed, while it is almost unchanged when lithium is intercalated (i.e. with graphene on top of it). Looking at the projected density of states we constructed a rather simple model explaining this behavior which seems to be general.

**4:54PM V26.00013 Semiconducting graphene and its incommensurate SiC interface<sup>1</sup>**, MATTHEW CONRAD, MEREDITH NEVIUS, FENG WANG, Georgia Tech, KATHERINE JINKINS, Univ Wisconsin, ARLENSI CELIS, Univ Paris-Sud, MAYA NAIR, ALESSANDRO COATI, AMINA TALEB-IBRAHIMI, SOLEIL, ANTONIO TEJEDA, Univ Paris-Sud, PAUL MICELI, Univ Missouri, EDWARD CONRAD, Georgia Tech — The development of a viable form of semiconducting graphene has been the goal since the onset of graphene research. Using improved growth techniques, we show that the first epitaxial graphene layer grown on SiC(0001) (the buffer layer) is semiconducting. With ARPES, we found that the buffer layer has a band gap > 0.5eV. At present, no existing theory explains the observed band structure. This is in part due to a corresponding lack of detailed structural studies of the buffer. Using SXRD, we show that the buffer layer is not the commensurate ( $6\sqrt{3} \times 6\sqrt{3}$ )R30° structure assumed for the past four decades. Rather, it is tensile strained and interacts with a strongly modulated SiC interface layer. The buffer-interface layer pair is well ordered, yet incommensurate with bulk SiC. We also find that the buffer evolves during the growth process and reverts to a near commensurate phase with a large RMS roughness when a monolayer forms. These structural changes correspond with changes in the band structure that demonstrate the importance of the incommensurate phase in producing semiconducting graphene.

<sup>1</sup>Support: NSF DMR-1401193, 1005880, 0934142 and the Partner Univ. Fund: French Embassy.

**5:06PM V26.00014 Band parameters of 2D semiconductor heterostructures determined by micro-ARPES**, PAUL NGUYEN, Department of Physics, University of Washington, NEIL WILSON, Department of Physics, University of Warwick, PASQUAL RIVERA, KYLE SEYLER, Department of Physics, University of Washington, ALEXEY BARINOV, Sincrotrone Elettra Trieste, GEETHA BALAKRISHNAN, Department of Physics, University of Warwick, XIAODONG XU, DAVID COBDEN, Department of Physics, University of Washington — Heterostructures made by stacking monolayers of different 2D materials can have unique properties, such as hosting long-lived polarized interlayer excitons. Understanding these depends on knowledge of the band parameters of both the separate monolayers and the hetero-bilayer. Interlayer hybridization can also produce distinct electronic structure dependent on the relative monolayer crystal orientation. The most powerful technique for determining such properties is angle-resolved photoemission (ARPES), which can now be applied to micron-scale samples at the Spectromicroscopy Elettra Trieste beamline. Using this new facility, combined with careful sample design, we have studied heterostructures of WSe<sub>2</sub>, MoSe<sub>2</sub>, WS<sub>2</sub> and graphene. We determined band offsets, effective masses, and spin-orbit splittings with an energy resolution <50 meV. Interestingly, the bands near the gamma-point in hetero-bilayers oriented near zero degrees are not a superposition of those in the isolated monolayers, but exhibit an additional higher band. However, the valence band edge remains at the K-point, which together with the band offsets is consistent with measurements of strong luminescence from interlayer excitons in MoSe<sub>2</sub>/WSe<sub>2</sub>.

**5:18PM V26.00015 Angle- and spin-resolved photoemission spectroscopy study of monolayer semiconducting transition metal dichalcogenides**, WEI YAO, ERYIN WANG, HUAQING HUANG, Tsinghua Univ, TAICHI OKUDA, Hiroshima Synchrotron Radiation Center, CHAOXIN LIU, Pennsylvania State University, WENHUI DUAN, SHUYUN ZHOU, Tsinghua Univ — Monolayer transition-metal dichalcogenides (TMDs) receive significant attention due to their intriguing physical properties for both fundamental research and potential applications in electronics, optoelectronics, spintronics, and so on. In particular, the multiple degrees of freedom in these materials (e.g. spin, valley and layer) are coupled with each other, providing various ways to control their properties. Here we report the electronic and spin structural studies of a monolayer semiconducting transition metal dichalcogenide thin film using Angle-resolved photoemission spectroscopy (ARPES) and Spin-Resolved ARPES.

**Thursday, March 17, 2016 2:30PM - 5:30PM —**

**Session V27 DCMP: Mixed Valence and Kondo Physics** 326 - Priscilla Rosa, Los Alamos National Laboratory

## 2:30PM V27.00001 The isostructural $\alpha-\gamma$ phase transition in Cerium: a DFT+DMFT study.

BERNARD AMADON, THOMAS APPLENCOURT, ALEXIS GEROSSIER, JORDAN BIEDER, CEA, DAM, DIF, F-91297 Arpajon, France, FABIEN BRUNEVAL, CEA, DEN, Service de Recherches de Metallurgie Physique, F-91191 Gif-sur-Yvette, France, JULES DENIER, CEA, DAM, DIF, F-91297 Arpajon, France — We present a study of the electronic structure and structural properties of the  $\alpha-\gamma$  isostructural first order phase transition in cerium. Because of strong local electronic interactions due to 4f electrons, Density Functional Theory is not able to describe it. We thus use the combination of DFT and Dynamical Mean Field Theory, as implemented in ABINIT to understand and describe the transition:

Firstly, we use the constrained Random Phase Approximation to compute the effective interaction in cerium and discuss the validity of this approximation [1]. Secondly, we use this interaction to clarify the orbital mechanism of the transition: we thus discuss the validity of different models [2].

Thirdly, we compute the electronic free energy for the transition and discuss the role of entropy and spin orbit coupling [3,4].

Finally, we put in perspective our results with respect to recent calculations.

[1] B. Amadon, T. Applencourt, and F. Bruneval PRB 89, 125110 (2014)

[2] B. Amadon and A. Gerossier PRB 91, 161103(R) (2015)

[3] J. Bieder and B. Amadon PRB 89, 195132 (2014)

[4] B. Amadon, J. Denier and J. Bieder (unpublished)

## 2:42PM V27.00002 Simulation of the X-ray Emission Spectrum from Early Lanthanides<sup>1</sup>, WEI-

TING CHIU, University of California, Davis, CHUNJING JIA, BRIAN MORITZ, TOM DEVEREAUX, SIMES, SLAC National Accelerator Laboratory and Stanford University, MAGNUS LIPP, Condensed Matter and Materials Division, LLNL, DEVON MORTENSEN, GERALD SEIDLER, University of Washington, RICHARD SCALETTAR, University of California, Davis — For decades it has been known that certain Lanthanide metals, such as cerium and praseodymium, exhibit a volume collapse transition at a critical pressure. The volume change correlates with charge transfer from 4f orbitals to higher energy conduction bands due small differences in energy. To date, high pressure X-ray emission measurements have enabled the determination of the bare 4f moment of Lanthanide metals.<sup>2</sup> In particular at the  $L_{\gamma_1}$  emission line, the intensity of a satellite peak captures the behavior of the 4f electrons across the volume collapse transition. Here we use exact diagonalization for an atomic model of the Lanthanides, including orbital site energies and core-, valence-, and conduction-band multiplet interactions to simulate the x-ray emission spectrum. The multiple interactions are derived from atomic structure calculations, augmented by effective 4f-to-conduction-band hybridization term. The Kondo screening effect from the conduction electrons at high pressure changes the 4f occupation, resulting in a change of the satellite peak intensity, which well reproduces the experimental findings in the early Lanthanide metals.

<sup>1</sup> Supported by NNSA grant number: DE-NA0002908

<sup>2</sup>M. J. Lipp *et al.*, PRL **109**, 195705(2012).

## 2:54PM V27.00003 Systematic investigation of structural, transport, magnetic and thermodynamic properties of hexagonal $R_2Pt_6Al_{15}$ ( $R = Y, La-Nd, Sm-Lu$ ) series.<sup>1</sup>, SOHAM MANNI, Q. LIN,

S. L. BUD'KO, P. C. CANFIELD, Ames Laboratory/ Iowa State University, Ames, IA 50011, USA — We have synthesized single crystals of new hexagonal intermetallic series of compounds  $R_2Pt_6Al_{15}$  with  $R = Y, La-Nd, Sm-Lu$ . Structural analysis have confirmed hexagonal  $P6_3/mmc$  crystal structure with ordered R-site. Magnetic, transport and heat capacity measurements show that most of the members of the series order antiferromagnetically at low temperature with highest  $T_N = 7.5$  K for  $Gd_2Pt_6Al_{15}$  and moments are along c-axis except  $Dy_2Pt_6Al_{15}$  and  $Ho_2Pt_6Al_{15}$ .  $Ce_2Pt_6Al_{15}$  does not order, but shows insulating behavior with a strong divergence in heat capacity divided by temperature ( $C/T$ ). Mixed valence state of  $Eu^{2+}/Eu^{3+}$  state has been observed in  $Eu_2Pt_6Al_{15}$  with antiferromagnetic ordering below 3 K. Magnetic entropy and crystal electric field are analyzed for all the members from the magnetic contribution of heat capacity. This series of compounds serves a unique example of a rare earth series with only one rare earth (R) site having hexagonal point-symmetry.

<sup>1</sup>This research is funded by the Gordon and Betty Moore Foundations EPiQS Initiative through Grant GBMF4411 and by U.S. Department of Energy under Contract No. DE-AC02-07CH11358.

## 3:06PM V27.00004 Epitaxial growth and *in situ* ARPES of ultrathin $YbAl_3$ thin films, SHOVIK

CHATTERJEE, DARRELL SCHLOM, KYLE SHEN, Cornell Univ —  $YbAl_3$  is a well-known intermediate valence compound that shows emergence of Fermi liquid behavior below a coherence temperature of  $\sim 34K - 40K$ . Transport, thermodynamic and photoemission measurements have established limitations of Single Impurity Anderson model in describing this material system, suggesting the importance of lattice effects. However, microscopic mechanisms underlying these properties are yet to be properly understood, one reason being that the direct experimental determination of its electronic band structure is still lacking. In this talk I will present our recent efforts in stabilizing thin films of  $YbAl_3$  and *in situ* angle-resolved photoemission spectroscopy (ARPES) of these films. With the aid of an Al buffer layer crystalline, phase pure and fully oriented epitaxial thin films can be grown with sub-nm surface roughness. By using ARPES, we, for the first time have been able to map out its band structure and Fermi surface. Moreover, by growing ultra thin films we have been able to drive this material system towards its 2D limit. Evolution of its electronic structure with temperature and dimensionality will be discussed.

## 3:18PM V27.00005 Entanglement entropy near Kondo-destruction quantum critical points,

TATHAGATA CHOWDHURY, CHRISTOPHER WAGNER, KEVIN INGERSANT, Univ of Florida, JEDEDIAH PIXLEY, University of Maryland — Entanglement entropy is a measure of quantum-mechanical entanglement across the boundary created by partitioning a system into two subsystems. We study this quantity in Kondo impurity models that feature Kondo-destruction quantum critical points (QCPs). Recent work [1] has shown that the entanglement entropy between a Kondo impurity of spin  $S_{imp}$  and its environment is pinned at its maximum possible value  $S_e = \ln(2S_{imp} + 1)$  throughout the Kondo phase. In the Kondo-destroyed phase, where the impurity spin acquires a nonzero expectation value  $M_{loc}$ ,  $S_e = \ln(2S_{imp} + 1) - a(S_{imp})M_{loc}^2$  irrespective of the properties of the host. Here, we report numerical renormalization-group results for Kondo models with a pseudogapped density of states under a different partition that separates the impurity and on-site conduction electrons from the rest of the system. Now, the entanglement entropy is affected by the nature of the environment beyond the information contained in  $M_{loc}$ , but  $S_e$  still contains a critical part that exhibits power-law behavior in the vicinity of the Kondo-destruction QCP. [1] J. H. Pixley *et al.*, Phys. Rev. B **91**, 245122 (2015).

## 3:30PM V27.00006 Entanglement across different cuts along the Wilson chain for the pseudo-gap Anderson model, CHRISTOPHER WAGNER, TATHAGATA CHOWDHURY, KEVIN INGERSANT, University of Florida, JEDEDIAH PIXLEY,

University of Maryland — Entanglement entropy measures the quantum entanglement of a pure state across the boundary created by partitioning a system into two subsystems. The entanglement entropy between an Anderson impurity and a pseudogapped conduction band displays nonuniversal behavior near the Kondo-destruction quantum critical point (QCP), but in the ordered phase contains a critical component proportional to the square of the order parameter [1]. Here we report calculations of the entanglement entropy for other partitions of the system. Specifically, within the numerical renormalization group formulation of the problem, we consider partitions where one subsystem is composed of the impurity plus the first few sites in the Wilson-chain representation of the conduction band, sites that represent the electronic states spatially localized closest to the impurity. By calculating the reduced density matrix for the subsystem containing the impurity, we study the behavior of the entanglement entropy across the parameter space of the model, with particular focus on the vicinity of the Kondo-destruction QCP. [1] J. H. Pixley, T. Chowdhury, M. T. Mienikowski, J. Stephens, C. Wagner, and K. Ingersant, Phys. Rev. B **91**, 245122 (2015)

**3:42PM V27.00007 Skyrmion defects of antiferromagnet and competing singlet orders of a Kondo-Heisenberg model on honeycomb lattice** , CHIA-CHUAN LIU, Rice Univ, PALLAB GOSWAMI, University of Maryland, QIMIAO SI, Rice Univ — The competition between antiferromagnetism and proximate singlet orders is the common feature of many heavy fermion compounds. Depending on the context, the singlet order can be described by static Kondo singlets, unconventional superconductivity, site or bond centered charge orders, or more exotic density waves. This competition between singlet and triplet orders can give rise to exotic quantum critical points or even an intervening non-Fermi liquid phase. It is a fundamentally important but challenging problem to develop a general scheme for identifying the competing singlet orders from the antiferromagnetically ordered side and vice versa. We study this problem on a honeycomb lattice, and approach it starting from the Kondo-destroyed antiferromagnetic phase. We show how the topological defects of the antiferromagnetic order parameter can give rise to competing singlet orders in the presence of itinerant fermions. We identify translational symmetry breaking singlet orders and static Kondo singlets as gapped collective excitations inside the skyrmion core. Our results provide non-perturbative insight into the global phase diagram of heavy fermion compounds.

**3:54PM V27.00008 Charge density wave instability in the periodic Anderson model with electron-phonon interaction<sup>1</sup>** , ENZHI LI, Department of Physics and Astronomy, Louisiana State University , PENG ZHANG, Xi'an Jiaotong University, KA-MING TAM, SHUXIANG YANG, JUANA MORENO, MARK JARRELL, Department of Physics and Astronomy, Louisiana State University — We study the periodic Anderson model with the conduction electrons coupled to phonons. It has been shown by using the dynamical mean field theory that the model contains two phases, the Kondo singlet phase for strong hybridization and the local moment phase for weak hybridization. In the hybridization-temperature plane, these two phases are separated by a first order phase transition line which terminates at a second order phase transition point. We calculated the susceptibilities for various possible orderings for the model. We found that the charge density wave ordering is robust at low temperature and for weak hybridization. The second order critical point is screened out by the formation of CDW. It is probable that the two phases should be Kondo singlet phase and CDW phase.

<sup>1</sup>Work supported by the NSF EPSCoR Cooperative Agreement No. EPS-1003897 with additional support from the Louisiana Board of Regents.

**4:06PM V27.00009 The entanglement structure of the Kondo singlet in energy space** , CHUN YANG, ADRIAN FEIGUIN, Physics department of Northeastern University — We unveil the entanglement structure of the Kondo singlet in energy space by studying the contribution of each individual free electron eigenstate. This is a problem of two spins coupled to a bath, where the bath is formed by the remaining conduction electrons. Being a mixed state, we resort to the "concurrence" as a good measure of entanglement. Using the density matrix renormalization group and analytical variational calculations with the Yoshida wave-function, and slave bosons, we find a distinct transition between weak and strong coupling regimes characterized by very different entanglement distributions. We discuss implications to the theory of the Kondo cloud.

**4:18PM V27.00010 Kondo phase shift at the zero-bias anomaly of quantum point contacts** , BORIS BRUN, CNRS, Institut Neel & Univ. Grenoble Alpes, Grenoble, France, FREDERICO MARTINS, SBASTIEN FANIEL, BENOIT HACKENS, IMCN/NAPS, Univ. catholique de Louvain, Belgium, ANTONELLA CAVANNA, CHRISTIAN ULYSSE, ALBDELKARIM OUEGHY, ULF GENNSER, DOMINIQUE MAILLY, CNRS, Laboratoire de photonique et de nanostructures, Marcoussis, France, PASCAL SIMON, Laboratoire de Physique des solides, Univ. de Paris-Sud, Orsay, France, SERGE HUANT, CNRS, Institut Neel & Univ. Grenoble Alpes, Grenoble, France, VINCENT BAYOT, IMCN/NAPS, Univ. catholique de Louvain, Belgium, MARC SANQUER, CEA, INAC-SPSMS & Univ Grenoble Alpes, Grenoble, France, HERMANN SELLIER, CNRS, Institut Neel & Univ. Grenoble Alpes, Grenoble, France — The Kondo effect is the many-body screening of a local spin by a cloud of electrons at very low temperature. It has been proposed as an explanation of the zero-bias anomaly in quantum point contacts where interactions drive a spontaneous charge localization. However, the Kondo origin of this anomaly remains under debate, and additional experimental evidence is necessary. Here we report on the first phase-sensitive measurement of the zero-bias anomaly in quantum point contacts using a scanning gate microscope to create an electronic interferometer. We observe an abrupt shift of the interference fringes by half a period in the bias range of the zero-bias anomaly, a behavior which cannot be reproduced by single-particle models. We instead relate it to the phase shift experienced by electrons scattering off a Kondo system. Our experiment therefore provides new evidence of this many-body effect in quantum point contacts.

**4:30PM V27.00011 Full counting statistics for current through each channel of orbital degenerate Anderson impurity with exchange interactions** , RUI SAKANO, ISSP, the university of Tokyo, AKIRA OGURI, YUNORI NISIKAWA, Department of physics, Osaka city university — We study non-equilibrium currents, current fluctuations and cross-correlations of the currents through Kondo-correlated quantum dots at low applied bias-voltages, using full counting statistics. To elucidate impact of dot-site interaction to these current properties in crossover between noninteracting and some Kondo states, renormalized perturbation theory or local Fermi liquid theory are employed. The exact form of the cumulant generating function up to third order of bias-voltage is derived in term of renormalized parameters. Specifically, crossover behavior of the Fano factor (ratio between noise and current) and current crosscorrelations for two-fold orbital case is discussed with using computed renormalized parameters by numerical renormalization group.

**4:42PM V27.00012 Voltage quench dynamics of a Kondo system** , ANDREY ANTIPOV, QIAOYUAN DONG, EMANUEL GULL, Univ of Michigan - Ann Arbor — We examine the dynamics of a correlated quantum dot in the mixed valence regime. We perform numerically exact calculations of the current after a quantum quench from equilibrium by rapidly applying a bias voltage in a wide range of initial temperatures. The current exhibits short equilibration times and saturates upon the decrease of temperature at all times, indicating Kondo behavior both in the transient regime and in steady state. The time-dependent current saturation temperature connects the equilibrium Kondo temperature to a substantially increased value at voltages outside of linear response. These signatures are directly observable by experiments in the time-domain.

**4:54PM V27.00013 NMR spin relaxation rates in the Heisenberg bilayer** , TIAGO MENDES, UFRJ / UC Davis, NICHOLAS CURRO, RICHARD SCALETTAR, UC Davis, THEREZA PAIVA, RAIMUNDO R. DOS SANTOS, UFRJ — One of the striking features of heavy fermions is the fact that in the vicinity of a quantum phase transition these systems exhibit the breakdown of Fermi-liquid behavior and superconductivity. Nuclear magnetic resonance (NMR) experiments play an important role in the study of these phenomena. Measurements of NMR spin relaxation rates and Knight shift, for instance, can be used to probe the electronic spin susceptibility of these systems. Here we studied the NMR response of the Heisenberg bilayer model. In this model, it is well known that the increase of the interplane coupling between the planes,  $J_{\text{perp}}$ , suppresses the antiferromagnetic order at a quantum critical point (QCP). We use stochastic series expansion (SSE) and the maximum-entropy analytic continuation method to calculate the NMR spin lattice relaxation rate  $1/T_1$  and the spin echo decay  $1/T_{2G}$  as function of  $J_{\text{perp}}$ . The spin echo decay,  $T_{2G}$  increases for small  $J_{\text{perp}}$ , due to the increase of the order parameter, and then vanishes abruptly in the QCP. The effects of  $J_{\text{perp}}$  dilution disorder in the QCP and the relaxation rates are also discussed. This research was supported by the NNSA grant number DE-NA 0002908, and Ciência sem fronteiras program/CNPQ.

**5:06PM V27.00014 4f metals (compounds) under High Pressure (and Temperature): f-electron Correlation Physics**, MAGNUS LIPP, ZSOLT JENEI, HYUNCHAE CYNN, WILLIAM EVANS, Lawrence Livermore National Laboratory, PHYSICS DIVISION TEAM — The physics of 4f-electron correlation governs the behavior of the most interesting group in the periodic table, the rare-earth elements. Arguably the most celebrated example is cerium with its iso-structural (fcc) volume collapse (VC) from the  $\gamma$ - to the  $\alpha$ -phase ending in a critical point. Close to the VC cerium is even auxetic since its Poisson's ratio becomes negative. Radiography tells us that both phases continue on into the melt, possibly separated by a first order transition. The presence of the f-electron can be interrogated via X-ray emission spectroscopy of the satellite intensity of the  $L\gamma$  radiation. Across the VC it experiences a step-like drop which could be interpreted as a discontinuous decrease of the 4f-moment or occupancy. The theoretical models (Hubbard-Mott or Kondo) explain these phenomena with the behavior of the f-electrons themselves or their spin but the contribution of the lattice-phonons also plays an important part. However, its share in the entropy change across the VC decreases with temperature. This work was performed under the auspices of the US DOE by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. The X-ray studies were performed at HPCAT (Sector 16), APS/ANL. HPCAT is supported by CIW, CDAC, UNLV and LLNL through funding from DOE-NNSA, DOE-BES and NSF. APS is supported by DOE-BES, under Contract No. DE-AC02-06CH11357.

**5:18PM V27.00015 Multi-pole orders and Kondo screening: Implications for quantum phase transitions in multipolar heavy-fermion systems**, HSIN-HUA LAI, EMILIAN NICA, QIMIAO SI, Department of Physics and Astronomy, Rice University — Motivated by the properties of the heavy-fermion  $\text{Ce3Pd20Si6}$  compound [1] which exhibits both antiferro-magnetic (AFM) and antiferro-quadrupolar (AFQ) orders, we study a simplified quantum non-linear sigma model for spin-1 systems [2], with generalized multi-pole Kondo couplings to conduction electrons [3]. We first consider the case when an  $\text{SU}(3)$  symmetry relates the spin and quadrupolar channels. We then analyze the effect of breaking the  $\text{SU}(3)$  symmetry, so that the interaction parameters in the spin and quadrupolar sectors are no longer equivalent, and different stages of Kondo screenings are allowed. A renormalization group analysis [4] is used to analyze the interplay between the Kondo effect and the AFM/AFQ orders. Our work paves the way for understanding the global phase diagram in settings beyond the prototypical spin- cases. We also discuss similar considerations in the non-Kramers systems such as the heavy fermion compound  $\text{PrV2Al20}$  [5]. [1]Custers et al, Nat.Mater. 11, 189 (2012). [2]A. Smerald et. al., Phys. Rev. B 88, 184430 (2013); Phys. Rev. B 91, 174402 (2015). [3]O. Parcollet et. al., Phys. Rev. Lett. 79, 4665 (1997); Phys. Rev. B 58, 3794 (1998) [4]Yamamoto S.J. and Q. Si, Phys. Rev. B 81, 205106 (2010). [5]Y. Shimura et. al., Phys. Rev. B 91, 241102(R) (2015)

## Thursday, March 17, 2016 2:30PM - 5:30PM – Session V28 DCMF: Josephson and Superconducting Proximity Effect 327 -

**2:30PM V28.00001 Topological phase transition of a Josephson junction and its dynamics**, JIMMY HUTASOIT, MARCO MARCIANI, BRIAN TARASINSKI, CARLO BEENAKKER, Lorentz Institute, Leiden University — A Josephson junction formed by a superconducting ring interrupted by a semiconductor nanowire can realize a zero-dimensional class D topological superconductor. By coupling the Josephson junction to a ballistic wire and altering the strength of the coupling, one can drive this topological superconductor through a topological phase transition. We study the compressibility of the junction as a probe of the topological phase transition. We also study the dynamics of the phase transition by studying the current pulse injected into the wire.

**2:42PM V28.00002 Combined gate-tunable Josephson junctions and normal state transport in  $\text{Bi}_2\text{Te}_3$  topological insulator thin films<sup>1</sup>**, PROSPER NGABONZIZA, MARTIN, P STEHNO, University of Twente, HIROAKI MYOREN, Saitama University, ALEXANDER BRINKMAN, University of Twente — In recent years, extensive efforts have been made to improve the coupling between topological insulators and s-wave superconductors in topological insulator Josephson devices (TIJDs). Despite significant progress, essential questions remain open such as the bulk contribution to the Josephson critical current or the existence (and number) of  $4\pi$ -periodic bound states (Majoranas) in TIJDs. To address these issues, we fabricated  $\text{Nb}/\text{Bi}_2\text{Te}_3/\text{Nb}$  Josephson junctions alongside Hall bar devices on MBE-grown  $\text{Bi}_2\text{Te}_3$  topological insulator thin films. Using the  $\text{SrTiO}_3$  [111] substrate as a gate dielectric, we tuned the carrier density electrostatically and measured the Josephson supercurrent and the normal state transport properties of our thin film devices. We identify three gate voltage ranges with distinct behavior: A region of intermediate gate bias where the measured quantities change rapidly with the applied electric field, and two saturation regions for large bias of either polarity. We discuss carrier distribution and band alignment in the material as well as implications for the effective Josephson coupling in TIJDs.

<sup>1</sup>This work is financially supported by the Dutch Foundation for Fundamental Research on Matter (FOM), the Netherlands Organization for Scientific Research (NWO), and by the European Research Council (ERC)

**2:54PM V28.00003 Quantum Phase Slips in Topological Josephson Junction Rings**, ROSA RODRIGUEZ MOTA, McGill University, SMITHA VISHVESHVARA, University of Illinois at Urbana-Champaign, TAMI PEREG-BARNEA, McGill University — We study quantum phase slip processes (QPS) in a ring of N topological superconducting islands joined by Josephson junctions and threaded by magnetic flux. In this array, neighboring islands interact through the usual charge  $2e$  Josephson tunneling and the Majorana assisted charge  $e$  tunneling.<sup>1</sup> When the charging energy associated with the island's capacitance is zero, the energy vs. flux relation of the system is characterized by parabolas centered around even or odd multiples of the superconducting flux quantum, depending on the parity of the system. For small but non-zero charging energy, quantum fluctuations can lead to tunneling between these classical states.<sup>2</sup> In this work, we calculate the amplitude of these tunneling processes, commonly known as quantum phase slips. We also add gate voltages to our system and study how the amplitude of QPS in these topological Josephson array is modified by Aharonov-Casher interference effects.

<sup>1</sup>A.Y. Kitaev, Phys.-Usp. 44, 131 (2001).

<sup>2</sup>K. A. Matveev, A. I. Larkin, and L. I. Glazman., Phys. Rev. Lett. 89, 096802 (2002).

**3:06PM V28.00004 Detecting evidence for chiral superconductivity in  $\text{Sr}_2\text{RuO}_4$  through the use of Josephson junctions**, BRIAN ZAKRZEWSKI, Y. A. YING, XINXIN CAI, SHAUN MILLS, N. E. STALEY, Pennsylvania State University, Y. XIN, National High Magnetic Field Laboratory, DAVID FOBES, TIJIANG LIU, ZHI-QIANG MAO, Tulane University, YING LIU, Pennsylvania State University —  $\text{Sr}_2\text{RuO}_4$  is predicted to be an odd-parity, spin-triplet superconductor, possibly featuring a doubly degenerate chiral order parameter, which leads to the presence of chiral edge currents, domains, and domain walls. We fabricated Josephson junctions on ramps cut by focused ion beam as well as on naturally cleaved edges of micron thick crystals of  $\text{Sr}_2\text{RuO}_4$  using Al as the conventional superconductor electrode. The sensitivity of these Josephson junctions to a magnetic flux penetrating the junction and the domain dependent intrinsic phase of the superconducting order parameter make them a powerful tool for probing the effects of chiral superconductivity mentioned above. We will present the methodology as well as preliminary measurements and discuss the implications of our results.

**3:18PM V28.00005 Switching Current Distributions in Superconductor–Topological Insulator–Superconductor Junctions**, ANDREW MURPHY, CAN ZHANG, ERIK HUERMILLER, Univ of Illinois - Urbana, SEONGSHIK OH, Rutgers University, JAMES ECKSTEIN, DALE VAN HARLINGEN, ALEXEY BEZRYADIN, Univ of Illinois - Urbana — It has been proposed that localized Majorana fermion (MF) modes can exist in lateral Josephson junctions with a 3D-topological insulator barrier at locations at which the phase difference across the junction is an odd multiple of  $\pi$ . These states enter the junctions bound to the nodes of the Josephson vortices as a perpendicular magnetic field is increased. Each mode contributes a local  $4\pi$ -periodic  $\sin(\varphi/2)$ -component to the junction's current-phase relation, adding to the usual  $\sin(\varphi)$  dependence. The sign of this new term encodes the parity of the Majorana pair. As a way to detect these states and measure their parity, we study the distribution of switching currents in Nb-Bi<sub>2</sub>Se<sub>3</sub>-Nb junctions fabricated on thin Bi<sub>2</sub>Se<sub>3</sub> films in which the superconductivity is induced by a pair of closely spaced Nb electrodes. We expect that such measurements will be sensitive to the parity of the MFs, yielding a splitting of the distribution. Preliminary measurements of the critical current distributions show the onset of unusual features when the magnetic field is increased which we are analyzing to determine if they may arise from Majorana fermions in the junctions.

**3:30PM V28.00006 Signature of topological transition in InAs nanowire Josephson junctions**, ELIA STRAMBINI, J. PAAJASTE, M. AMADO, S. RODDARO, NEST, CNR-NANO and Scuola Normale Superiore, Pisa, Italy, P. SAN-JOSE, R. AGUADO, ICMN-CSIC, Madrid, Spain, S. BERGERET, CFM-MPC, San Sebastian, Spain, D. ERCOLANI, L. SORBA, F. GIAZZOTTO, NEST, CNR-NANO and Scuola Normale Superiore, Pisa, Italy — The coupling of a conventional s-wave superconductors to semiconductors with strong spin-orbit (SO) coupling, like e. g. InAs or InSb nanowires (NWs), gives rise to unconventional p-wave superconductivity that may become a topological superconductor (TS), which is a natural host for exotic edge modes with Majorana character. Recently the enhancement of the critical supercurrent  $I_c$  in a strong SO semiconducting Josephson junction (JJ) have been proposed as a new evidence of the sought-after Majorana bound states.<sup>1</sup> Here we report on the first observation of the colossal  $I_c$  enhancement induced by an external magnetic field on a mesoscopic JJ formed by InAs NWs and Ti/Al leads. This anomalous enhancement appears precisely above a threshold magnetic field  $B_{th}$  orthogonal to the substrate and in junctions of different lengths, suggesting that the origin of the enhancement is intrinsic, i.e. it is not related to geometrical resonances in the junction. None of the standard phenomenon known in JJ, including e. g. Fraunhofer patterns or  $\pi$ -junction behavior, can explain this colossal enhancement while a topological transition at  $B_{th}$  is qualitatively compatible with the observed phenomenology.

<sup>1</sup>Phys.Rev.Lett. **112**, 137007 (2014)

**3:42PM V28.00007 Band structure of topological insulators from noise measurements in tunnel junctions**, JUAN PEDRO CASCALES SANDOVAL, Massachusetts Institute of Technology, ISIDORO MARTINEZ, Universidad Autnoma de Madrid, RUBEN GUERRERO, IMDEA-Nanociencia, CUI-ZU CHANG, FERHAT KATMIS, JAGADEESH MOODERA, Massachusetts Institute of Technology, FARKHAD ALIEV, Universidad Autnoma de Madrid — The unique properties of spin-polarized surface or edge states in topological insulators (TIs) make these quantum coherent systems interesting from the point of view of both fundamental physics and their implementation in low power spintronic devices. Here we present such a study in TIs, through tunnelling and noise spectroscopy utilizing TI/Al<sub>2</sub>O<sub>3</sub>/Co tunnel junctions with bottom TI electrodes of either Bi<sub>2</sub>Te<sub>3</sub> or Bi<sub>2</sub>Se<sub>3</sub>. We demonstrate that features related to the band structure of the TI materials show up in the tunnelling conductance and even more clearly through low frequency noise measurements. The bias dependence of  $1/f$  noise reveals peaks at specific energies corresponding to band structure features of the TI. TI tunnel junctions could thus simplify the study of the properties of such quantum coherent systems that can further lead to the manipulation of their spin-polarized properties for technological purposes.

**3:54PM V28.00008 Quantum interferences and edge states in Bismuth based Josephson junctions**, ANIL MURANI, SHAMASHIS SENGUPTA, ALIK KASUMOV, SOPHIE GUERON, HLENE BOUCHIAT, Laboratoire de Physique des Solides, MESO GROUP TEAM — We have investigated proximity induced superconductivity in single crystal bismuth nanowires connected to superconducting electrodes with a high critical field. I will specially report recent results on nanowires whose crystalline orientation could be determined by electron diffraction. At low temperature a supercurrent is measured which persists up to the critical field of the electrodes and exhibits sample dependent fast squid-like oscillations (period one to few hundred gauss) modulated by slower (few thousand Gauss) oscillations. We attribute this striking result to the appearance of 1D topological edge channels on special surfaces of Bi due to its strong spin-orbit coupling, in addition to a strong Zeeman effect caused by an unusually high g-factor.

**4:06PM V28.00009 Quantum transport in topological insulator nanoribbon field effect and Josephson devices**, MORTEZA KAYYALHA, Purdue University, LUIS JAUREGUI, Purdue University, Harvard University, ALEKSANDER KAZAKOV, Purdue University, MICHAEL PETTES, University of Connecticut, IRENEUSZ MIOTKOWSKI, Purdue University, LI SHI, University of Texas at Austin, LEONID ROKHINSON, YONG CHEN, Purdue University — The spin-helical topological surface states (TSS) of topological insulators have attracted great attention in the past few years as an excellent platform to study topological transport and other exotic physics such as Majorana fermions. Here we present experiments studying quantum transport of TSS in topological insulator nanoribbon (TINR) field effect devices with normal as well as superconducting contacts. In Bi<sub>2</sub>Te<sub>3</sub> NRs with normal contacts, we observe that the conductance vs. axial magnetic field exhibits Aharonov-Bohm (AB) oscillations with an alternating phase of zero and  $\pi$ , depending periodically on the Fermi momentum  $k_F$  tuned by an applied back-gate voltage, consistent with the 1D sub-band structure formed by circumferentially quantized TSS [1]. We also investigated the Josephson effects in BiSbTeSe<sub>2</sub> TINRs with superconducting Nb contacts. We measured the gate voltage and temperature dependence of the supercurrent and multiple Andreev reflections (MAR), to probe phase coherent transport via TSS. [1] L. A. Jauregui et al., arxiv:1503.00685.

**4:18PM V28.00010 Multi-terminal Josephson junctions as topological matter**, ROMAN-PASCAL RIWAR, MANUEL HOUZET, JULIA S. MEYER, Univ. Grenoble Alpes & CEA, INAC-SPSMS, F-38000 Grenoble, France, YULI V. NAZAROV, Kavli Institute of Nanoscience, TU Delft, NL-2628 CJ, Delft, The Netherlands — Topological materials and their unusual transport properties are now at the focus of modern experimental and theoretical research. Their topological properties arise from the bandstructure determined by the atomic composition of a material and as such are difficult to tune and naturally restricted to  $\leq 3$  dimensions. Here we demonstrate that  $n$ -terminal Josephson junctions with conventional superconductors may provide novel realizations of topology in  $n - 1$  dimensions, which have similarities, but also marked differences with existing 2D or 3D topological materials. For  $n \geq 4$ , the Andreev subgap spectrum of the junction can accommodate Weyl singularities in the space of the  $n - 1$  independent superconducting phases, which play the role of bandstructure quasimomenta. The presence of these Weyl singularities enables topological transitions that are manifested experimentally as changes of the quantized transconductance between two voltage-biased leads, the quantization unit being  $4e^2/h$ .

**4:30PM V28.00011 Towards all electrical control of topological Josephson junctions and Majorana zero modes via spin-orbit interactions**, XIN LIU, School of Physics and Wuhan National High Magnetic Field Center, Huazhong University of Science and Technology, Wuhan, Hubei 430074, China, XIAOPENG LI, Condensed Matter Theory Center and Joint Quantum Institute, Department of Physics, University of Maryland, College Park, MD 20742-4111, USA, XIONG-JUN LIU, International Center for Quantum Materials and School of Physics, Peking University, Beijing 100871, China, DONG-LING DENG, Condensed Matter Theory Center and Joint Quantum Institute, Department of Physics, University of Maryland, College Park, MD 20742-4111, USA — We study the current-phase relation of topological Josephson junctions with spin-orbit interactions, and show that the coupling between Majorana zero modes (MZMs) can be controlled via gate tunable spin-orbit couplings (SOCs). The spin-triplet pairings in the presence of MZMs at the two ends of a one-dimensional topological superconductor, are shown to have a  $\pi$  phase difference, from which a Josephson  $\pi$ -junction can be created. This  $\pi$  phase is unambiguously manifested to be a spin-dependent superconducting phase, dubbed spin-phase. We demonstrate that SOC can induce such spin-phase in spin-triplet superconducting condensates which can tune the MZM coupling energy and allow a finite topological Josephson current without a magnetic flux in superconducting circuits. We further establish the linkage between this Josephson current and the fermion parity in a topological Josephson junction and propose an all-electronically controlled superconductor-semiconductor hybrid circuit to detect the non-Abelian nature of MZMs.

**4:42PM V28.00012 Mean-field description of topological charge  $4e$  superconductors**, VICTORIA GABRIELE, JING LUO, JEFFREY C. Y. TEO, University of Virginia — BCS superconductors can be understood by a mean-field approximation of two-body interacting Hamiltonians, whose ground states break charge conservation spontaneously by allowing non-vanishing expectation values of charge  $2e$  Cooper pairs. Topological superconductors, such as one-dimensional  $p$ -wave wires, have non-trivial ground states that support robust gapless boundary excitations. We construct a four-body Hamiltonian in one dimension and perform a mean-field analysis. The mean-field Hamiltonian is now quartic in fermions but is still exactly solvable. The ground state exhibits 4-fermion expectation values instead of Cooper pair ones. There also exists a topological phase, where the charge  $4e$  superconductor carries exotic zero energy boundary excitations.

**4:54PM V28.00013 Scattering states of the Majorana-bound-state-supporting vortices at the interface of a topological insulator and an s-wave superconductor**, ADAM DURST, Hofstra University — We consider an isolated vortex in the 2D proximity-induced superconducting state formed at the interface of a 3D topological insulator (TI) and an s-wave superconductor (sSC). Prior calculations of the bound states of this system famously revealed a zero-energy state that is its own conjugate, a Majorana fermion bound to the vortex core. We calculate, not the bound states, but the scattering states of this system, and ask how the spin-momentum-locked massless Dirac form of the single-particle Hamiltonian, inherited from the TI surface, affects the cross section for scattering Bogoliubov quasiparticles from the vortex. As in the case of an ordinary superconductor, this is a two-channel problem with the vortex mixing particle-like and hole-like excitations. And as in the ordinary case, the same-channel differential cross section diverges in the forward direction due to the Aharonov-Bohm effect, resulting in an infinite total cross section but finite transport and skew cross sections. We calculate the transport and skew cross sections numerically, via a partial wave analysis, as a function of both quasiparticle excitation energy and chemical potential. Novel effects emerge as particle-like or hole-like excitations are tuned through the Dirac point.

**5:06PM V28.00014 Observation of superconductivity induced by a point contact on 3D Dirac semimetal  $\text{Cd}_3\text{As}_2$  crystals.**<sup>1</sup>, HE WANG, HUICHAO WANG, HAIWEN LIU, HONG LU, WUHAO YANG, SHUANG JIA, XIONGJUN LIU, XINCHENG XIE, JIAN WEI, JIAN WANG, Peking Univ — The 3D Dirac semimetal state is located at the topological phase boundary and can potentially be driven into other topological phases including topological insulator, topological metal and the long-pursuit topological superconductor states. Crystalline  $\text{Cd}_3\text{As}_2$  has been proposed and proved to be one of 3D Dirac semimetals which can survive in atmosphere. By precisely controlled point contact (PC) measurements, we observe the exotic superconductivity in the vicinity of the point contact region on the surface of  $\text{Cd}_3\text{As}_2$  crystal, which might be induced by the local pressure in the out-of-plane direction from the metallic tip for PC. The observation of zero bias conductance peak (ZBCP) and double conductance peaks (DCPs) symmetric to zero bias further reveals  $p$ -wave like unconventional superconductivity in  $\text{Cd}_3\text{As}_2$ . Considering the special topological property of the 3D Dirac semimetal, our findings may indicate that the  $\text{Cd}_3\text{As}_2$  crystal under certain conditions is a candidate of topological superconductor, which is predicted to support Majorana zero modes or gapless Majorana edge/surface modes on the boundary depending on the dimensionality of the material.

<sup>1</sup>This work was financially supported by the National Basic Research Program of China (Granted Nos.2012CB927400)

**5:18PM V28.00015 Induced gap in topological materials from the superconducting proximity effect**, CHING-KAI CHIU, WILLIAM COLE, Condensed Matter Theory Center, University of Maryland — Topological superconductivity has been of considerable interest lately, with several proposed experimental realizations in solid state systems. A heterostructure of s-wave superconductor and 3D topological insulator is one of the more promising platforms, with topological superconductivity realized on the "naked" surface of the topological insulator through the superconducting proximity effect. We theoretically study the induced superconducting gap on the naked surface. Adjusting the Fermi level above the bulk gap (which is the case in experiments), our results for the induced superconducting gap are in agreement with that probed in thin topological insulators ( $<10\text{nm}$ ) in the experiments (Nat. Phys. 10, 943-950 (2014) and Phys. Rev. Lett. 112, 217001 (2014)). We further predict the gap in thick topological insulators ( $>10\text{nm}$ ). This work is supported by LPS-MPO-CMTC, Microsoft Q, and JQI-NSF-PFC.

**Thursday, March 17, 2016 2:30PM - 5:30PM —**

**Session V29 DCMP: Weyl Semimetals: Theory and Experiments** 328 - Rudro Biswas, Purdue University

**2:30PM V29.00001 Topological Nodal-Line Fermions in the Non-Centrosymmetric Spin-Orbit Metal  $\text{PbTaSe}_2$ .**<sup>1</sup>, GUANG BIAN, Princeton University, PRINCETON TEAM — We report on the existence of topological nodal-line states in the non-centrosymmetric compound single-crystalline  $\text{PbTaSe}_2$  with strong spin-orbit coupling. Remarkably, the spin-orbit nodal lines in  $\text{PbTaSe}_2$  are not only protected by the reflection symmetry but also characterized by an integer topological invariant. Our detailed angle-resolved photoemission measurements, first-principles simulations and theoretical analysis illustrate the physical mechanism underlying the formation of the topological nodal-line states and associated surface states. Our work paves the way towards exploring the exotic properties of the topological nodal-line fermions in condensed matter systems and, potentially, the rich physics arising from the interplay between the topological nodal-line states and the emergent superconductivity in this compound.

<sup>1</sup>Work at Princeton University and Princeton-led synchrotron-based ARPES measurements were supported by the Gordon and Betty Moore Foundations EPiQS Initiative through grant GBMF4547 (Hasan) and by U.S. Department of Energy DE-FG-02-05ER46200.

**2:42PM V29.00002 Magnetic structure and its role in the possible Weyl state in topological semimetal  $\text{Sr}_{1-y}\text{Mn}_{1-z}\text{Sb}_2$  ( $0 < y, z < 0.1$ )**<sup>1</sup>, QIANG ZHANG, Louisiana State Univ - Baton Rouge, HUIBO CAO, Oak Ridge National Laboratory, JINYU LIU, Tulane University, ALAN TENNANT, Oak Ridge National Laboratory, JOHN DITUSA, Louisiana State Univ - Baton Rouge, ZHIQIANG MAO, Tulane University — Very recently, Liu et al ([arxiv.org/pdf/1507.07978](https://arxiv.org/pdf/1507.07978), (2015)) discovered the first magnetic topological semimetal  $\text{Sr}_{1-y}\text{Mn}_{1-z}\text{Sb}_2$  ( $0 < y, z < 0.1$ ), in which a possible Weyl state arising from time reversal symmetry breaking is expected. However, the origin of ferromagnetic (FM) behavior of this material has not been clarified. By employing the neutron diffraction at the four-circle diffractometer HB3A, HFIR, we found a long-range FM order with Mn moments along  $b$ -axis below  $T_C = 565$  K, followed by another magnetic transition to a canted  $C$ -type antiferromagnetic (AFM) order at  $T_{FM-AFM} = 304$  K. In the canted  $C$ -type AFM state, the Mn moments are aligned with the  $a$ -axis along with a canting toward the  $b$ -axis, leading to a net FM moment lying along the  $b$ -axis. The Mn moments along the  $a$ - and  $b$ -axes at 5 K are found to be 3.789(3) and 0.741(4)  $\mu_B$ , respectively. The discovered FM order in  $\text{Sr}_{1-y}\text{Mn}_{1-z}\text{Sb}_2$ , either the FM ordering at  $304 < T < 565$  K or the FM component of the canted AFM order for  $T < 304$  K, is sufficient to break time-reversal symmetry likely creating a Weyl semimetal.

<sup>1</sup>This work is supported by the U.S. Department of Energy under EPSCoR Grant No. DE-SC0012432 with additional support from the Louisiana Board of Regents.

**2:54PM V29.00003 An optical investigation of the Magnetic Weyl semi-metal candidate  $\text{YbMnBi}_2$** , DIPANJAN CHAUDHURI, BING CHENG, Department of Physics and Astronomy, Johns Hopkins University, QUINN D. GIBSON, ROBERT J. CAVA, Department of Chemistry, Princeton University, N. PETER ARMITAGE, Department of Physics and Astronomy, Johns Hopkins University — The discovery of Dirac and Weyl fermions in condensed matter systems has sparked tremendous interest in both condensed matter and high energy physics communities alike. While the existence of Dirac electrons in graphene and topological insulator materials is now well established, only a handful of experiments provide direct evidence of Weyl fermions in non-centrosymmetric systems. Moreover, the theoretically predicted Weyl fermions in magnetic materials with strong spin-orbit coupling have continued to be elusive. A potent candidate for a Weyl semimetal with broken time reversal symmetry (TRS) and antiferromagnetic ordering is the newly discovered  $\text{YbMnBi}_2$  compound. Although the complete magnetic structure of this material is still unknown, preliminary ARPES measurements are consistent with TRS breaking and a Weyl fermionic band dispersion. In this work, we investigate  $\text{YbMnBi}_2$  single crystal with FTIR spectroscopy and study its low energy electrodynamic response. The energy scale of IR light is ideally suited to probe for the linear band dispersion of these materials close to the Weyl points. Temperature dependent optical conductivity calculations reveal crucial information on the fundamental scattering processes in these materials.

**3:06PM V29.00004 Scanning tunneling microscopic investigation of the topological surface of a Weyl semimetal**<sup>1</sup>, HAO ZHENG, department of Physics, Princeton University — Weyl semimetals are believed to open the next era of condensed matter physics after graphene and topological insulators because they provide the first ever realization of Weyl fermions in all physics and extend the classification of topological phases beyond insulators. For many years, experimental studies have been held back due to the absence of material realization of the Weyl semimetal state. Very recently, the first Weyl semimetal has been experimentally discovered in TaAs class of materials. So far only preliminary ARPES and transport experiments have been reported. In this talk, we will present some interesting results of the scanning tunneling microscopy/spectroscopy (STM/STS) study on a Weyl semimetal.

<sup>1</sup>The work at Princeton were supported by the Gordon and Betty Moore Foundations EPIQS Initiative through grant GBMF4547 (Hasan) and by U.S. Department of Energy DE-FG-02-05ER46200

**3:18PM V29.00005 SdH oscillations and pressure effect of the Weyl semimetal NbAs**, YONGKANG LUO, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, N. J. GHIMIRE, Argonne National Laboratory, Argonne, Illinois 60439, USA, M. WARTENBE, HONGCHUL CHOI, M. NEUPANE, R. D. MCDONALD, E. D. BAUER, JIANXIN ZHU, J. D. THOMPSON, F. RONNING, Los Alamos National Laboratory, Los Alamos, NM 87545, USA — Via angular Shubnikov-de Hass (SdH) quantum oscillations measurements, we determine the Fermi surface topology of NbAs. The SdH oscillations consist of two frequencies, corresponding to two Fermi surface extrema: 20.8 T ( $\alpha$ -pocket) and 15.6 T ( $\beta$ -pocket). The analysis shows that the  $\beta$ -pocket has a Berry phase of  $\pi$  and a small effective mass 0.033  $m_0$ , indicative of a nontrivial topology; whereas the  $\alpha$ -pocket has a trivial Berry phase of 0 and a heavier effective mass 0.066  $m_0$ . Subtle changes can be seen in the  $\rho_{xx}(T)$  profiles with pressure up to 2.31 GPa. The Fermi surfaces undergo an anisotropic evolution under pressure, while the topological features of the two pockets remain unchanged. Specific heat measurements reveal a small Sommerfeld coefficient  $\gamma_0 = 0.09(1)$  mJ/(mol $\cdot$ K<sup>2</sup>) and a large Debye temperature,  $\Theta_D = 450(9)$  K, confirming a “hard” crystalline lattice that is stable under pressure. We also studied the Kadowaki-Woods ratio of this low-carrier-density massless system,  $R_{KW} = 3.210^4 \Omega \text{ cm mol}^{-1} \text{ K}^2 \text{ J}^{-2}$ . After accounting for the small carrier density in NbAs, this  $R_{KW}$  indicates a suppressed transport scattering rate relative to other metals. **References:** [1] N. J. Ghimire et al., J. Phys.: Condens. Matter **27**, 152201 (2015) [2] Y. Luo et al., arXiv: 1506.01751 (2015) [3] Y. Luo et al., arXiv: 1510.08538 (2015)

**3:30PM V29.00006 Topological semimetal  $\text{Sr}_{1-y}\text{Mn}_{1-z}\text{Sb}_2$** , JINYU LIU, JIN HU, Tulane Univ, DAVID GRAF, National High Magnetic Field Lab, S.M.A. RADMANESH, D.J. ADAMS, Univ. of New Orleans, Y.L. ZHU, G.F. CHEN, X. LIU, J. WEI, Tulane Univ, I. CHIORESCU, National High Magnetic Field Lab & Florida State Univ., L. SPINU, Univ. of New Orleans, Z.Q. MAO, Tulane Univ — Recent discoveries of topological Weyl semimetals in noncentrosymmetric monpnictides TX ( $T=\text{Ta/Nb}$ ,  $X=\text{As/P}$ ) [1-4] and photonic crystals [5] have generated immense interests since they represent new topological states of quantum matter. Time reversal symmetry (TRS) breaking Weyl semimetal was also recently reported in  $\text{YbMnBi}_2$  [6]. In this talk, we report a new type of topological semimetal phase arising from two-dimensional Sb layers in  $\text{Sr}_{1-y}\text{Mn}_{1-z}\text{Sb}_2$  ( $y, z < 0.1$ ), which coexists with ferromagnetism. Through quantum transport measurements on this material, we reveal remarkable signatures of relativistic fermions, including light effective quasiparticle mass, high carrier mobility, a  $\pi$  Berry phase and valley polarized interlayer conduction. Given  $\text{Sr}_{1-y}\text{Mn}_{1-z}\text{Sb}_2$  shows ferromagnetism, it offers a wonderful opportunity to explore the TRS breaking Weyl state. [1]. H. Weng et al., Phys. Rev. X **5**, 011029, (2015). [2]. S.M. Huang et al., Nature Commun. **6**, (2015). [3]. S.Y. Xu et al., Science **349**, 613-617 (2015). [4]. B.Q. Lv et al., Phys. Rev. X **5**, 031013, (2015). [5]. L. Lu et al., Science **349**, 622-624 (2015). [6] S. Borisenko et al., arXiv:1507.04847, (2015). [7] J.Y. Liu et al., arXiv:1507.07978, (2015).

**3:42PM V29.00007 Chiral magnetic effect in  $\text{ZrTe}_5$** , QIANG LI, CHENG ZHANG, GENDA GU, T. VALLA, Brookhaven National Lab, DMITRI KHARZEEV, Brookhaven National Lab and Stony Brook University, I. PLETIKOSIC, Princeton University — The chiral magnetic effect is the generation of electric current induced by chirality imbalance in the presence of magnetic field. Here we report on the measurement of magneto-transport in zirconium pentatelluride,  $\text{ZrTe}_5$  that provides a strong evidence for the chiral magnetic effect. Our angle-resolved photoemission spectroscopy experiments show that this material's electronic structure is consistent with a 3D Dirac semimetal. We observe a large negative magnetoresistance when magnetic field is parallel with the current. The measured quadratic field dependence of the magnetoresistance is a clear indication of the chiral magnetic effect. The observed phenomenon stems from the effective transmutation of Dirac semimetal into a Weyl semimetal induced by the parallel electric and magnetic fields that represent a topologically nontrivial gauge field background. We expect that chiral magnetic effect may emerge in a wide class of materials that are near the transition between the trivial and topological insulators.

**3:54PM V29.00008 Optical evidence for a Weyl semimetal state in pyrochlore  $\text{Eu}_2\text{Ir}_2\text{O}_7$** <sup>1</sup>, ANDREI SUSHKOV, JOHANNES HOFMANN, GREGORY JENKINS, DENNIS DREW, Department of Physics, University of Maryland, USA, JUN ISHIKAWA, SATORU NAKATSUJI, Institute for Solid State Physics, University of Tokyo, Japan — Possible realization of a Weyl semimetallic state with the broken time-reversal symmetry in pyrochlore iridates is still under debate. In the absence of ARPES and neutron data, optical evidence become very important. We found that the THz optical conductivity and temperature dependence of the free carrier response in pyrochlore  $\text{Eu}_2\text{Ir}_2\text{O}_7$  match the predictions for a Weyl semimetal and suggest novel Dirac liquid behavior. The interband optical conductivity vanishes continuously at low frequencies signifying a semimetal. The metal-semimetal transition at  $T_N = 110$  K is manifested in the Drude spectral weight, which is independent of temperature in the metallic phase, and which decreases smoothly in the ordered phase. The temperature dependence of the free carrier weight below  $T_N$  is in good agreement with theoretical predictions for a Weyl semimetal. The fit of experimental Drude weight yields a Fermi velocity  $4 \times 10^7$  cm/s, a logarithmic renormalization scale  $\Lambda_L \approx 600$  K, and require a Fermi temperature of  $\sim 100$  K associated with residual unintentional doping to account for the low temperature optical response and dc resistivity.

<sup>1</sup>This work was supported by grants: NSF DMR-1104343 and 1066293, DOE ER46741-SC0005436, LPS-MPO-CMTC, the Japanese Society for the Promotion of Science R2604, and Grants-in-Aid for Scientific Research 25707030.

**4:06PM V29.00009 Weak Topological Insulators and Composite Weyl Semimetals:  $\beta\text{-Bi}_4\text{X}_4$  ( $\text{X}=\text{Br}, \text{I}$ )**, FAN ZHANG, CHENG-CHENG LIU, Univ of Texas, Dallas, JIN-JIAN ZHOU, YUGUI YAO, Beijing Institute of Technology — While strong topological insulators (STI) have been experimentally realized soon after their theoretical predictions, a weak topological insulator (WTI) has yet to be unambiguously confirmed. A major obstacle is the lack of distinct natural cleavage surfaces to test the surface selective hallmark of WTI. With a new scheme, we discover that  $\text{Bi}_4\text{X}_4$  ( $\text{X}=\text{Br}, \text{I}$ ), stable or synthesized before, can be WTI with two natural cleavage surfaces, where two anisotropic Dirac cones stabilize and annihilate, respectively. We further find four surface state Lifshitz transitions under charge doping and two bulk topological phase transitions under uniaxial strain. Near the WTI-STI transition, there emerges a novel Weyl semimetal phase, in which the Fermi arcs generically appear at both cleavage surfaces whereas the Fermi circle only appears at one selected surface.

**4:18PM V29.00010 STM studies of Weyl semimetals**, HIROYUKI INOUE, ANDRAS GYENIS, SEONG WOO OH, JIAN LI, ZHI JUN WANG, ANDREI BERNEVIG, Princeton University, NI NI, University of California at Los Angeles, ALI YAZDANI, Princeton University — Weyl semimetal exhibits a new gapless topological phase, which is characterized by an even number of band touching points of two non-degenerate bands in the bulk, called Weyl nodes. The surfaces of these compounds are expected to harbor topologically protected surface states with disconnected Fermi surfaces, called Fermi arcs, which connect surface projections of the Weyl nodes with opposing Chern numbers. Among the theoretically predicted Weyl semimetals, there have been several experimental reports on the presence of Fermi arcs in inversion-symmetry-broken monoarsenides, such as TaAs. In this talk, we will present atomic-scale imaging and spectroscopic mapping of the electronic properties of TaAs and other Weyl semimetal candidates. Such measurements have the potential to directly visualize the Fermi arc surface states of these compounds and to probe their properties. This work is supported by ARO and NSF.

**4:30PM V29.00011 Noncentrosymmetric Line-Node Dirac semimetal  $\text{CaAgX}$  ( $\text{X}=\text{P}, \text{As}$ )**, AI YAMAKAGE, Department of Applied Physics, Nagoya University, YUICHI YAMAKAWA, Department of Physics, Nagoya University, YUKIO TANAKA, YOSHIHIKO OKAMOTO, Department of Applied Physics, Nagoya University — Noncentrosymmetric ternary pnictide  $\text{CaAgX}$  ( $\text{X}=\text{P}, \text{As}$ ) is shown to be a topological line-node semimetal protected solely by mirror-reflection symmetry. The band gap vanishes on a circle in momentum space and surface states emerge within the circle. The  $Z_2$  topological invariant  $\nu$  related to the surface states is defined from the Berry phase and mirror-reflection symmetry. Extending this study to spin-orbit coupled systems reveals that, compared with  $\text{CaAgP}$ , a substantial band gap is induced in  $\text{CaAgAs}$  by large spin-orbit interaction. The resulting states are a topological insulator, in which the  $Z_2$  topological invariant is given by 1;000. We have found that the  $Z_2$  topological invariants  $\nu_0, \nu_1, \nu_2$ , and  $\nu_3$  for time-reversal-invariant insulators without spatial-inversion symmetry and with mirror-reflection symmetry are calculated from the  $Z_2$  invariant  $\nu$  for a line node in the absence of spin-orbit interaction. Namely, line-node Dirac semimetals protected by mirror-reflection symmetry turn into strong topological insulators owing to spin-orbit interaction. [AY, Y. Yamakawa, Y. Tanaka, and Y. Okamoto, arXiv:1510.00202]

**4:42PM V29.00012 Signature of Instability of Chiral Fermion in Ultraquantum Weyl Semimetal TaAs**, CHENGLONG ZHANG, BING-BING TONG, ZHUJUN YUAN, SHUANG JIA, CHI ZHANG, Peking University — In the compound of Tantalum Monoarsenide (TaAs), the novel Weyl fermions are hosted. In our high mobility single crystal samples, the Shubnikov-de Haas oscillations are distinct below the quantum limit ( $B \sim 10$  T). Beyond the quantum limit, within the configuration-B (electric field  $\mathbf{E} \parallel \mathbf{B}$ -fields), we observed the novel quantum phase transitions in the  $\rho_{zz}$ -measurements, which may come from the nesting of the vector over a wide range of B-T plane. Due to the similarity to those observed density wave phases or the excitonic states in three-dimensional graphite semimetal, the novel phase may from many body effect beyond the quantum limit. However, in the other measurements ( $R_{xx}$  in configuration-A:  $\mathbf{E} \perp \mathbf{B}$ -fields), the novel quantum phase transition does not exist. In general, our results on the density wave phase support its non-trivial topological order.

**4:54PM V29.00013 Optical spectroscopy study of Weyl Semimetal NbP**, JEREMY YANG, YUXUAN JIANG, Georgia Institute of Technology, ZHILING DUN, HAIDONG ZHOU, University of Tennessee, DMITRY SMIRNOV, National High Magnetic Field Laboratory, ZHIGANG JIANG, Georgia Institute of Technology — Weyl semimetals have attracted much interest lately because of its unique band structure, where conduction band and valence band touch at discrete points. Here, we report on optical spectroscopy study of Weyl semimetal NbP, seeking evidence for the existence of Weyl fermions. Specifically, using Raman spectroscopy we investigate the anisotropic response of Raman-active phonon modes in NbP and compare with Quantum Espresso simulations. Using magneto-infrared spectroscopy in a high magnetic field up to 17.5T, we observe several Landau level transitions and compare with the theoretical model of three-dimensional massless Dirac/Weyl fermions. By combining our data with low-temperature magneto-transport measurement, the magnetic field dispersion of Landau levels in NbP is obtained.

**5:06PM V29.00014 Non-stoichiometry and Defects in the Weyl Semimetals TaAs, TaP, NbAs, and NbP**<sup>1</sup>, TIGLET BESARA, DANIEL A. RHODES, KUAN-WEN CHEN, QUI ZHANG, BIN ZHENG, YAN XIN, LUIS BALICAS, RYAN E. BAUMBACH, THEO SIEGRIST, National High Magnetic Field Laboratory / Florida State University — We report on a structural study of the Weyl semimetals TaAs, TaP, NbAs, and NbP, utilizing diffraction techniques (single crystal x-ray diffraction and energy dispersive spectroscopy) and imaging techniques (transmission electron microscopy). We observe defects of various degrees, leading to non-stoichiometric single crystals of all four semimetals. While TaP displays a very large pnictide deficiency with composition  $\text{TaP}_{0.83(3)}$  and stacking faults accompanied by anti-site disorder and site vacancies, TaAs displays transition metal deficiency with composition  $\text{Ta}_{0.92(2)}\text{As}$  and a high density of stacking faults. NbP also displays pnictide deficiency, yielding composition  $\text{NbP}_{0.95(2)}$ , and lastly, NbAs display very little deviation from a 1:1 composition,  $\text{NbAs}_{1.00(3)}$ , and is therefore recommended to serve as the model compound for these semimetals.

<sup>1</sup>DOE-BES #DE-SC0008832 (TB & TS), NSF DMR-1157490 (NHMFL)

**5:18PM V29.00015 Chiral Magnetic Effect in Condensed Matter<sup>1</sup>**, TONICA VALLA, QIANG LI, Brookhaven National Laboratory, DMITRI KHARZEEV, Brookhaven National Laboratory and Stony Brook University, CHENG ZHANG, YUAN HUANG, Brookhaven National Laboratory, IVO PLETIKOSIC, Brookhaven National Laboratory and Princeton University, ALEXEI FEDOROV, Lawrence Berkeley National Laboratory, RUIDAN ZHONG, JOHN SCHNEELOCH, GENDA GU, Brookhaven National Laboratory — The chiral magnetic effect (CME) is the generation of electric current induced by chirality imbalance in the presence of magnetic field - a macroscopic manifestation of the quantum anomaly in relativistic field theory of chiral fermions. The recent discovery of Dirac and Weyl semimetals opened a fascinating possibility to study this phenomenon in condensed matter experiments. Magneto-transport in  $\text{ZrTe}_5$  shows a strong evidence for CME. Our ARPES experiments show that this material's electronic structure is consistent with a highly anisotropic 3D Dirac semimetal. We observe a large negative magnetoresistance in parallel magnetic field, with the quadratic field dependence of the magneto-conductance - a clear indication of the CME.

<sup>1</sup>This work is supported by the US Department of Energy and ARO

**Thursday, March 17, 2016 2:30PM - 5:30PM –**  
**Session V30 DMP: Charge Transfer and Electron Gases at Oxide Interfaces** 329 - Uli Aschauer, ETH Zurich

**2:30PM V30.00001 Charge transfer and emergent phenomena of oxide heterostructures<sup>1</sup>**, HANGHUI CHEN, Columbia Univ — Charge transfer is a common phenomenon at oxide interfaces. We use first-principles calculations to show that via heterostructuring of transition metal oxides, the electronegativity difference between two dissimilar transition metal ions can lead to high level of charge transfer and induce substantial redistribution of electrons and ions. Notable examples include i) enhancing correlation effects and inducing a metal-insulator transition [1]; ii) tailoring magnetic structures and inducing interfacial ferromagnetism [2]; iii) engineering orbital splitting and inducing a non-cuprate single-orbital Fermi surface [3]. Utilizing charge transfer to induce emergent electronic/magnetic/orbital properties at oxide interfaces is a robust approach. Combining charge transfer with quantum confinement and epitaxial strain provides an appealing prospect of engineering electronic structure of artificial oxide heterostructures. [1] H. Chen, A. J. Millis and C. A. Marianetti, PRL 111, 116403 (2013) [2] H. Chen, H. Park, A. J. Millis and C. A. Marianetti, PRB 90, 245138 (2014) [3] H. Chen, D. P. Kumah, A. S. Disa, F. J. Walker, C. H. Ahn, and S. Ismail-Beigi, PRL 110, 186402 (2013)

<sup>1</sup>This research was supported by National Science Foundation under Grant No. DMR-1120296.

**3:06PM V30.00002 Structural and electronic properties of  $\text{Sr}(\text{Zr,Ti})\text{O}_3$  alloys for use in oxide heterostructures<sup>1</sup>**, LEIGH WESTON, University of California, Santa Barbara, ANDERSON JANOTTI, University of Delaware, Newark, XIANGYUAN CUI, The University of Sydney, BURAK HIMMETOGLU, University of California, Santa Barbara, CATHERINE STAMPFL, The University of Sydney, CHRIS G. VAN DE WALLE, University of California, Santa Barbara —  $\text{Sr}(\text{Ti,Zr})\text{O}_3$  alloys are promising materials for use in oxide heterostructures, however the fundamental properties of this system have not yet been characterized. Using hybrid density functional calculations, we study the electronic and structural properties of ordered  $\text{SrTi}_x\text{Zr}_{1-x}\text{O}_3$  alloys at  $x=0, 0.25, 0.5, 0.75$ , and 1. As Ti is added to  $\text{SrZrO}_3$ , the lattice parameter is reduced according to Vegard's law, while the band gap shows a large bowing and is sensitive to the Ti distribution. For  $x=0.5$ , arranging the Ti and Zr atoms into a  $1\times 1$   $\text{SrZrO}_3/\text{SrTiO}_3$  superlattice along the [001] direction leads to a highly dispersive single band at the conduction-band minimum (CBM) that is absent in the parent compounds, and a direct gap close to that of pure  $\text{SrTiO}_3$ . This is explained by the splitting of the Ti  $3d\ t_{2g}$  states in the reduced symmetry of the superlattice, lowering the band originating from the Ti  $3d_{xy}$  orbitals. The lifting of the orbital degeneracy around the CBM suppresses scattering due to electron-phonon interactions. We propose that short-period  $\text{SrZrO}_3/\text{SrTiO}_3$  superlattices could be exploited to engineer the band structure and improve carrier mobility compared to bulk  $\text{SrTiO}_3$ .

<sup>1</sup>This work was supported by NSF, ONR and ARC.

**3:18PM V30.00003 Direct observation of induced ferromagnetism in  $\text{SrTiO}_3$  quantum wells confined in  $\text{GdTiO}_3$  heterostructures**, RYAN NEED, BRANDON ISAAC, University of California Santa Barbara, Materials Department, BRIAN KIRBY, JULIE BORCHERS, NIST Center for Neutron Research, SUSANNE STEMMER, STEPHEN WILSON, University of California Santa Barbara, Materials Department — Complex oxide thin film heterostructures with charge transfer at the interface provide a uniquely tunable environment in which to study the physics of highly-correlated and quantum-confined electron systems. Previous studies using magnetoresistance measurements had suggested that thin  $\text{SrTiO}_3$  layers become ferromagnetic when grown between thicker  $\text{GdTiO}_3$  layers. Here we report the direct observation of induced ferromagnetism in  $\text{SrTiO}_3$  quantum wells using polarized neutron reflectometry (PNR). Four  $\text{GdTiO}_3/\text{SrTiO}_3$  superlattice structures with varying  $\text{SrTiO}_3$  layer thickness were grown epitaxially on LSAT (001) substrates by hybrid molecular beam epitaxy. Chemical and magnetic depth-profiles were refined using a combination of x-ray and polarized neutron reflectivity measurements taken at temperatures ranging from 4-300K. We observed a critical thickness below which the  $\text{SrTiO}_3$  layer have non-zero magnetism in the center of the well. These results are in excellent agreement with the previous magnetoresistance measurements and provide the first direct observation of induced-magnetism in this system.

**3:30PM V30.00004 Intrinsic Electronic Confinement at Conducting Oxide Interfaces**, DANFENG LI, STEFANO GARIGLIO, WEI LIU, ALEXANDRE FTE, MARGHERITA BOSELLI, DQMP, University of Geneva, MARC GABAY, LPS, Universit Paris-Sud, JEAN-MARC TRISCONE, DQMP, University of Geneva, DQMP COLLABORATION, LPS COLLABORATION — The discovery of a two-dimensional electron liquid (2DEL), confined at the interface between the two band insulators  $\text{LaAlO}_3$  (LAO) and  $\text{SrTiO}_3$  (STO) has generated tremendous research interest [1]. The 2DEL confinement lifts the degeneracy of Ti  $t_{2g}$  orbitals and promotes exotic physical properties [2]. A previous study [3] has demonstrated that a 2DEL is also observed when LAO is alloyed with STO ( $(\text{La,Al})_{1-x}(\text{Sr,Ti})_x\text{O}_3$  (LASTO: $x$ )). The threshold thickness required for the onset of conductivity scales with  $x$ . We present here a study of magnetotransport and superconductivity at the (LASTO:0.5)/STO interface. The thickness of the 2DEL, measured using perpendicular and parallel critical fields is larger than the one at the LAO/STO interface. This change is due to a modification on the confining potential linked to a reduced charge transfer that is scaling as  $1/x$ . This study supports an intrinsic origin to the formation of the 2DEL in the LAO/STO system. [1] A. Ohtomo, H. Y. Hwang, Nature **427**, 423 (2004). [2] P. Zubko, S. Gariglio, M. Gabay, P. Ghosez, and J.-M. Triscone, Annual Review of Condensed Matter Physics **2**, 141 (2011). [3] M.L. Reinle-Schmitt, C. Cancellieri, D. Li, D. Fontaine, M. Medarde, E. Pomjakushina, C.W. Schneider, S. Gariglio, P. Ghosez, J.-M. Triscone, and P.R. Willmott, Nature Communications **3**, 932 (2012).

**3:42PM V30.00005 Beyond GaAs: Room-Temperature Intersubband Absorption in SrTiO<sub>3</sub>/LaAlO<sub>3</sub> Multiple Quantum Wells**, JOHN ORTMANN, NISH NOOKALA, University of Texas at Austin, QIAN HE, Oak Ridge National Lab, AGHAM POSADAS, University of Texas at Austin, ALBINA BORISEVICH, Oak Ridge National Lab, MIKHAIL BELKIN, ALEX DEMKOV, University of Texas at Austin — With the recent advancements in oxide thin film fabrication, it is possible to design and grow oxide quantum well heterostructures whose well depths far exceed those of traditional GaAs-based quantum wells. Here, we discuss the design, fabrication, structural quality, and optical properties of MBE-grown SrTiO<sub>3</sub>/LaAlO<sub>3</sub> multiple quantum wells. These oxide quantum wells have a conduction band offset of greater than 2eV, as measured by X-ray photoelectron spectroscopy. We present simulations of the confined states within the wells and demonstrate the feasibility of driving intersubband transitions whose energies exceed 1eV. Furthermore, we demonstrate the excellent crystalline quality of these heterostructures via X-ray diffraction spectra and STEM-HAADF imaging and present evidence of atomic-scale control of the structures. Finally, we present room-temperature FTIR spectra demonstrating the first-reported evidence of intersubband absorption in SrTiO<sub>3</sub>/LaAlO<sub>3</sub> multiple quantum wells and discuss the possibility of oxide quantum well-based devices.

**3:54PM V30.00006 Constriction based superconducting quantum interference devices at the LaAlO<sub>3</sub>/SrTiO<sub>3</sub> interface**, EMRE MULAZIMOGLU, SRIJIT GOSWAMI, ANA M. R. V. L. MONTEIRO, Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands, ROMAN WOELBING, DIETER KOELLE, REINHOLD KLEINER, Physikalisches Institut - Experimentalphysik II, Eberhard Karls Universität Tuebingen, Germany, YAROSLAV BLANTER, LIEVEN M. K. VANDERSYPEN, ANDREA D. CAVIGLIA, Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands — The two-dimensional (2D) superconductor formed at the interface between LaAlO<sub>3</sub> (LAO) and SrTiO<sub>3</sub> (STO) has been studied extensively and shows many intriguing properties. However, to date there exist no measurements which are sensitive to the phase of the superconducting order parameter, a fundamental prerequisite to understand the microscopic mechanism of the superconductivity. Here, we realize superconducting quantum interference devices (SQUIDs) at the LAO/STO interface. Using nanoscale patterning, we define sub-100 nm physical constrictions, which serve as weak links between superconducting reservoirs. The SQUIDs show clear flux-periodic oscillations in the critical current. Back gate and temperature dependent studies, in combination with numerical simulations, show that the low superfluid density of this 2D superconductor results in an exceptionally large, gate controllable kinetic inductance of the SQUID. This ability to perform phase-sensitive measurements opens up a completely new approach to study this unique interfacial superconductor.

**4:06PM V30.00007 Electrostatically defined superconducting quantum interference devices at the LaAlO<sub>3</sub>/SrTiO<sub>3</sub> interface**, SRIJIT GOSWAMI, EMRE MULAZIMOGLU, ANA MONTEIRO, Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands, ROMAN WOELBING, DIETER KOELLE, REINHOLD KLEINER, Physikalisches Institut - Experimentalphysik II, Eberhard Karls Universität Tuebingen, Germany, YAROSLAV BLANTER, LIEVEN VANDERSYPEN, ANDREA CAVIGLIA, Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands — Two-dimensional superconductivity at the LaAlO<sub>3</sub> (LAO)/ SrTiO<sub>3</sub> (STO) interface can be controlled via the field effect, whereby a global back gate can be used to systematically tune the critical temperature ( $T_c$ ) of the bulk superconductor. Here, we exploit this sensitivity of  $T_c$  to the field effect to create an electrostatically defined superconducting quantum interference device (SQUID) at the LAO/STO interface. The device consists of a superconducting loop with nanoscale local top gates on each arm. By controllably depleting carriers below the gates we create a SQUID with two identical Josephson junctions (JJs), giving rise to flux-periodic oscillations in the critical current. Furthermore, by independently tuning the two JJs we create an asymmetric SQUID, which allows us to accurately estimate an extremely large kinetic inductance of about 60nH. While other examples of gate-tunable JJs do exist, they necessarily involve physical interfaces between two dissimilar materials. In contrast, our gate-defined SQUIDs are unique in that the entire device is made from a single superconductor with purely electrostatic interfaces.

**4:18PM V30.00008 Aharanov-Bohm quantum interference in LaAlO<sub>3</sub>/SrTiO<sub>3</sub> Hall bar structures<sup>1</sup>**, PATRICK IRVIN, SHICHENG LU, ANIL ANNADI, GUANGLEI CHENG, MICHELLE TOMCZYK, MENGCHEN HUANG, JEREMY LEVY, University of Pittsburgh, HYUNGWOO LEE, CHANG-BEOM EOM, University of Wisconsin-Madison — Aharanov-Bohm (AB) interference can arise in transport experiments when magnetic flux threads through two or more transport channels. The existence of this behavior requires long-range ballistic transport and is typically observed only in exceptionally clean materials. We observe AB interference in wide ( $w \sim 100$  nm) channels created at the LaAlO<sub>3</sub>/SrTiO<sub>3</sub> interface using conductive AFM lithography. Interference occurs above a critical field  $B \sim 4$  T and increases in magnitude with increasing magnetic field. The period of oscillation implies a ballistic length that greatly exceeds the micron-scale length of the channel, consistent with Fabry-Perot interference in 1D channels. The conditions under which AB oscillations are observed will be discussed in the context of the electron pairing mechanism in LaAlO<sub>3</sub>/SrTiO<sub>3</sub>.

<sup>1</sup>We gratefully acknowledge financial support from AFOSR (FA9550-10-1-0524 (JL), FA9550-12-1-0268 (JL), and FA9550-12-1-0342 (CBE)) and NSF (DMR-1124131 (JL), DMR-1104191 (JL), and DMR-1234096 (CBE))

**4:30PM V30.00009 Dimensionality effects on superconductivity in LaAlO<sub>3</sub>/SrTiO<sub>3</sub> nanostructures<sup>1</sup>**, ANIL ANNADI, SHICHENG LU, GUANGLEI CHENG, MICHELLE TOMCZYK, MENGCHEN HUANG, PATRICK IRVIN, University of Pittsburgh, HYUNGWOO LEE, CHANG-BEOM EOM, University of Wisconsin-Madison, JEREMY LEVY, University of Pittsburgh — We investigate electron transport, especially superconductivity, in LaAlO<sub>3</sub>/SrTiO<sub>3</sub> nanostructures with respect to the dimensionality by creating channels with widths varying from nanometers to micrometers using c-AFM lithography. Superconducting properties such as upper critical magnetic field and critical current are compared as a function of electron doping (gating) and temperature. The superconducting properties among these devices show a marked deviation from naive scaling expectations. We discuss the results in regard to ferroelastic domains and possible edge/boundary mode transport scenarios.

<sup>1</sup>We gratefully acknowledge financial support from following agencies and grants: AFOSR FA9550-10-1-0524 (JL, CBE), AFOSR FA9550-12-1-0057 (JL, CBE), NSF DMR-1104191 (JL), ONR N00014-15-1-2847 (JL).

**4:42PM V30.00010 Quantum Oscillations at LaTiO<sub>3</sub>/SrTiO<sub>3</sub> Interfaces<sup>1</sup>**, MICHAEL VEIT, YURI SUZUKI, Stanford University — Emergent metallic behavior at the interface of the Mott insulator LaTiO<sub>3</sub> and the band insulator SrTiO<sub>3</sub> was observed for the first time more than a decade ago. Since then the metallicity has been explained in terms of charge redistribution at the interface combined with lattice relaxation. However to date, Shubnikov de Haas oscillations have not been reported in this two dimensional metallic system. For ultrathin (3-4 unit cells) LaTiO<sub>3</sub> thin films on SrTiO<sub>3</sub>, we report the observation of Shubnikov-de Haas oscillations whose frequency corresponds to a small Fermi pocket. Surprisingly the oscillation are only observed between 1 and 4 T. Above this range, the quantum limit is reached for this pocket so no more oscillations are observed. A Berry's phase of  $\pi$  is also detected in these oscillations. Additionally a strong in-plane anisotropic magnetoresistance was measured in the heterostructures which, along with the Berry's phase, is attributed to a giant Rashba coupling at the interface.

<sup>1</sup>This work is funded by a National Security Science Engineering Faculty Fellowship of the Department of Defense under N00014-15-1-0045

**4:54PM V30.00011 Impact of electric-field-dependent dielectric constants on two-dimensional electron gases in complex oxides<sup>1</sup>**, CHRIS VAN DE WALLE, HARTWIN PEELAERS, KARTHIK KRISHNASWAMY, LUKE GORDON, DANIEL STEIAUF, ANNA SARWE, ANDERSON JANOTTI, Univ of California - Santa Barbara — A high-density two-dimensional electron gas (2DEG) can be formed at interfaces of complex oxides. The electric field in the vicinity of the interface depends on the dielectric properties of the material as well as on the electron distribution. However, electric fields can strongly modify the dielectric constant of SrTiO<sub>3</sub> (STO) as well as other complex oxides. Solving the electrostatic problem thus requires a self-consistent approach in which the dielectric constant varies according to the local magnitude of the field. We have implemented the field dependence of the dielectric constant in a Schrodinger-Poisson solver and use the SrTiO<sub>3</sub>/GdTiO<sub>3</sub> interface as an example to discuss the importance of taking this field dependence into account when modeling interfaces of complex oxides [1].

[1] H. Peelaers, K. Krishnaswamy, L. Gordon, D. Steiauf, A. Sarwe, A. Janotti, and C. G. Van de Walle, Appl. Phys. Lett. **107**, 183505 (2015).

<sup>1</sup>This work was supported by ONR and LEAST.

**5:06PM V30.00012 Nanomechanical probes of sketched LaAlO<sub>3</sub>/SrTiO<sub>3</sub> single-electron transistors<sup>1</sup>**, JESSICA MONTONE, FENG BI, MENGCHEN HUANG, PATRICK IRVIN, JEREMY LEVY, University of Pittsburgh, HYUNGWOO LEE, CHANG-BEOM EOM, University of Wisconsin-Madison — The interface of LaAlO<sub>3</sub>/SrTiO<sub>3</sub> presents a locally tunable metal-insulator transition that can be utilized to create complex nanostructures. Using conducting AFM lithography techniques, we can create a variety of nanoscale devices such as sketched single-electron transistors (SketchSETs)<sup>2</sup>. Due to the piezoelectric properties of LaAlO<sub>3</sub>/SrTiO<sub>3</sub>, there exists the possibility of locally modulating the local electron density using the pressure applied by an AFM tip. Some of the most interesting properties are only observed at cryogenic temperature. For this purpose we utilize a cryogenic AFM system. I will describe our efforts to perform nanomechanical imaging of conductive structures, which can be helpful in mapping the electronic properties of oxide nanostructures.

<sup>1</sup>We gratefully acknowledge support from NSF DMR-1104191 (JL, CBE), NSF NASA PA Space Grant Consortium (JM).

<sup>2</sup>G. Cheng, *et. al*, Nature Nanotechnology **6**, 343 (2011).

**5:18PM V30.00013 Density-functional modelling of electron energy-loss spectra for LaAlO<sub>3</sub>/SrTiO<sub>3</sub> quantum well**, MIRI CHOI, LINGYUAN GAO, The University of Texas, QIAN HE, ALBINA BORISEVICH, Oak Ridge National Laboratory, ALEXANDER A. DEMKOV, The University of Texas — LaAlO<sub>3</sub>/SrTiO<sub>3</sub> quantum wells (QW) are grown by molecular beam epitaxy (MBE). The conduction band alignment is investigated using electron energy loss spectroscopy (EELS). We model the EELS spectrum using first-principle calculations. To account for the core-hole effect, the Z+1 approximation is adopted. Site-projected unoccupied p and d densities of states (pDOS) are extracted and compared with the experimental O K and Ti L edges that correspond to 1s to 2p and 2p to 3d transitions, respectively. Results for bulk LaAlO<sub>3</sub> (LAO) and SrTiO<sub>3</sub> (STO) are discussed first and then the quantum well case is analyzed. We investigate the orbital character of the conduction band states in a QW. We find that in LAO/STO QW, there are evanescent Ti-originated states in the LAO layer and relate them with the peak at EELS front edge.

**Thursday, March 17, 2016 2:30PM - 5:42PM —**

**Session V31 DCP: Plasmonics and Beyond III: Materials and Structures** 331 - F. Javier Garcia de Abajo, Barcelona Institute of Science

**2:30PM V31.00001 Three-dimensional topological insulator based nanospaser**, HARI PAUDEL, VADYM APALKOV, MARK STOCKMAN, Georgia State Univ — After the discovery of spaser, now it has been possible to deliver optical energy beyond the diffraction limit and generate an intense source of optical field. Spaser is a nanoplasmonic counter part of laser. One of the major advantages of spaser is the size: spaser is truly a nanoscopic device whose size can be made smaller than skin depth of the material to a size as small as the nonlocality radius. Recently, an electrically pumped graphene based nanospaser has been proposed that operates in the mid-infrared frequency (Apalkov & Stockman). Here we propose an optically pumped nanospaser based on 3-dimensional topological insulator (3D TI) materials such as Bi<sub>2</sub>Se<sub>3</sub> that operates at an energy equal to the bulk bandgap energy and uses the surface as a source for plasmons and its bulk as a gain medium. The population inversion is obtained in the bulk and radiative energy of exciton recombination is transferred to surface plasmons of the same material to stimulate spasing action. As this spaser operates in the mid-infrared spectral region, it can be a useful device for number of applications such as nanoscopy, nanolithography, nanospectroscopy, and semi-classical information processing.

**2:42PM V31.00002 Light Scattering by Spheroids<sup>1</sup>**, YA-MING XIE, Beijing Computational Science Research Center, Beijing 100094, China, XIA JI, LSEC, Institute of Computational Mathematics, Chinese Academy of Sciences, Beijing 100190, China — Nowadays, with the development of technology, particles with size at nanoscale have been synthesized in experiments. It is noticed that anisotropy is an unavoidable problem in the production of nanospheres. Besides, nonspherical nanoparticles have also been extensively used in experiments. Comparing with spherical model, spheroidal model can give a better description for the characteristics of nonspherical particles. Thus the study of analytical solution for light scattering by spheroidal particles has practical implications. By expanding incident, scattered, and transmitted electromagnetic fields in terms of appropriate vector spheroidal wave functions, an analytic solution is obtained to the problem of light scattering by spheroids. Unknown field expansion coefficients can be determined with the combination of boundary conditions and rotational-translational addition theorems for vector spheroidal wave functions. Based on the theoretical derivation, a Fortran code has been developed to calculate the extinction cross section and field distribution, whose results agree well with those obtained by FDTD simulation.

<sup>1</sup>This research is supported by the National Natural Science Foundation of China No. 91230203

**2:54PM V31.00003 Optical response of metal nanojunctions driven by single atom motion: influence of quantized electron transport on nanoplasmonics<sup>1</sup>**, DANIEL SANCHEZ-PORTAL, FEDERICO MARCHESIN, Centro de Física de Materiales de San Sebastián CSIC-UPV/EHU and DIPC, Spain, PETER KOVAL, Donostia International Physics Center (DIPC), Spain, MARC BARBRY, JAVIER AIZPURUA, Centro de Física de Materiales de San Sebastián CSIC-UPV/EHU and DIPC, Spain — The correlation between transport properties across sub-nanometric metallic gaps and the optical response of the system is a complex effect that, similarly to the near-field enhancement [1], is determined by fine atomic-scale details in the junction structure. Using ab initio calculations, we present here a study of the simultaneous evolution of the structure and the optical response of a plasmonic junction as the two Na<sub>380</sub> clusters forming the cavity approach and retract. Atomic reorganizations are responsible for a large hysteresis of the optical response. The system exhibits a jump-to-contact instability during the approach, and the formation of an atom-sized neck across the junction during retraction. Due to the quantization of the conductance in metal nanocontacts, atomic-scale reconfigurations play a crucial role in determining the optical response. We observe abrupt changes in the intensities and spectral positions of the dominating plasmon resonances, and find a one-to-one correspondence between these jumps and those of the quantized transport across the neck. These results point out to an unforeseen connection between transport and optics at the atomic scale, which is at the frontier of current optoelectronics. [1] M. Barbry, et al., Nano Letters **354**, 216 (2015)

<sup>1</sup>We acknowledge support from MINECO (Grants FIS2013-14481-P and MAT2013-46593-C6-2-P), UPV/EHU and Gipuzkuako Foru Aldundia

**3:06PM V31.00004 Condensed Matter in Ultrafast and Superstrong Fields: Attosecond Phenomena**, MARK STOCKMAN, Center for Nano-Optics (CeNO) and Department of Physics and Astronomy, Georgia State University, Atlanta, GA 30302 — We present our latest results for a new class of phenomena in condensed matter optics when a strong optical field 1-3 V/Å changes a solid within optical cycle [1-7]. Such a pulse drives ampere-scale currents in dielectrics and adiabatically controls their properties, including optical absorption and reflection, extreme UV absorption, and generation of high harmonics [8] in a non-perturbative manner on a 100-as temporal scale. Applied to a metal, such a pulse causes an instantaneous and, potentially, reversible change from the metallic to semimetallic properties. We will also discuss our latest theoretical results on graphene that in a strong ultrashort pulse field exhibits unique behavior [9, 10]. New phenomena are predicted for buckled two-dimensional solids, silicene and germanene [11]. These are fastest phenomena in optics unfolding within half period of light. They offer potential for petahertz-bandwidth signal processing, generation of high harmonics on a nanometer spatial scale, etc.

References  
M. Durach et al., Phys. Rev. Lett. 105, 086803 (2010). [2] M. Durach et al., Phys. Rev. Lett. 107, 086602 (2011). [3] A. Schiffrin et al., Nature 493, 70 (2013). [4] M. Schultze et al., Nature 493, 75 (2013). [5] V. Apalkov, and M. I. Stockman, Phys. Rev. B 88, 245438 (2013). [6] V. Apalkov, and M. I. Stockman, Phys. Rev. B 86, 165118 (2012). [7] F. Krausz, and M. I. Stockman, Nat. Phot. 8, 205 (2014). [8] T. Higuchi, M. I. Stockman, and P. Hommelhoff, Phys. Rev. Lett. 113, 213901 (2014). [9] H. K. Kelardeh, V. Apalkov, and M. I. Stockman, Phys. Rev. B 90, 085313 (2014). [10] H. K. Kelardeh, V. Apalkov, and M. I. Stockman, Phys. Rev. B 91, 045439 (2015). [11] H. K. Kelardeh, V. Apalkov, and M. I. Stockman, Phys. Rev. B 92, 045413 (2015).

**3:42PM V31.00005 Nobel metal alloyed thin-films with optical properties on demand**, CHEN GONG, MARINA S. LEITE, Department of Materials Science and Eng., Institute for Research in Electronics and Applied Physics, Univ. of Maryland, College Park, MD 20742 — Metallic materials with tunable optical responses can enable the unprecedented control of optoelectronic and nanophotonic devices with enhanced performance, such as thin-film solar cells, metamaterials and metasurfaces for tunable absorbers and optical filters, among others. Here we present the alloying of noble metals, Ag, Au and Cu, to develop a novel class of material with optical response not achieved by pure metals. We fabricate binary mixtures with controlled chemical composition by co-sputtering. Ellipsometry and surface plasmon polariton coupling angle measurements are in excellent agreement when determining the real part of the dielectric function ( $\epsilon_1$ ). Surprisingly, in some cases, a mixture provides a material with higher surface plasmon polariton quality factor than the corresponding pure metals. Our approach paves the way to implement metallic nanostructures with tunable absorption/transmission, overcoming the current limitation of the dielectric function of noble metals.

**3:54PM V31.00006 Metal alloyed nanostructures with tunable optical properties.**, MARIAMA REBELLO SOUSA DIAS, CHEN GONG, GARRETT WESSLER, MARINA LEITE, Department of Material Science and Eng. Institute for Research in Electronics and Applied Physics - Univ. of Maryland, College Park, MD 20742 — Pure metal nanostructures (Ns) have been widely used to enhance the optical response of optoelectronic devices, ranging from photovoltaics to broadband absorbers. However, their use is limited by their fixed optical properties. The development of metallic materials with modulated optical response could lead to a new class of Ns for optoelectronic devices with enhanced performance. In this work, we simulated and measured the optical response of binary mixtures of silver (Ag), gold (Au) and aluminum (Al) nanoparticles. We resolved the broadband forward scattering of these alloyed nanoparticles when applied to solar cells by finite-difference time-domain (FDTD) calculations. For a realistic prediction, we used the measured dielectric function of thin-films with identical chemical composition. We demonstrate that, in some cases, an alloy can outperform their pure metal counterparts, e.g.  $\text{Ag}_{0.5}\text{Au}_{0.5}$  shows increased light absorption at 800 nm than pure Au and Ag. The optical response of the alloyed Ns and its dependence with size and composition is measured by transmission and near-field scanning optical microscopy (NSOM). The use of alloyed metals as building blocks for broadband absorbers, where a large imaginary part of the dielectric function is desired, will also be discussed.

**4:06PM V31.00007 Emission and propagation of hyperbolic phonon polaritons in hexagonal boron nitride**, SIYUAN DAI, University of California, San Diego, QIONG MA, YAFANG YANG, Massachusetts Institute of Technology, JEREMY ROSENFELD, MICHAEL GOLDFLAM, ALEX MCLEOD, University of California, San Diego, TROND ANDERSEN, Massachusetts Institute of Technology, ZHE FEI, MENGKUN LIU, ZHIYUAN SUN, YINMING SHAO, University of California, San Diego, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Japan, MARK THIEMENS, University of California, San Diego, FRITZ KEILMANN, Ludwig-Maximilians-Universitt and Center for Nanoscience, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology, MICHAEL FOGLER, D. N. BASOV, University of California, San Diego — Using scattering-type scanning near-field optical microscope (s-SNOM), we studied various kinds of emission and propagation of hyperbolic phonon polaritons (HP2s) in hexagonal boron nitride (hBN). The systematic study via real-space nano-imaging reveals the emission mechanisms and propagating properties of HP2s excited by crystal edges, artificial structures, surface defects and impurities. Compared with traditional s-SNOM tip emitter, the polaritons from new emitters reported in this work possess longer propagation length and can be artificially manipulated on the hBN surface. Our work may benefit the future applications and engineering of HP2s using convenient emitters which are analogous to collective modes in other materials.

**4:18PM V31.00008 Nano-photonic phenomena in van der Waals atomic layered materials**, DMITRI BASOV, UCSD — Layered van der Waals (vdW) crystals reveal diverse classes of light-matter modes (polaritons) including: surface plasmon polaritons in graphene, hyperbolic phonon polaritons in boron nitride, exciton polaritons in  $\text{MoS}_2$ , Cooper pair plasmon polaritons in high-Tc cuprates, topological plasmon polaritons and many others. Polaritons in vdW materials are of considerable technological interest. For example, polaritonic modes enable sub diffractional focusing and imaging in infrared frequencies. Applications apart, infrared nano-imaging of propagating polaritons facilitates experimental access to new physics of vdW materials not attainable with conventional spectroscopic methods. I will discuss two recent experiments performed in our group that utilize unique virtues of polaritons. Nano-imaging of plasmon polaritons in moire superlattices formed in graphene on boron nitride has allowed us to establish the important features of the electronic structure of this interesting from of graphene. Pump-probe hyper-spectral images of non-equilibrium plasmon polaritons in graphene revealed novel aspects of carrier relaxation.

**4:54PM V31.00009 Unveiling nanometric plasmons optical properties with advanced electron spectroscopy in the Scanning Transmission Electron Microscope**, MATHIEU KOCIAK, Centre National de la Recherche Scientifique — Since the pioneering work of Yamamoto[1], the use of electron spectroscopy such as Cathodoluminescence (CL) and Electron Energy Loss Spectroscopy (EELS) in a Scanning (Transmission) Electron Microscope (STEM) has considerably helped improving our understanding of the optical properties of metallic nanoparticles. The resemblance of spectroscopic signals from electron and pure optical techniques leads to the intuition that both types of techniques are very close, an idea theoretically discussed by F.J. Garcia de Abajo and coworkers[2]. However, it is also quite intuitive that CL and EELS should be different. For example, EELS helps detecting any sort of modes while CL can only detect radiative ones. On the other hand, even between optical spectroscopy techniques, clear differences such as energy shifts or spectral shapes changes are expected in the case of plasmons. The lack of adapted instrumentation capable of performing combined EELS and CL, as well as theoretical developments allowing to account for the generic difference between EELS and CL and their optical counterparts impeached a comprehensive understanding of plasmons physics with the otherwise amazing electron spectroscopies. In this talk, I will present recent experimental results showing combined EELS and CL spectral mapping of plasmonic properties for nanoparticles with several shapes (triangles [3], cubes, stars) and composition (gold, silver, aluminum). Helped with different theoretical tools [3,4], I will try to show how these results can be related to their optical counterparts (extinction, scattering), and what type of physical insights can be gained from these combined measurements. Finally, if time allows, pointing the weaknesses of state-of-the-art CL and EELS (in terms of spectral range and/or spectral resolution), I will present EELS results obtained on highly monochromated electron beams that could cope with these limitations. [1] N. Yamamoto, K. Araya, and F. Garca de Abajo, Phys. Rev. B 64, (2001). [2] F. Garca de Abajo and M. Kociak, Phys. Rev. Lett. 100, (2008). [3] A. Losquin, L. F. Zagonel, V. Myroshnychenko, B. Rodriguez-Gonzalez, M. Tenc, L. Scarabelli, J. Frstner, L. M. Liz-Marzn, F. J. G. de Abajo, O. Stphan, and M. Kociak, Nano Lett. 15, 1229 (2015). [4] A. Losquin and M. Kociak, ACS Photonics 2, 1619 (2015).

**5:30PM V31.00010 GaAs/InAs quantum dot exciton and trion excitation via nearby plasmonic waveguides**, MATT SEATON, YANWEN WU, USC Columbia, DAN GAMMON, ALLAN BRACKER, NRL, WU OPTICS GROUP TEAM, NRL TEAM — An open area of research in quantum plasmonics is the detailed characterization of the interaction between plasmonic structures and single quantum emitters. We observe the indirect excitation of excitons and trions in MBE grown GaAs/InAs quantum dots embedded in a Schottky structure by nearby plasmons. The samples, grown on heavily doped N-type GaAs, were coated with a thin Cr layer to provide an electrical gate, through which we observe the photoluminescence spectrum of the different exciton charge states. Through spatially resolved photoluminescence spectroscopy, we verify the QD signature by laser pumping of surface plasmons in Ag thin film plasmonic waveguides near the dots. The waveguides were lithographically defined and embedded in the QD layer of the substrate via wet chemical etching and thermal vapor deposition. The characteristic PL spectra of the dots were collected and observed a large distance away from the excitation point, on the order of ten microns.

**Thursday, March 17, 2016 2:30PM - 5:18PM —**

**Session V32 DCP: Chemical Physics of Extreme Environments II** 332 - Timothy Zwier, Purdue University

**2:30PM V32.00001 Kinetics, mechanisms and products of reactions of Criegee intermediates.**<sup>1</sup>, ANDREW ORR-EWING, University of Bristol — The atmospheric ozonolysis of alkenes such as isoprene produces Criegee intermediates which are increasingly recognized as important contributors to oxidation chemistry in the Earth's troposphere. Stabilized Criegee intermediates are conveniently produced in the laboratory by ultraviolet photolysis of diiodoalkanes in the presence of O<sub>2</sub>, and can be detected by absorption spectroscopy using their strong electronic bands in the near ultraviolet region. We have used these techniques to study a wide range of reactions of Criegee intermediates, including their self-reactions, and reactions with carboxylic acids and various other trace atmospheric constituents. In collaboration with the Sandia National Laboratory group led by Drs C.A. Taatjes and D.L. Osborn, we have used photoionization and mass spectrometry methods, combined with electronic structure calculations, to characterize the products of several of these reactions. Our laboratory studies determine rate coefficients for the Criegee intermediate reactions, many of which prove to be fast. In the case of reactions with carboxylic acids, a correlation between the dipole moments of the reactants and the reaction rate coefficients suggests a dipole-capture controlled reaction and allows us to propose a structure-activity relationship to predict the rates of related processes. The contributions of these various Criegee intermediate reactions to the chemistry of the troposphere have been assessed using the STOCHEM-CRI global atmospheric chemistry model.

<sup>1</sup>This work was supported by NERC grant NE/K004905/1.

**3:06PM V32.00002 Direct Measurement of the Unimolecular Decay Rate of Criegee Intermediates to OH Products.**<sup>1</sup>, FANG LIU, YI FANG, University of Pennsylvania, STEPHEN KLIPPENSTEIN, Argonne National Laboratory, ANNE MCCOY, University of Washington Seattle, MARSHA LESTER, University of Pennsylvania — Ozonolysis of alkenes is an important non-photolytic source of OH radicals in the troposphere. The production of OH radicals proceeds through formation and unimolecular decay of Criegee intermediates such as syn-CH<sub>3</sub>CHOO and (CH<sub>3</sub>)<sub>2</sub>CCOO. These alkyl-substituted Criegee intermediates can undergo a 1,4-H transfer reaction to form an energized vinyl hydroperoxide species, which breaks apart to OH and vinoxy products. Recently, this laboratory used IR excitation in the C-H stretch overtone region to initiate the unimolecular decay of syn-CH<sub>3</sub>CHOO and (CH<sub>3</sub>)<sub>2</sub>CCOO Criegee intermediates, leading to OH formation. Here, direct time-domain measurements are performed to observe the rate of appearance of OH products under collision-free conditions utilizing UV laser-induced fluorescence for detection. The experimental rates are in excellent agreement with statistical RRKM calculations using barrier heights predicted from high-level electronic structure calculations. Accurate determination of the rates and barrier heights for unimolecular decay of Criegee intermediates is essential for modeling the kinetics of alkene ozonolysis reactions, a significant OH radical source in atmospheric chemistry, as well as the steady-state concentration of Criegee intermediates in the atmosphere.

<sup>1</sup>This research was supported through the National Science Foundation under grant CHE-1362835.

**3:18PM V32.00003 Probing neutral atmospheric collision complexes with anion photoelectron imaging.**<sup>1</sup>, CAROLINE JARROLD, None — Photodetachment of anionic precursors of neutral collision complexes offers a way to probe the effects of symmetry-breaking collision events on the electronic structure of normally transparent molecules. We have measured the anion photoelectron imaging (PEI) spectra of a series of O<sub>2</sub><sup>-</sup> · X complexes, where X is a volatile organic molecule with atmospheric relevance, to determine how the electronic properties of various X molecules affect the low-lying electronic structure of neutral O<sub>2</sub> undergoing O<sub>2</sub> – X collisions. The study was motivated by the catalog of vibrational and electronic absorption lines induced by O<sub>2</sub>–O<sub>2</sub>, O<sub>2</sub>–N<sub>2</sub>, and other collisions. The energies of electronic features observed in the anion PEI spectra of O<sub>2</sub><sup>-</sup> · X (X = hexane, hexene, isoprene and benzene) relative to O<sub>2</sub><sup>-</sup> PEI spectroscopic features indicate that photodetachment of the anion does indeed access a repulsive part of the O<sub>2</sub> – X potential. In addition, the spectra of the various complexes show an interesting variation in the intensities of transitions to the excited O<sub>2</sub>(<sup>1</sup>Δ<sub>g</sub>) · X and O<sub>2</sub>(<sup>1</sup>Σ<sub>g</sub><sup>+</sup>) · X states relative to the ground O<sub>2</sub>(<sup>3</sup>Σ<sub>g</sub><sup>-</sup>) · X state. With X = non-polar species such as hexane, the relative intensities of transitions to the triplet and singlet states of O<sub>2</sub> · X are very similar to those of isolated O<sub>2</sub>, while the relative intensity of the singlet band decreases and becomes lower in energy relative to the triplet band for X = polar molecules. A significant enhancement in the intensities of the singlet bands is observed for complexes with X = isoprene and benzene, both of which have low-lying triplet states. The role of the triplet states in isoprene and benzene, and the implications for induced electronic absorption in O<sub>2</sub> undergoing collisions with these molecules, are explored.

<sup>1</sup>National Science Foundation NSF CHE 1265991

**3:54PM V32.00004 Photoelectron Spectroscopy of Transition Metal Hydride Cluster Anions and Their Roles in Hydrogenation Reactions**, XINXING ZHANG, KIT BOWEN, Johns Hopkins University — The interaction between transition metals and hydrogen has been an intriguing research topic for such applications as hydrogen storage and catalysis of hydrogenation and dehydrogenation. Special bonding features between TM and hydrogen are interesting not only because they are scarcely reported but also because they could help to discover and understand the nature of chemical bonding. Very recently, we discovered a PtZnH<sub>5</sub><sup>-</sup> cluster which possessed an unprecedented planar pentagonal coordination between the H<sub>5</sub><sup>-</sup> moiety and Pt, and exhibited special σ-aromaticity. The H<sub>5</sub><sup>-</sup> kernel as a whole can be viewed as a η<sup>5</sup>-H<sub>5</sub> ligand for Pt. As the second example, an H<sub>2</sub> molecule was found to act as a ligand in the PdH<sub>3</sub><sup>-</sup> cluster, in which two H atoms form a η<sup>2</sup>-H<sub>2</sub> type of ligation to Pd. These transition metal hydride clusters were considered to be good hydrogen sources for hydrogenation. The reactions between Pth<sub>n</sub><sup>-</sup> and CO<sub>2</sub> were investigated. We observed formate in the final product H<sub>2</sub>Pt(HCO<sub>2</sub>)<sup>-</sup>.

**4:06PM V32.00005 Total Cross Section Measurements and Velocity Distributions of Hyper-thermal Charge Transfer in  $\text{Xe}^{2+} + \text{N}_2^1$** , MICHAEL HAUSE, Boston College Institute of Scientific Research, BENJAMIN PRINCE, RAYMOND BEMISH, Air Force Research Laboratory — Guided-ion beam measurements of the charge exchange (CEX) cross section for  $\text{Xe}^{2+} + \text{N}_2$  are reported for collision energies ranging from 0.3 to 100 eV in the center-of-mass frame. Measured total XS decrease from  $69.5 \pm 0.3$  Angstroms<sup>2</sup> (Angs.) at the lowest collision energies to 40 Angs.<sup>2</sup> at 100 eV. The product  $\text{N}_2^+$  CEX cross section is similar to the total CEX cross section while those of the dissociative product,  $\text{N}^+$ , are less than 1Angs.<sup>2</sup> for collision energies above 9 eV. The product  $\text{N}_2^+$  CEX cross section measured here are much larger than the total optical emission-excitation cross sections for the  $\text{N}_2^+$  (*A*) and (*B*) state products determined previously in the chemiluminescence study of Prince and Chiu suggesting that most of the  $\text{N}_2^+$  products are in the *X* state. Time-of-flight (TOF) spectra of both the  $\text{Xe}^+$  and  $\text{N}_2^+$  products suggest two different CEX product channels. The first leaves highly-vibrationally excited  $\text{N}_2^+$  products with forward scattered  $\text{Xe}^+$  (LAB frame) and releases between 0.35 to 0.6 eV translational energy for collisions below 17.6 eV. The second component decreases with collisional energy and leaves backscattered  $\text{Xe}^+$  and low-vibrational states of  $\text{N}_2^+$ . At collision energies above 17.6 eV, only charge exchange involving minimal momentum exchange remains in the TOF spectra.

<sup>1</sup>AFOSR 13RV07COR

**4:18PM V32.00006 Aerosol droplets: Nucleation dynamics and photokinetics<sup>1</sup>**, RUTH SIGNORELL, Laboratory of Physical Chemistry, ETH Zurich — This talk addresses two fundamental aerosol processes that play a pivotal role in atmospheric processes: The formation dynamics of aerosol particles from neutral gas phase precursors and photochemical reactions in small aerosol droplets induced by ultraviolet and visible light. Nucleation is the rate determining step of aerosol particle formation. The idea behind nucleation is that supersaturation of a gas leads to the formation of a critical cluster, which quickly grows into larger aerosol particles. We discuss an experiment for studying the size and chemical composition of critical clusters at the molecular level. Much of the chemistry happening in planetary atmospheres is driven by sunlight. Photochemical reactions in small aerosol particles play a peculiar role in this context. Sunlight is strongly focused inside these particles which leads to a natural increase in the rates of photochemical reactions in small particles compared with the bulk. This ubiquitous phenomenon has been recognised but so far escaped direct observation and quantification. The development of a new experimental setup has finally made it possible to directly observe this nanofocusing effect in droplet photokinetics.

<sup>1</sup>This work was supported by the Swiss National Science Foundation (SNSF) and ETH Zurich.

**4:54PM V32.00007 Single Scattering Albedo of fresh biomass burning aerosols measured using cavity ring down spectroscopy and nephelometry<sup>1</sup>**, SOLOMON BILILIGN, SUJEETA SINGH, MARC FIDDLER, NCAT State University, DAMON SMITH, High Point University, BILILIGN RESEARCH GROUP TEAM — An accurate measurement of optical properties of aerosols is critical for quantifying the effect of aerosols on climate. Uncertainties still persist and measurement results vary significantly. The factors that affect measurement accuracy and the resulting uncertainties of the extinction-minus-scattering method are evaluated using a combination of cavity ring-down spectroscopy (CRDS) and integrating nephelometry and applied to measure the optical properties of fresh soot (size 300 and 400 nm) produced from burning of pine, red oak and cedar. We have demonstrated a system that allows measurement of optical properties at a wide range of wavelengths, which can be extended over most of the solar spectrum to determine “featured” absorption cross sections as a function of wavelength. SSA values measured were nearly flat ranging from 0.45 to 0.6. The result also demonstrates that SSA of fresh soot is nearly independent of wavelength of light in the 500-680 wavelength range with a slight increase at longer wavelength. The values are within the range of measured values both in the laboratory and in field studies for fresh soot

<sup>1</sup>The work is supported by the Department of Defense grant W911NF-11-1-0188

**5:06PM V32.00008 Catching Conical Intersections in the Act; Monitoring Transient Electronic Coherences by Attosecond Stimulated X-Ray Raman Signals<sup>1</sup>**, KOCHISE BENNETT, MARKUS KOWALEWSKI, KONSTANTIN DORFMAN, SHAUL MUKAMEL, University of California, Irvine — Conical intersections (CIs) dominate the pathways and outcomes of virtually all photochemical molecular processes. Despite extensive experimental and theoretical effort, CIs have not been directly observed yet and the experimental evidence is inferred from fast reaction rates and vibrational signatures. We show that short X-ray pulses can directly detect the passage through a CI with the adequate temporal and spectral sensitivity. The non-adiabatic coupling that exists in the region of a CI redistributes electronic population but also generates electronic coherence. This coherent oscillation can then be detected via a coherent Raman process that employs a composite femtosecond/attosecond X-ray pulse. This technique, dubbed Transient Redistribution of Ultrafast Electronic Coherences (TRUECARS) is reminiscent of Coherent Anti-Stokes Raman Spectroscopy (CARS) in that a coherent oscillation is set in motion and then monitored, but differs in that the dynamics is electronic (CARS generally observes nuclear dynamics) and the coherence is generated internally by passage through a region of non-adiabatic coupling rather than by an externally applied laser.

<sup>1</sup>Support provided by U.S. Department of Energy through Award No. DE-FG02-04ER15571, the National Science Foundation (Grant No CHE-1361516), and the Alexander von Humboldt foundation through the Feodor Lynen program.

**Thursday, March 17, 2016 2:30PM - 5:30PM —**  
**Session V33 DPOLY: Block Copolymer Thin Films: Directed Self-Assembly** 336 - Gila Stein, University of Houston

**2:30PM V33.00001 Log-rolling block copolymers cylinders**, SO YOUN KIM, YE CHAN KIM, DONG HYUP KIM, NA KYUNG KWON, Ulsan National Institute of Science and Technology, RICHARD A. REGISTER, Princeton University — Shear has been the most effective method to create long range order of micro- or nano- structures in soft materials. When shear is applied, soft particles or polymers tend to align along the shear direction to minimize the viscous dissipation, thus transverse (so-called log-rolling) alignment is unfavored. In this study, for the first time we report the transverse alignment of cylinder-forming block copolymers. Poly(styrene-*b*-methyl methacrylate), PS-PMMA, can form a metastable hemicylinder structure when confined in a thin film, and this hemicylinder structure can align either along the shear direction, or transverse to the shear direction (log-rolling), depending on the shearing temperature. This unusual log-rolling behavior is explained by the different chain mobility of the two blocks in PS-PMMA; the rigidity of core cylinder is the critical parameter determining the direction of shear alignment.

**2:42PM V33.00002 Laser Zone Annealing - Accelerated Route to Self-Assembled Nanostructures<sup>1</sup>**, PAWEL MAJEWSKI, KEVIN YAGER, ATIKUR RAHMAN, CHARLES BLACK, Brookhaven National Laboratory — We present Laser Zone Annealing – a novel technique of accelerated self-assembly of block copolymer thin films utilizing laser light. In our approach, the laser beam, focused to a narrow line, is rastered across the polymer film coated on the light-absorbing substrate, inducing rapid and highly localized temperature transients in the film. By coupling our method with soft-shear, we demonstrate monolithic alignment of various cylinder-forming block copolymers over extremely short timescales. We utilize the aligned block copolymer films as templates for inorganic nanomaterials patterning. After delivery of inorganic precursors via aqueous or gaseous route, the polymer matrix is ashed leading to extremely well-ordered arrays of inorganic, metallic or semiconducting nanowires. Subsequently, we demonstrate how more complex nanostructures can be created with LZA including multilayered nanomeshes with symmetries beyond the conventional motifs accessible by native block copolymers. We investigate a perspective use of the inorganic arrays as transparent conductors or chemical sensors and characterize their anisotropic electro-optical properties.

<sup>1</sup>Research carried out in part at the Center for Functional Nanomaterials, Brookhaven National Laboratory, which is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886.

**2:54PM V33.00003 Block Copolymer Directed Self-Assembly Approaches for Doping Planar and Non-Planar Semiconductors.**, BHOOSHAN POPERE, Univ of California - Santa Barbara, BORIS RUSS, Univ of California - Berkeley, ANDREW HEITSCH, The Dow Chemical Company, PETER TREFONAS, Dow Electronic Materials, RACHEL SEGALMAN, Univ of California - Santa Barbara — As electronic circuits continue to shrink, reliable nanoscale doping of functional devices presents new challenges. While directed self-assembly (DSA) of block copolymers (BCPs) has enabled excellent pitch control for lithography, controlling the 3D dopant distribution remains a fundamental challenge. To this end, we have developed a BCP self-assembly approach to confine dopants to nanoscopic domains within a semiconductor. This relies on the supramolecular encapsulation of the dopants within the core of the block copolymer (PS-*b*-P4VP) micelles, self-assembly of these micelles on the substrate, followed by rapid thermal diffusion of the dopants into the underlying substrate. We show that the periodic nature of the BCP domains enables precise control over the dosage and spatial position of dopant atoms on the technologically relevant length scales (10-100 nm). Additionally, as the lateral density of 2D circuit elements approaches the Moore's limit, novel 3D architectures have emerged. We have utilized our BCP self-assembly approach towards understanding the self-assembly of our micelles directed by such nanoscale non-planar features. We show that the geometric confinement imposed by the hard feature walls directs the assembly of these micelles.

**3:06PM V33.00004 Directed Nanoscale Assembly of Graphene Based Materials**, SANG OUK KIM, National Creative Research Initiative Center for Multi-Dimensional Directed Nanoscale Assembly, Department of Materials Science & Engineering, KAIST — Graphene based materials, including fullerene, carbon nanotubes and graphene, are two-dimensional polymeric materials consisting of sp<sup>2</sup> hybrid carbons. Those carbon materials have attracted enormous research attention for their outstanding material properties along with molecular scale dimension. The optimized utilization of those materials in various application fields inevitably requires the subtle controllability of their structures and properties. In this presentation, our research achievements associated to directed nanoscale assembly of B- or N-doped graphene based materials will be introduced. Graphene based materials can be efficiently processed into various three-dimensional structures via self-assembly principles. Those carbon assembled structures with extremely large surface and high electro-conductivity are potentially useful for energy and environmental applications. Aqueous dispersion of graphene oxide shows liquid crystalline phase, whose spontaneous molecular ordering is useful for display or fiber spinning. Along with the structure control by directed nanoscale assembly, substitutional doping of graphene based materials with B- or N- can be attained via various chemical treatment methods. The resultant chemically modified carbon materials with tunable workfunction, charge carrier density and enhanced surface activity could be employed for various nanomaterials and nanodevices for improved functionalities and performances.

**3:42PM V33.00005 Direct Immersion Solvent Annealing of Nano-filled Block Copolymer Films**, MELANIE LONGANECKER, ARVIND MODI, Univ of Akron, GUANGCUI YUAN, SUSHIL SATIJA, National Institute of Standards and Technology, JOONA BANG, Korea University, ALAMGIR KARIM, Univ of Akron, UNIVERSITY OF AKRON TEAM, NATIONAL INSTITUTE OF TECHNOLOGY COLLABORATION, KOREA UNIVERSITY COLLABORATION — The addition of nanoparticles to polymer films is a strategic approach to enhance film properties such as optical, thermal, hardness, conductivity, permeability etc. with inorganic components while maintaining an easily processable polymer matrix. To this end, the “annealing” of block copolymers while immersed directly in a chamber of solvent is examined to determine its efficacy in ordering nano-filled block copolymer films. Previously we have shown that it is possible to order neat block copolymer films in a mixture of solvents, and this research follows up that work. Specifically, we observe and utilize the effects of direct immersion solvent annealing (DIA) on lamellar poly(styrene-*b*-methyl methacrylate) thin films with loadings of gold nanoparticles as high as 25 percent by mass. Neutron reflection confirms that DIA is a viable technique applicable to ordering these highly loaded, nano-filled block copolymer systems. Some notable differences exist with respect to results on conservation of domain spacing that may be beneficial to film barrier properties, accomplished with minimal disruption of order and fast kinetics that is compatible with roll-to-roll techniques.

**3:54PM V33.00006 Effects of ultra-fast solvent evaporation in solvent vapor annealed cylinder-forming block polymer thin films**, A. BARUTH, G. NELSON, C. DRAPES, J. WONG, M. GRANT, Creighton Univ, Omaha, NE — Despite continued advances in directed self-assembly of block polymer thin films via solvent vapor annealing, a standardized process remains absent. There remain several complicating factors, notably solvent evaporation rate. Recent theoretical models point to this rate dominating the propagation of a given morphology into the bulk of a thin film following nucleation from the free surface. During this drying process, the film undergoes a competition between thermodynamically driven phase separation and kinetically controlled chain mobility. We, among others, have demonstrated that faster solvent removal can enhance propagation down to the substrate. Perpendicularly aligned cylinders are one illustrative example. To further quantify this effect, and look at ultra-fast time scales, we have constructed a solvent vapor annealing chamber that computer-controls evaporation times down to 15 ms. *In situ* spectral reflectance, with 10 ms temporal resolution, monitors the swelling and evaporation. We will present results on cylinder-forming polystyrene-*block*-polylactide thin films swollen to near disorder with tetrahydrofuran, followed by immediate solvent evaporation. Our data reveals control over evaporation times, ranging from 15 ms to several seconds, and the discovery of various evaporation types, previously undetected, including linear, exponential and combinations. Furthermore, atomic force micrographs correlate surface morphologies (both free and substrate) of the resultant films with each evaporation condition. Funded by Nebraska EPSCoR.

**4:06PM V33.00007 Fabrication of nanoporous block copolymer films using highly selective solvents and non-solvent extraction**, CHANGHUI YE, BRYAN VOGT, The University of Akron — Nanoporous polymeric films with high porosity are necessary for some applications, such as anti-reflective coating. A simple and relatively environmental benign method is developed to fabricate nanoporous block copolymer thin film with tunable porosity up to 69% based on selective solvent swelling of the majority phase and subsequent rapid extraction with a miscible non-solvent (water). Poly(butylnorbornene)-*block*-poly(hydroxyhexafluoroisopropyl norbornene) (BuHFA) is used to generate these porous thin films due to its high T<sub>g</sub> (>300 °C) and the selectivity of primary alcohols towards HFA. The porosity of these nanoporous films is highly dependent on the solvent quality for HFA. The modulus of the as-prepared nanoporous BuHFA thin films with the porosity from 0% to 69% was investigated by surface wrinkling and a scaling law of modulus versus density was obtained. These nanoporous thin films act as anti-reflective coatings and an increase in transmittance from approximately 92% to 99.1% (average for the full range of visible light) was obtained for double-side coated glass slides. This methodology is simple and highly tunable; extension to other block copolymer systems is likely possible if sufficient solubility contrast between segments exists.

**4:18PM V33.00008 Tracking Solvent Distribution in Block Polymer Thin Films with In Situ Solvent Vapor Annealing during Neutron Scattering**, CAMERON SHELTON, University of Delaware, RONALD JONES, JOSEPH DURA, National Institute of Standards and Technology, THOMAS EPPS, University of Delaware — Solvent vapor annealing (SVA) is a potential route to controlling the self-assembly of block polymer nanostructures in thin film geometries as it harnesses the ability to tune substrate surface, free surface, and polymer-polymer interactions simultaneously. However, the effect of parameters such as solvent preference and solvent partial pressure on nanostructure self-assembly is still poorly understood. Herein, we quantified the degree of preferential segregation of d-benzene into polystyrene domains of cylinder-forming poly(styrene-*b*-isoprene-*b*-styrene) as a function of film thickness and solvent partial pressure. Additionally, measurable changes in lateral domain spacing, vertical layer spacing, film thickness, and the number of stacked domains at set partial pressures were used to determine how solvent-polymer interactions affected nanostructure reorganization. These in situ experiments were conducted with a combination of small-angle neutron scattering (SANS) and neutron reflectivity (NR), which allowed us to obtain a 3-D profile of solvent distribution and nanostructure self-assembly. By studying the underlying solvent-polymer interactions, this work provides an improved understanding of the mechanisms responsible for nanostructure reorganization during SVA.

**4:30PM V33.00009 Continuous and patterned deposition of functional block copolymer thin films using electrospray**, KRISTOF TOTH, HANQIONG HU, Yale University, MYUNGWOONG KIM, Inha University, PADMA GOPALAN, University of Wisconsin, MICHAEL LOEWENBERG, CHINEDUM OSUJI, Yale University — The delivery of sub-micron droplets of dilute polymer solutions to a heated substrate by electrospray deposition (ESD) enables precisely controlled and continuous growth of block copolymer (BCP) thin films. The ESD process overcomes many shortcomings of spin coating deposition, including the batch nature of the process, loss of potentially valuable polymer, limitations of solvent choice, and large time scales of annealing. We report that high substrate temperatures led to vertically oriented cylindrical microdomains of poly(styrene-*b*-methyl methacrylate) (PS-*b*-PMMA) at the film surface independent of the solvent composition and deposition rates utilized. Conversely, low substrate temperatures resulted in morphologies that were more sensitive to these parameters, with poorly ordered films of globular structures. We also report on the new possibility for patterned deposition of BCP films by spatially varying the electric field at the substrate using an underlying charged grid. To overcome surface charging, a novel alternating current electrospray process is proposed for deposition on non-conductive surfaces.

**4:42PM V33.00010 Formation of Lamellar Heterolattices in Block Copolymer Thin Films by Sequential Electrospray Deposition**<sup>1</sup>, YOUNGWOONG CHOO, HANQIONG HU, KRISTOF TOTH, CHINEDUM OSUJI, Yale University — Electrospray deposition (ESD) of block copolymers (BCPs) on a heated substrate provides precise control over the formation of BCP thin films. This continuous deposition process allows one to fabricate heterogeneously assembled thin films by altering the deposition materials. Here, we demonstrate such the sequential ESD of lamellae-forming poly(styrene-*b*-4-vinylpyridine) BCPs with differing molecular weights and explore the morphology of the composite films. The resulting structure of the heterolattice interface was a strong function of temperature. Sharp interfaces with abrupt changes in the lamellar period ( $L_0$ ) were observed at lower deposition temperatures (150 - 170 °C), while higher temperature (190 °C) produced a smooth variation in the lamellar period from one molecular weight to the next. Furthermore, the ordering kinetics of a secondary layer which was deposited onto the primary layer could be substantially enhanced depending on the molecular weight of the polymer present in the underlying primary layer. We elucidate these findings in the context of temperature and molecular weight dependent diffusion dynamics of the polymers in the melt which control the inter-mixing of the layers.

<sup>1</sup>We gratefully acknowledge funding by NSF DRM-1410568

**4:54PM V33.00011 Hierarchical assembled nanostructures of hydrogen-bonded supramolecular block copolymer thin films.**<sup>1</sup>, XIAOFANG CHEN, YONGCHEN CAI, Soochow University — Controlling the microdomain orientation and long-range ordering in block copolymer thin films is very important in a number of applications, such as nanotemplate, nanoporous thin film, and data storage media. The hierarchical assemblies of block copolymers PS-*b*-P4VP with dendronized small molecules (DM) hydrogen-bonded onto P4VP blocks were investigated in thin films after solvent vapor annealing. P4VP/DM could form lamellar or hexagonal columnar structure with the periodicity around 8 nm, depending on the stoichiometry of the complex. Hierarchical assemblies of PS-*b*-P4VP(DM)<sub>x</sub>, including lamellae-within-lamellae, cylinder-within-lamellae, and cylinder-within-cylinder, were simultaneously ordered and oriented in thin films, which have been studied systematically with the help of AFM, TEM and GISAXS technologies. The orientation of supramolecular assembly depends on the P4VP(DM) fraction and can be tailored by varying the DM to P4VP ratio. Structural transitions from cylinders of (P4VP/DM), lamellae, to cylinders of PS could be achieved by simply increasing the ratio of DM to 4VP units in block copolymer systems.

<sup>1</sup>This work was supported by the National Natural Science Foundation of China (21174003 and 21474073)

**5:06PM V33.00012 Azobenzene photoswitching as a tool for controlling block copolymer self-assembly in dip-coated thin films**, JAANA VAPAAVUORI, JOSU GROSRENAUD, KATERYNA BOROZENKO, CHRISTIAN PELLERIN, GERALDINE BAZUIN, University of Montreal, DEPARTMENT OF CHEMISTRY, UNIVERSITY OF MONTREAL TEAM — Understanding how to control the characteristics of microphase-separated block copolymer thin films is of crucial importance for developing nanotechnological applications, such as producing nanoscale lithography templates for the electronics industry. The supramolecular complexation of small molecules selectively to one of the blocks in suitable block copolymers enables modulating the block volume fractions and thereby controlling the type of surface morphology obtained in thin films. In this contribution, we show that the morphology of dip-coated polystyrene-*b*-poly(4-vinylpyridine) polymer films containing a hydrogen-bonding azobenzene guest can be further controlled using light as an external in situ stimulus during the dip-coating procedure. A change from spherical to cylindrical morphology was demonstrated when the geometry of the azobenzene units was switched by illumination at 365 nm. Film thickness measurements revealed that the thickness of the films can also be tailored by light, since films prepared under irradiation are significantly thicker than non-irradiated ones. The photochemical requirements to guide the choice of azobenzene molecule and the nature of the solvent used will be discussed in view of an optimal material combination for easily directable systems.

**5:18PM V33.00013 Crystallization induced block copolymer assembly at curved liquid-liquid interface**, HAO QI, TIAN ZHOU, HAO ZHOU, CHRISTOPHER LI, Drexel University, SOFT MATERIALS LAB TEAM — In a selected solvent, amphiphilic block copolymers can self-assemble into various micelle structures which find widespread applications in nanomedicine. Herein we report a directed assembly of poly(L-lactide acid)-*b*-poly(ethylene glycol) (PLLA-*b*-PEG) at curved oil/water interfaces. Oil droplets were dispersed in water phase upon sonication with amphiphilic PLLA-*b*-PEG as the surfactant. Subsequent crystallization of PLLA segments resulted in the formation of lamellosomes consisting of crystalline PLLA shell and densely-grafted (approx. 1 chain/nm<sup>2</sup>) PEG layer. The structure, morphology, and mechanical properties of these unique polymer ensembles were investigated using transmission electron microscopy and atomic force microscopy. Detailed formation mechanism will be discussed in detail.

**Thursday, March 17, 2016 2:30PM - 5:30PM –**  
Session V34 DPOLY DCOMP: Where Simulation, Theory, and Experiments Meet Across Length Scales II 337 - David Simmons, University of Akron

**2:30PM V34.00001 What drives hydrophobic polymer collapse and re-entry transitions in miscible good solvents?**<sup>1</sup> , FRANCISCO RODRIGUEZ ROPERO, TIMIR HAJARI, NICO F. A. VAN DER VEGT, Tech Univ Darmstadt — Herein, we study co-nonsolvency of poly(*N*-isopropylacrylamide) (PNiPAM) in methanol aqueous solutions. Our results show that both the coil-to-globule transition at low methanol concentrations and the globule-to-coil re-entrance at high methanol concentrations are entropy driven. At low alcohol content, methanol preferentially binds to the PNiPAM globule and drives polymer collapse. Rather than being driven by electrostatic, hydrogen bonding or bridging-type interactions with the globule, preferential methanol binding is found to result from a significant increase of the chain configurational entropy, stabilizing methanol-enriched globular structures over wet globular structures in neat water. The globule-to-coil re-entrance at high methanol concentrations is instead driven by changes in solvent-excluded volume of the coil and globular states imparted by a decrease in solvent density with increasing methanol content of the solution. The co-nonsolvency mechanism proposed in this contribution provides a new angle on how to develop Coarse Grained simulation models for responsive soft matter systems. Moreover, several of the solvation effects described in this contribution can be incorporated in theories for cosolvent-induced conformational transitions in dilute polymer solutions.

<sup>1</sup>This research was supported by the German Research Foundation (DFG) within the Collaborative Research Center "Multiscale Simulation Methods for Soft Matter Systems" (SFB-TRR146).

**2:42PM V34.00002 Co-non-solvency: Depletion forces or preferential adsorption?** , CARLOS MARQUES, Institut Charles Sadron, CNRS, TIAGO OLIVEIRA, PAULO NETZ, Universidade Federal do Rio Grande do Sul, Brazil, TORSTEN STUEHN, DEBASHISH MUKHERJI, KURT KREMER, Max-Planck-Institute for Polymer Research, Germany — Co-non-solvency is a phenomenon that occurs when a polymer is added to a mixture of two (perfectly) miscible and competing good solvents. As a result, the same polymer collapses into a globule within intermediate mixing ratios. More interestingly, polymer collapses despite the fact that the solvent quality remains good or even gets increasingly better by the addition of the better cosolvent [1]. This puzzling phenomenon, where the solvent quality is completely decoupled from the polymer conformation, is driven by strong local preferential adsorption of the better cosolvent to the polymer [1,2,3]. Because a polymer collapses in good solvent, the depletion forces, that are responsible for standard poor solvent collapse, do not play any role in describing co-non-solvency [4]. [1] D. Mukherji and K. Kremer, *Macromolecules* (2013). [2] D. Mukherji, C. M. Marques, and K. Kremer, *Nature Communications* (2014). [3] D. Mukherji, C. M. Marques, T. Stuehn and K. Kremer, *Journal of Chemical Physics* (2015). [4] T. E. de Oliveira, P. A. Netz, D. Mukherji, and K. Kremer, *Soft Matter* (2015).

**2:54PM V34.00003 Depleting depletion: Polymer swelling in poor solvent mixtures** , DEBASHISH MUKHERJI, Max-Planck-Institute for Polymer Research, CARLOS MARQUES, Institut Charles Sadron, CNRS, TORSTEN STUEHN, KURT KREMER, Max-Planck-Institute for Polymer Research — A polymer collapses in a solvent when the solvent particles dislike monomers more than the repulsion between monomers. This leads to an effective attraction between monomers, also referred to as depletion induced attraction. This attraction is the key factor behind standard polymer collapse in poor solvents. Strikingly, even if a polymer exhibits poor solvent condition in two different solvents, it can also swell in mixtures of these two poor solvents. This collapse-swelling-collapse scenario is displayed by poly(methyl methacrylate) (PMMA) in aqueous alcohol. Using molecular dynamics simulations of a thermodynamically consistent generic model and theoretical arguments, we unveil the microscopic origin of this phenomenon. Our analysis suggests that a subtle interplay of the bulk solution properties and the local depletion forces reduces depletion effects, thus dictating polymer swelling in poor solvent mixtures.

**3:06PM V34.00004 Effects of dipolar interactions in polymer brushes** , RAJEEV KUMAR, Oak Ridge National Laboratory — Effects of dipolar interactions on structure of polymer brushes are studied using a combination of semi-analytical theory, numerical simulations based on the self-consistent field theory (SCFT) and experiments. In this talk, insights obtained by studying brushes in the presence and absence of various polar solvents will be discussed. Possibility of vertical phase segregation in planar polymer brushes immersed in polar solvents and interpenetration as well as forces between opposing brushes will be discussed.

**3:42PM V34.00005 Molecular dynamics simulations of poly (ethylene oxide) hydration and conformation in solutions.**<sup>1</sup> , UDAYA DAHAL, DDept. of Physics and Inst. of Mat. Sci., Univ of Connecticut, ELENA DORMIDONTOVA, Dept. of Physics and Inst. of Mat. Sci., Univ of Connecticut — Polyethylene oxide (PEO) is one of the most actively used polymers, especially in biomedical applications due to its high hydrophilicity, biocompatibility and potency to inhibit protein adsorption. PEO solubility and conformation in water depends on its capability to form hydrogen bonds. Using atomistic molecular dynamics simulations we investigated the details of water packing around PEO chain and characterized the type and lifetime of hydrogen bonds in aqueous and mixed solvent solutions. The observed polymer chain conformation varies from an extended coil in pure water to collapsed globule in hexane and a helical-like conformation in pure isobutyric acid or isobutyric acid –water mixture in agreement with experimental observations. We'll discuss the implications of protic solvent arrangement and stability of hydrogen bonds on PEO chain conformation and mobility.

<sup>1</sup>This research is supported by NSF (DMR-1410928)

**3:54PM V34.00006 A Coarse-Grained Model for Thermoresponsive Poly(*N*-isopropylacrylamide)** , LAUREN J ABBOTT, MARK J STEVENS, Sandia National Laboratories — Poly(*N*-isopropylacrylamide) (PNIPAM) is a thermoresponsive polymer that undergoes a phase transition at its lower critical solution temperature (LCST). Although atomistic simulations have been effective to study PNIPAM single chains in solution, they are limited in reaching longer length- and time-scales. In this work, a coarse-grained (CG) model is developed for PNIPAM that captures its thermoresponsive behavior. Nonbonded parameters are fit to experimental thermodynamic data, with minor adjustments to provide better agreement with radial distribution functions from atomistic simulations. Bonded parameters are fit to probability distributions from atomistic simulations using multi-centered Gaussian-based potentials. The temperature-dependent potentials derived for the CG model in this work properly capture the coil-globule transition of PNIPAM single chains and yield a chain-length dependence consistent with atomistic simulations and experiment. The self-assembly of PNIPAM surfactants is also explored. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

**4:06PM V34.00007 A Coarse Grained Model for Methylcellulose: Spontaneous Ring Formation at Elevated Temperature**, WENJUN HUANG, RONALD LARSON, Univ of Michigan - Ann Arbor — Methylcellulose (MC) is widely used as food additives and pharma applications, where its thermo-reversible gelation behavior plays an important role. To date the gelation mechanism is not well understood, and therefore attracts great research interest. In this study, we adopted coarse-grained (CG) molecular dynamics simulations to model the MC chains, including the homopolymers and random copolymers that models commercial METHOCEL A, in an implicit water environment, where each MC monomer modeled with a single bead. The simulations are carried using a LAMMPS program. We parameterized our CG model using the radial distribution functions from atomistic simulations of short MC oligomers, extrapolating the results to long chains. We used dissociation free energy to validate our CG model against the atomistic model. The CG model captured the effects of monomer substitution type and temperature from the atomistic simulations. We applied this CG model to simulate single chains up to 1000 monomers long and obtained persistence lengths that are close to those determined from experiment. We observed the chain collapse transition for random copolymer at 600 monomers long at 50C. The chain collapsed into a stable ring structure with outer diameter around 14nm, which appears to be a precursor to the fibril structure observed in the methylcellulose gel observed by Lodge *et al.* in the recent studies. Our CG model can be extended to other MC derivatives for studying the interaction between these polymers and small molecules, such as hydrophobic drugs.

**4:18PM V34.00008 Modeling helical polymer brushes using self-consistent field theory (SCFT)**<sup>1</sup>, JYOTI MAHALIK, BOBBY SUMPTER, RAJEEV KUMAR, Oak Ridge National Lab — We investigate structure of helical polymer brushes in terms of segment density distribution and local helical ordering using SCFT. A flexible chain model with vector potential was used to model liquid crystalline-like ordering in the brushes. The effects of surface grafting density, polymer molecular weight and the solvent quality on the brush structure were investigated. For densely grafted polymer brushes or the brushes made up of high molecular weight polymers, immersed in good quality solvent, stronger orientational ordering was found near the edge of the brushes (i.e., far from the grafting surface). Furthermore, an increase in the orientational ordering near the grafted end was found with decrease in solvent quality or decrease in molecular weight and decrease in surface grafting density.

<sup>1</sup>Computer Science and Mathematics Division, Oak Ridge National Laboratory

**4:30PM V34.00009 The effects of bonded interactions on the structural phase properties of flexible elastic homopolymer**, KAI QI, BENJAMIN LIEWEHR, TOMAS KOCI, BUSARA PATTANASIRI, MATTHEW WILLIAMS, MICHAEL BACHMANN, The Univ of Georgia — By means of advanced parallel-tempering replica-exchange Monte Carlo methods we systematically examine the effects of an asymmetric bond potential between the bonded monomers on the structural formations of an elastic flexible polymer model. Employing microcanonical inflection-point analysis and conformational analysis based on a suitable set of structural order parameters, we identify diverse structural phases in the low-temperature region of the microcanonical hyperphase diagram. In addition to the icosahedral phase occurring if the symmetry of the bonded interaction is broken by strong bonded Lennard-Jones potential, amorphous structures with bihexagonal cores appear for small values of the asymmetry control parameter in the bond potential. Another remarkable feature is the observation of the hierarchy of freezing transitions associated with the formation of the surface layer after nucleation.

**4:42PM V34.00010 Crystal Growth in Lennard-Jones Mixtures: A Model System to Study Generic Effects in Biomineralization Processes**, MARC RADU, KURT KREMER, Max Planck Institute for Polymer Research — In various scientific fields regulating the growth of crystalline structures and tuning their morphologies plays an important role. E.g. in pharmaceutical delivery the crystallization of a supersaturated drug solution is inhibited by the addition of stimuli-responsive polymers. While past simulation studies rather focused on a detailed understanding of the binding modes of specific additives to likewise specific crystal surfaces here we investigate the characteristics of a generic model system in which we modify the growth mechanisms and the emerging shapes of Lennard-Jones crystallites by tuning the specific interaction parameters and/or adding polymer chains - represented by linear bead-spring molecules - to the system. We performed molecular dynamics simulations on samples containing a crystalline phase embedded in a supersaturated solution applying an adaptive simulation scheme in order to keep the chemical potential difference between the solid and the surrounding liquid constant. We report on different crystal properties depending on a systematic variation of simulation parameters as the solvent content, the solubility and the density of polymer chains. We analyze our results by means of various approaches within the framework of non-equilibrium statistical physics.

**4:54PM V34.00011 ABSTRACT WITHDRAWN** —

**5:06PM V34.00012 Thermodynamics of polymer nematics described with a worm-like chain model: particle-based simulations and SCF theory calculations**, CRISTINA GRECO, Max Planck Institute for Polymer Research, Mainz, Germany, YING YIANG, School of Chemistry and Environment, Center of Soft Matter Physics and Its Applications, BeiHang University, Beijing, China, KURT KREMER, Max Planck Institute for Polymer Research, Mainz, Germany, JEFF CHEN, Department of Physics and Astronomy, University of Waterloo, Canada, KOSTAS DAOULAS, Max Planck Institute for Polymer Research, Mainz, Germany — Polymer liquid crystals, apart from traditional applications as high strength materials, are important for new technologies, e.g. Organic Electronics. Their studies often invoke mesoscale models, parameterized to reproduce thermodynamic properties of the real material. Such top-down strategies require advanced simulation techniques, predicting accurately the thermodynamics of mesoscale models as a function of characteristic features and parameters. Here a recently developed model [1] describing nematic polymers as worm-like chains interacting with soft directional potentials is considered. We present a special thermodynamic integration scheme delivering free energies in particle-based Monte Carlo simulations of this model, avoiding thermodynamic singularities. Conformational and structural properties, as well as Helmholtz free energies are reported as a function of interaction strength. They are compared with state-of-art SCF calculations [2] invoking a continuum analog of the same model, demonstrating the role of liquid-packing and fluctuations. [1] P. Gemnden and K.Ch. Daoulas, Soft Matter 2015, 11, 532; [2] Y. Jiang and J.Z.Y. Chen, Macromolecules 2010, 43, 10668.

**5:18PM V34.00013 Molecular Dynamics Modeling of Dielectric Polarization and Ferroelectricity in Poly(vinylidene fluoride) and Related Polymers**<sup>1</sup>, JEFFREY CALAME, Naval Research Laboratory, Washington, DC 20375 — Molecular dynamics studies of the dielectric polarization response of a constrained bond length and bond angle, united-atom-based model of lamellar crystals of poly(vinylidene fluoride) (PVDF) are reported. Classical ferroelectricity is observed in PVDF, and when variations in the basic PVDF-like interaction parameters are allowed, a transition between classical and relaxor ferroelectricity is found to depend systematically on the polymer repeat unit dipole moment and on the united atom radius of the non-CH<sub>2</sub> functional group. The effects of step and ramp electric field reversal are studied. A complicated sequence of reorientation processes occurs over a wide range of time scales, including a weak, temperature-independent response of 1-2 ps duration associated with local torsional motion, followed by a slow-rising delay regime lasting 10s of ns or longer that involves trans-gauche (TG) transitions in the amorphous phase. After the delay, a large-amplitude primary reorientation occurs over a relatively short additional duration (0.1 to 2 ns), which is due to rotation of large sub-segments in the crystalline phase with few TG transitions. The overall sequence concludes with a slow terminal rise lasting several 100s of ns involving an improvement in crystalline order.

<sup>1</sup>Work supported by the U.S. Office of Naval Research

**Thursday, March 17, 2016 2:30PM - 5:30PM –**

**Session V35 DBIO GSOF GSNP: Active Matter: Collective Phenomena in Living Systems V**

338 - Thierry Mora, ENS and CNRS

**2:30PM V35.00001 Questioning the activity of active matter: the case of bird flocks** , THIERRY MORA, ALEKSANDRA WALCZAK, Ecole normale supérieure and CNRS, LORENZO DEL CASTELLO, University of Rome and CNR, FRANCESCO GINELLI, University of Aberdeen, STEFANIA MELILLO, LEONARDO PARISI, MASSIMILIANO VIALE, ANDREA CAVAGNA, IRENE GIARDINA, University of Rome and CNR — Animal flocking is a natural instance of active matter. What makes flocks active is the rearrangement of neighborhoods, which constantly remodels the network of interactions between individuals in the group, keeping the system out of equilibrium. Despite the predicted importance of this reshuffling, its true impact for natural flocks is not well understood. Here we analyse films of flocks of starlings with a novel statistical inference technique based on dynamical maximum entropy to measure the parameters of flock alignment - alignment strength, interaction range, and noise. We show that birds align their flight orientations must faster than they change neighbors. In the statistical mechanics sense, this means that flocks remain adiabatically in equilibrium, allowing for a rigorous analogy with equilibrium systems of interacting spins, and we show that an inference method based on equilibrium assumptions gives fully consistent results.

**2:42PM V35.00002 Linear response to leadership, effective temperature and decision making in flocks.** , DANIEL PEARCE, LUCA GIOMI, Univ of Leiden — The Vicsek model is the prototypical system for studying collective behavior of interacting self propelled particles (SPPs). It has formed the basis for models explaining the collective behavior of many active systems including flocks of birds and swarms of insects. To the standard Vicsek model we introduce a small angular torque to a subset of the particles and observe how this effects the direction of polarisation of the entire swarm. This is analogous to a few informed birds trying to lead the rest of a large flock by initiating a turn. We find a linear response to this perturbation and fluctuations that are in agreement with fluctuation dissipation theorem. This allows the identification of an effective temperature for the Vicsek model that follows a power law with the noise amplitude. The linear response can also be extended to the process of decision-making, wherein flocks must decide between the behaviors of two competing subgroups of individuals.

**2:54PM V35.00003 Fluctuation Spectra Underlie the Behavior of Non-equilibrium Systems** , ALPHA LEE, Harvard University, DOMINIC VELLA, University of Oxford, JOHN WETTLAUFER, Yale University — A diverse set of important physical phenomena, ranging from hydrodynamic turbulence to the collective behaviour of bacteria, are intrinsically far from equilibrium. Despite their ubiquity, there are few general theoretical results that describe these non-equilibrium steady states. Here we argue that a generic signature of non-equilibrium systems is nontrivial fluctuation spectra. Based on this observation, we derive a general relation for the force exerted by a non-equilibrium system on two embedded walls. We find that for a narrow, unimodal spectrum, the force depends solely on the width and the position of the peak in the fluctuation spectrum, and will oscillate between repulsion and attraction. We demonstrate the generality of our framework by examining two apparently disparate examples: the Maritime Casimir effect and recent simulations of active Brownian particles. A key implication of our work is that important non-equilibrium interactions are encoded within the fluctuation spectrum. In this sense the noise becomes the signal.

**3:06PM V35.00004 Visual perturbations and the collective dynamics of fish schools** , JULIA GIANNINI, JAMES PUCKETT, Gettysburg College — We investigate the dynamics of the collective behaviors exhibited in a laboratory fish school. Using an artificial light gradient with varies both spatially and temporally, we investigate the competition between individual locomotion and local polarization arising from social interactions between individuals. We will discuss how our work informs current agent-based models on the interplay between social interactions and heterogeneous environments.

**3:18PM V35.00005 The influence of following on bidirectional flow through a doorway<sup>1</sup>** , AMY GRAVES, RACHEL DIAMOND, EDUARD SAAKASHVILI, Swarthmore College — Pedestrian dynamics is a subset of the study of self-propelled particles. We simulate two species of pedestrians undergoing bidirectional flow through a narrow doorway. Using the Helbing-Monlr-Farkas-Vicsek Social Force Model, our pedestrians are soft discs that experience psychosocial and physical contact forces. We vary the following parameter which determines the degree to which a pedestrian matches its direction of movement to the average of nearby, same-species pedestrians. Current density, efficiency and statistics of bursts and lags are calculated. These indicate that choosing different following parameters for each species affects the efficacy of transport - greater following being associated with lower efficacy. The information entropy associated with velocity and the long time tails of the complementary CDF of lag times are additional indicators of the dynamical consequences of following during bidirectional flow.

<sup>1</sup>Acknowledgement is made to the donors of the ACS Petroleum Research Fund, and the Vandervelde-Cheung Fund of Swarthmore College

**3:30PM V35.00006 Collective dynamics of sperm in viscoelastic fluid<sup>1</sup>** , CHIH-KUAN TUNG, <sup>1,2</sup>, BENEDICT B. HARVEY, <sup>2</sup>, ALYSSA G. FIORE, <sup>1</sup>, FLORENCIA ARDON, SUSAN S. SUAREZ, <sup>2</sup>, MINGMING WU, Depts of <sup>1</sup>Biological and Environmental Engineering; <sup>2</sup>Biomedical Sciences, Cornell University — Collective dynamics in biology is an interesting subject for physicists, in part because of its close relations to emergent behaviors in condensed matter, such as phase separation and criticality. However, the emergence of order is often less drastic in systems composed of the living cells, sometimes due to the natural variability among individual organisms. Here, using bull sperm as a model system, we demonstrate that the cells migrate collectively in viscoelastic fluids, exhibiting behavior similar to flocking. This collectiveness is greatly reduced in similarly viscous Newtonian fluids, suggesting that the cell-cell interaction is primarily a result of the elastic property or the memory effect of the fluids, instead of pure hydrodynamic interactions. Unlike bacterial swarming, this collectiveness does not require a change in phenotype of the cells; therefore, it is a better model system for physicists.

<sup>1</sup>Supported by NIH grant 1R01HD070038.

**3:42PM V35.00007 To be decided by speaker** , MADAN RAO, National Centre for Biological Sciences(TIFR) — No abstract available.

**4:18PM V35.00008 Critical phenomena in active matter<sup>1</sup>**, MATTEO PAOLUZZI, M CRISTINA MARCHETTI, Syracuse Univ, CLAUDIO MAGGI COLLABORATION, UMBERTO MARINI BETTOLO MARCONI COLLABORATION, NICOLETTA GNAN COLLABORATION — A collection of active agents can organize in phases with structural properties remarkably similar to those of ordinary materials, such as active gases, liquids and glasses. These phases are formed, however, out of equilibrium, where the machinery of equilibrium statistical mechanics cannot be applied. It has recently been shown that models of particles with Gaussian colored noise can capture some of the nonequilibrium behavior of active Brownian particles, including motility-induced phase separation. By using the Unified Gaussian Colored Noise Approximation (UCNA) it has been possible to obtain an equilibrium-like probability distribution function and an effective free energy for active Brownian particles. Here we employ UCNA to examine the effect of colored noise on mean-field order-disorder transitions. Starting with a  $\varphi^4$  Landau model that undergoes a second-order phase transition as a function of a tuning parameter, we calculate the shift in transition due to colored noise as a function of the noise amplitude and correlation time  $\tau$ . We find that the transition line exhibits reentrance as a function of  $\tau$ . The mean-field theoretical predictions are compared with Molecular Dynamics simulations of active Lennard-Jones particles.

<sup>1</sup>We acknowledge support from NSF-DMR-1305184.

**4:30PM V35.00009 Long-range Acoustic Interactions in Insect Swarms: An Adaptive Gravity Model**, DAN GORBONOS, REUVEN IANCONESCU, Department of Chemical Physics, The Weizmann Institute of Science, JAMES G. PUCKETT, Department of Physics, Gettysburg College, RUI NI, Department of Mechanical and Nuclear Engineering, The Pennsylvania State University, NICHOLAS T. OUELLETTE, Department of Civil and Environmental Engineering, Stanford University, NIR S. GOV, Department of Chemical Physics, The Weizmann Institute of Science — The collective motion of groups of animals emerges from the net effect of the interactions between individual members of the group. In many cases, such as birds, fish, or ungulates, these interactions are mediated by sensory stimuli that predominantly arise from nearby neighbors. But not all stimuli in animal groups are short range. Here, we consider mating swarms of midges, which interact primarily via long-range acoustic stimuli. We exploit the similarity in form between the decay of acoustic and gravitational sources to build a model for swarm behavior. By accounting for the adaptive nature of the midges acoustic sensing, we show that our adaptive gravity model makes mean-field predictions that agree well with experimental observations of laboratory swarms. Our results highlight the role of sensory mechanisms and interaction range in collective animal behavior. The adaptive interactions that we present here open a new class of equations of motion, which may appear in other biological contexts.

**4:42PM V35.00010 Synchronization of self-propelled units carrying an internal oscillator**, DEMIAN LEVIS, IGNACIO PAGONABARRAGA, ALBERT DIAZ-GUILERA, Univ de Barcelona — We address the question of how self-propulsion, and the dynamical patterns emerging from it, affects the synchronization of motile physical entities, like moving cells synchronizing their intracellular genetic oscillators. In order to do that, we introduce a simple model of self-propelled hard disks moving in 2D carrying an internal variable which follows a Kuramoto dynamics. We find that, in the absence of particle-particle interactions, self-propulsion promotes the synchronization of the particles up to a saturation threshold that we identify with the parameters of the model. However, the presence of steric interactions give rise to an optimal self-propulsion for synchronization as a consequence of the clustering of the particles. This new effect shows that the interplay between the oscillators coupling and the topology of the underlying network, arising from particle interactions, plays an important role for the performance of mobile systems. We single out several dynamic regimes controlled by different processes that we describe. We analyse the relaxation of the system and show that synchronization proceeds through a mechanism that, despite being out-of-equilibrium, verifies the dynamical scaling hypothesis.

**4:54PM V35.00011 Statistical Mechanics of Collective Transport by Ants**, ITAI PINKOVIEZKY, Department of Chemical Physics, Weizmann Institute of Science, AVIRAM GELBLUM, EHUD FONIO, Department of Physics of Complex Systems, Weizmann Institute of Science, ABHIJIT GHOSH, NIR GOV, Department of Chemical Physics, Weizmann Institute of Science, OFER FEINERMAN, Department of Physics of Complex Systems, Weizmann Institute of Science — Collective decisions and cooperation within groups are essential for the survival of many species. Conflicts within the group must be suppressed but conformism may render the system unresponsive to new information. Collective transport by ants is therefore an ideal model system to study how animal groups optimize these opposing requirements. We combine experiments and theory to characterize the collective transport. The ants are modeled as binary Ising spins, representing the two roles ants can perform during transport. It turns out that the ants poise themselves collectively near a critical point where the response to a newly attached ant is maximized. We identify the size as being proportional to an inverse effective temperature and thus the system can exhibit a mesoscopic transition between order and disorder by manipulating the size. Constraining the cargo with a string makes the system behave as a strongly non-linear pendulum. Theoretically we predict that a Hopf bifurcation occurs at a critical size followed by a global bifurcation where full swings emerge. Remarkably, these theoretical predictions were verified experimentally.

**5:06PM V35.00012 Dynamics of fire ant aggregations**, MICHAEL TENNENBAUM, DAVID HU, ALBERTO FERNANDEZ-NIEVES, Georgia Inst of Tech — Fire ant aggregations are an inherently active system. Each ant harvests its own energy and can convert it into motion. The motion of individual ants contributes non-trivially to the bulk material properties of the aggregation. We have measured some of these properties using plate-plate rheology, where the response to an applied external force or deformation is measured. In this talk, we will present data pertaining to the aggregation behavior in the absence of any external force. We quantify the aggregation dynamics by monitoring the rotation of the top plate and by measuring the normal force. We then compare the results with visualizations of 2D aggregations.

**5:18PM V35.00013 Extensional Rheology of Fire Ant Aggregates<sup>1</sup>**, SCOTT FRANKLIN, MATTHEW KERN, Rochester Institute of Technology, SULISAY PHONEKEO, DAVID HU, Georgia Tech — We explore the extensional rheology and self-healing of fire ant (*Solenopsis invicta*) aggregations, mechanically entangled ensembles used to form rafts, bivouacs or bridges. Macroscopic experiments create quasi-two dimensional piles and measure the force required to impose a constant end-velocity. This force fluctuates, reminiscent of similar experiments on geometrically cohesive granular materials. Heterogeneous chains develop, with isolated ants often the sole link between top and bottom. Finally, the maximum pile strength scales sub-linearly with the number of ants, with the maximum force per ant decreasing as the pile grows. We reproduce these behaviors with a simple model that represents ants feet as discs connected by a spring (the "leg"). Discs move randomly, and stick to one another when in contact. Discs in contact un-stick at random with a probability that decreases as the spring (leg) is stretched, modeling an ant's tendency to hold on longer when stretched. Simulations qualitatively reproduces the fluctuating force, chain formation and sublinear scaling of maximum force with particle number and give insight into underlying mechanisms that govern the ants' behaviors.

<sup>1</sup>Funded in part by NSF DMR 1133722

**Thursday, March 17, 2016 2:30PM - 5:30PM —**  
**Session V36 GSOF: Disordered and Glassy Systems (Non-Polymeric)** 339 - Colm Kelleher, New York University

**2:30PM V36.00001 Injecting a droplet into a quasi-2D jammed emulsion: Fluctuations and rearrangements**, ERIC R. WEEKS, XIA HONG, Physics Dept., Emory University — We experimentally study the dynamic response of a quasi-two-dimensional emulsion to a slowly growing injected droplet. Our area fractions range from  $\phi = 0.77 - 0.99$ , such that the droplets are in most cases in contact with one another and are in many cases highly deformed. There is no dependence of the average flow behavior on distance to the inflation droplet, or on polydispersity or packing fraction of the emulsions. However, the fluctuations of velocity increase as the packing fraction increases. The magnitude of the fluctuations appears similar in both monodisperse, moderately ordered samples and bidisperse, disordered samples.

**2:42PM V36.00002 Densest packings of hard spheres in a cylinder**, LIN FU, WILLIAM STEINHARDT, HAO ZHAO, JOSHUA SOCOLAR, PATRICK CHARBONNEAU, Duke University — Densely packing hard spheres (HS) within a cylinder is remarkably complex. Little is known about the densest achievable packings when the cylinder diameter,  $D$ , is larger than 2.85 times the sphere diameter,  $s$ . Here, we extend the identification of the densest packings up to  $D = 4.00s$  by adapting Torquato-Jiao's adaptive-shrinking-cell formulation and sequential-linear-programming technique to this geometry. We identify 17 new structures, almost all of them chiral. Beyond  $D$ , approx  $2.85s$ , most of the structures consist of an outer shell and of an inner core that compete for being close packed. In some cases the shell adopts a periodic configuration that is optimal and the stacking of core spheres within it is quasiperiodic, while in other cases a direct interplay between the two layers is observed. For some packings the very distinction between the core and shell vanishes, which results in exotic geometries, including some that are a three-dimensional extension of packing hard disks in a circle. In order to connect our results with experiments on comparable systems, we also consider the ease with which these structures assemble. Using kinetic Monte Carlo simulations, we find that some of the structures promptly assemble while others simply do not.

**2:54PM V36.00003 Labyrinthine phase and slow dynamics in a driven magnetic granular medium**, SIMON MERMINOD, TIMOTHEE JAMIN, ERIC FALCON, MICHAEL BERHANU, Matter and Complex Systems (MSC), University Paris Diderot, CNRS, Paris, DIVISION OF NON-EQUILIBRIUM PHYSICS TEAM — Labyrinthine patterns arise in two-dimensional physical systems submitted to competing interactions, ranging from the fields of solid-state physics to hydrodynamics. Here we experimentally investigate a labyrinthine phase in an out-of-equilibrium system constituted of vibrated granular particles. Once sufficiently magnetized, they self-organize into short chains of particles in contact and randomly orientated. We quantitatively characterize the transition from a granular gas state to a labyrinthine phase, and we explain the formation of these chains using a simple model. Interestingly, the labyrinthine phase does not display any steady state: its morphology evolves with the aging time on very long timescales. Experiments suggest that here, slow dynamics involves strong structural rearrangements and therefore is comparable to slow dynamics in structural glasses. We characterize this aging process and evaluate to what extent this analogy holds.

**3:06PM V36.00004 From Gelation and Glass Transition of Colloidal Systems to Polymers**, CHARLES HAN, ICCAS and IAS of SZU, GUANGCUI YUAN, ICCAS, HE CHENG, ICCAS and IHEP — Charles C. Han, Guangcui Yuan and He Cheng Joint Laboratory of Polymer Science and Materials, ICCAS, Beijing, China and Institute for Advanced Study, Shenzhen University, Shenzhen, China Aggregation and gelation behavior of mixed suspensions of polystyrene microspheres and poly(N-isopropylacrylamide) microgels have been studied. In dilute microsphere suspensions, with increasing concentration of microgel (MG), microspheres (MS) first aggregated with each other through the bridging of the microgels, then dispersed individually when saturated adsorption was achieved, and finally depletion clusters formed at even higher concentrations of microgel. In concentrated microsphere suspensions, with saturated MG adsorption, a state transition from attractive glass to repulsive glass can be observed. This type of system can be viewed as a molecular model system which has a long range repulsive interaction potential and a short range attractive potential. A comparison between the glass transition of the colloidal systems and the glass transition of polymeric systems can be made.

**3:18PM V36.00005 Relaxation and self-diffusion of supercooled liquids derived from picosecond timescale dynamics**, MARCUS CICERONE, MIAOCHAN ZHI, BRANDON BLAKELY, MADHUSUDAN TYAGI, NIST — We use neutron scattering and nonlinear optical measurements to investigate ps-ns timescale dynamics in liquid, supercooled liquid, and glassy states. The experimental observables show evidence of dynamic heterogeneity on this timescale that supports a facilitated dynamics picture. We obtain a direct measure of the concentration of molecular excitations, or mobile regions, as a function of time and temperature. Using a model [1] broadly consistent with that proposed by Chandler and co-workers [2], we are able to quantitatively predict self-diffusion rates and Stokes Einstein violation deep in the supercooled regime directly from ps timescale and Angstrom - nanometer length scale measurements for all systems we have investigated. The model we employ also provides a clear physical mechanism for the Johari-Goldstein relaxation process. [1] M.T. Cicerone, Q. Zhong & M. Tyagi, PRL 113 117801 (2014). [2] J. P. Garrahan & D. Chandler, Coarse-grained microscopic model of glass formers, PNAS 100, 9710 (2003).

**3:30PM V36.00006 In search of a Corresponding state description of the thermodynamics and dynamics of complex fluids.**, TAMOGHNA DAS, National Institute of Standards and Technology & University of Maryland, MAHESH BANDI, Okinawa Institute of Science and Technology Graduate University, JACK DOUGLAS, National Institute of Standards and Technology — Long ago, Pitzer introduced a scheme for characterizing the relative "complexity" of fluids based on a consideration of the temperature dependence of the second virial coefficient at low temperature, where this property is sensitive to the form of the inter-molecular potential. "Simple" fluids, in this classification scheme, are those that satisfy a common "corresponding states" in which the properties (eg. shape of the phase boundary, surface tension etc.) obey a universal reduced variable scaling description. This idea was pioneered by van der Waals based on his equation of states describing the pressure of gases. Many real fluids are not "simple" in the sense that the molecules have complex shapes and interact with a combination of short-range and long-range directional interactions having different spatial interaction ranges. These features lead to these fluids being classified as "complex". We show that an effective reduced variable description for a model complex fluid can be achieved by defining a reduced variable involving the second virial coefficient. We further show that a recent reduced variable description of the dynamics and thermodynamics of glass-forming liquids derives from the same principle.

**3:42PM V36.00007 Short-Time Glassy-like Dynamics Observed in Viscous Protein Solutions with Competing Potential Features.**, NORMAN WAGNER, DOUG GODFRIN, University of Delaware, YUN LIU, University of Delaware/NCNR NIST — Structures in concentrated protein solutions caused by the combination of short-range attraction (SA) and long-range repulsion (LR) have been extensively studied due to their importance in understanding therapeutic protein formulations and the phase behavior in general. Despite extensive studies of kinetically arrested states in colloidal systems with short-range attraction, less is understood for the effect of an additional longer-range repulsion on model colloidal systems with a SA interaction. Highly purified lysozyme is used as a model experimental system due to its stable globular structure and SALR interactions at low ionic strength that can be quantitatively modeled. The fluid microstructure and protein short time self diffusion are measured across a broad range of conditions by small angle neutron scattering (SANS) and neutron spin echo (NSE), respectively. Newtonian liquid behavior is observed at all concentrations, even with an increase of zero shear viscosity by almost four orders of magnitude with increasing concentration. However, dynamic measurements demonstrate a sub-diffusive regime at relatively short time scales for concentrated samples at low temperature. The formation of a heterogeneous density distribution is shown to produce localized regions of high density that reduce protein motion, giving it a glassy-like behavior at the short time scale. This heterogeneity occurs at the length scale associated with the intermediate range order driven by the competing potential features, distinguishable from heterogeneous colloidal gels.

### **3:54PM V36.00008 Combined Effects of Media Disorderedness and Tracer Shape on the Trend of Translation-Rotation Decoupling in Two-Dimensional Binary Colloids**

**YOUNGHOON OH, JEONGMIN KIM, BONG JUNE SUNG**, Department of Chemistry, Sogang University, Seoul 987-654, Korea — While translational diffusion of tracers often violates the Stokes-Einstein relation, the rotational diffusion of tracers follows the Debye-Stokes-Einstein relation faithfully in the glass-forming materials. A previous study revealed that in two-dimensional (2D) monodisperse colloids, as the dynamics of media became heterogeneous in 2D hexatic phase, the tracer shape and the local media structure affected the translation-rotation decoupling trend significantly [1]: the rotation of tracers was enhanced compared to the translation for square tracers but was rather suppressed for diamond tracers. The shape dependency of rotation originated from the similarity in structure between the local hexagonal media structure and the tracer shape. Unlike in 2D monodisperse colloids where the liquid-to-hexatic phase transition takes place, in 2D binary colloids, a phase transition from the liquid to either solid or glass depends on the disorderedness that is controlled by size and number ratios. We present simulation results on the combined effects of the tracer shape and the local media disorderedness on the translation-rotation decoupling, which relates closely to the nature of glass transition. [1] J. Kim and B. J. Sung, Phys. Rev. Lett. 115, 158302 (2015)

### **4:06PM V36.00009 Spatio-temporal correlations in Coulomb clusters**

**AMIT GHOSAL, BISWARUP ASH**, Indian Institute of Science Education and Research-Kolkata, Mohanpur Campus, India-741246, **JAYDEB CHAKRABARTI**, S. N. Bose National Centre for Basic Sciences, Kolkata, India-700098 — Dynamical response of Coulomb-particles in nanoclusters are investigated at different temperatures characterizing their solid-like (Wigner molecule) and liquid-like behavior. The density correlations probe spatio-temporal relaxation, uncovering distinct behavior at multiple time scales in these systems. They show a stretched-Gaussian or stretched-exponential spatial decay at long times in circular and irregular traps. Interplay of confinement and long-range nature of interactions yields spatially correlated motion of the particles in string-like paths, leaving the system heterogeneous even at long times. While particles in a 'solid' flow producing dynamic heterogeneities, their random motion in 'liquid' defies central limit theorem. Distinguishing the two confinements, temperature dependent motional signatures serve as a criterion for the crossover between 'solid' and 'liquid'. The irregular Wigner molecule turns into a nearly homogeneous liquid over a much wider temperature window compared to the circular case. The temperature dependence of different relaxation time scales builds crucial insights. A phenomenological model, relating the unusual dynamics to the heterogeneous nature of the diffusivities in the system, captures much of the subtleties of our numerical simulations.

### **4:18PM V36.00010 Glassy Spin Dynamics in Buckled Colloidal Crystal<sup>1</sup>**

**DI ZHOU, FENG WANG, YILONG HAN**, Department of Physics, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong — Geometric frustration arises when lattice structure prevents simultaneous minimization of local interaction energies. It leads to highly degenerate ground states and complex behaviors in frustrated magnetic materials. Here we experimentally studied buckled 1.5-layer colloidal NIPA microgel crystals confined between parallel plates. Spheres buckled up and down are analogous to antiferromagnetic Ising spins. These spins on the distorted triangular lattice exhibit glassy dynamics at low temperatures. In particular, a spin only has 13 nearest-neighbor configurations, which enables to reveal the correlation between structures and dynamical heterogeneity. Soft modes also localize at high-energy regions. Further, we compared the colloidal spin system with kinetic constrained models (KCMs) and observed dynamical facilitation behaviors including excitations lines in space-time. Similar structures and glassy dynamics are also observed in our simulation of Coulomb charges on a triangular lattice.

<sup>1</sup>The work was supported by grant RGC-GRF601613.

### **4:30PM V36.00011 Experiments reveal different dynamics in two and three dimensions near the colloidal glass transition**

**SKANDA VIVEK**, Emory University, **COLM KELLEHER, PAUL CHAIKIN**, New York University, **ERIC WEEKS**, Emory University — We use microscopy to study both 3D and quasi-2D colloidal systems as they approach their glass transitions. We use two different bidisperse 2D systems, one of which has hard particles and the other which has particles interacting with long range dipolar interactions. The 3D system also has hard interactions (3D data obtained from Narumi, et al. Soft Matter 2011). In the 3D data, we observe significant plateaus in the mean square displacement curves, in contrast to 2D. This indicates stronger transient localization in 3D. In both 2D systems, as we approach the glass transition, we observe decoupling between translational time scales and time scales for structural reorientation. In 3D, these time scales always remain coupled. Finally, in 2D we observe large clusters of particles moving in parallel directions, but similar clusters are markedly smaller in 3D. In both 2D systems, these clusters become larger on approaching the glass transition. We attribute the observed decoupling of translational and bond-orientational times in 2D to the presence of these large directional clusters. Overall, our results are in good qualitative agreement with recent simulation results [Flenner and Szamel, Nature Communications 2015].

### **4:42PM V36.00012 Measuring heterogenous stress fields in a 3D colloidal glass**

**NEIL LIN, MATTHEW BIERBAUM**, Cornell University, **MAX BI**, Rockefeller University, **JAMES SETHNA**, **ITAI COHEN**, Cornell University — Glass in our common experience is hard and fragile. But it still bends, yields, and flows slowly under loads. The yielding of glass, a well documented yet not fully understood flow behavior, is governed by the heterogenous local stresses in the material. While resolving stresses at the atomic scale is not feasible, measurements of stresses at the single particle level in colloidal glasses, a widely used model system for atomic glasses, has recently been made possible using Stress Assessment from Local Structural Anisotropy (SALSA). In this work, we use SALSA to visualize the three dimensional stress network in a hard-sphere glass during start-up shear. By measuring the evolution of this stress network we identify local-yielding. We find that these local-yielding events often require only minimal structural rearrangement and as such have most likely been ignored in previous analyses. We then relate these micro-scale yielding events to the macro-scale flow behavior observed using bulk measurements.

### **4:54PM V36.00013 Mean-field description of plastic flow in amorphous solids**

**JIE LIN**, New York University, **MATTHIEU WYART**, EPFL — Failure and flow of amorphous materials are central to various phenomena including earthquakes and landslides. There is accumulating evidence that the yielding transition between a flowing and an arrested phase is a critical phenomenon, but the associated exponents are not understood, even at a mean-field level where the validity of popular models is debated. Here we solve a mean-field model that captures the broad distribution of the mechanical noise generated by plasticity, whose behavior is related to biased Lévy flights near an absorbing boundary. We compute the exponent  $\theta$  characterizing the density of shear transformation  $P(x) \sim x^\theta$ , where  $x$  is the stress increment beyond which they yield. We find that after an isotropic thermal quench,  $\theta = 1/2$ . However,  $\theta$  depends continuously on the applied shear stress, this dependence is not monotonic, and its value at the yield stress is not universal. The model rationalizes previously unexplained observations, and captures reasonably well the value of exponents in three dimensions. These results support that it is the true mean-field model that applies in large dimension, and raise fundamental questions on the nature of the yielding transition.

**5:06PM V36.00014 Rearrangement dynamics in colloidal particle packings identified through local structure and machine-learning<sup>1</sup>**, ZOEY S. DAVIDSON, TIM STILL, MATTHEW D. GRATALE, XIAO GUANG MA, SAMUEL S. SCHOENHOLZ, DANIEL M. SUSSMAN, A.J. LIU, A.G. YODH, University of Pennsylvania — We explore the connection between measures of local structure and particle rearrangements in soft thermal quasi-two-dimensional colloidal systems employing a machine learning approach. Local structure is characterized by two and three point structure functions that measure radial and angular distributions of particles, and rearrangements are identified by a measure of change in average colloidal particle position. By generating labeled training data, we can extract the features of these functions that contribute to the likelihood of a rearrangement. In particular, we use a machine-learning algorithm to construct a decision function in the form of a scalar field we call softness that with high accuracy labels regions of particles more likely to rearrange. Thus, we can predict dynamic rearrangements from the instantaneous local structure. The softness field remains a good predictor when we vary the packing fraction between training and test data sets. In glassy samples, the softness field can identify aging as particles become less likely to undergo cage rearrangements.

<sup>1</sup>We gratefully acknowledge financial support through NSF DMR12-05463, MRSEC DMR11-20901, NASA NNX08AO0G, and DE-FG02-05ER46199.

**5:18PM V36.00015 A Generic Microscopic Theory for the Universality of TTLS Meissner-Berret Ratio of Amorphous Solid**, DI ZHOU, ANTHONY LEGGETT, Univ of Illinois - Urbana — Tunneling-two-level-system (TTLS) has successfully explained several experimental results for amorphous solid which do not exist in crystalline counterparts. However longitudinal and transverse phonon-TTLS coupling constants' ratio  $\gamma_l/\gamma_t$  has been found to lie between 1.5 and 1.6 for 13 different amorphous solids which cannot be explained within TTLS model. In this paper by developing an interacting generic block model with random stress tensors, we show the universality essentially comes from interaction between generic blocks, independent of the material's microscopic structure. In the appendix we also give a detailed correction for non-elastic stress-stress interaction coefficient  $\Lambda_{ijkl}^{(ss')}$  derived by Joffrin and Levelut.

**Thursday, March 17, 2016 2:30PM - 5:30PM –**

**Session V37 GSOF DBIO: Soft Mechanics in Biological Systems** 340 - Itai Cohen, Cornell University

**2:30PM V37.00001 State transitions of actin cortices in vitro and in vivo**, TZER HAN TAN, Massachusetts Inst of Tech-MIT, KINNERET KEREN, Technion-Israel Institute of Technology, FRED MACKINTOSH, University of Amsterdam, CHRISTOPH SCHMIDT, Goettingen University, NIKTA FAKHRI, Massachusetts Inst of Tech-MIT — Most animal cells are enveloped by a thin layer of actin cortex which governs the cell mechanics. A functional cortex must be rigid to provide mechanical support while being flexible to allow for rapid restructuring events such as cell division. To satisfy these requirements, the actin cortex is highly dynamic with fast actin turnover and myosin-driven contractility. The regulatory mechanism responsible for the transition between a mechanically stable state and a restructuring state is not well understood. Here, we develop a technique to map the dynamics of reconstituted actin cortices in emulsion droplets using IR fluorescent single-walled carbon nanotubes (SWNTs). By increasing crosslinker concentration, we find that a homogeneous cortex transitions to an intermediate state with broken rotational symmetry and a globally contractile state which further breaks translational symmetry. We apply this new dynamic mapping technique to cortices of live starfish oocytes in various developmental stages. To identify the regulatory mechanism for steady state transitions, we subject the oocytes to actin and myosin disrupting drugs.

**2:42PM V37.00002 Direct measurement of local material properties within living embryonic tissues**, FRIEDHELM SERWANE, ALESSANDRO MONGERA, PAYAM ROWGHANIAN, DAVID KEALHOFER, ADAM LUCIO, ZACHARY HOCKENBERRY, OTGER CAMPÀS, University of California, Santa Barbara — The shaping of biological matter requires the control of its mechanical properties across multiple scales, ranging from single molecules to cells and tissues. Despite their relevance, measurements of the mechanical properties of sub-cellular, cellular and supra-cellular structures within living embryos pose severe challenges to existing techniques. We have developed a technique that uses magnetic droplets to measure the mechanical properties of complex fluids, including in situ and in vivo measurements within living embryos across multiple length and time scales. By actuating the droplets with magnetic fields and recording their deformation we probe the local mechanical properties, at any length scale we choose by varying the droplets' diameter. We use the technique to determine the subcellular mechanics of individual blastomeres of zebrafish embryos, and bridge the gap to the tissue scale by measuring the local viscosity and elasticity of zebrafish embryonic tissues. Using this technique, we show that embryonic zebrafish tissues are viscoelastic with a fluid-like behavior at long time scales. This technique will enable mechanobiology and mechano-transduction studies in vivo, including the study of diseases correlated with tissue stiffness, such as cancer.

**2:54PM V37.00003 The role of anisotropy in cell morphology**, KOEN SCHAKENRAAD, WIM POMP, Univ of Leiden, ROELAND MERKS, Univ of Leiden, Centrum Wiskunde en Informatica Amsterdam, THOMAS SCHMIDT, LUCA GIOMI, Univ of Leiden — The shape of adhering cells is determined by the interplay between contractile forces, arising from the cytoskeleton, and the resistance of the underlying substrate. In particular, experiments with fibroblasts on an elastic micro-pillar array show that fibroblasts possess a high degree of orientational order of the actin stress fibers. This anisotropy causes the shape of the cell edge to deviate from the shape of cells with an isotropic cytoskeleton. We present a model that describes the contractility of the cytoskeleton as a combination of directed forces, in the direction of stress fibers, and isotropic forces. We found that cell morphology is described by an anisotropic generalization of the Young-Laplace law, which describes the cell edges as parts of an ellipse. Experiments on the shape of and adhesion forces on fibroblasts show good agreement with our model. Our work highlights the strong coupling between the organization of the internal cytoskeleton and the shapes and forces on the outside of the cell.

**3:06PM V37.00004 Role of forces and of micromechanics of biopolymers in the cellular process of cell division**, MARIA KILFOIL, University of Massachusetts, Amherst — No abstract available.

**3:42PM V37.00005 Hydraulic fracture and resilience of epithelial monolayers under stretch**, MARINO ARROYO, Univ Politecnica de Catalunya, ALESSANDRO LUCANTONIO, GIOVANNI NOSELLI, SISAInternational School for Advanced Studies, LAURA CASARES, Institute for Bioengineering of Catalonia (IBEC) / Univ Politecnica de Catalunya, ANTONIO DESIMONE, SISAInternational School for Advanced Studies, XAVIER TREPAT, Institute for Bioengineering of Catalonia (IBEC) — Epithelial monolayers are very simple and prevalent tissues. Their functions include delimiting distinct physicochemical containers and protecting us from pathogens. Epithelial fracture disrupts the mechanical integrity of this barrier, and hence compromises these functions. Here, we show that in addition to the conventional fracture resulting from excessive tissue tension, epithelia can hydraulically fracture under stretch as a result of the poroelastic nature of the matrix [1]. We will provide experimental evidence of this counterintuitive mechanism of fracture, in which cracks appear under compression. Intriguingly, unlike tensional fracture, which is localized and catastrophic, hydraulic epithelial fracture is distributed and reversible. We will also describe the active mechanisms responsible for crack healing, and the physical principles by which the poroelastic matrix contributes to this resilient behavior [2]. [1] Casares et al., Nature Materials, 14, 343-351 (2015) [2] Lucantonio et al., Physical Review Letters, 115, 188105 (2015)

**3:54PM V37.00006 Mechanics and crack formation in the extracellular matrix with articular cartilage as a model system<sup>1</sup>**, SARAH KEARNS, Rochester Institute of Technology, JESSE SILVERBERG, Harvard University, LAWRENCE BONASSAR, ITAI COHEN, Cornell University, MOUMITA DAS, Rochester Institute of Technology — We investigate the mechanical structure-function relations in the extracellular matrix (ECM) with focus on crack formation and failure. As a model system, our study focuses on the ECM in articular cartilage (AC), the tissue that covers the ends of bones, and distributes load in joints including in the knees, shoulders, and hips. The strength, toughness, and crack resistance of native articular cartilage is unparalleled in materials made by humankind. This mechanical response is mainly due to its ECM. The ECM in AC has two major mechanobiological components: a network of the biopolymer collagen and a flexible aggrecan gel. We model this system as a biopolymer network embedded in a swelling gel, and investigate the conditions for the formation and propagation of cracks using a combination of rigidity percolation theory and energy minimization approaches. Our results may provide useful insights into the design principles of the ECM as well as of biomimetic hydrogels that are mechanically robust and can, at the same time, easily adapt to cues in their surroundings.

<sup>1</sup>This work was partially supported by a Cottrell College Science Award

**4:06PM V37.00007 Fiber networks amplify active stress**, MARTIN LENZ, PIERRE RONCERAY, LPTMS, CNRS, Univ. Paris-Sud, Universit Paris-Saclay, 91405 Orsay, France, CHASE BROEDERSZ, Arnold-Sommerfeld-Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universitt, Mnchen, Theresienstrasse 37, D-80333 — Large-scale force generation is essential for biological functions such as cell motility, embryonic development, and muscle contraction. In these processes, forces generated at the molecular level by motor proteins are transmitted by disordered fiber networks, resulting in large-scale active stresses. While fiber networks are well characterized macroscopically, this stress generation by microscopic active units is not well understood. I will present a comprehensive theoretical study of force transmission in these networks. I will show that the linear, small-force response of the networks is remarkably simple, as the macroscopic active stress depends only on the geometry of the force-exerting unit. In contrast, as non-linear buckling occurs around these units, local active forces are rectified towards isotropic contraction and strongly amplified. This stress amplification is reinforced by the networks' disordered nature, but saturates for high densities of active units. I will show that our predictions are quantitatively consistent with experiments on reconstituted tissues and actomyosin networks, and that they shed light on the role of the network microstructure in shaping active stresses in cells and tissue.

**4:18PM V37.00008 A micro-mechanical model to determine changes of collagen fibrils under cyclic loading**, MICHELLE L CHEN, Johns Hopkins University, MONICA E. SUSILO, JEFFREY A. RUBERTI, Northeastern University, THAO D. NGUYEN, Johns Hopkins University — Dynamic mechanical loading induces growth and remodeling in biological tissues. It can alter the degradation rate and intrinsic mechanical properties of collagen through cellular activity. Experiments showed that repeated cyclic loading of a dense collagen fibril substrate increased collagen stiffness and strength, lengthened the substrate, but did not significantly change the fibril areal fraction or fibril anisotropy (Susilo, et al. Collagen Network Hardening Following Cyclic Tensile Loading, Interface Focus, submitted). We developed a model for the collagen fibril substrate (Tonge, et al. A micromechanical modeling study of the mechanical stabilization of enzymatic degradation of collagen tissues, Biophys J, in press.) to probe whether changes in the fibril morphology and mechanical properties can explain the tissue-level properties observed during cyclic loading. The fibrils were modeled as a continuous distribution of wavy elastica, based on experimental measurements of fibril density and collagen anisotropy, and can experience damage after a critical stress threshold. Other mechanical properties in the model were fit to the stress response measured before and after the extended cyclic loading to determine changes in the strength and stiffness of collagen fibrils.

**4:30PM V37.00009 Confined semiflexible biopolymers suppress fluctuations of soft membrane tubes**, STEVEN ABEL, SINA MIRZAEIFARD, University of Tennessee, Knoxville — Membrane nanotubes are tubular membrane structures that contain actin and connect cells over long distances. Disrupting the actin cytoskeleton abrogates membrane nanotubes, making them an interesting model system for studying membrane-biopolymer interactions. In this study, we use Monte Carlo computer simulations to investigate tubular, elastic membrane structures with and without semiflexible polymers confined inside. At small values of membrane bending rigidity, fluid membranes adopt irregular, highly fluctuating shapes while non-fluid membranes maintain extended tube-like structures. With increasing bending rigidity, fluid membranes exhibit a local maximum in specific heat that is coincident with a transition to extended tube-like structures. We further find that confining a semiflexible polymer within a fluid membrane tube suppresses membrane shape fluctuations and reduces the specific heat of the membrane. Polymers with a sufficiently large persistence length can significantly deform the membrane tube, leading to localized bulges in the membrane that accommodate regions in which the polymer forms loops. Analytical calculations of the energies of idealized polymer-membrane configurations provide additional insight into the formation of polymer-induced membrane deformations.

**4:42PM V37.00010 Force distributions in disordered fiber networks**, KNUT HEIDEMANN, Institute for Numerical and Applied Mathematics, Georg-August-Universitaet, Goettingen, ABHINAV SHARMA, FLORIAN REHFELDT, CHRISTOPH F SCHMIDT, Third Institute of Physics – Biophysics, Georg-August-Universitaet, Goettingen, MAX WARDETZKY, Institute for Numerical and Applied Mathematics, Georg-August-Universitaet, Goettingen — Disordered filamentous networks determine the mechanical response of many materials in nature. Due to the filamentous character of these networks, the strain field, and hence the force distributions, can be highly inhomogeneous. Large local stresses can result in an increased susceptibility for local rearrangements due to rupture or unbinding events. In our study, we introduce a quantitative measure to characterize the emergence of highly stressed one-dimensional paths, so-called force chains, in three-dimensional nonlinear fiber networks. Furthermore, we provide an analytical approach, based on graph theory, that quantitatively describes the force distributions in one-dimensional periodic spring networks. Our analytical results are in excellent agreement with our extensive numerical simulations.

**4:54PM V37.00011 Role of differential physical properties in the collective mechanics and dynamics of tissues<sup>1</sup>**, MOUMITA DAS, Rochester Institute of Technology — Living cells and tissues are highly mechanically sensitive and active. Mechanical stimuli influence the shape, motility, and functions of cells, modulate the behavior of tissues, and play a key role in several diseases. In this talk I will discuss how collective biophysical properties of tissues emerge from the interplay between differential mechanical properties and statistical physics of underlying components, focusing on two complementary tissue types whose properties are primarily determined by (1) the extracellular matrix (ECM), and (2) individual and collective cell properties. I will start with the structure-mechanics-function relationships in articular cartilage (AC), a soft tissue that has very few cells, and its mechanical response is primarily due to its ECM. AC is a remarkable tissue: it can support loads exceeding ten times our body weight and bear 60+ years of daily mechanical loading despite having minimal regenerative capacity. I will discuss the biophysical principles underlying this exceptional mechanical response using the framework of rigidity percolation theory, and compare our predictions with experiments done by our collaborators. Next I will discuss ongoing theoretical work on how the differences in cell mechanics, motility, adhesion, and proliferation in a co-culture of breast cancer cells and healthy breast epithelial cells may modulate experimentally observed differential migration and segregation. Our results may provide insights into the mechanobiology of tissues with cell populations with different physical properties present together such as during the formation of embryos or the initiation of tumors.

<sup>1</sup>This work was partially supported by a Cottrell College Science Award

**Thursday, March 17, 2016 2:30PM - 5:30PM —**  
Session V38 DPOLY DBIO: Mechanics of Biopolymers: Single Polymer Dynamics 341 - Alex Levine, UCLA

**2:30PM V38.00001 Non-continuum correlated intermolecular dynamical displacements in entangled biopolymer solutions.** , KENNETH S. SCHWEIZER, ZACHARY E. DELL, BOYCE TSANG, LINGXIANG JIANG, University of Illinois at Urbana-Champaign, STEVE GRANICK, IBS Center for Soft and Living Matter — Understanding correlated intermolecular motion is important in biology and of fundamental interest in polymer physics. We performed real space measurements of the correlated dynamical displacements of a pair of biopolymers in entangled F-actin solutions over mesoscopic and continuum length scales, and on time scales beyond the entanglement crossover but much shorter than the reptation time. A microscopic theory is constructed based on generalizing a recent force-level statistical mechanical approach for predicting the separation-dependent, non-hydrodynamic relative friction of a pair of colloids in polymer melts [1] and in dense suspensions [2]. In the mesoscopic time regime, individual biopolymers move by reptation, and the dynamically-emergent intermolecular correlation hole is proposed as the mechanism for inducing non-hydrodynamic collective Fickian motion. Non-continuum cross correlations are predicted to dominate for inter-polymer separations up to the rod length (~15 microns), beyond which a crossover to hydrodynamic behavior occurs. The theoretical results agree well with our measurements at different observation times and physical mesh values. [1] Yamamoto, Schweizer, J.Chem.Phys.139,064907(2013); [2] Dell, Tsang, Jian, Granick, Schweizer, Phys.Rev.E, in press, 2015

**2:42PM V38.00002 Force fluctuation in a semiflexible loop** , JAMES WATERS, HAROLD KIM, Georgia Institute of Technology, HAROLD KIM TEAM — DNA-binding proteins can regulate genetic expression by holding two sites in close proximity, forming a closed loop. Such complexes may require strong bending of DNA segments on the order of one persistence length or less. Both this elastic bending and the thermal fluctuations of the DNA molecule are necessary to describe the resulting behavior. To explore this problem, we consider a discrete model of a wormlike chain, kept in the fixed extension ensemble. By using a novel method to sample conformations in both position and momentum space, we can obtain a distribution of constraint forces as a function of chain length, extension, and flexibility. Our coarse-grained model allows us to explore the space of these parameters more efficiently than a detailed molecular dynamics approach. We find that increasing contour length decreases average force by relieving bending stress, but that the additional freedom allows fluctuations in the constraint force to increase. This implies that the probability of large forces may go up even as the mean goes down, impacting the lifetime of such bound states in a way unforeseen by purely equilibrium methods.

**2:54PM V38.00003 Watching entangled circular DNA in real time with super-resolution** , AH-YOUNG JEE, HYEONGJU KIM, STEVE GRANICK, Institute for Basic Science — In this talk, we will show how we unraveled the conformational dynamics of entangled ring-shaped polymers in network, which is one of the most well-known problems in polymer physics, using deep imaging based on super-resolution fluorescence imaging, stimulated emission depletion (STED) microscopy. By using home-written software, we obtained the statistics of each of the hundreds of molecules, mapping out a large statistical distribution. Through inspection we not only found some aspects of the classic understanding of polymers, but some surprising aspects as well.

**3:06PM V38.00004 Single Molecule Dynamics of Branched DNA Polymers** , DANIELLE MAI, CHARLES SING, CHARLES SCHROEDER, Univ of Illinois - Urbana — This work focuses on extending the field of single polymer dynamics to topologically complex polymers. Here, we report the direct observation of DNA-based branched polymers. Recently, we recently demonstrated a two-step synthesis method to generate star, H-shaped, and comb polymers for single molecule visualization. Following synthesis, we use single-color or dual-color single molecule fluorescence microscopy to directly visualize branched polymer dynamics in flow, in particular tracking side branches and backbones independently. In this way, our imaging method allows for characterization of molecular properties, including quantification of polymer contour length and branch distributions. Moving beyond characterization, we use molecular rheology and single molecule techniques to study the dynamics of single branched polymers in flow. Here, we utilize precision microfluidics to directly observe branched DNA polymer conformations during transient stretching, steady-state extension, and relaxation from high stretch. We specifically measure backbone end-to-end distance as a function of time. Experiments and Brownian dynamics simulations show that branched polymer relaxation is a strong function of the number of branches and position of branch points along the main chain backbone.

**3:18PM V38.00005 Single polymer dynamics of linear and architecturally complex chains in semi-dilute solutions** , KAIWEN HSIAO, Univeristy of Illinois at Urbana Champaign, YANFEI LI, GREGORY MCKENNA, Texas Tech University, CHARLES SCHROEDER, Univeristy of Illinois at Urbana Champaign — The interplay between polymer topology and concentration gives rise to complex dynamics due to inter- and intramolecular interactions. We use a molecular level approach to study the threading behavior for linear and ring polymers near equilibrium and in non-linear flows. A semi-dilute solution of linear DNA chains is doped with fluorescently labeled ring polymers (circular DNA plasmids), and this material is used to study the dynamics of rings in semi-dilute solutions of linear chains. Single molecule fluorescence microscopy in combination with a custom-built microfluidic trapping system is used to study collective polymer dynamics at the molecular level, which allows us to precisely control flow rates and accumulated fluid strain applied to single polymer. We performed step-strain experiments on ring polymer in linear semi-dilute polymer solutions undergoing deformation in planar extensional flow. In comparison to our previous work on semi-dilute linear chains, ring polymers exhibit large fluctuations in fractional extension at steady state extension, indicating strong interactions with the background polymer solution. Transient stretching dynamics of ring polymer is inhibited in semi-dilute linear background, similar to our previous observation in linear systems. Our findings show that topology and concentration play a strong role on polymer chain dynamics in non-equilibrium flow.

**3:30PM V38.00006 Study of mechanical properties of DNA in E. coli cells by fluorescence correlation spectroscopy** , RUDRA KAFLE, Worcester Polytechnic Institute, MOLLY LIEBESKIND, JENS-CHRISTIAN MEINERS, University of Michigan — Mechanical quantities like the elasticity of cells are conventionally measured by directly probing them mechanically. Measurements of these quantities for subcellular structures in living cells are almost impossible this way. We use fluorescence correlation spectroscopy (FCS) to measure such mechanical quantities in chromosomal DNA in *E. coli* cells. We present methods to address complexities of live-cell FCS such as photobleaching, and calculate the viscoelastic moduli from the FCS data. We compare the measured viscoelastic moduli of live cells with those that are ATP-depleted to stop all molecular motor action and find substantial differences. Active processes are stopped in ATP-depleted cells and hence the bacterial DNA appears to become stiffer and the surrounding intracellular medium more viscous. We also compare our results with the FCS data obtained from the lambda DNA solution in various concentrations to mimic the cellular environment.

**3:42PM V38.00007 Single Polymer Dynamics under Large (LAOE) Flow** , YUECHENG ZHOU<sup>1</sup>, CHARLES M. SCHROEDER, Univ of Illinois - Urbana — Imaging and particle manipulation have enabled the direct observation of single polymer dynamic flow. The vast majority of single polymer studies, however, has focused on chain dynamics using single polymer dynamics in non-idealized model flows, there is a clear need to implement more complicated amplitude oscillatory shear (LAOS) was widely used to study the linear and nonlinear viscoelasticity. In this work, we directly probe single polymer dynamics using oscillatory extensional flow in precisely large and small amplitude sinusoidal oscillatory extensional flow in a cross-slot microfluidic device where polymer chains are trapped at the stagnation point. In this flow, polymer chains are stretched, squeezed, and rotated in a transient manner. Using this technique, we studied the dynamics and coil-stretch transition of polymer chains as a function of the Weissenberg number (Wi) and Deborah number (De). Moreover, we use Brownian dynamics simulation to map a wide range of conditions to non-linear unsteady-states. Our results reveal a critical Wi at the coil-stretch transition.

**3:54PM V38.00008 Large-scale structural transitions in supercoiled DNA revealed by coarse-grained simulations**, BRAD KRAJINA, ANDREW SPAKOWITZ, Stanford Univ — Topological constraints, such as DNA supercoiling, play an integral role in genomic regulation and organization in living systems. However, physical understanding of the principles that underlie DNA structure and organization at biologically-relevant length-scales remains a formidable challenge. We develop a coarse-grained simulation approach for predicting equilibrium conformations of supercoiled DNA. With this approach, we study the conformational transitions that arise due to supercoiling across the full range of supercoiling densities that are commonly explored by living systems. Simulations of ring DNA molecules with lengths up to the scale of topological domains in the E. coli chromosome (~10 kilobases) reveal large-scale structural transitions elicited by supercoiling, resulting in 3 supercoiling conformational regimes: chiral coils, extended plectonemes, and branched hyper-supercoils. These results capture the non-monotonic relationship of size versus degree of supercoiling observed in experimental sedimentation studies of supercoiled DNA, and our results provide a physical explanation of the structural transitions underlying this behavior.

**4:06PM V38.00009 Jamming of Knots along a Tensioned Chain**, PATRICK DOYLE, VIVEK NARSIMHAN, C. BENJAMIN RENNER<sup>1</sup>, Massachusetts Institute of Technology — In the limit of very long chains, coiled polymers almost always self-entangle and form knots. In this study, we characterize the motion of these knots along the chain contour when the chain is under very high tension. In this regime, we find that the knot exhibits glassy physics. For example, instead of moving continuously along the contour, the knot becomes kinetically trapped in long-lived, metastable states. This caging phenomenon follows Poisson statistics, and thus the long-time dynamics of the knot are diffusive. We quantify the long-time diffusivity of knots of various topologies, and we find that the diffusivity decays exponentially with increasing chain tension. The rate-of-decay of these transport properties is relatively insensitive to the knot's topology, which can be explained by examining the energy landscape of the self-reptation moves of the knot along the chain. Finally, we examine the role of bending and excluded volume interactions on this jamming phenomenon. Bending plays the biggest role in determining the onset of jamming, but the corrugation of the excluded volume interactions solely determines the rate-of-decay of the knot's transport properties.

<sup>1</sup>Now at Liquiglide

**4:18PM V38.00010 Activity induced phase separation in particles and (bio)polymers**, ALEXANDER GROSBERG, New York University — It was recently shown that the non-equilibrium steady state of the mixture of two types of particles exposed to two different thermostats can phase separate (A.Y.Grosberg, J.-F.Joanny, PRE, v. **91**, 032118, 2015). similar result is valid also in the case when particles in question are monomers of two different polymer chains, or blocks of a co-polymer. We discuss the implications of these results for the physics of chromatin.

**4:54PM V38.00011 Electrophoresis of semiflexible heteropolymers and the “hydrodynamic Kuhn length”**, MYKYTA V. CHUBYNSKY, GARY W. SLATER, Department of Physics, University of Ottawa, Canada — Semiflexible polymers, such as DNA, are rodlike for short lengths and coil-like for long lengths. For purely geometric properties, such as the end-to-end distance, the crossover between these two behaviors occurs when the polymer length is on the order of the Kuhn length. On the other hand, for the hydrodynamic friction coefficient it is easy to see by comparing the expressions for a rod and a coil that the crossover should occur at the polymer length, termed by us the *hydrodynamic Kuhn length* [1], which is larger than the ordinary Kuhn length by a logarithmic factor that can be quite significant. We show that for the problem of electrophoresis of a heteropolymer consisting of several blocks of (in general) different stiffnesses, both of these length scales can be important depending on the details of the problem. [1] M. V. Chubynsky and G. W. Slater, *Macromolecules* 48 (2015) 5899.

**5:06PM V38.00012 Viscoelastic dynamics in a system of two actin filaments under stress**, ARJAN ERIK BOERMA, ERIK VAN DER GIESSEN, Univ of Groningen, STEFANOS PAPANIKOLAOU, Johns Hopkins University — The viscoelasticity of cytoskeleton networks is experimentally well-established but still lacks a consistent theoretical description. We present a novel minimal model that consists of two semi-flexible filaments coupled by cross-linkers, whose dynamics are described by Grand Canonical Monte Carlo. The mechanical properties are captured in the continuum and solved through an athermal finite-element approach. We discuss the phase diagram of the model and the emergence of viscoelastic behavior: the variation of the dynamic modulus as a function of loading frequency and density of cross-linkers, in thermodynamically and biologically realistic settings.

**5:18PM V38.00013 How to Concentrate Genomic Length DNA in a Microfabricated Array**, YU CHEN, Princeton University, EZRA ABRAMS, CHRISTIAN BOLES, Sage Science Inc., JONAS PEDERSEN, HENRIK FLYVBJERG, Danish Technical University, JAMES STURM, ROBERT AUSTIN, Princeton University — We demonstrate that a microfabricated bump array can concentrate genomic-length DNA molecules efficiently at continuous, high flow velocities, up to 40  $\mu\text{m/s}$ , if the single-molecule DNA globule has a sufficiently large shear modulus.. Increase in the shear modulus is accomplished by compacting the DNA molecules to minimal coil-size using polyethylene glycol (PEG) derived depletion forces. We map out the sweet spot where concentration occurs as a function of PEG concentration, flow speed, and bump array parameters using a combination of theoretical analysis and experiment. Purification of DNA from enzymatic reactions for next-generation DNA-sequencing libraries will be an important application of this development.

**Thursday, March 17, 2016 2:30PM - 5:30PM —**

**Session V39 DBIO GSNP: Inference in Biophysics** 342 - David Schwab, Northwestern University

**2:30PM V39.00001 Self-Organized Information Processing in Neuronal Networks: Replacing Layers in Deep Networks by Dynamics**, CHRISTOPH KIRST, Rockefeller University — It is astonishing how the sub-parts of a brain co-act to produce coherent behavior. What are mechanism that coordinate information processing and communication and how can those be changed flexibly in order to cope with variable contexts? Here we show that when information is encoded in the deviations around a collective dynamical reference state of a recurrent network the propagation of these fluctuations is strongly dependent on precisely this underlying reference. Information here 'surfs' on top of the collective dynamics and switching between states enables fast and flexible rerouting of information. This in turn affects local processing and consequently changes in the global reference dynamics that re-regulate the distribution of information. This provides a generic mechanism for self-organized information processing as we demonstrate with an oscillatory Hopfield network that performs contextual pattern recognition. Deep neural networks have proven to be very successful recently. Here we show that generating information channels via collective reference dynamics can effectively compress a deep multi-layer architecture into a single layer making this mechanism a promising candidate for the organization of information processing in biological neuronal networks.

**2:42PM V39.00002 The learnability of critical distributions**, DAVID SCHWAB, Northwestern University, JOHANNAH TORRENCE, University of Chicago, GIACOMO TORLAI, ROGER MELKO, University of Waterloo, STEPHANIE PALMER, University of Chicago — Many biological systems, including some neural population codes, have been shown empirically to sit near a critical point. Here we study the learnability of such codes. We first construct networks of interacting binary neurons with random, sparse interactions (i.e. a Erdos-Renyi graph) of uniform strength. We then characterize the discriminability of those interactions from data samples by performing a direct coupling analysis and thresholding the direct information between each pair of neurons to predict the presence or absence of an interaction. By sweeping through threshold values, we compute the area under the ROC curve as a measure of discriminability of the interactions. We show that the resulting discriminability is maximized when the original distribution is at its critical point. We next trained deep neural networks to discriminate between samples drawn from two nearby temperatures in the 2D Ising model. We find distinct signatures of decoding performance in the vicinity of the critical point. This technique may be useful for detecting phase transitions in models without an a priori identified order parameter.

**2:54PM V39.00003 Machine learning phases of matter**, JUAN CARRASQUILLA, MILES SToudenMIRE, Perimeter Inst for Theo Phys, ROGER MELKO, Perimeter Inst for Theo Phys and University of Waterloo — We show how the technology that allows automatic teller machines read hand-written digits in cheques can be used to encode and recognize phases of matter and phase transitions in many-body systems. In particular, we analyze the (quasi-)order-disorder transitions in the classical Ising and XY models. Furthermore, we successfully use machine learning to study classical Z2 gauge theories that have important technological application in the coming wave of quantum information technologies and whose phase transitions have no conventional order parameter.

**3:06PM V39.00004 Using chaos to model random symbols for improved unsupervised information processing**<sup>1</sup>, SUMONA MUKHOPADHYAY<sup>2</sup>, HENRY LEUNG<sup>3</sup>, Department of Electrical and Computer Engineering, University of Calgary — We present theoretical analyses that may allow strengthening the connection between chaotic dynamical system and information processing. The analytical and empirical studies prove that computing with chaos and nonlinear characterization of information improves unsupervised information processing. Traditional supervised techniques for information retrieval from noisy environment achieve optimal performance. However, the need for training symbols is an inefficient strategy. We prove that with a chaotic generator as an information source, unsupervised performance is close to that of supervised with a white Gaussian stochastic process. Analytical results show that unsupervised technique using chaotic symbolic dynamics is equivalent to that of supervised when using random symbolic information. We conclude from the concepts of measure theory and ergodic theory, that random symbolic information can be modeled by a chaotic dynamical system via symbolic dynamics. We observe that the performance of unsupervised information retrieval is equivalent to that of supervised, when random symbolic information and a dynamical representation of it are used in conjunction. This fact enables to apply nonlinear dynamics to design improved communication systems.

<sup>1</sup>This research is supported by Alberta Innovates Technology Futures doctoral scholarship

<sup>2</sup>PhD student

<sup>3</sup>Professor

**3:18PM V39.00005 Anatomy of a Spin: The Information-Theoretic Structure of Classical Spin Systems**, RYAN JAMES, VIKRAM VIJAYARAGHAVAN, JAMES CRUTCHFIELD, Univ of California - Davis — Collective organization in matter plays a significant role in its expressed physical properties. Typically, it is detected via an order parameter, appropriately defined for a given system's observed emergent patterns. Recent developments in information theory suggest how to quantify collective organization in a system- and phenomenon-agnostic way: decompose the system's thermodynamic entropy density into a localized entropy, that solely contained in the dynamics at a single location, and a bound entropy, that stored in space as domains, clusters, excitations, or other emergent structures. We compute this decomposition and related quantities explicitly for the nearest-neighbor Ising model on the 1D chain, the Bethe lattice with coordination number  $k = 3$ , and the 2D square lattice, illustrating its generality and the functional insights it gives near and away from phase transitions. In particular, we consider the roles that different spin motifs play (cluster bulk, cluster edges, and the like) and how these affect the dependencies between spins.

**3:30PM V39.00006 Global Characterization of Model Parameter Space Using Information Topology**, MARK TRANSTRUM, Brigham Young University — A generic parameterized model is a mapping between parameters and data and is naturally interpreted as a prediction manifold embedded in data space. In this interpretation, known as Information Geometry, the Fisher Information Matrix (FIM) is a Riemannian metric that measures the identifiability of the model parameters. Varying the experimental conditions (e.g., times at which measurements are made) alters both the FIM and the geometric properties of the model. However, several global features of the model manifold (e.g., edges and corners) are invariant to changes in experimental conditions as long as the FIM is not singular. Invariance of these features to changing experimental conditions generates an "Information Topology" that globally characterizes a model's parameter space and reflects the underlying physical principles from which the model was derived. Understanding a model's information topology can give insights into the emergent physics that controls a system's collective behavior, identify reduced models and describe the relationship among them, and determine which parameter combinations will be difficult to identify for various experimental conditions.

**3:42PM V39.00007 Statistical Physics of High Dimensional Inference**<sup>1</sup>, MADHU ADVANI, SURYA GANGULI, Stanford University — To model modern large-scale datasets, we need efficient algorithms to infer a set of  $P$  unknown model parameters from  $N$  noisy measurements. What are fundamental limits on the accuracy of parameter inference, given limited measurements, signal-to-noise ratios, prior information, and computational tractability requirements? How can we combine prior information with measurements to achieve these limits? Classical statistics gives incisive answers to these questions as the measurement density  $\alpha = \frac{N}{P} \rightarrow \infty$ . However, modern high-dimensional inference problems, in fields ranging from bio-informatics to economics, occur at finite  $\alpha$ . We formulate and analyze high-dimensional inference analytically by applying the replica and cavity methods of statistical physics where data serves as quenched disorder and inferred parameters play the role of thermal degrees of freedom. Our analysis reveals that widely cherished Bayesian inference algorithms such as maximum likelihood and maximum a posteriori are suboptimal in the modern setting, and yields new tractable, optimal algorithms to replace them as well as novel bounds on the achievable accuracy of a large class of high-dimensional inference algorithms.

<sup>1</sup>Thanks to Stanford Graduate Fellowship and Mind Brain Computation IGERT grant for support

**3:54PM V39.00008 Compression and regularization with the information bottleneck**, DJ STROUSE, Princeton University, DAVID SCHWAB, Northwestern University — Compression fundamentally involves a decision about what is relevant and what is not. The information bottleneck (IB) by Tishby, Pereira, and Bialek formalized this notion as an information-theoretic optimization problem and proposed an optimal tradeoff between throwing away as many bits as possible, and selectively keeping those that are most important. The IB has also recently been proposed as a theory of sensory gating and predictive computation in the retina by Palmer et al. Here, we introduce an alternative formulation of the IB, the deterministic information bottleneck (DIB), that we argue better captures the notion of compression, including that done by the brain. As suggested by its name, the solution to the DIB problem is a deterministic encoder, as opposed to the stochastic encoder that is optimal under the IB. We then compare the IB and DIB on synthetic data, showing that the IB and DIB perform similarly in terms of the IB cost function, but that the DIB vastly outperforms the IB in terms of the DIB cost function. Our derivation of the DIB also provides a family of models which interpolates between the DIB and IB by adding noise of a particular form. We discuss the role of this noise as a regularizer.

**4:06PM V39.00009 A novel method for the precise determination of step times and sizes in counting large numbers of photobleaching events** , KONSTANTINOS TSEKOURAS, STEVE PRESSE, Indiana University - Purdue University Indianapolis — Counting of photobleaching steps is of importance in the investigation of many open problems in biophysics. Current methods of counting photo- bleaching steps cannot directly account for fluorophore photophysical behaviors such as fluorophore self-quenching, blinking and flickering. Our Bayesian approach to the counting problem allows for fluorophore blinking and reactivation as well as for multiple simultaneous photobleaching events and is neither computational resource- nor time- heavy. We detail the methods applicability and limitations and present examples of application in photobleach event counting.

**4:18PM V39.00010 Assessing the limits of hidden Markov model analysis for multi-state particle tracks in living systems** , DYLAN YOUNG, Clarkson Univ — Particle tracking offers significant insight into the molecular mechanics that govern the behavior of living cells. The analysis of molecular trajectories that transition between different motive states, such as diffusive, driven and tethered modes, is of considerable importance, with even single trajectories containing significant amounts of information about a molecule's environment and its interactions with cellular structures such as the cell cytoskeleton, membrane or extracellular matrix. Hidden Markov models (HMM) have been widely adopted to perform the segmentation of such complex tracks, however robust methods for failure detection are required when HMMs are applied to individual particle tracks and limited data sets. Here, we show that extensive analysis of hidden Markov model outputs using data derived from multi-state Brownian dynamics simulations can be used for both the optimization of likelihood models, and also to generate custom failure tests based on a modified Bayesian Information Criterion. In the first instance, these failure tests can be applied to assess the quality of the HMM results. In addition, they provide critical information for the successful design of particle tracking experiments where trajectories containing multiple mobile states are expected.

**4:30PM V39.00011 Inferring phenomenological models of Markov processes from data<sup>1</sup>** , CATALINA RIVERA, ILYA NEMENMAN, Emory Univ — Microscopically accurate modeling of stochastic dynamics of biochemical networks is hard due to the extremely high dimensionality of the state space of such networks. Here we propose an algorithm for inference of phenomenological, coarse-grained models of Markov processes describing the network dynamics directly from data, without the intermediate step of microscopically accurate modeling. The approach relies on the linear nature of the Chemical Master Equation and uses Bayesian Model Selection for identification of parsimonious models that fit the data. When applied to synthetic data from the Kinetic Proofreading process (KPR), a common mechanism used by cells for increasing specificity of molecular assembly, the algorithm successfully uncovers the known coarse-grained description of the process. This phenomenological description has been noticed previously, but this time it is derived in an automated manner by the algorithm.

<sup>1</sup>James S. McDonnell Foundation Grant No. 220020321

**4:42PM V39.00012 Probing self similar structures by studying the frequency of directional changes<sup>1</sup>** , ALI TABELI, University of Northern Iowa, STANISLAV BUROV, Bar Ilan University, ANDREW MILBRANDT, KYLE SPURGEON, University of Northern Iowa — It has been shown that in two and higher dimension, when the time series of individual particle trajectories exist, the distribution of relative angles of motion between successive time intervals of random motions provides information about stochastic processes, which is beyond the information obtained from studying mean squared displacement. We show that this distribution is a useful measure, which provides supplementary information about the structural properties of the media that a random walker is diffusing. We compare the behavior of this measure for common self-similar structures. We show that the distribution of relative angles is a good measure to discriminate different complex structural geometries.

<sup>1</sup> EPSCoR capacity building grant and UNI summer fellowship

**4:54PM V39.00013 Diffusion, Backward In Time: A Universal Inversion Scheme** , DERVIS VURAL, VU NGUYEN, University of Notre Dame — A sugar cube placed in a cup of tea will erode and eventually dissolve. Given the initial shape of the sugar block, it is trivial to predict its final distribution. However, the opposite problem of determining the initial state, given a final one is extremely difficult. A surprising number of seemingly unrelated topics in biology are the same one in disguise: Inverting diffusion on a network. Here we present a method that will identify the origin of a stochastic biological diffusion process, regardless of the forward model. We will then discuss potential implications to evolution, neuroscience, aging biology, and epidemiology.

**5:06PM V39.00014 Inferring biological dynamics in heterogeneous cellular environments** , STEVE PRESS, IUPUI — In complex environments, it often appears that biomolecules such as proteins do not diffuse normally. That is, their mean square displacement does not scale linearly with time. This anomalous diffusion happens for multiple reasons: proteins can bind to structures and other proteins; fluorophores used to label proteins may flicker or blink making it appear that the labeled protein is diffusing anomalously; and proteins can diffuse in differently crowded environments. Here we describe methods for learning about such processes from imaging data collected inside the heterogeneous environment of the living cell. Refs.: "Inferring Diffusional Dynamics from FCS in Heterogeneous Nuclear Environments" Konstantinos Tsekouras, Amanda Siegel, Richard N. Day, Steve Press\*, Biophys. J. , 109, 7 (2015). "A data-driven alternative to the fractional Fokker-Planck equation" Steve Press\*, J. Stat. Phys.: Th. and Exptl. , P07009 (2015).

**5:18PM V39.00015 Discovering cell types in flow cytometry data with random matrix theory** , YANG SHEN, Chemical Physics Graduate Program, University of Maryland, ROBERT NUSSENBLATT, Laboratory of Immunology, National Eye Institute, National Institutes of Health, WOLFGANG LOSERT<sup>1</sup>, Chemical Physics Graduate Program, University of Maryland — Flow cytometry is a widely used experimental technique in immunology research. During the experiments, peripheral blood mononuclear cells (PBMC) from a single patient, labeled with multiple fluorescent stains that bind to different proteins, are illuminated by a laser. The intensity of each stain on a single cell is recorded and reflects the amount of protein expressed by that cell. The data analysis focuses on identifying specific cell types related to a disease. Different cell types can be identified by the type and amount of protein they express. To date, this has most often been done manually by labelling a protein as expressed or not while ignoring the amount of expression. Using a cross correlation matrix of stain intensities, which contains both information on the proteins expressed and their amount, has been largely ignored by researchers as it suffers from measurement noise. Here we present an algorithm to identify cell types in flow cytometry data which uses random matrix theory (RMT) to reduce noise in a cross correlation matrix. We demonstrate our method using a published flow cytometry data set. Compared with previous analysis techniques, we were able to rediscover relevant cell types in an automatic way.

<sup>1</sup>Department of Physics, University of Maryland, College Park, MD 20742

**Thursday, March 17, 2016 2:30PM - 5:42PM —**  
**Session V40 GSNP GSOFD DBIO: Robophysics: Physics Meets Robotics I** 343 - Chen Li, Johns Hopkins University

**2:30PM V40.00001 Geometric mechanics for modelling bioinspired robots locomotion: from rigid to continuous (soft) systems**, FREDERIC BOYER, MATHIEU POREZ, Ecole des Mines de Nantes, FEDERICO RENDA, Khalifa University — This talk presents recent geometric tools developed to model the locomotion dynamics of bio-inspired robots. Starting from the model of discrete rigid multibody systems we will rapidly shift to the case of continuous systems inspired from snakes and fish. To that end, we will build on the model of Cosserat media. This extended picture of geometric locomotion dynamics (inspired from fields' theory) will allow us to introduce models of swimming recently used in biorobotics. We will show how modeling a fish as a one-dimensional Cosserat medium allows to recover and extend the Large Amplitude Elongated Body theory of J. Lighthill and to apply it to an eel-like robot. In the same vein, modeling the mantle of cephalopods as a two dimensional Cosserat medium will build a basis for studying the jet propelling of a soft octopus like robot.

**2:42PM V40.00002 Geometric Mechanics Reveals Optimal Complex Terrestrial Undulation Patterns**, CHAOHUI GONG, Carnegie Mellon University, HENRY ASTLEY, PERRIN SCHIEBEL, Georgia Institute of Technology, JIN DAI, MATTHEW TRAVERS, Carnegie Mellon University, DANIEL GOLDMAN, Georgia Institute of Technology, HOWIE CHOSSET, Carnegie Mellon University, CMU TEAM, GT TEAM — Geometric mechanics offers useful tools for intuitively analyzing biological and robotic locomotion. However, utility of these tools were previously restricted to systems that have only two internal degrees of freedom and in uniform media. We show kinematics of complex locomotors that make intermittent contacts with substrates can be approximated as a linear combination of two shape bases, and can be represented using two variables. Therefore, the tools of geometric mechanics can be used to analyze motions of locomotors with many degrees of freedom. To demonstrate the proposed technique, we present studies on two different types of snake gaits which utilize combinations of waves in the horizontal and vertical planes: sidewinding (in the sidewinder rattlesnake *C. cerastes*) and lateral undulation (in the desert specialist snake *C. occipitalis*). *C. cerastes* moves by generating posteriorly traveling body waves in the horizontal and vertical directions, with a relative phase offset equal to  $\pm \frac{\pi}{2}$  while *C. occipitalis* maintains a  $\frac{\pi}{2}$  offset of a frequency doubled vertical wave. Geometric analysis reveals these coordination patterns enable optimal movement in the two different styles of undulatory terrestrial locomotion. More broadly, these examples demonstrate the utility of geometric mechanics in analyzing realistic biological and robotic locomotion.

**2:54PM V40.00003 Optimal bipedal interactions with dynamic terrain: synthesis and analysis via nonlinear programming**, CHRISTIAN HUBICKI, DANIEL GOLDMAN, AARON AMES, Georgia Institute of Technology — In terrestrial locomotion, gait dynamics and motor control behaviors are tuned to interact efficiently and stably with the dynamics of the terrain (i.e. terradynamics). This controlled interaction must be particularly thoughtful in bipeds, as their reduced contact points render them highly susceptible to falls. While bipedalism under rigid terrain assumptions is well-studied, insights for two-legged locomotion on soft terrain, such as sand and dirt, are comparatively sparse. We seek an understanding of how biological bipeds stably and economically negotiate granular media, with an eye toward imbuing those abilities in bipedal robots. We present a trajectory optimization method for controlled systems subject to granular intrusion. By formulating a large-scale nonlinear program (NLP) with reduced-order resistive force theory (RFT) models and jamming cone dynamics, the optimized motions are informed and shaped by the dynamics of the terrain. Using a variant of direct collocation methods, we can express all optimization objectives and constraints in closed-form, resulting in rapid solving by standard NLP solvers, such as IPOPT. We employ this tool to analyze emergent features of bipedal locomotion in granular media, with an eye toward robotic implementation.

**3:06PM V40.00004 Geometric Mechanics for Continuous Swimmers on Granular Material**, JIN DAI, Carnegie Mellon Univ, HOSSEIN FARAJI, Oregon State University, PERRIN SCHIEBEL, Georgia Institute of Technology, CHAOHUI GONG, MATTHEW TRAVERS, Carnegie Mellon Univ, ROSS HATTON, Oregon State University, DANIEL GOLDMAN, Georgia Institute of Technology, HOWIE CHOSSET, Carnegie Mellon Univ, THE BIOROBOTICS LAB COLLABORATION, LABORATORY FOR ROBOTICS AND APPLIED MECHANICS (LRAM) COLLABORATION, COMPLEX RHEOLOGY AND BIOMECHANICS LAB COLLABORATION — Animal experiments have shown that *Chionactis occipitalis* (N=10) effectively undulating on granular substrates exhibits a particular set of waveforms which can be approximated by a sinusoidal variation in curvature, i.e., a serpenoid wave. Furthermore, all snakes tested used a narrow subset of all available waveform parameters, measured as the relative curvature equal to 5.00.3, and number of waves on the body equal to 1.80.1. We hypothesize that the serpenoid wave of a particular choice of parameters offers distinct benefit for locomotion on granular material. To test this hypothesis, we used a physical model (snake robot) to empirically explore the space of serpenoid motions, which is linearly spanned with two independent continuous serpenoid basis functions. The empirically derived height function map, which is a geometric mechanics tool for analyzing movements of cyclic gaits, showed that displacement per gait cycle increases with amplitude at small amplitudes, but reaches a peak value of 0.55 body-lengths at relative curvature equal to 6.0. This work signifies that with shape basis functions, geometric mechanics tools can be extended for continuous swimmers.

**3:18PM V40.00005 A Cosserat-based formulation for elastic, axisymmetric shells with implications to the pulsed-jetting propulsion of soft-bodied aquatic vehicles**, FEDERICO RENDA, Khalifa University Robotics Institute, Khalifa University, FRANCESCO GIORGIO-SERCHI, Southampton Marine and Maritime Institute, University of Southampton, FREDERIC BOYER<sup>1</sup>, Institut de Recherche en Communication et Cybernetique de Nantes, Ecole des Mines de Nantes — We take the cue from recent development in geometric-based modelling in order to describe the dynamics of a novel soft-structured aquatic vehicle. The Cosserat-like formulation for an axisymmetric, elastic shell subject to concentrated dynamic loadings lends itself to the case of this new vehicle, recently designed by the authors, which consists of a shell of rubber-like materials undergoing sequential stages of inflation and deflation in order to propel itself in water via pulsed-jetting. The experiments performed on the existing robotic prototypes are used for the validation of the geometric model. This is eventually employed for deriving an accurate measure of the efficiency of propulsion which explicitly accounts for the elastic energy involved during the propulsion routine. The model yields a-priori estimations of swimming efficiency based on vehicle specifications and mode of actuation. These provide invaluable information for both design optimization and control, as well as a means to study the biomechanics of soft-bodied aquatic organisms.

<sup>1</sup>Presenting author

**3:30PM V40.00006 Reverse engineering the euglenoid movement: from unicellular swimmers to bio-inspired robots.**<sup>1</sup>, ANTONIO DESIMONE, GIOVANNI NOSELLI, SISSA-International School for Advanced Studies, MARINO ARROYO, Universitat Politècnica de Catalunya — Euglenids are unicellular organisms living in freshwater, which are capable of moving either by beating a flagellum, or by executing dramatic shape changes. These are accomplished thanks to a complex structure made of interlocking pellicle strips, microtubules, and motor proteins. Relative sliding of the pellicle strips, suitably orchestrated, can cause the propagation of a bulge along the body, hence generating a propulsive force. We study the mechanisms by which the sliding of pellicle strips leads to shape control and locomotion, by means of both theory (through the mechanics of active surfaces and its coupling to computational fluid dynamics for the surrounding fluid) and experimental observations. Moreover, we implement them into a new concept of a surface with programmable shape, obtained by assembling 3d-printed strips in a construct mimicking the biological template. We explore the range of possible geometries achievable by actuating these surfaces, to assess their potential in soft robotics applications. The subtle balance between constraints and flexibility leads to a wide variety of shapes that can be obtained with relatively simple controls, similar to the notion of morphological computation in biological systems.

<sup>1</sup>ERC Advanced Grant 340685 (MicroMotility)

### **3:42PM V40.00007 Robotics and Biology: Lets get Physical** , HOWIE CHOSET, Carnegie Mellon University —

Our research group investigates the core fundamentals of locomotion as it exists in biology and as it applies to locomoting robotic systems. Initially, our work advanced techniques found in geometric mechanics to design cyclic controllers, often called gaits, for snake robots, highly articulated mechanisms that can thread through tightly packed spaces to access locations people cannot. We had considerable success in designing snake robot gaits, but found our systems stymied in terrains characterized by sandy substrates. Sandy terrains and other granular media pose a challenge to snake robots because it is unclear how the mechanism interacts with environment: we cannot simply assume the robot is on hard-ground nor in a fluid. Simulating granular interactions can prove to be computationally intractable for real-time use on the robots. Therefore, we developed experimental tools that allowed us to sieve out models of the locomoting systems operating on granular media. We were then able to bring these models into harmony with the elegant formulation of our geometric mechanics approach. This allowed us to derive adaptive controllers for our snake robots in sandy terrains, and enabled us to gain deeper insight into of how biological systems move over similar terrains as well.

### **4:18PM V40.00008 Bio-inspired robot design for viscous fluids** , GRACE MA, TYLER LIPMAN, SUNGHWAN

JUNG, Virginia Tech — Many modern micro-robots are designed for biomedical applications to transport drugs to targets or to operate tests in the body for diagnosis. However, most micro-robots simply mimic the morphology and the propulsive mechanism of micro-organisms without understanding the underlying physics of low-Re swimming. Two types of swimming motions have been observed in micro-organisms; stresslet and source-dipole swimming. The stresslet swimmer (e.g. *E. coli*) uses a rotating helical appendage, whereas the source-dipole swimmer (e.g. *Paramecium*) creates surface velocity for propulsion. Using this principle, we designed a robot to swim in very viscous fluids either by rotating a helix or creating surface velocity, simply by changing the orientation of the appendage. Further, we will discuss the performance of this robot (swimming speed and rotation speed) with respect to the number, winding angle, and radius of helices in a very viscous fluid.

### **4:30PM V40.00009 A microfluidic two-pump system inspired by liquid feeding in mosquitoes**

, ANDREW MARINO, Virginia Tech, ANGELA GOAD, Carroll County High School, MARK STREMLER, JOHN SOCHA, SUNGHWAN JUNG, Virginia Tech — Mosquitoes feed on nectar and blood using a two-pump system in the head—a smaller cibarial pump in line with a larger a pharyngeal pump, with a valve in between. To suck, mosquitoes transport the liquid (which may be a multi-component viscous fluid, blood) through a long micro-channel, the proboscis. In the engineering realm, microfluidic devices in biomedical applications, such as lab-on-a-chip technology, necessitate implementing a robust pump design to handle clogging and increase flow control compared to a single-pump system. In this talk, we introduce a microfluidic pump design inspired by the mosquito's two-pump system. The pumping performance (flow rate) in presence of impurities (air bubbles, soft clogs) is quantified as a function of phase difference and volume expansion of the pumps, and the elasticity of the valve.

### **4:42PM V40.00010 Propulsion of a two-sphere swimmer** , DAPHNE KLOTS, Department of Applied and Physical

Sciences, University of North Carolina at Chapel Hill, KYLE BALDWIN, RICHARD HILL, ROGER BOWLEY, MICHAEL SWIFT, School of Physics and Astronomy, University of Nottingham, UK — We describe experiments and simulations demonstrating the propulsion of a neutrally-buoyant macroscopic swimming robot that consists of a pair of spheres attached by a spring, immersed in a vibrating fluid. The vibration of the fluid induces relative motion of the spheres which, for sufficiently large amplitudes, can lead to motion of the center of mass of the two spheres. We find that the swimming speed obtained from both experiment and simulation agree and collapse onto a single curve if plotted as a function of the streaming Reynolds number, suggesting that the propulsion is related to streaming flows. There appears to be a critical onset value of the streaming Reynolds number for swimming to occur. We observe a change in the streaming flows as the Reynolds number increases, from that generated by two independent oscillating spheres to a collective flow pattern around the swimmer as a whole. The mechanism for swimming is traced to a strengthening of a jet of fluid in the wake of the swimmer.

### **4:54PM V40.00011 Microstructural view of burrowing with a bioinspired digging robot** , KERSTIN

NORDSTROM, Mount Holyoke College, DAN DORSCH, Massachusetts Institute of Technology, WOLFGANG LOSERT, University of Maryland, AMOS WINTER, V, Massachusetts Institute of Technology — RoboClam is a burrowing technology inspired by *Ensis directus*, the Atlantic razor clam. Atlantic razor clams should only be strong enough to dig a few centimeters into the soil, yet they burrow to over 70 cm. The animal uses a clever trick to achieve this: by contracting its body, it agitates and locally fluidizes the soil, reducing the drag and energetic cost of burrowing. RoboClam technology, which is based on the digging mechanics of razor clams, may be valuable for subsea applications that could benefit from efficient burrowing, such as anchoring, mine detonation, and cable laying. We directly visualize the movement of soil grains during the contraction of RoboClam, using a novel index-matching technique along with particle tracking. We show that the size of the failure zone around contracting RoboClam can be theoretically predicted from the substrate and pore fluid properties, provided that the timescale of contraction is sufficiently large. We also show that the nonaffine motions of the grains are a small fraction of the motion within the fluidized zone, affirming the relevance of a continuum model for this system, even though the grain size is comparable to the size of RoboClam.

### **5:06PM V40.00012 Bipedal locomotion in granular media** , MARK KINGSBURY, TINGNAN ZHANG, DANIEL

GOLDMAN, Georgia Inst of Tech — Bipedal walking, locomotion characterized by alternating swing and double support phase, is well studied on ground where feet do not penetrate the substrate. On granular media like sand however, intrusion and extrusion phases also occur. In these phases, relative motion of the two feet requires that one or both feet slip through the material, degrading performance. To study walking in these phases, we designed and studied a planarized bipedal robot (1.6 kg, 42 cm) that walked in a fluidized bed of poppy seeds. We also simulated the robot in a multibody software environment (Chrono) using granular resistive force theory (RFT) to calculate foot forces. In experiment and simulation, the robot experienced slip during the intrusion phase, with the experiment presenting additional slip due to motor control error during the double support phase. This exaggerated slip gave insight (through analysis of ground reaction forces in simulation) into how slip occurs when relative motion exists between the two feet in the granular media, where the foot with higher relative drag forces (from its instantaneous orientation, rotation, relative direction of motion, and depth) remains stationary. With this relationship, we generated walking gaits for the robot to walk with minimal slip.

### **5:18PM V40.00013 Obstacle traversal and self-righting of bio-inspired robots reveal the physics of multi-modal locomotion** , CHEN LI, RONALD FEARING, ROBERT FULL, University of California, Berkeley —

Most animals move in nature in a variety of locomotor modes. For example, to traverse obstacles like dense vegetation, cockroaches can climb over, push across, reorient their bodies to maneuver through slits, or even transition among these modes forming diverse locomotor pathways; if flipped over, they can also self-right using wings or legs to generate body pitch or roll. By contrast, most locomotion studies have focused on a single mode such as running, walking, or jumping, and robots are still far from capable of life-like, robust, multi-modal locomotion in the real world. Here, we present two recent studies using bio-inspired robots, together with new locomotion energy landscapes derived from locomotor-environment interaction physics, to begin to understand the physics of multi-modal locomotion. (1) Our experiment of a cockroach-inspired legged robot traversing grass-like beam obstacles reveals that, with a terradynamically “streamlined” rounded body like that of the insect, robot traversal becomes more probable by accessing locomotor pathways that overcome lower potential energy barriers. (2) Our experiment of a cockroach-inspired self-righting robot further suggests that body vibrations are crucial for exploring locomotion energy landscapes and reaching lower barrier pathways. Finally, we posit that our new framework of locomotion energy landscapes holds promise to better understand and predict multi-modal biological and robotic movement.

**5:30PM V40.00014 Swarming Bristle-Bots: Exploring Properties of Active Matter** , MARTIN B. FORSTNER, DAMIAN BEASOCK, Syracuse University — Active Matter describes an ubiquitous class of non-equilibrium systems that encompasses a diverse range of phenomena in the living and non-living realm. Examples are microscopic bio-filaments and their associated motor proteins, flocks of birds and fish, vibrated rods and disks, or nanoscale colloids actuated by catalytic activity on their surface. What unifies these systems is that they are all composed of self-driven units. In consequence, these systems are not driven into non-equilibrium by energy input at their boundary, but by local energy injection. As fascinating as these systems are, there are currently barely any laboratory systems that allow for controlled experiments in dry active matter. That is, systems not immersed in a fluid that can be observed without specialized equipment. Here we present a two-dimensional 'active matter' system consisting of hundreds of macroscopic (~0.05 m long), modified, commercially available bristle-bots. We show that this swarm of toys classifies as active matter as it exhibits properties such as dynamic phase separation. Because of their straight forward implementation, their size and controllability, such swarms can not only answer scientific questions, but they have great potential as educational tools in teaching labs and classrooms.

**Thursday, March 17, 2016 2:30PM - 5:30PM –**  
**Session V41 DBIO DPOLY DCOMP: Physics of Proteins: Mechanics and Forces** 344 - Tom Chou,  
University of California, Los Angeles

**2:30PM V41.00001 Rationally designing the mechanical properties of protein hydrogels** , YI CAO, Nanjing University — Naturally occurring biomaterials possess diverse mechanical properties, which are critical to their unique biological functions. However, it remains challenging to rationally control the mechanical properties of synthetic biomaterials. Here we provide a bottom-up approach to rationally design the mechanical properties of protein-based hydrogels. We first use atomic force microscope (AFM) based single-molecule force spectroscopy to characterize the mechanical stability of individual protein building blocks. We then rationally design the mechanical properties of hydrogels by selecting different combination of protein building blocks of known mechanical properties. As a proof-of-principle, we demonstrate the engineering of hydrogels of distinct extensibility and toughness. This simple combinatorial approach allows direct translation of the mechanical properties of proteins from the single molecule level to the macroscopic level and represents an important step towards rationally designing the mechanical properties of biomaterials.

**3:06PM V41.00002 Nonlinear elasticity of disordered fiber networks** , JINGCHEN FENG, Bioengineering Department and Center for Theoretical Biological Physics, Rice University, Houston TX, 77251-1892, USA., HERBERT LEVINE, Bioengineering Department and Center for Theoretical Biological Physics, Rice University, Houston TX, 77251-1892, USA, XIAOMING MAO, Department of Physics, University of Michigan, Ann Arbor MI 48109-1040, USA., LEONARD M. SANDER, Physics & Complex Systems, University of Michigan, Ann Arbor MI 48109-1040, USA. — One of the most striking mechanical properties in disordered biopolymer gels is strong nonlinearities. In the case of athermal gels (such as collagen- I) the nonlinearity has long been associated with a crossover from a bending dominated to a stretching dominated regime of elasticity. The physics of this crossover is related to the existence of a central-force isostatic point and to the small bending modulus for most gels. This crossover induces scaling behavior for the elastic moduli. In particular, for linear elasticity such a scaling law has been demonstrated by Broedersz et al. We generalize the scaling to the nonlinear regime with a two-parameter scaling law involving three critical exponents. We do numerical testing of the scaling law for two disordered lattice models, and find a good scaling collapse for the shear modulus in both the linear and nonlinear regimes. We compute all the critical exponents for the two lattice models and discuss the applicability of our results to real systems.

**3:18PM V41.00003 Mechanosensing by tethered membrane channels** , BENEDIKT SABASS, HOWARD A. STONE, Mechanical and Aerospace Engineering, Princeton University — Force-gated membrane channels are a paradigm of biological mechanosensing. These channels are often tethered to cytoskeletal elements, which allows direct transmission of the mechanical signal. How force at tethers leads to channel opening is unknown. Here, we focus on the generic role of membrane-channel interaction for gating. We propose a scaling relation, linking protein deformation under force to membrane energy. A minute conical deformation during gating leads to an elastic energy gain that far exceeds the thermal energy. Force thresholds for gating are in the experimentally inferred range and are robust against changes of membrane tension. We also study a detailed model for membrane-mediated interactions among channels. In general, interactions reduce the force threshold, leading to cooperatively enhanced gating.

**3:30PM V41.00004 Group transfer theory of single molecule imaging experiments in the F-ATPase biomolecular motor** , SANDOR VOLKAN-KACSO, RUDOLPH MARCUS, California Institute of Technology — I describe a chemo-mechanical theory to treat single molecule imaging and "stalling" experiments on the F-ATPase enzyme. This enzyme is an effective stepping biomolecular rotary motor with a rotor shaft and a stator ring. Using group transfer theoretical approach the proposed structure-based theory couples the binding transition of nucleotides in the stator subunits and the physics of torsional elasticity in the rotor. The twisting of the elastic rotor domain acts as a perturbation upon the driving potential, the Gibbs free energy. In the theory, without the use of adjustable parameters, we predict the rate and equilibrium constant dependence of steps such as ATP binding and phosphate release as a function of manipulated rotor angle. Then we compare these predictions to available data from stalling experiments. Besides treating experiments, the theory can provide guides for atomistic simulations, which could calculate the reorganization parameter and the torsional spring constant. The framework is generic and I discuss its application to other single molecule experiments, such as controlled rotation and other biomolecular motors, including motor-DNA complexes and linear motors.[PNAS, Early Edition, Oct. 19, 2015, doi: 10.1073/pnas.1518489112]

**3:42PM V41.00005 Fluorescent ATP analog mant-ATP reports dynein activity in the isolated *Chlamydomonas* axoneme** , MARIA FEOFILOVA, JONATHON HOWARD, Yale University — Eukaryotic flagella are long rod-like extensions of cells, which play a fundamental role in single cell movement, as well as in fluid transport. Flagella contain a highly evolutionary conserved mechanical structure called the axoneme. The motion of the flagellum is generated by dynein motor proteins located all along the length of the axoneme. How the force production of motors is controlled spatially and temporally is still an open question. Therefore, monitoring dynein activity in the axonemal structure is expected to provide novel insights in regulation of the beat. We use high sensitivity fluorescence microscopy to monitor the binding and hydrolysis kinetics of the fluorescently labeled ATP analogue mant-ATP (2'-(3')-O-(N-methylanthraniloyl) adenosine 5'-triphosphate), which is known to support dynein activity. By studying the kinetics of mant-ATP fluorescence, we identified distinct mant-ATP binding sites in the axoneme. The application of this method to axonemes with reduced amounts of dynein, showed evidence that one of the sites is associated with binding to dynein. In the future, we would like to use this method to find the spatial distribution of dynein activity in the axoneme.

**3:54PM V41.00006 Limiting Speed of the Bacterial Flagellar Motor** , JASMINE NIRODY, University of California, Berkeley, RICHARD BERRY, University of Oxford, GEORGE OSTER, University of California, Berkeley — The bacterial flagellar motor (BFM) drives swimming in a wide variety of bacterial species, making it crucial for several fundamental biological processes including chemotaxis and community formation. Recent experiments have shown that the structure of this nanomachine is more dynamic than previously believed. Specifically, the number of active torque-generating units (stators) was shown to vary across applied loads. This finding invalidates the experimental evidence reporting that limiting (zero-torque) speed is independent of the number of active stators. Here, we put forward a model for the torque generation mechanism of this motor and propose that the maximum speed of the motor increases as additional torque-generators are recruited. This is contrary to the current widely-held belief that there is a universal upper limit to the speed of the BFM. Our result arises from the assumption that stators disengage from the motor for a significant portion of their mechanochemical cycles at low loads. We show that this assumption is consistent with current experimental evidence and consolidate our predictions with arguments that a processive motor must have a high duty ratio at high loads.

**4:06PM V41.00007 A mechanochemical model for myosin VI**, RIINA TEHVER, AMANDA JACK, Denison University, IAN LOWE, University of Pennsylvania — Myosin VI is a motor protein that transports cellular cargo along actin filaments. This transport takes place as a result of a coordinated mechano-chemical cycle that is controlled by external variables including imposed force and nucleotide concentrations. We present a model that captures the different dynamic pathways that myosin VI can take in response to these variables. The results of our model for experimentally observable quantities, such as the motor velocity or run length, agree with available experimental data, and we can also make predictions beyond the tested regimes. Using the model, we study how myosin VI reacts to its environment and test its operational efficiency.

**4:18PM V41.00008 Talin mediated force transmission and mechanosensing<sup>1</sup>**, JIE YAN, Department of Physics and Mechanobiology Institute, Natl Univ of Singapore, MINGXI YAO, Mechanobiology Institute, Natl Univ of Singapore, BENJAMIN GOULT, School of Biosciences, University of Kent, UK, MICHAEL SHEETZ, Department of Biological Sciences, Columbia University; Mechanobiology Institute, Natl Univ of Singapore — Cells adhere to extracellular matrix (ECM) through focal adhesion. Talin is a cytoplasmic adapter protein that links the actin cytoskeleton to focal adhesion, playing a central role in regulation of cell spreading and migration. Talin's functions depend on the binding of talin rod domains to a cytoplasmic protein vinculin in a force dependent manner. By stretching full-length talin rod using magnetic tweezers, we have determined the force-dependent unfolding and refolding rates of subdomains in talin rod. Kinetics simulations based on these rates have revealed that talin rod can serve as a force buffer, capable of maintaining tension in talin in a range of 5-10 pN over a wide range of extension change of talin rod from 50 nm to 400 nm. Further, this level of force is found able to expose the cryptic vinculin-binding sites, promoting subsequent binding of the head domain of vinculin with a nano Molar affinity. Such a force-sensitive interaction between talin rod and vinculin is described by a force-dependent dissociation constant derived based on the mechanical stability of the talin rod domains. Together, these results provide important insights into the mechanosensing at focal adhesion that is crucial for cells to sense and respond to their microenvironments.

<sup>1</sup>The research is supported by the National Research Foundation of Singapore through Mechanobiology Institute and NRF Investigatorship to YJ

**4:30PM V41.00009 Directly measuring single molecule heterogeneity in proteins and RNA using force spectroscopy**, MICHAEL HINCZEWSKI, Case Western Reserve University, CHANGBONG HYEON, Korea Institute for Advanced Study, DEVARAJAN THIRUMALAI, Institute For Physical Science and Technology, University of Maryland, College Park — One of the most intriguing results of single molecule experiments on proteins and nucleic acids is the discovery of functional heterogeneity: the observation that complex cellular machines exhibit multiple, biologically active conformations. The structural differences between these conformations may be subtle, but each distinct state can be remarkably long-lived, with stochastic interconversions occurring only at macroscopic timescales, fractions of a second or longer. Though we now have proof of functional heterogeneity in a handful of systems—enzymes, motors, adhesion complexes—identifying and measuring it remains a formidable challenge. We show that evidence of this phenomenon is more widespread than previously known, encoded in data collected from some of the most well-established single molecule techniques: AFM or optical tweezer pulling experiments. We present a theoretical procedure for analyzing distributions of rupture/unfolding forces recorded at different pulling speeds. This results in a single parameter, quantifying the degree of heterogeneity, and also leads to bounds on the equilibration and conformational interconversion timescales. Our work suggests experimental approaches for estimating the timescales of these fluctuations with unprecedented accuracy.

**4:42PM V41.00010 Bayesian Uncertainty Quantification for Bond Energies and Mobilities Using Path Integral Analysis**, PAK-WING FOK, University of Delaware, JOSHUA CHANG, Ohio State University, TOM CHOU, UCLA, UCLA-OSU-UD BIOMATH GROUP COLLABORATION — Dynamic single-molecule force spectroscopy is often used to distort bonds. The resulting responses, in the form of rupture forces and trajectories of displacements, are used to reconstruct bond potentials. Such approaches often rely on simple parameterizations of one-dimensional bond potentials and/or large amounts of trajectory data. Parametric approaches typically fail at inferring complicated bond potentials with multiple minima, while piecewise estimation may not guarantee smooth results. Existing techniques also do not address spatial variations in the diffusivity that may arise from inhomogeneous coupling to other degrees of freedom in the macromolecule. To address these challenges, we develop an empirical Bayesian approach that incorporates data and regularization terms into a path integral. All experimental and statistical parameters in our method are estimated from the data. Upon testing our method on simulated data, our regularized approach requires less data and allows simultaneous inference of both complex bond potentials and diffusivities. We show that the accuracy of the reconstructed bond potential is sensitive to the spatially varying diffusivity and accurate reconstruction can be expected only when both are simultaneously inferred.

**4:54PM V41.00011 Base-by-Base Counting of Nucleotide Incorporations by DNA Polymerase**, MACKENZIE W. TURVEY, O. TOLGA GUL, KAITLIN M. PUGLIESE, DENYS O. MARUSHCHAK, ARITH J. RAJAPAKSE, GREGORY A. WEISS, PHILLIP G. COLLINS, University of California, Irvine — Previously, the catalytic cycle of DNA polymerase has been recorded by tethering single polymerase molecules to single-walled carbon nanotube field effect transistors (FETs) [1]. As the polymerase incorporates nucleotides into a single-stranded DNA template, it generates electrical signals in the SWCNT-FET. Here, we investigate the accuracy of this electronic method by using low concentrations (<10 nM) of DNA template, such that the signal consists of long, diffusion-limited pauses interrupted by template binding and a burst of nucleotide incorporation events. By counting the events generated by as few as 10 template molecules, template length has been correctly determined with <1 base pair resolution. Furthermore, differing template lengths can be identified and correctly enumerated in solutions containing mixtures of templates. Processivity of the Klenow Fragment of DNA polymerase currently limits read lengths to 50-100 base pairs, but the FET technique should work equally well with longer-processivity polymerases. 1. T.J. Olsen, et. al., "Electronic Measurements of Single-Molecule Processing by DNA polymerase I (Klenow fragment)," JACS 135, 7855 (2013).

**5:06PM V41.00012 Sequence and Structure Dependent DNA-DNA Interactions**, BENJAMIN KOPCHICK, XIANGYUN QIU, The George Washington University — Molecular forces between dsDNA strands are largely dominated by electrostatics and have been extensively studied. Quantitative knowledge has been accumulated on how DNA-DNA interactions are modulated by varied biological constituents such as ions, cationic ligands, and proteins. Despite its central role in biology, the sequence of DNA has not received substantial attention and "random" DNA sequences are typically used in biophysical studies. However, ~50% of human genome is composed of non-random-sequence DNAs, particularly repetitive sequences. Furthermore, covalent modifications of DNA such as methylation play key roles in gene functions. Such DNAs with specific sequences or modifications often take on structures other than the canonical B-form. Here we present series of quantitative measurements of the DNA-DNA forces with the osmotic stress method on different DNA sequences, from short repeats to the most frequent sequences in genome, and to modifications such as bromination and methylation. We observe peculiar behaviors that appear to be strongly correlated with the incurred structural changes. We speculate the causalities in terms of the differences in hydration shell and DNA surface structures.

**5:18PM V41.00013 *In vivo* Studies of VEGFR2 Interactions in the Presence and Absence of VEGF<sup>1</sup>**, CHRISTOPHER KING, DR. KALINA HRISTOVA, Johns Hopkins Univ — Vascular Endothelial Growth Factor Receptor 2 (VEGFR2) is a receptor tyrosine kinase (RTK) that is critical for vasculogenesis and angiogenesis. Enhanced VEGFR2 signaling is often correlated with malignancy. Recently, it was shown that full-length VEGFR2 exists in a monomer-dimer equilibrium in the absence of bound VEGF. Thus, the canonical model of RTK activation does not seem to adequately describe the behavior of VEGFR2 in the cell membrane. In order to understand the role that VEGFR2 extracellular domain plays in unliganded dimerization in live cells, we utilize Fully Quantified Spectral Imaging (FSI) to probe the interactions of VEGFR2 mutant constructs with rationally truncated EC domains. In addition, we investigate the stoichiometry of ligand binding to VEGFR2 EC domain as a function of VEGF concentration and total receptor expression.

<sup>1</sup>Supported by NSF MCB 1157687 and NIH GM068619 (to KH) and NSF Graduate Research Fellowship DGE-1232825 (to CK)

## Thursday, March 17, 2016 2:30PM - 5:30PM –

### Session V42 DPOLY: Polymer Architecture, Control of Structure and Dynamics in Polyolefins

345 - Lin Wang, The Dow Chemical Company

#### 2:30PM V42.00001 Melt structure and self-nucleation of ethylene copolymers<sup>1</sup>, RUFINA G ALAMO,

Florida State University, FAMU-FSU College of Engineering, Tallahassee, FL 32310 USA — A strong memory effect of crystallization has been observed in melts of random ethylene copolymers well above the equilibrium melting temperature. These studies have been carried out by DSC, x-ray, TEM and optical microscopy on a large number of model, narrow, and broad copolymers with different comonomer types and contents. Melt memory is correlated with self-seeds that increase the crystallization rate of ethylene copolymers. The seeds are associated with molten ethylene sequences from the initial crystals that remain in close proximity and lower the nucleation barrier. Diffusion of all sequences to a randomized melt state is a slow process, restricted by topological chain constraints (loops, knots, and other entanglements) that build in the intercrystalline region during crystallization. Self-seeds dissolve above a critical melt temperature that demarcates homogeneity of the copolymer melt. There is a critical threshold level of crystallinity to observe the effect of melt memory on crystallization rate, thus supporting the correlation between melt memory and the change in melt structure during copolymer crystallization. Unlike binary blends, commercial ethylene-1-alkene copolymers with a range in inter-chain comonomer composition between 1 and about 15 mol % display an inversion of the crystallization rate in a range of melt temperatures where narrow copolymers show a continuous acceleration of the rate. With decreasing the initial melt temperature, broadly distributed copolymers show enhanced crystallization followed by a decrease of crystallization rate. The inversion demarcates the onset of liquid-liquid phase separation (LLPS) and a reduction of self-nuclei due to the strong thermodynamic drive for molecular segregation inside the binodal. The strong effect of melt memory on crystallization rate can be used to identify liquid-liquid phase separation in broadly distributed copolymers, and offers strategies to control the state of copolymer melts in ways of technological relevance for melt processing of LLDPE and other random olefin copolymers. References: B. O. Reid, et al, *Macromolecules* 46, 6485-6497, 2013 H. Gao, et al, *Macromolecules* 46, 6498-6506, 2013 A. Mamun et al, *Macromolecules* 47, 7958-7970, 2014 X. Chen et al, *Macromol. Chem. Phys.* 216, 1220–1226, 2015 M. Ren et al, *Macromol. Symp.* 356, 131–141, 2015

<sup>1</sup>Work supported by the NSF (DMR1105129)

#### 3:06PM V42.00002 Crystal Structures of Precise Functional Copolymers: Atomistic Molecular Dynamics Simulations and Comparisons with Experiments, EDWARD B. TRIGG, University of Pennsylvania, MARK J. STEVENS, Sandia National Laboratories, KAREN I. WINEY, University of Pennsylvania — Layered crystal structures have been observed in linear poly(ethylene-co-acrylic acid) in which the carboxylic acid groups are placed precisely every 21 carbon atoms along the backbone. The alkane segments form structures resembling orthorhombic polyethylene crystals, while the acid groups form continuous domains that may act as pathways for ion conduction. Further details of the crystal structure have been difficult to elucidate experimentally, but could be important for understanding structure-property relationships. Here, two classes of crystal structures are evaluated via atomistic molecular dynamics: extended chain structures, wherein the polymer backbones are highly extended in near-trans conformations, and adjacent reentry structures, wherein the polymer backbones conform in adjacent reentry loops near the site of each covalently-bonded acid group. Energies of relaxed structures and hydrogen bonding states are compared, and X-ray scattering and other experimental data is compared with the simulation results.

#### 3:18PM V42.00003 Modeling neutron scattering in disperse, nonuniformly labeled commercial polyolefins, BRIAN HABERSBERGER, KYLE HART, DAVID GILLESPIE, TIANZI HUANG, Dow Chemical Co — In spite of their chemically simple monomer elements, understanding of many structural, thermodynamic, and other aspects of polyolefins has remained elusive. Scattering studies on polyolefins are challenged by their nearly identical density in the melt, requiring the use of deuterium-labeling to provide contrast for small-angle neutron scattering (SANS). Until recently, labeling of commercial polyolefins has been prohibitively costly, leading SANS investigations on polyolefins to focus on non-disperse model systems. Commercial polyolefins often have broad molecular weight and composition distributions, and such dispersity plays an important role in their rheology, crystallization, and mechanical properties. Recent reports have described facile hydrogen-deuterium exchange reactions that preserve the chain architecture of polyolefins. However, such exchange is not uniformly distributed across the chain population. Here, we report a generalized application of the Random Phase Approximation prediction for SANS from homogeneous polymer blends to account for such dispersity. A Monte-Carlo method is used to calculate the deuterium distribution that corresponds to SANS measurements. These methods provide powerful tools for probing the structure of disperse polymer architectures.

#### 3:30PM V42.00004 Time-resolved WAXD studies on the crystallization of semicrystalline/graphene nanocomposites, MAYA ENDOH, Stony Brook Univ, SHOTARO NISHITSUJI, Yamagata Univ, TAD KOGA, MIRIAN RAFAILOVICH, Stony Brook Univ — Graphene is one layer of carbon atoms, which has good electronic, thermal conductivity, and mechanical properties. By adding graphene to semicrystalline polymers such as polyethylene (PE) and isotactic polypropylene (iPP), the mechanical and electrical properties of the polymers are significantly improved. To further achieve high performance of semicrystalline polymer/graphene nanocomposites, it is important to investigate the relationship between the crystalline structure of the polymer and the mechanical property of the nanocomposites. In this study, the effect of graphene on the crystallization behavior of PE and iPP was investigated by using time-resolved wide angle X-ray diffraction (WAXD). The in situ WAXD results on the melt-crystallization process showed that the crystalline structures of all the samples remained the same as the pure bulk, while both the rate and degree of the crystallinity increased. We will discuss the detailed structure information along with DSC and mechanical test results.

#### 3:42PM V42.00005 Porous Polyolefin Films via Polymer Blends, CHRIS MACOSKO, University of Minnesota — Porous polymer films have broad application including battery separators, membrane supports and filters. Polyolefins are attractive for these applications because of their solvent resistance, low electrical and thermal conductivity, easy fabrication and cost. We will describe fabrication of porous films using cocontinuous blends of a polyolefin with another polymer which can be readily removed with a solvent. Methods to image and control the cocontinuous morphology will be presented. Bell, J. R., K. Chang, C. R. Lopez-Barron, C. W. Macosko, and D. C. Morse, "Annealing of cocontinuous polymer blends: effect of block copolymer molecular weight and architecture," *Macromolecules* 43, 5024-5032 (2010). Lopez-Barron, C. R., and C. W. Macosko, "Direct measurement of interface anisotropy of bicontinuous structures via 3D image analysis," *Langmuir* 26, 14284-14293 (2010). Trifkovic, M., A. T. Hedegaard, K. Huston, M. Sheikhzadeh, and C. W. Macosko, "Porous films via PE/PEO cocontinuous blends," *Macromolecules* 45, 6036-6044 (2012). Hedegaard, A.T., L.L. Gu and C. W. Macosko, "Effect of Extensional Viscosity on Cocontinuity of Immiscible Polymer Blends" *J. Rheol.* 59, 1397-1417 (2015).

#### 4:18PM V42.00006 Quantifying tie-molecule content in semicrystalline polymers, AMANDA MCDERMOTT, CHAD SNYDER, NIST - Natl Inst of Stds & Tech, PAUL DESLAURIERS, Chevron Phillips Chemical Co., RONALD JONES, NIST - Natl Inst of Stds & Tech — Tie molecules bridging adjacent crystalline lamellae in semicrystalline polymers strongly impact mechanical properties, but they remain difficult to characterize. We demonstrate a new method of measuring tie-chain content: applying equilibrium swelling theory to small-angle neutron scattering patterns from semicrystalline polyethylene films whose interlamellar amorphous regions are swollen with deuterated organic solvent in a vapor-flow sample environment. To aid in validating the measurement, measured tie-chain content is compared with a primary structural parameter (PSP2) that is calculated from molecular architecture and correlates with slow crack growth behavior. Agreement is favorable for a linear polyethylene and a series of ethylene-hexene copolymers. Recent applications of the technique are also discussed.

## 4:30PM V42.00007 ABSTRACT WITHDRAWN —

### 4:42PM V42.00008 Understanding the Evolution in Meso/Nanostructure in UHMWPE Fibers

, PRESTON MCDANIEL, JOSEPH DEITZEL, JOHN GILLESPIE, Univ of Delaware — Ultra-high-molecular-weight polyethylene (UHMWPE) fibers are increasingly used in composite armor applications. Understanding the complex sub-filament structure which ultimately dictates macroscopic mechanical performance is important as a materials by design approach is taken. In this work, the meso/nanostructure of fibers is studied through a series of atomic force microscopy, X-ray diffraction, and tomography techniques. Fibers with varying thermomechanical processing histories and macroscopic mechanical properties are examined to correlate the evolution of structure with fiber mechanical response in both tension and transverse compression. This work spotlights the sub-filament structural hierarchy in the fiber. The study of nanoscale fibril geometry and crystal structure provides some insight into the load pathways within the fiber, while the identification of a three-dimensional fibrillar network indicates the presence of complex mechanical interactions throughout. The presence and geometry of mesoscale voids in highly drawn fibers is discussed, and tomography results are presented to further understand their distribution throughout the fiber. Finally, the presence of these features are explored in the context of their influence on the energy dissipative capabilities at the fiber level.

### 4:54PM V42.00009 Unfolding of Isotactic Polypropylene under Uniaxial Stretching

, JIA KANG, TOSHIKAZU MIYOSHI, Univ of Akron, AKIHIRO KAMIMURA, AKIHIRO OTSUBO COLLABORATION — Despite numerous investigations on polymer processing, understanding the deformation mechanisms of semicrystalline polymer under uniaxial stretching is still challenging. In this work,  $^{13}\text{C}$ - $^{13}\text{C}$  Double Quantum (DQ) NMR was applied to trace the structural evolution of  $^{13}\text{C}$ -labeled isotactic polypropylene (iPP) chains inside the crystallites stretched to engineering strain ( $\epsilon$ ) of 21 at 100 C. DQ NMR based on spatial proximity of  $^{13}\text{C}$  labeled nuclei proved conformational changes from the folded chains to the locally extended chains induced by stretching. By combining experimental findings with literature results on molecular dynamics, it was concluded that transportation of the crystalline chains plays a critical role to achieve large deformability of iPP.

### 5:06PM V42.00010 Deformation across length scales in polyolefines: effect of the chain microstructure on the polymorphism, phase transitions and morphological changes.

, FINIZIA AURIEMMA, CLAUDIO DE ROSA, ROCCO DI GIROLAMO, ANNA MALAFRONTÉ, MIRIAM SCOTI, Dipartimento di Scienze Chimiche- Universit di Napoli Federico II-Complesso Monte Sant' Angelo- via Cintia-80126 Napoli — The transformations related to phase changes of the crystals, and at lamellar length scales by effect of tensile deformation are studied in the case of some isotactic polypropylene samples having high molecular mass, polydispersity index  $\approx 2$ , and stereodefects at different concentrations and with a uniform distribution. The stress induced transformations are followed in real time during stretching through wide and small angle X-ray scattering measurements. The data analysis evidences that during the transformations of the spherulitic into the fibrillar morphology, stress-induced phase transitions occurring during plastic deformation are regulated by the same factors that govern the textural and morphological changes, that is the ability of the entangled amorphous chains to transmit the stress and the intrinsic stability of the lamellar crystals. Since the relative stability of the different polymorphic forms involved in the structural transformations and the intrinsic flexibility of the chains depend on the stereoregularity, precise correlations between the stereoregularity of the chains, and the deformation behavior are outlined, paving the way for understanding the material properties at molecular level.

### 5:18PM V42.00011 Topological Constraints on Chain-Folding Structure of Semicrystalline Polymer as Studied by $^{13}\text{C}$ - $^{13}\text{C}$ Double Quantum NMR<sup>1</sup>

, YOULEE HONG, TOSHIKAZU MIYOSHI, The university of akron — Chain-folding process is a prominent feature of long polymer chains during crystallization. Over the last half century, much effort has been paid to reveal the chain trajectory. Even though various chain-folding models as well as theories of crystallization at molecule levels have been proposed, they could be not reconciled due to the limited experimental evidences. Recent development of double quantum NMR with selective isotope labeling identified the chain-trajectory of  $^{13}\text{C}$  labeled *isotactic* poly(1-butene). The systematic experiments covered a wide range of parameters, i.e. kinetics, concentration, and molecular weight ( $M_w$ ). It was demonstrated that i) adjacent re-entry site was invariant as a function of crystallization temperature ( $T_c$ ), concentration, and  $M_w$ , ii) long-range order of adjacent re-entry sequence is independence of kinetics at a given concentration while it decreased with increasing the polymer concentration at a given  $T_c$  due to the increased interruption between the chains, and iii) high  $M_w$  chains led to the multilayer folded structures in single crystals, but the melt state induced the identical short adjacent sequences of long and short polymer over a wide range of  $T_c$  due to the entanglements. The behaviors indicated that the topological restriction plays significant roles in the chain-folding process rather than the kinetics. The proposed framework to control the chain-folding structure presents a new perspective into the chain organization by either the intra- or inter-chain interaction.

<sup>1</sup>National Science Foundation Grants DMR-1105829 and 1408855

## Thursday, March 17, 2016 2:30PM - 5:30PM —

Session V43 GSNP: Wave Chaos: Theory and Applications 346 - Gabriele Gradoni, University of Nottingham

### 2:30PM V43.00001 Modeling Transmission Line Networks Using Quantum Graphs<sup>1</sup>

, TRYSTAN KOCH, THOMAS ANTONSEN, Univ of Maryland-College Park — Quantum graphs—one dimensional edges, connecting nodes, that support propagating Schrödinger wavefunctions—have been studied extensively as tractable models of wave chaotic behavior (Smilansky and Gnutzmann 2006, Berkolaiko and Kuchment 2013). Here we consider the electrical analog, in which the graph represents an electrical network where the edges are transmission lines (Hul et. al. 2004) and the nodes contain either discrete circuit elements or intricate circuit elements best represented by arbitrary scattering matrices. Including these extra degrees of freedom at the nodes leads to phenomena that do not arise in simpler graph models. We investigate the properties of eigenfrequencies and eigenfunctions on these graphs, and relate these to the statistical description of voltages on the transmission lines when driving the network externally. The study of electromagnetic compatibility, the effect of external radiation on complicated systems with numerous interconnected cables, motivates our research into this extension of the graph model.

<sup>1</sup>Work supported by the Office of Naval Research (N0014130474) and the Air Force Office of Scientific Research.

### 2:42PM V43.00002 Experimental Study of Quantum Graphs with Microwave Networks<sup>1</sup>

, ZIYUAN FU, TRYSTAN KOCH, THOMAS ANTONSEN, EDWARD OTT, STEVEN ANLAGE, University of Maryland, College Park, WAVE CHAOS TEAM — An experimental setup consisting of microwave networks is used to simulate quantum graphs. The networks are constructed from coaxial cables connected by T junctions. The networks are built for operation both at room temperature and superconducting versions that operate at cryogenic temperatures. In the experiments, a phase shifter is connected to one of the network bonds to generate an ensemble of quantum graphs by varying the phase delay. The eigenvalue spectrum is found from S-parameter measurements on one-port graphs. With the experimental data, the nearest-neighbor spacing statistics and the impedance statistics of the graphs are examined. It is also demonstrated that time-reversal invariance for microwave propagation in the graphs can be broken without increasing dissipation significantly by making nodes with circulators. Random matrix theory (RMT) successfully describes universal statistical properties of the system.

<sup>1</sup>We acknowledge support under contract AFOSR COE Grant FA9550-15-1-0171

## **2:54PM V43.00003 Numerical and experimental studies of the elastic enhancement factor of 2D open systems<sup>1</sup>**

, LESZEK SIRKO, MAŁGORZATA BIAŁOUS, VITALII YUNKO, SZYMON BAUCH, MICHAŁ ŁAWNICZAK, Institute of Physics Polish Academy of Sciences, al. Lotników 32/46, 02-668 Warszawa, Poland — We present the results of numerical and experimental studies of the elastic enhancement factor  $W$  for microwave rough and rectangular cavities simulating two-dimensional chaotic and partially chaotic quantum billiards in the presence of moderate absorption strength. We show that for the frequency range  $\nu = 15.0 - 18.5$  GHz, in which the coupling between antennas and the system is strong enough, the values of  $W$  for the microwave rough cavity lie below the predictions of random matrix theory and on average they are above the theoretical results of V. Sokolov and O. Zhirov, Phys. Rev. E, **91**, 052917 (2015). We also show that the enhancement factor  $W$  of a microwave rectangular cavity coupled to the external channels via microwave antennas, simulating a partially chaotic quantum billiard [1], calculated by applying the Potter-Rosenzweig model with  $\kappa = 2.8 \pm 0.5$  is close to the experimental one. Our numerical and experimental results suggest that the enhancement factor can be used as a measure of internal chaos which can be especially useful for systems with significant openness or absorption. [1] M. Ławniczak, M. Białous, V. Yunko, S. Bauch, and L. Sirko, Phys. Rev. E **91**, 032925 (2015).

<sup>1</sup>This work was partially supported by the Ministry of Science and Higher Education grants N N202 130239 and UMO-2013/09/D/ST2/03727.

## **3:06PM V43.00004 Statistical Model of Wave Transport in Systems with Coexisting Chaotic and Regular Phase Space Regions.**

, EDWARD OTT, University of Maryland — We study the statistics of the input-output properties of wave systems in which ray trajectories that are regular and chaotic coexist (i.e., ‘mixed systems’). The transport is expressed as a summation over eigenmodes (energy states) where the eigenmodes can typically be classified as either regular or chaotic. By appropriate characterization of regular and chaotic contributions, we obtain predictions for the transport as characterized by impedance or scattering matrices. We test these predictions by comparison with numerical calculations for a specific example. [Collaborators: M.-J. Lee, T.M. Antonsen, and K. Ma]

## **3:42PM V43.00005 Radiation of complex and noisy sources within enclosures<sup>1</sup>**

, GABRIELE GRADONI, STEPHEN CREAGH, GREGOR TANNER, University of Nottingham — Predicting the radiation of complex electromagnetic sources inside semi-open cavities and resonators with arbitrary geometry is a challenging topic both for physics and for engineering. We have exploited a Perron-Frobenius operator to propagate field-field correlation functions of complex and extended sources in free-space. The formula is based on a phase-space picture of the electromagnetic field, using the Wigner distribution function, and naturally captures evanescent as well as diffracted waves. This approach can be extended to study the propagation of correlation functions within cavities, with the ray-dynamical map given by the geometry of the cord connecting a point of the boundary to another. While ray methods provide an efficient way to predict average values of the correlation matrix elements, the use of random matrix theory approaches allows efficient characterisation of statistical fluctuations around these averages. Universal relations are derived and tested in the presence of dissipation for quantum maps and billiard systems. The use of this formalism is discussed in the contexts of open systems with surface roughness. The theory and achieved results are of interest in the simulation of next-generation of wireless communications.

<sup>1</sup>Work supported by the UK Engineering and Physical Sciences Research Council

## **3:54PM V43.00006 FDTD simulations of the losses in complex electromagnetic cavities<sup>1</sup>**

, FRANCO MOGLIE, LUCA BASTIANELLI, VALTER MARIANI PRIMIANI, Università Politecnica delle Marche - DII, Ancona, EMC TEAM — The simulations of complex electromagnetic cavities like reverberation chambers (RC) require a massive parallel computer to accurately account the complex three dimensional geometry. A parallel finite-difference time-domain (FDTD) code optimized for a massive parallel computer could lose its efficiency if the losses are concentrated in some part of the computation volume. For example, the simulation of the finite conductivity of the cavity metallic walls requires a significant overcharge for the computer processors that handle the boundary part of the global computational domain. Our in-house parallel FDTD code replaces the volumetric losses in every cell of the grid instead of the Ohmic losses on the walls. In this contribution, we evaluate the difference in the field distribution inside the cavity due to this replacement. Moreover, we compare the common RC statistics like the number of stirrer uncorrelated positions and the field uniformity, and the resources required for the two methods are reported and discussed. Finally, the numerical results will be compared with the measurements of the RC in our laboratory with a volume of 60 m<sup>3</sup> and plated steel walls in the frequency range 0.2-1.0 GHz, that includes the transition from the undermoded to the overmoded region.

<sup>1</sup>We acknowledge PRACE for awarding us access to resource FERMI based in Italy at CINECA

## **4:06PM V43.00007 Conductance and Transmittance of waves through a chaotic cavity (or, equivalently, quantum dot) results in regularization of tunneling rates**

, LOUIS PECORA, DONG HO WU, CHRISTOPHER KIM, Naval Research Lab — Tunneling rates in closed, double well quantum or wave systems in two dimensions or higher are radically different between wells with classically regular or chaotic behavior [1]. Wells with regular dynamics have tunneling rates that fluctuate by several orders of magnitude as a function of energy or frequency. Wells with chaotic dynamics have fluctuations smaller than one order of magnitude (a regularization of the fluctuations). We examine a more realistic experimental system, a single well with two channels with tunneling barriers at their junctions with the wells. Former theories for conductance in quantum dots will not apply here. We developed a theory, which uses proper boundary conditions at the barriers and yields the scattering matrix. Results show that the transmission rates fluctuate by orders of magnitude in the regular-shaped well, but are greatly reduced (regularized) for the chaotic-shaped well. We will show experimental results that test these theoretical findings for microwave transmission through a chaotic-shaped cavity, which is made of copper and has two ports with tunneling barriers. [1] Chaos regularization of quantum tunneling rates, L. M. Pecora, H. Lee, D-H. Wu, T. Antonsen, M-J. Lee, and E. Ott, Phys. Rev. E **83**, 065201(R) (2011)

## **4:18PM V43.00008 Time Reversed Electromagnetics as a Novel Method for Wireless Power Transfer**

, ANU CHALLA, ECE Department, University of Maryland, STEVEN M. ANLAGE, Physics and ECE Departments, University of Maryland, TESLA TEAM<sup>1</sup> — Taking advantage of ray-chaotic enclosures, time reversal has been shown to securely transmit information via short-wavelength waves between two points, yielding noise at all other sites. In this presentation, we propose a method to adapt the signal-focusing technique to electromagnetic signals in order to transmit energy to portable devices. Relying only on the time-reversal invariance properties of waves, the technique is unencumbered by the inversely-proportional-to-distance path loss or precise orientation requirements of its predecessors, making it attractive for power transfer applications. We inject a short microwave pulse into a complex, wave-chaotic chamber and collect the resulting long time-domain signal at a designated transceiver. The signal is then time reversed and emitted from the collection site, collapsing as a time-reversed replica of the initial pulse at the injection site. When amplified, this reconstruction is robust, as measured through metrics of peak-to-peak voltage and energy transfer ratio. We experimentally demonstrate that time reversed collapse can be made on a moving target, and propose a way to selectively target devices through nonlinear time-reversal.

<sup>1</sup>University of Maryland Gemstone Team TESLA: Frank Cangialosi, Anu Challa, Tim Furman, Tyler Grover, Patrick Healey, Ben Philip, Brett Potter, Scott Roman, Andrew Simon, Liangcheng Tao, Alex Tabatabai

**4:30PM V43.00009 Enhancement of coherent terahertz beam with chaotic electrodes in a photoconductive antenna**, DONG HO WU, BENJAMIN GRABER, LOUIS PECORA, CHRISTOPHER KIM, U.S. Naval Research Laboratory — We investigated terahertz beam emission from photoconductive antennas containing various shapes of electrodes. With a pair of curved (e.g. concave shape) electrodes it appears that electrons (mostly thermal electrons) follow chaotic trajectories, which keep the electrons away from the surface plasma so that the surface plasma can coherently oscillates without being disrupted by thermal electrons, resulting a slightly increased coherent terahertz power. For an emitter with a pair of ripple electrodes, the classical Poincare surface section map using Birkoff coordinate tends to exhibit chaotic sea and KAM islands if the ripple amplitude becomes comparable to the electrode gap, indicating considerable electron bunching in between the ripple electrodes. Our data show that, when the bunched electrons are stimulated by terahertz pulses, the emitter produces additional spontaneous coherent terahertz beams, which is known as Dicke effect. We will discuss details of our experiments and results.

**4:42PM V43.00010 Controlling and enhancing high frequency collective electron dynamics in superlattices by chaos-assisted miniband transport**, MARK FROMHOLD, MARK GREENAWAY, NATALIA ALEXEEVA, University of Nottingham, ALEXANDER BALANOV, Loughborough University, OLEG MAKAROVSKY, AMALIA PATANE, University of Nottingham, MARAT GAIFULLIN, FEO KUSMARTSEV, Loughborough University — We show in both measurements and calculations that a tilted magnetic field can transform the structure and THz dynamics of charge domains in a biased semiconductor superlattice (SL) [1]. In SLs, at critical field values, when the Bloch frequency equals the cyclotron frequency corresponding to the magnetic field component along the SL axis, the semiclassical electron motion changes abruptly from localized stable trajectories to unbounded chaotic paths, which propagate rapidly through the SL. This delocalisation of the electron creates a series of sharp resonant peaks in drift velocity-field characteristics, which were detected in previous DC current-voltage measurements. We show that these additional peaks can create multiple propagating charge domains, shaped by both the strength and tilt angle of the magnetic field. As a result, the tilted magnetic field generates AC currents whose magnitude and frequencies are far higher than with no magnetic field applied. Chaos-assisted single-electron transport induced by the interplay between cyclotron and Bloch motion therefore provides a mechanism for controlling the collective dynamics of miniband electrons, and thus enhancing the high frequency response of SLs. References: [1] N. Alexeeva et. al. Phys. Rev. Lett. 109, 024102 (2012)

**4:54PM V43.00011 Light transport in dense composite media: role of near-field coupling**, ROXANA REZVANI NARAGHI, CREOL and Department of Physics, University of Central Florida, SERGEY SUKHOV, CREOL, University of Central Florida, JUAN JOS SENZ, Condensed Matter Physics Center, Universidad Autnoma de Madrid and Donostia International Physics Center, Paseo Manuel Lardizabal 4, ARISTIDE DOGARIU, CREOL, University of Central Florida — In scattering media, optical waves comprise both homogeneous and evanescent components. At very high concentrations of scatterers, particles are located in close proximity and interact through evanescent near fields. Thus, in this regime the energy is not only carried by propagating waves but it also evolves through evanescent coupling between individual scatterers. We have shown that in dense composite media additional transmission channels open because of these near-field interactions between close proximity scatterers and, consequently, a new regime of transport emerges. This is clearly beyond simple descriptions of scatterers acting independently of their environment and framed in terms of far-field characteristics such as Mie cross-sections. We will show that, because in the dense media the energy can transfer through both diffusion and evanescent channels, the total transmittance is  $T = T_{CS} + T_{NF} = 1/L(l_{CS}^* + l_{NF}^*)$ . Correcting the total transmission in this manner is appealing because it is done in terms of physically meaningful and measurable quantities such a near-field (NF) scattering cross-section  $\sigma_{NF}$ .

**5:06PM V43.00012 Complexity of knotting in chaotic 3D eigenfunctions**, ALEXANDER TAYLOR, MARK DENNIS, University of Bristol — Quantised vortices occur generically in disordered 3D complex scalar fields, forming a geometrically complex and statistically random large scale tangle even in systems with very different origins of complexity such as turbulent superfluids, optical volume speckle, the quantum eigenfunctions of chaotic 3D cavities, and liquid crystal phases. Although all such systems are random and fractal on large scales [1], it has previously been established that topological measures such as the probability of vortices knotting or linking with one another are sensitive to the local physics. We use the wave chaos as a universal model system with just one physical lengthscale, the wavelength, beyond which its vortices are Brownian. To access finite-volume realisations of wavefields, vortices are traced numerically in three different random degenerate eigenfunction systems, each approximating the random isotropic limit but with different constraints and symmetries that significantly impact topological statistics even at high energies. By a simple mode counting argument, we observe that the probability of a generic eigenfunction containing a knotted vortex line reaches 50% by around its 1000-3000th mode. [1] A J Taylor and M R Dennis, *J Phys A* **47** 465101 (2014)

**5:18PM V43.00013 Supersymmetric sigma model of disordered, isotropic, elastic media<sup>1</sup>**, DOUGLAS PHOTIADIS, Naval Research Laboratory — The supersymmetry method proposed by Efetov in 1983 has been enormously successful at describing a broad range of phenomena involving disorder, providing a framework for understanding and going beyond the successes of random matrix theory and allowing a calculation of the slowing of diffusion as the Anderson transition is approached. The original model described the propagation of a scalar wave in a disordered medium, and subsequent work extended these ideas to classical waves, optical or elastic, with the approximation that the wave propagation can be similarly described by a scalar theory. Such a theory cannot however account correctly for scattering between different polarizations. A direct attempt to derive a supersymmetric model describing elastic waves results in a non-renormalizable field theory, and poses substantial difficulties. We have obtained a supersymmetric sigma model by considering the dual model which describes a generalized superstress field. The model enables one to fully account for the different wave types and polarizations in the medium. We will present our recent results in this area, including model predictions for the obtained diffusion constants, and the effects of renormalization to first order.

<sup>1</sup>This research was funded by the Office of Naval Research.

**Thursday, March 17, 2016 2:30PM - 5:30PM –**

**Session V44 GQI: Quantum Information and Communication 347 - Mark Wilde, Louisiana State University**

**2:30PM V44.00001 Second-Order Asymptotics for the Classical Capacity of Image-Additive Quantum Channels**, MARCO TOMAMICHEL, University of Sydney — We study non-asymptotic fundamental limits for transmitting classical information over memoryless quantum channels, i.e. we investigate the amount of classical information that can be transmitted when a quantum channel is used a finite number of times and a fixed, non-vanishing average error is permissible. Specifically we consider the classical capacity of quantum channels that are image-additive, including all classical to quantum channels, as well as the product state capacity of arbitrary quantum channels. In both cases we show that the non-asymptotic fundamental limit admits a second-order approximation that illustrates the speed at which the rate of optimal codes converges to the Holevo capacity as the blocklength tends to infinity. The behavior is governed by a new channel parameter, called channel dispersion, for which we provide a geometrical interpretation.

**3:06PM V44.00002 Quantum Coding with Finite Resources** , MARIO BERTA, Caltech — The quantum capacity of a memoryless channel determines the maximal rate at which we can code reliably over asymptotically many uses of the channel. Here we argue that this asymptotic characterization is often insufficient in practice where decoherence severely limits our ability to manipulate large quantum systems in the encoder and decoder. For all practical purposes we should instead focus on the optimal trade-off between three parameters: the rate of the code, the size of the quantum devices at the encoder and decoder, and the fidelity of the transmission. Towards this goal, we find approximate and exact characterizations of this tradeoff for various channels, including dephasing, depolarizing and erasure channels. In each case the tradeoff is parametrized by the capacity and a second channel parameter, the quantum channel dispersion. In the process we develop several general bounds that are valid for all finite-dimensional quantum channels and can be computed efficiently.

**3:42PM V44.00003 Experimental loophole-free Bell inequality violation using electron spins separated by 1.3 km** , B HENSEN, H BERNIEN, A E DRÉAU, A REISERER, N KALB, M S BLOK, J RUITENBERG, R F L VERMEULEN, R N SCHOUTEN, QuTech & Kavli Inst. of Nanoscience, Delft Univ. of Tech. The Netherlands, C ABELLÁN, W AMAYA, V PRUNERI, M W MITCHELL, ICFO-Institut de Ciències Fotoniques, The Barcelona Inst. of Sc. and Tech., Spain, M MARKHAM, D J TWITCHEN, Element Six Innovation, Didcot, Oxfordshire, UK, D ELKOUS, S WEHNER, QuTech, Delft Univ. of Tech., The Netherlands, T H TAMINIAU, R HANSON, QuTech & Kavli Inst. of Nanoscience, Delft Univ. of Tech. The Netherlands — 50 years ago[1], John Bell proved that no theory of nature that obeys locality and realism can reproduce all the predictions of quantum theory. Numerous Bell inequality tests have been reported, however, all experiments reported so far required additional assumptions to obtain a contradiction with local realism, resulting in loopholes. Here we will present[2] a Bell experiment that is free of any such additional assumption. We use an event-ready scheme that enables the generation of robust entanglement between distant electron spins. Efficient spin read-out avoids the fair-sampling assumption, while the use of fast random-basis selection and spin read-out combined with a spatial separation of 1.3 km ensure the required locality conditions. We performed 245 trials that tested the CHSH-Bell inequality  $S \leq 2$  and found  $S = 2.42 \pm 0.20$ . A null-hypothesis test yields a probability of  $P \leq 0.039$  that a local-realist model for space-like separated sites could produce data with a violation at least as large as we observe, even when allowing for memory in the devices. [1] J.S. Bell, Physics 1, 195-200, (1964) [2] Hensen et al. Nature 526, 682 (2015)

**3:54PM V44.00004 Beating the Classical Limits of Information Transmission using a Quantum Decoder** , AKIB KARIM, ZIXIN HUANG, ROB CHAPMAN, University of Sydney, RMIT University, MARCO TOMAMICHEL, STEVE FLAMMIA, University of Sydney, ALBERTO PERUZZO, University of Sydney, RMIT University — Reliable transmission of information over a noisy channel is a fundamental challenge in communication theory. The emergence of quantum technologies has created a new class of strategies that allow for message recovery greater than purely classical methods. Despite this, for minimal uses of the channel, finding such schemes remains a challenge. We investigate the amplitude damping channel which describes physical systems that suffer energy loss such as in cavity quantum electrodynamics or spin chain excitations. We derive and experimentally demonstrate the fundamental limit for message recovery possible with only classical methods. We then propose a quantum decoder and experimentally demonstrate message recovery past this classical limit. We use polarisation-encoded photonic qubits. The post-amplitude damping states are generated by an unbalanced Mach-Zehnder interferometer and entanglement is accomplished with a linear optical probabilistic controlled z gate. Our quantum decoder uses a single entangling gate at the receiver where other similar schemes rely on both the sender and the receiver having quantum devices. Our results present an advance in discovering the quantum capabilities of finite resource communications, with specific regard to the amplitude damping channel.

**4:06PM V44.00005 Quantum Key Distribution based on Silicon Integrated Photonic Devices** , DARIUS BUNANDAR, NICHOLAS HARRIS, ZHESHEN ZHANG, Massachusetts Inst of Tech-MIT, RAN DING, TOM BAEHR-JONES, MICHAEL HOCHBERG, Coriant Advanced Technology Group, JEFFREY SHAPIRO, FRANCO WONG, DIRK ENGLUND, Massachusetts Inst of Tech-MIT — We present a compact quantum key distribution (QKD) transmitter near a 1550-nm wavelength using microring modulators implemented on a silicon-on-insulator photonics platform. The transmitter generates time-bin based qubits with a temporal FWHM of 940 ps and an extinction ratio beyond 16 dB. We prove the feasibility of the transmitter with a coherent one-way QKD protocol, where the bit string is encoded in the arrival time of the time-bin qubits and possible eavesdropping is monitored via the interference visibility of neighboring time-bin qubits<sup>1</sup>. The receiver consists of an asymmetric beamsplitter, which provides a random choice of measurement basis, followed by either a superconducting nanowire single-photon detector (SNSPD) or an unbalanced Michelson interferometer with SNSPDs. This experiment demonstrates the feasibility of high-speed QKD based on CMOS-compatible silicon photonics integrated circuits.

<sup>1</sup>B. Korzh, C. C. W. Lim, R. Houlmann, N. Gisin, M. J. Li, D. Nolan, B. Sanguinetti, R. Thew, and H. Zbinden, Nature Photonics **9**, 163–168 (2015)

**4:18PM V44.00006 Quantum Versus Classical Advantages in Secret Key Distillation (and Their Links to Quantum Entanglement)** , ERIC CHITAMBAR, BENJAMIN FORTESCUE, Southern Illinois University Carbondale, MIN-HSIU HSIEH, University of Technology Sydney — We consider the extraction of shared secret key from correlations that are generated by either a classical or quantum source. In the classical setting, two honest parties (Alice and Bob) use public discussion and local operations to distill secret key from some distribution  $p_{XYZ}$  that is shared with an unwanted eavesdropper (Eve). In the quantum settings, the correlations  $p_{XYZ}$  are delivered to the parties as either an incoherent mixture of orthogonal quantum states or as coherent superposition of such states. Here we demonstrate that the classical and quantum key rates are equivalent when the correlations are generated incoherently in the quantum setting. For coherent sources, we next show that the rates are incomparable, and in fact, their difference can be arbitrarily large in either direction. However, we identify a large class of non-trivial distributions that possess the following properties: (i) Eve's advantage is always greater in the quantum source than classically, and (ii) for the entanglement shared in the coherent source, the so-called entanglement cost/squashed entanglement/relative entropy of entanglement can all be computed. We thus present a rare instance in which various entropic entanglement measures of a quantum state can be explicitly computed.

**4:30PM V44.00007 Unstructured quantum key distribution** , PATRICK COLES, ERIC METODIEV, NORBERT LUTKENHAUS, University of Waterloo — Quantum key distribution (QKD) allows for communication with security guaranteed by quantum theory. The main theoretical problem in QKD is to calculate the secret key rate for a given protocol. Analytical formulas are known for protocols with a high degree of symmetry, since symmetry simplifies the analysis. However, experimental imperfections break symmetries, hence the effect of imperfections on key rates is difficult to estimate. Furthermore, it is an interesting question whether (intentionally) asymmetric protocols could outperform symmetric ones. In this work, we develop a robust numerical approach for calculating the key rate for arbitrary discrete-variable QKD protocols. Ultimately this will allow researchers to study “unstructured” protocols, i.e., those that lack symmetry. Our approach relies on transforming the key rate calculation to the dual optimization problem, which dramatically reduces the number of parameters and hence the calculation time. We illustrate our method by investigating some unstructured protocols for which the key rate was previously unknown.

#### 4:42PM V44.00008 A Contextuality Based Quantum Key Distribution Protocol<sup>1</sup> , JAMES TROUPE,

The University of Texas at Austin — In 2005 Spekkens presented a generalization of noncontextuality that applies to imperfect measurements (POVMs) by allowing the underlying hidden variable model to be indeterministic. In addition, unlike traditional Bell-Kochen-Specker noncontextuality, HV models of a single qubit were shown to be *contextual* under this definition. Thus, not all single qubit POVM measurement outcomes can be modeled classically. Recently M. Pusey showed that, under certain conditions, exhibiting an anomalous weak value (i.e. values outside the eigenspectrum of the observable) implies contextuality. We will present a new single qubit prepare and measure QKD protocol that uses observation of anomalous weak values of particular observables to estimate the quantum channel error rate and certify the security of the channel. We also argue that it is the “degree” of contextuality of the noisy qubits exiting the channel that fundamentally determine the secure key rate. A benefit of this approach is that the security does not depend on the fair sampling assumption, and so is not compromised by Eve controlling Bob’s measurement devices. Thus, it retains much of the benefit of “Measurement Device Independent” QKD protocols while only using single photon preparations and measurements.

<sup>1</sup>Supported by the Office of Naval Research under grant N00014-15-1-2225.

#### 4:54PM V44.00009 Investigation of physical implementation of one-way quantum repeaters with multilevel systems , SRERAMAN MURALIDHARAN, CHANG-LING ZOU, LINSHU LI, JIANMING WEN, LIANG JIANG, Yale University

— Error correcting codes of multilevel systems have been shown to be resource efficient for the correction of erasure errors. One way quantum repeaters based on multilevel systems offer ultrafast key generation rates, while consuming lower resources than qubit based schemes (arxiv:1504.08054). On the other hand, they are technologically demanding. Here, we identify the key technological requirements needed for the implementation of quantum repeaters with multilevel systems and propose different experimental techniques that can be used to overcome the difficulties. We propose a generalized Duan-Kimble scheme for the generation of error correcting codes of multilevel systems with time-bin qudits.

#### 5:06PM V44.00010 Long distance quantum communication using continuous variable encoding

, LINSHU LI, VICTOR V. ALBERT, Yale University, MARIOS MICHAEL, Cambridge University, SRERAMAN MURALIDHARAN, CHANGLING ZOU, LIANG JIANG, Yale University — Quantum communication enables faithful quantum state transfer between different parties and protocols for cryptographic purposes. However, quantum communication over long distances (>1000km) remains challenging due to optical channel attenuation. This calls for investigation on developing novel encoding schemes that correct photon loss errors efficiently. In this talk, we introduce the generalization of multi-component Schrödinger cat states [1] and propose to encode quantum information in these cat states for ultrafast quantum repeaters [2,3]. We detail the quantum error correction procedures at each repeater station and characterize the performance of this novel encoding scheme given practical imperfections, such as coupling loss. A comparison with other quantum error correcting codes for bosonic modes will be discussed. [1] M. Mirrahimi, Z. Leghtas, V. V. Albert, S. Touzard, R. J. Schoelkopf, L. Jiang, and M. H. Devoret, New J. Phys. 16, 045014 (2014). [2] S. Muralidharan, J. Kim, N. Lütkenhaus, M. D. Lukin, and L. Jiang, Phys. Rev. Lett. 112, 250501 (2014). [3] S. Muralidharan, L. Li, J. Kim, N. Lütkenhaus, M. D. Lukin, and L. Jiang, arXiv:1509.08435

#### 5:18PM V44.00011 Quantum Secure Direct Communication in a noisy environment: Theory and Experiment<sup>1</sup> , GUI LU LONG, Tsinghua University

— Quantum communication holds promise for absolutely security in secret message transmission. Quantum secure direct communication (QSDC) is an important branch of the quantum communication in which secret messages are sent directly over a quantum channel with security[Phys. Rev. A 65 , 032302 (2002)]. QSDC offers higher security and is instantaneous in communication, and is a great improvement to the classical communication mode. It is also a powerful basic quantum communication primitive for constructing many other quantum communication tasks such as quantum bidding, quantum signature and quantum dialogue and so on. Since the first QSDC protocol proposed in 2000, it has become one of the extensive research focuses. In this talk, the basic ideas of QSDC will be reviewed, and major QSDC protocols will be described, such as the efficient-QSDC protocol, the two-step QSDC protocol, the one-time-pad QSDC protocol, the high-dimensional QSDC protocol and so on. Experimental progress is also developing steadily, and will also be reviewed. In particular, the quantum one-time-pad QSDC protocol has recently been successfully demonstrated experimentally[arXiv:1503.00451].

<sup>1</sup>Work supported by China National Natural Science Foundation, the Ministry of Science and Technology of China

## Thursday, March 17, 2016 2:30PM - 5:42PM –

Session V45 GQI: Semiconductor Qubits: Optical and Microwave Control 348 - Jake Taylor, NIST/JQI/QuICS

#### 2:30PM V45.00001 Generation of heralded entanglement between distant quantum dot hole spins , AYMERIC DELTEIL, Institute of Quantum Electronics, ETH Zurich

— Entanglement plays a central role in fundamental tests of quantum mechanics as well as in the burgeoning field of quantum information processing. Particularly in the context of quantum networks and communication, some of the major challenges are the efficient generation of entanglement between stationary (spin) and propagating (photon) qubits, the transfer of information from flying to stationary qubits, and the efficient generation of entanglement between distant stationary (spin) qubits. In this talk, I will present such experimental implementations achieved in our team with semiconductor self-assembled quantum dots.

Not only are self-assembled quantum dots good single-photon emitters, but they can host an electron or a hole whose spin serves as a quantum memory, and then present spin-dependent optical selection rules leading to an efficient spin-photon quantum interface. Moreover InGaAs quantum dots grown on GaAs substrate can profit from the maturity of III-V semiconductor technology and can be embedded in semiconductor structures like photonic cavities and Schottky diodes.

I will report on the realization of heralded quantum entanglement between two semiconductor quantum dot hole spins separated by more than five meters. The entanglement generation scheme relies on single photon interference of Raman scattered light from both dots. A single photon detection projects the system into a maximally entangled state. We developed a delayed two-photon interference scheme that allows for efficient verification of quantum correlations. Moreover the efficient spin-photon interface provided by self-assembled quantum dots allows us to reach an unprecedented rate of 2300 entangled spin pairs per second, which represents an improvement of four orders of magnitude as compared to prior experiments carried out in other systems. Our results extend previous demonstrations in single trapped ions or neutral atoms, in atom ensembles and nitrogen vacancy centers to the domain of artificial atoms in semiconductor nanostructures that allow for on-chip integration of electronic and photonic elements. This work lays the groundwork for the realization of quantum repeaters and quantum networks on a chip.

### 3:06PM V45.00002 Polarisation singularities in disordered photonic crystal waveguides for on-chip spin-photon entanglement.

, DARYL BEGGS, BEN LANG, ANDREW YOUNG, RUTH OULTON, University of Bristol — A polarisation singularity occurs at a position in a vector field where one of the parameters of the local polarisation ellipse (handedness, eccentricity or orientation) becomes singular. With the vector nature of electromagnetic fields, optics is an obvious place for the study of polarisation singularities, and they can be found in systems ranging from tightly focused beams to speckle fields. Here we demonstrate that photonic crystal waveguides support on-chip polarisation singularities. As Bloch waves, the eigenmodes of photonic crystal waveguides possess a strong longitudinal, as well as transverse, component of their electric field. The spatial dependence of both these components and the phase between them ensures a rich and complex polarisation landscape in the waveguide. Recently, the use of polarisation singularities found in photonic crystal waveguides is generating much interest for integrated quantum information applications, as they can couple the spin-states of electrons confined to quantum dots to the optical modes of the waveguide. For example, at a circular-point (C-point), the sign of the local helicity is governed by the propagation direction of the optical mode, which allows for spin-photon coupling to one direction only. However, any real system will inevitably contain imperfections, and it is not obvious that the polarisation singularities will persist in the disordered waveguides. Here, we use calculations of the eigenmodes of disordered waveguides to demonstrate that the polarisation singularities persist far beyond realistically expected levels of disorder.

**3:18PM V45.00003 Optical control of Berry phase in a diamond spin qubit<sup>1</sup>**, CHRISTOPHER G. YALE, F. JOSEPH HEREMANS, BRIAN B. ZHOU, DAVID D. AWSCHALOM, Institute for Molecular Engineering, University of Chicago, ADRIAN AUER, GUIDO BURKARD, Department of Physics, University of Konstanz — Geometric phase, a fascinating quantum mechanical phenomenon that arises from cyclic state evolution, is a promising avenue to realize fault-tolerant quantum information processing. Here, we demonstrate an all-optical approach to accumulate a geometric phase, or Berry phase, within a solid-state spin qubit, the nitrogen-vacancy center in diamond<sup>2</sup>. With stimulated Raman adiabatic passage (STIRAP), we evolve two light fields to cycle the resulting dark state of a low temperature lambda system in a 'tangerine slice' trajectory that we examine through time-resolved state tomography. This type of trajectory acquires a Berry phase which we then measure through phase comparison to a reference state. We then probe the limits of this control as a result of adiabatic breakdown for short timescales and unintended excitation driven by far-detuned optical fields that accumulate for long timescales. We also investigate the intrinsic resilience of this Berry phase to noise introduced into the system, which is the focus of the following talk. As an all-optical approach, this geometric control represents a pathway to the development of optical geometric gates in the solid state.

<sup>1</sup>This work is supported by the AFOSR, the NSF, and the German Research Foundation.

<sup>2</sup>C. G. Yale\*, F. J. Heremans\*, B. B. Zhou\*, A. Auer, G. Burkard, D. D. Awschalom, arXiv:1507.08993 (2015).

### 3:30PM V45.00004 Robustness of optically-controlled Berry phase in a diamond spin qubit<sup>1</sup>

BRIAN B. ZHOU, CHRISTOPHER G. YALE, F. JOSEPH HEREMANS, DAVID D. AWSCHALOM, Institute for Molecular Engineering, University of Chicago, Chicago, IL 60637, ADRIAN AUER, GUIDO BURKARD, Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — The intrinsic noise resilience of geometric phases has motivated their application as an alternative protocol for realizing high fidelity quantum operations. Using stimulated Raman adiabatic passage (STIRAP) to cyclically evolve the dark state of a lambda system, we demonstrate all-optical control over Berry phase for a single spin in the solid state, the nitrogen vacancy center in diamond [1]. Here we introduce both phase and amplitude noise into the optical control fields for a class of 'tangerine slice' trajectories on the Bloch sphere. We examine the response of Berry phase to scaling of the noise amplitude and adiabatic cycle time, finding Berry phase to be unaffected by deviations parallel to the trajectory and to increase in robustness for long cycle times. Moreover, our noise resilience is independent of the value of the accumulated Berry phase, a property that differs from the behavior of circular trajectories investigated by prior microwave techniques. We also discuss potential improvements to our work.

[1] C. G. Yale\*, F. J. Heremans\*, B. B. Zhou\*, A. Auer, G. Burkard, D. D. Awschalom, arXiv:1507.08993 (2015).

<sup>1</sup>This work is supported by the AFOSR, NSF, and German Research Foundation.

### 3:42PM V45.00005 Quantum nanophotonics: Controlling a photon with a single spin<sup>1</sup>

EDO WAKS, Univ of Maryland-College Park — The implementation of quantum network and distributive quantum computation relies on strong interactions between stationary matter qubits and flying photons. The spin of a single electron confined in a quantum dot is considered as a promising matter qubit as it possesses microsecond coherence time and allows picosecond timescale control using optical pulses. The quantum dot spin can also interact with a photon by controlling the optical response of a strongly coupled cavity. In this talk I will discuss our recent work on an experimental realization of a spin-photon quantum phase switch using a single spin in a quantum dot strongly coupled to a photonic crystal cavity. We show large modulation of the cavity reflection spectrum by manipulating the spin states of the quantum dot, which enables us to control the quantum state of a reflected photon. We also show the complementary effect where the presence of a single photon switches the quantum state of the spin. The reported spin-photon quantum phase operation can switch spin or photon states in picoseconds timescale, representing an important step towards GHz semiconductor based quantum logic devices on-a-chip and solid-state implementations of quantum networks.

<sup>1</sup>Shuo Sun, Hyochul Kim, Glenn Solomon, co-authors

### 4:18PM V45.00006 A quantum phase switch between a solid state spin and a photon

, SHUO SUN, HYOCHUL KIM, University of Maryland College Park, GLENN SOLOMON, National Institute of Standards and Technology, EDO WAKS, University of Maryland-College Park — The implementation of quantum network and distributive quantum computation relies on strong interactions between stationary matter qubits and flying photons. The spin of a single electron confined in a quantum dot is considered as a promising matter qubit as it possesses microsecond coherence time and allows picosecond timescale control using optical pulses. The quantum dot spin can also interact with a photon by controlling the optical response of a strongly coupled cavity. In this talk I will discuss our recent work on an experimental realization of a spin-photon quantum phase switch using a single spin in a quantum dot strongly coupled to a photonic crystal cavity. We show large modulation of the cavity reflection spectrum by manipulating the spin states of the quantum dot, which enables us to control the quantum state of a reflected photon. We also show the complementary effect where the presence of a single photon switches the quantum state of the spin. The reported spin-photon quantum phase operation can switch spin or photon states in picoseconds timescale, representing an important step towards GHz semiconductor based quantum logic devices on-a-chip and solid-state implementations of quantum networks.

### 4:30PM V45.00007 Efficient generation of indistinguishable single photons on-demand at telecom wavelengths

, JEHYUNG KIM, TAO CAI, Univ of Maryland-College Park, CHRISTOPHER RICHARDSON, RICHARD LEAVITT, Laboratory for Physical Science, EDO WAKS, Univ of Maryland-College Park — Highly efficient single photon sources are important building blocks for optical quantum information processing. For practical use and long-distance quantum communication, single photons should have fiber-compatible telecom wavelengths. In addition, most quantum communication applications require high degree of indistinguishability of single photons, such that they exhibit interference on a beam splitter. However, deterministic generation of indistinguishable single photons with high brightness remains a challenging problem in particular at telecom wavelengths. We demonstrate a telecom wavelength source of indistinguishable single photons using an InAs/InP quantum dot in a nanophotonic cavity. To obtain the efficient single quantum dot emission, we employ the higher order mode in L3 photonic crystal cavity that shows a nearly Gaussian transverse mode profile and results in out-coupling efficiency exceeding 46 % and unusual bright single quantum dot emission exceeding 1.5 million counts per second at a detector. We also observe Purcell enhanced spontaneous emission rate as large as 4 and high linear polarization ratio of 0.96 for the coupled dots. Using this source, we generate high purity single photons at 1.3  $\mu\text{m}$  wavelength and demonstrate the indistinguishable nature of the emission using a two-photon interference measurement.

**4:42PM V45.00008 Quantum Dot Device Design Optimization for Resonator Coupling<sup>1</sup>**, CAMERON KING, S. N. COPPERSMITH, MARK FRIESEN, University of Wisconsin, Madison — Coupling a semiconductor quantum dot qubit to a superconducting resonator broadens the possibilities for interqubit communication and potentially allows integration of quantum dots with other qubit systems. The major technological hurdle that must be overcome is reaching the strong coupling limit, where the coupling frequency between the resonator and the qubit is larger than both the qubit decoherence rate and the photon loss rate of the resonator. In this work, we examine optimization of the quantum dot device design. Using the Thomas-Fermi approximation in conjunction with a metallic dot capacitive model, we focus on improving the capacitive coupling between a resonator gate and a quantum dot while decreasing the cross-coupling to nearby dots. Through these simulations, we find that the optimization follows an intuitive geometric relation.

<sup>1</sup>This work was supported in part by ARO (W911NF-12-0607), NSF (PHY-1104660), and ONR (N00014-15-1-0029).

**4:54PM V45.00009 A Dressed Spin Qubit in Silicon<sup>1</sup>**, ARNE LAUCHT, RACHPON KALRA, JUAN DEHOLLAIN, STEPHANIE SIMMONS, JUHA MUHONEN, FAHD MOHIYADDIN, SOLOMON FREER, FAY HUDSON, UNSW Australia, KOHEI ITOH, Keio University, DAVID JAMIESON, JEFF MCCALLUM, University of Melbourne, ANDREW DZURAK, ANDREA MORELLO, UNSW Australia — Coherent dressing of a quantum two-level system has been demonstrated on a variety of systems, including atoms, self-assembled quantum dots, and superconducting quantum bits, and can be demonstrated by measuring Rabi oscillations, or a Mollow triplet in the spectrum. It can be used to gain access to a new quantum system with improved properties - a different and tunable level splitting, faster and easier control, and longer coherence times. In our work we investigate the properties of the dressed, donor-bound electron spin in silicon, and probe its potential for the use as quantum bit in scalable architectures. Here, the two dressed spin-polariton levels constitute the quantum bit. The dressed qubit can be coherently driven with an oscillating magnetic field, an oscillating electric field, by frequency modulating the driving field, or by a simple detuning pulse. We measure coherence times of  $T_2^* = 2.4$  ms and  $T_2 = 9$  ms (Hahn echo), one order of magnitude longer than those of the undressed qubit.

<sup>1</sup>This research was funded by the ARC Centre of Excellence for Quantum Computation and Communication Technology (project number CE110001027) and the US Army Research Office (W911NF-13-1-0024).

**5:06PM V45.00010 Gate sensing coherent charge oscillations in a silicon field-effect transistor.<sup>1</sup>**, M. FERNANDO GONZALEZ-ZALBA, Hitachi Cambridge Laboratory, UK, SERGEY SHEVCHENKO, B. Verkin Institute for Low Temperature Physics and Engineering, Ukraine, SYLVAIN BARRAUD, CEA-LETI, France, J. ROBERT JOHANSSON, CEMS, RIKEN, Japan, ANDREW FERGUSON, Cavendish Laboratory, UK, FRANCO NORI, CEMS, RIKEN, Japan, ANDREAS BETZ, Hitachi Cambridge Laboratory, UK — We report the observation of coherent charge oscillations in a double quantum dot formed in a silicon nanowire transistor detected via its dispersive interaction with a radio-frequency resonant circuit coupled via the gate. Differential capacitance changes at the inter-dot charge transitions allow us to monitor the state of the system in the strong-driving regime where we observe the emergence of Landau-Zener-Stückelberg-Majorana interference on the phase response of the resonator. A theoretical analysis of the dispersive signal demonstrates that quantum and tunnelling capacitance changes must be included to describe the qubit-resonator interaction. Furthermore, a Fourier analysis of the interference pattern reveals a charge coherence time,  $T_2 = 100$  ps. Our results demonstrate charge coherent control and readout in a simple silicon transistor and open up the possibility to implement charge and spin qubits in existing complementary metal-oxide-semiconductor technology.

<sup>1</sup>We thank FP7 318397, RIKEN iTHES project, AFOSR FA9550-14-1-0040, IMPACT program of JST and a Grant-in-Aid for Scientific Research.

**5:18PM V45.00011 Coplanar photonic bandgap resonators for low temperature electron and nuclear magnetic resonance spectroscopy**, A. J. SIGILLITO, A. M. TYRYSKHIN, S. A. LYON, Department of Electrical Engineering, Princeton University — In recent years, superconducting coplanar waveguide (CPW) resonators have become a useful tool for low temperature pulsed electron spin resonance (ESR), even at dilution refrigerator temperatures. Their small mode volumes make CPW resonators particularly well suited to measuring small numbers of spins near the resonator surface, since in this region the spin sensitivity is very high. While these resonators have proven useful for ESR at single microwave frequencies, it is difficult to also manipulate nuclear spins in electron-nuclear-double resonance (ENDOR) experiments, since manipulation of nuclear spins requires radio frequency (RF) magnetic fields. Ideally one would simply generate these fields by passing RF currents through the CPW, but because conventional CPW resonators are capacitively coupled, they will not transmit low-frequency RF currents. In this talk, we discuss the use of one dimensional photonic bandgap (PBG) resonators to overcome this challenge. PBG resonators are a promising alternative to conventional CPW resonators since they offer high quality factors at microwave frequencies, while simultaneously allowing transmission of nonresonant RF currents below the photonic bandgap. Here, we will discuss PBG resonator designs and present data showing their use for low temperature ESR of donors in <sup>28</sup>Si. Initial ENDOR results will also be presented.

**5:30PM V45.00012 Theory of nuclear spin dephasing and relaxation by optically illuminated nitrogen vacancy center.**, PING WANG, WEN YANG, Zhongguancun Software Park II, No. 10 West Dongbeiwang Road, Haidian District, Beijing 100094, China — Dephasing and relaxation of the nuclear spins coupled to the nitrogen-vacancy (NV) center during optical initialization and readout is an important issue for various applications of this hybrid quantum register. Here we present both an analytical description and a numerical simulation for this process, which agree reasonably with the experimental measurements. For the NV center under cyclic optical transition, our analytical formulas not only provide a clear physics picture, but also allows controlling the nuclear spin dissipation by tuning an external magnetic field. For more general optical pumping, our analytical formulas reveal significant contribution to the nuclear spin dissipation due to electron random hopping into/out of the  $m = 0$  (or  $m = \pm 1$ ) subspace. This contribution is not suppressed even under saturated optical pumping and/or vanishing magnetic field, thus providing a possible solution to the puzzling observation of nuclear spin dephasing in zero perpendicular magnetic field [M. V. G. Dutt *et al.*, Science **316**, 1312 (2007)]. It also implies that enhancing the degree of spin polarization of the nitrogen-vacancy center can reduce the effect of optical induced nuclear spin dissipation.

**Thursday, March 17, 2016 2:30PM - 4:30PM —**  
**Session V46 GIMS: Instrumentation IV** 311 - Chuck Mielke, LANL

**2:30PM V46.00001 Optimum Noise Reduction Methods for the Interior of Vehicles and Aircraft Cabins**, HASSON M. TAVOSSI, PH.D., Valdosta State University, Department of Physics, Astronomy & Geosciences — The most effective methods of noise reduction in vehicles and Aircraft cabins are investigated. The first goal is to determine the optimal means of noise mitigation without change in external shape of the vehicle, or aircraft cabin exterior such as jet engine or fuselage design, with no significant added weight. The second goal is to arrive at interior designs that can be retrofitted to the existing interiors, to reduce overall noise level for the passengers. The physical phenomena considered are; relaxation oscillations, forced vibrations with non-linear damping and sub-harmonic resonances. The negative and positive damping coefficients and active noise cancelations methods are discussed. From noise power-spectrum for a prototype experimental setup, the most energetic vibration modes are determined, that require the highest damping. The proposed technique will utilize the arrangement of uniformly distributed open Helmholtz resonators, with sound absorbing surface. They are tuned to the frequencies that correspond to the most energetic noise levels. The resonators dissipate noise energy inside the vehicle, or aircraft cabin, at the peak frequencies of the noise spectrum, determined for different vehicle or aircraft cabin, interior design models.

**2:42PM V46.00002 A Noninvasive In Vivo Glucose Sensor Based on Mid-Infrared Quantum Cascade Laser Spectroscopy**, ALEXANDRA WERTH, Princeton University, SABBIR LIAKAT, SRI International, LAURA XU, Yahoo Inc., CLAIRE GMACHL, Princeton University — Diabetes affects over 387 million people worldwide; a number which grows every year. The most common method of measuring blood glucose concentration involves a finger prick which for some can be a harrowing process. Therefore, a portable, accurate, noninvasive glucose sensor can significantly improve the quality of life for many of these diabetics who draw blood multiple times a day to monitor their glucose levels. We have implemented a noninvasive, mobile glucose sensor using a mid-infrared (MIR) quantum cascade laser (QCL), integrating sphere, and thermal electrically (TE) cooled detector. The QCL is scanned from 8 - 10 microns wavelength over which are distinct absorption features of glucose molecules with little competition of absorption from other molecules found in the blood and interstitial fluid. The obtained absorption spectra are analyzed using a neural network algorithm which relates the small changes in absorption to the changing glucose concentration. The integrating sphere has increased the signal-to-noise ratio from a previous design, allowing us to use the TE-cooled detector which increases mobility without loss of accuracy.

**2:54PM V46.00003 Temperature Coefficient of Secondary Electron Emission: A Novel Thermal Metrology**, MD. IMRAN KHAN, SEAN DANIEL LUBNER, University of California at Berkeley, DAVID FRANK OGLETREE, ED WONG, Molecular Foundry (Lawrence Berkeley National Laboratory), CHRIS DAMES, University of California at Berkeley — State of the art nanoscale temperature mapping techniques include Scanning Thermal Microscopy (SThM) and optical thermorefectance, though these have the challenges of requiring sample contact and being diffraction limited, respectively. Near field scanning optical microscopy (NSOM) can beat the diffraction limit but still cannot measure temperature at 10s of nanometer resolution. SEM is well known for topographic imaging but has not been previously used for thermal mapping. Past literature suggested that secondary electron yields might have a small temperature dependence due to electron-phonon scattering and/or temperature dependence of work function. We previously measured the temperature coefficient of secondary electron emission of several group IV and III-V semiconductors and found it to range from around 100 to 1000 ppm/K. Here, we utilize this to map a spatial temperature gradient in an SEM image. We implement a double-heater structure to produce a temperature gradient along the plane of a substrate. The primary electron beam is scanned across the sample's surface while the emitted (secondary plus backscattered) electron current and net absorbed sample currents are simultaneously recorded. The results demonstrate the ability to map a spatial temperature gradient.

**3:06PM V46.00004 Tomographic Reconstruction of Circularly Polarized High Harmonic Fields: 3D Attosecond Metrology**, CONG CHEN, ZHENSHENG TAO, JILA, University of Colorado Boulder, CARLOS HERNANDEZ-GARCA, Universidad de Salamanca, Spain, PIOTR MATYBA, ADRA CARR, RONNY KNUT, JILA, University of Colorado Boulder, OFER KFIR, Technion, Haifa, Israel, DIMITRY ZUSIN, CHRISTIAN GENTRY, PATRICK GRYCHTOL, JILA, University of Colorado Boulder, OREN COHEN, Technion, Haifa, Israel, LIUS PLAJA, Universidad de Salamanca, Spain, ANDREAS BECKER, AGNIESZKA JARON-BECKER, HENRY KAPTEYN, MARGARET MURNANE, JILA, University of Colorado Boulder — Bright, circularly polarized, extreme ultraviolet (EUV) and soft X-ray high harmonic beams can now be produced using counter-rotating circularly polarized driving laser fields. In the time domain, the field is predicted to emerge as a complex series of rotating linearly polarized bursts, varying rapidly in amplitude, frequency and polarization. Here, we extend attosecond metrology techniques to circularly polarized light for the first time by simultaneously irradiating a copper surface with circularly polarized high harmonic and linearly polarized infrared laser fields. The resulting temporal modulation of the photoelectron spectra carries essential phase information about the EUV field. Utilizing the polarization selectivity of the solid surface and by rotating the circularly polarized EUV field in space, we fully retrieve the amplitude and phase of the circularly polarized harmonics, allowing us to reconstruct one of the most complex coherent light fields produced to date.

**3:18PM V46.00005 Enhancement of photocurrent on few-layered  $p$ -WSe<sub>2</sub> FET by multi-terminal measurement<sup>1</sup>**, CARLOS GARCIA, Florida State University/NHMFL, NIHAR PRADHAN, NHMFL, JOSHUA HOLLEMAN, DANIEL RHODES, Florida State University/NHMFL, LUIS BALICAS, STEPHEN MCGILL, NHMFL — Recently, two dimensional materials particularly transition metal dichalcogenides (TMDs) have been extensively studied because of their strong light-matter interactions and extraordinary electrical and optical properties in field-effect transistors (FETs). We investigated the photocurrent response on few-layered  $p$ -WSe<sub>2</sub> and MoSe<sub>2</sub> FETs in a multi-terminal configuration using a 532 nm laser. Photogenerated current  $I_{ph}$  ( $= I_{light} - I_{dark}$ ) was measured as a function of optical power incident on the sample with varying source-drain bias,  $V_{ds}$ , and back gate voltage,  $V_{bg}$ . We observed a large enhancement of photocurrent in a four-terminal configuration compared to a two-terminal configuration. The measured two-terminal photoresponsivity ( $R$ ) and external quantum efficiency ( $EQE$ ) from our ~10 layers  $p$ -WSe<sub>2</sub> at applied  $V_{ds}$  = 1V and  $V_{bg}$  = 10V were ~18A/W and ~4000%, respectively. The  $R$  and  $EQE$  values increased to ~85 A/W and ~20000% respectively using a four-terminal configuration. Thus by using a multi-terminal configuration, one can observe an enhanced photocurrent response on few-layered TMDs for potential applications in photo-detection and optoelectronic circuits.

<sup>1</sup>Support by Army MURI W911NF-11-1-0362 and NSF DMR-1229217

**3:30PM V46.00006 Cavities for electron spin resonance: predicting the resonant frequency**, JOHN COLTON, KYLE MILLER, MICHAEL MEEHAN, ROSS SPENCER, Brigham Young University — Microwave cavities are used in electron spin resonance to enhance magnetic fields. Dielectric resonators (DRs), pieces of high dielectric material, can be used to tailor the resonant frequency of a cavity. However, designing cavities with DRs to obtain desired frequencies is challenging and in general can only be done numerically with expensive software packages. We present a new method for calculating the resonant frequencies and corresponding field modes for cylindrically symmetric cavities and apply it to a cavity with vertically stacked DRs. The modes of an arbitrary cavity are expressed as an expansion of empty cavity modes. The wave equation for  $D$  gives rise to an eigenvalue equation whose eigenvalues are the resonant frequencies and whose eigenvectors yield the electric and magnetic fields of the mode. A test against theory for an infinitely long dielectric cylinder inside an infinite cavity yields an accuracy better than 0.4% for nearly all modes. Calculated resonant frequencies are also compared against experiment for quasi-TE<sub>011</sub> modes in resonant cavities with ten different configurations of DRs; experimental results agree with predicted values with an accuracy better than 1.0%. MATLAB code is provided at <http://www.physics.byu.edu/research/coltonlab/cavityresonance>.

**3:42PM V46.00007 High magnetic field calibration using de Haas-van Alphen oscillations in polycrystalline copper<sup>1</sup>**, WILLIAM A. CONIGLIO, National High Magnetic Field Laboratory, ALAN F. WILLIAMS, ANNA YANNAKOPOULOS, Florida State University/National High Magnetic Field Laboratory, AUDREY GROCKOWIAK, STAN TOZER, National High Magnetic Field Laboratory — We provide a calibration for the de Haas-van Alphen (dHvA) frequency in polycrystalline copper, which may be used to standardize the measurement of magnetic fields, particularly in pulsed field environments, where direct observation of NMR is challenging. Using a reliable single-crystal model of the Fermi surface from coefficients that are traceable to a powder Al NMR reference, we computed Fermi surface extremal areas for evenly spaced directions around a sphere. Summing the peaks corresponding to extremal orbits according to the Lifshitz-Kosevich model, we arrive at a dHvA spectrum that corresponds to experimental observation. We find that actual maximum fields reached at the NHMFL-Pulsed Field Facility are slightly larger than previously determined.

<sup>1</sup>We appreciate generous primary support from the U. S. Department of Energy NNSA SSAA DE-NA0001979. The National High Magnetic Field Laboratory is supported by the National Science Foundation, U. S. Department of Energy, and the State of Florida.

**3:54PM V46.00008 NANONIS TRAMEA – A Quantum Transport Measurement System**, THORSTEN KAMPEN, ANDREAS THISSEN, OLIVER SCHAFF, ALESSANDRO PIODA, SPECS Surface Nano Analysis GmbH — Nanonis Tramea is a quantum leap with respect to increased speed for transport measurements taking research onto a new level. Measurements which took several hours in the past can now be done in minutes without compromising signal quality. Tramea uses its fast, high-resolution, high-precision and ultra-low-noise outputs and inputs to generate and acquire up to 20000 data points per second on 24 channels in parallel. This is not only up to 1000 × faster than typical measurement systems but it is also time deterministic with highest precision. Here, the time separation between points is constant so that artefacts caused by unequal point spacings in non-deterministic measurement systems are avoided. The emphasis here is the real-time relation. Tramea comes with a built-in interface which allows for control of the instruments' basic functions from any programming environment. For users requiring more functionality and higher speeds a full-featured LabVIEW-based programming interface or scripting module are available as add-on modules. Due to the modularity and flexibility of the hardware and software architecture of Tramea upgrades with standardized add-on modules are possible. Non-standard requests can still be handled by the various programming options.

**4:06PM V46.00009 Construction and  $^{13}\text{C}$  NMR signal-amplification efficiency of a dynamic nuclear polarizer at 6.4 T and 1.4 K<sup>1</sup>**, ANDHIKA KISWANDHI, PETER NIEDEBALSKI, CHRISTOPHER PARISH, SARAH FERGUSON, DAVID TAYLOR, GEORGE MCDONALD, LLOYD LUMATA, Univ of Texas, Dallas — Dissolution dynamic nuclear polarization (DNP) is a rapidly emerging technique in biomedical and metabolic imaging since it amplifies the liquid-state nuclear magnetic resonance (NMR) and imaging (MRI) signals by >10,000-fold. Originally used in nuclear scattering experiments, DNP works by creating a non-Boltzmann nuclear spin distribution by transferring the high electron ( $\gamma = 28,000 \text{ MHz/T}$ ) thermal polarization to the nuclear spins via microwave irradiation of the sample at high magnetic field and low temperature. A dissolution device is used to rapidly dissolve the frozen sample and consequently produces an injectable hyperpolarized liquid at physiologically-tolerable temperature. Here we report the construction and performance evaluation of a dissolution DNP hyperpolarizer at 6.4 T and 1.4 K using a continuous-flow cryostat. The solid and liquid-state  $^{13}\text{C}$  NMR signal enhancement levels of  $^{13}\text{C}$  acetate samples doped with trityl OX063 and 4-oxo-TEMPO free radicals will be discussed and compared with the results from the 3.35 T commercial hyperpolarizer.

<sup>1</sup>This work is supported by US Dept of Defense award no. W81XWH-14-1-0048 and Robert A. Welch Foundation grant no. AT-1877

**4:18PM V46.00010 Comparative Analysis of two Methods for High-Resolution Differential Conductance Measurement<sup>1</sup>**, DAVID CUSICK, Taylor University, MICHIO NAITO, Tokyo University of Agriculture and Technology, ROBERTO RAMOS, University of the Sciences — We compare two methods of differential conductance measurement. The first is a traditional method in which current and voltage data is acquired via four-wire measurement, then averaged and differentiated numerically. The second method calculates  $dI/dV$  in real time by superimposing a small DC signal  $dI$  on the input step function, alternating between addition and subtraction of the signal with each step, then averaging the small signal voltage response over three steps to obtain  $dV$ . This requires two instruments: a DC current source and a high-resolution voltmeter. Keithley Instruments has commercially promoted the Keithley 622x current source and 2182A nanovoltmeter as means to achieve this measurement; we therefore refer to it as the Keithley method. We compare the two methods by performing high-resolution measurements of the energy gap of  $\text{MgB}_2$  thin film Josephson junctions. We show that the Keithley method has advantages of cleaner data, easier implementation, and overall faster data collection, but may lack the traditional method's high resolution.

<sup>1</sup>R.C.R. acknowledges support from National Science Foundation Grant # DMR-1555775

**Thursday, March 17, 2016 2:30PM - 5:30PM —**  
**Session V47 DCMP: Dynamics of Surfaces, Adlayers, and Films** 312 - Brad Conrad, Appalachian State University

**2:30PM V47.00001 Area Determination of Electrodeposited Ni, Co, and NiCo Thin Films<sup>1</sup>**, MATTHEW GIRA, KEVIN TKACZ<sup>2</sup>, JENNIFER HAMPTON, Hope College — The surface area of electrodeposited thin films of Ni, Co, and NiCo was evaluated using electrochemical double-layer capacitance, electrochemical area measurements using the  $[\text{Ru}(\text{NH}_3)_6]^{3+}/[\text{Ru}(\text{NH}_3)_6]^{2+}$  redox couple, and topographic atomic force microscopy (AFM) imaging. The methods were compared to each other for each composition separately and for all the samples regardless of composition. Double-layer capacitance measurements were found to be positively correlated to the roughness factors determined by AFM topography. Electrochemical area measurements were less correlated with measured roughness factors and applicable only to two of the three compositions studied. The results indicate that *in situ* double-layer capacitance measurements are a practical, versatile technique for estimating the accessible surface area of a metal sample.

<sup>1</sup>This work supported by the NSF under Grants RUI-DMR-1104725, REU-PHY/DMR-1004811, MRI-CHE-1126462, MRI-CHE-0959282, and ARI-PHY-0963317 and by the Hope College Nyenhuis Faculty Development Fund.

<sup>2</sup>University of California, Irvine

**2:42PM V47.00002 Structure and Dynamics of the Au(111) Surface in an Electrochemical Environment<sup>1</sup>**, JOHN COLLINI, Rochester Institute of Technology, YIHUA LIU, Argonne National Laboratory, BRYANNE MCDONOUGH, MICHAEL PIERCE, Rochester Institute of Technology, HOYDOO YOU, Argonne National Laboratory, VLADIMIR KOMANICKY, Safarik University, ANDI BARBOUR, Brookhaven National Laboratory — The Au(111) surface possesses a well-known herringbone surface reconstruction pattern. However, the character of the reconstruction's response to external variables is not completely understood due to the limited amount of kinetics and dynamics studies of the surface in different environments. Here, we present *in-situ* x-ray scattering measurements from the Advanced Photon Source at Argonne National Laboratory of the Au(111) surface in a controllable electrochemical environment of weak NaF solution. Crystal truncation rod (CTR) measurements were taken to examine how the average surface properties and overall structure change with cell voltage. X-ray photon correlation spectroscopy (XPCS) measurements were also taken to examine how the dynamics of the surface change with voltage. The relation between applied potential, average kinetics, and microstate dynamics will be discussed.

<sup>1</sup>Funding provided by Research Corporation for Science Advancement. Work done at the Advanced Photon Source supported by the U.S. Department of Energy.

**2:54PM V47.00003 Atomic diffusion processes in heteroepitaxial metallic systems using SLKMC-II**, SYED ISLAMUDDIN SHAH, ALTAF KARIM, Department of Physics, COMSATS Institute of information technology, Park Road, Tar-lai Kalan, Islamabad 45550, Pakistan — We have examined the diffusion of small islands of Cu on Ag(111) surface using a self-learning kinetic Monte Carlo (SLKMC-II) [1] method with an improved pattern recognition scheme. Due to strain generated at the interface between metals with different bulk lattice constants, interesting single atom, multi-atom and concerted diffusion processes are automatically revealed in the simulations. Here we will report various processes for small islands in the case of Cu/Ag(111) system. Key processes responsible for island diffusion and their energetics together with trends in effective energy barriers as well as diffusion constants for small islands will also be provided. In addition to 2-D diffusion processes, as an application of SLKMC-II to the 3-dimensional heteroepitaxial systems, we will also report energy barriers of some of the 3-dimensional processes including down the A- and B-steps and exchange processes. [1] Syed Islamuddin Shah, et al., J. Phys.: Condens. Matter 24, 354004 (2012)

**3:06PM V47.00004 Nanotribological properties of water films adsorbing atop, and absorbing below, graphene layers supported by metal substrates<sup>1</sup>**, ZIJIAN LIU, C.K. CURTIS, North Carolina State University, R. STINE, P. SHEEHAN, Naval Research Laboratory, J. KRIM, North Carolina State University — The tribological properties of graphite, a common lubricant with known sensitivity to the presence of water, have been studied extensively at the macroscopic and microscopic scales. Although far less attention has been devoted to the tribological properties of graphene, it has been established that the tribological response to the presence of water is dissimilar from that of graphite.[1] We report here a quartz crystal microbalance study of the nanotribological properties of water films adsorbed/absorbed on graphene layers prepared by either chemical decomposition on nickel(111) substrates or transfer of freestanding graphene layers to aluminum substrates. Sliding friction levels of the water films were also measured for metal surfaces in the absence of a graphene layer. We observe very high friction levels for water adsorbed atop graphene on Ni(111) and very low levels for water on aluminum. For the case of graphene/aluminum, the data indicate that the water is absorbing between the graphene layer and the aluminum. Dissipation levels moreover indicate the presence of an interstitial water increases sliding friction between the graphene and the aluminum substrate. [1] D. Berman et al., Materials Today 17, 31 (2014)

<sup>1</sup>Work supported by NSF and NRL

**3:18PM V47.00005 Interfacial Assembly of Graphene Oxide Films.**, CAIN VALTIERREZ, Department of Physics, Augsburg College, ISSAM ISMAIL, CHRISTOPHER MACOSKO, Department of Chemical Engineering and Materials Science, University of Minnesota Twin Cities, BENJAMIN STOTTRUP, Department of Physics, Augsburg College — Controlled assembly of monolayer graphene-oxide (GO) films at the air/water interface is of interest for the development of transparent conductive thin films of chemically-derived graphene. We present experimental results from investigations of the assembly of polydisperse GO sheets at the air-water interface. GO nanosheets with lateral dimensions of greater than 10 microns were created using a modified Tour synthesis (Dimiev and Tour, 2014). GO films were generated with conventional Langmuir trough techniques to control lateral packing density. Film morphology was characterized *in situ* with Brewster angle microscopy. Films were transferred unto a substrate via the Langmuir-Blodgett deposition technique and imaged with fluorescence quenching microscopy. Through pH modulation of the aqueous subphase, it was found that GO's intrinsic surface activity to the interface increased with increasing subphase acidity. Finally, we found a dominant elastic contribution during uniaxial film deformation as measured by anisotropic pressure measurements. A. M. Dimiev, and J. M. Tour, "Mechanism of GO Formation," ACS Nano, 8, (2014)

**3:30PM V47.00006 Tuning friction with an external magnetic field: A Quartz Crystal Microbalance study of physisorbed oxygen monolayers and multilayers sliding on nickel substrates.<sup>1</sup>**, Z.B. FREDRICKS, K.M. STEVENS, B. ACHARYA, J. KRIM, North Carolina State University — The sliding friction levels of oxygen monolayer and multilayer films adsorbed on nickel close to the oxygen monolayer solid-liquid melting transition temperature have been monitored by means of a Quartz Crystal Microbalance (QCM) technique in the presence and absence of a weak external magnetic field. Friction levels for the monolayers in the presence of the field were observed to be half of those observed in the absence of a field. For thick films, the reduction was proportionately less, indicating an interfacial effect as the source of the magnetic sensitivity. While the presence of the field is expected to increase the normal force between the paramagnetic oxygen overlayer and the ferromagnetic substrate, the impact of this mechanism on friction appears to be minimal, or possibly masked by more dominant mechanisms. These include magnetically induced structural reorientation (magnetostriction), and/or realignment of adlayer spins in response to the applied field, both of which would reduce the physical or magnetic interfacial commensurability, thus lowering friction levels.

<sup>1</sup>Work supported by NSF DMR1310456

**3:42PM V47.00007 Effect of charges on the interaction of water with hematite<sup>1</sup>**, FABIO NEGREIROS RIBEIRO, LUANA PEDROZA, GUSTAVO DALPIAN, Universidade Federal do ABC — Hematite is one of the many types of iron oxide that is easily found in nature. It is most commonly used in catalysis and it is rarely present in its pristine form. The influence of charged defects in its properties is very important for the correct geometrical/electronic characterization in more realistic operative conditions, but very few studies focus explicitly on these defects in this system. In this work we perform first principles DFT+U calculations to determine the properties of a hematite slab when both dopant and electrons/holes are added. We focus on the differences between the geometrical/electronic properties between the neutral/charged surfaces and also study their interaction with water (molecule and liquid) by performing molecular dynamics simulations at room temperature. Our results indicate that electric charges strongly influence the properties of these surfaces, changing the binding energies and the molecular arrangement of the water molecules adsorbed on hematite. Negative charges induce a larger binding and favor the partial water dissociation, whereas positive charges weaken the binding energy. We will provide comparative results for different configurations of this system.

<sup>1</sup>FAPESP

**3:54PM V47.00008 Novel Transrotational Solid State Order Discovered by TEM in Crystallizing Amorphous Films<sup>1</sup>**, VLADIMIR KOLOSOV, Ural Federal University — Exotic thin crystals with unexpected **transrotational** microstructures [1] have been discovered by transmission electron microscopy (TEM) for crystal growth in thin (10-100 nm) amorphous films of different chemical nature (oxides, chalcogenides, metals and alloys) prepared by various methods. Primarily we use our TEM bend contour technique. The unusual phenomenon can be traced **in situ** in TEM column: dislocation independent regular internal bending of crystal lattice planes in a growing crystal. Such **transrotation** (unit cell **translation** is complicated by small **rotation** realized round an axis lying in the film plane) can result in strong regular lattice orientation gradients (up to 300 degrees per micrometer) of different geometries: cylindrical, ellipsoidal, toroidal, saddle, etc. Transrotation is increasing as the film gets thinner. Transrotational crystal resembles ideal single crystal enclosed in a curved space. Transrotational micro crystals have been eventually recognized by other authors in some vital thin film materials, i.e. PCMs for memory, silicides, SrTiO<sub>3</sub>. Atomic model and possible mechanisms of the phenomenon are discussed. New transrotational nanocrystalline model of amorphous state is also proposed. [1] V.Yu. Kolosov and A.R.Tholen, Acta Mater., 48 (2000) 1829.

<sup>1</sup>Support of RF Ministry of Education and Science is acknowledged

#### 4:06PM V47.00009 Successively Thresholded Domain Boundary Roughening Driven by Pinning Centers and Missing Bonds: Hard-Spin Mean-Field Theory Applied to $d=3$ Ising Magnets

, TOLGA CAGLAR, Sabanci University, A. NIHAT BERKER, Sabanci University and MIT — Hard-spin mean-field theory has recently been applied to Ising magnets, correctly yielding the absence and presence of an interface roughening transition respectively in  $d = 2$  and  $d = 3$  dimensions and producing the ordering-roughening phase diagram for isotropic and anisotropic systems. The approach has now been extended to the effects of quenched random pinning centers and missing bonds on the interface of isotropic and anisotropic Ising models in  $d = 3$  [1]. We find that these frozen impurities cause domain boundary roughening that exhibits consecutive thresholding transitions as a function of interaction anisotropy. For both missing-bond and pinning-center impurities, for moderately large values of the anisotropy, the systems saturate to the "solid-on-solid" limit, exhibiting a single universal curve for the domain boundary width as a function of impurity concentration.

[1] T. Caglar, A.N. Berker, arXiv:1509.01910 [cond-mat.stat-mech]

#### 4:18PM V47.00010 Atomic-Scale Mechanism for Hydrogenation of *o*-Cresol on Pt Catalysis<sup>1</sup>

, YAPING LI, University of Tulsa, ZHIMIN LIU, University of Oklahoma, WENHUA XUE, University of Tulsa, STEVEN CROSSLEY, University of Oklahoma, FRIEDERIKE JENTOFT, University of Massachusetts Amherst, SANWU WANG, University of Tulsa — Biofuels derived from lignocellulosic biomass have received significant attention lately due to increasing environmental concerns. With first-principles density-functional theory and *ab initio* molecular dynamic simulations, we investigated the atomic-scale mechanism of *o*-cresol hydrogenation on the Pt(111) surface. The formation of 2-methyl-cyclohexanone (the intermediate product) was found to involve two steps. The first step is the dehydrogenation, that is, the H atom in the hydroxyl group moves to the Pt surface. The second step is the hydrogenation, that is, the H atoms on Pt react with the carbon atoms in the aromatic ring. The first step involves a smaller barrier, suggesting that dehydrogenation occurs first, followed by hydrogenation of the ring. In particular, tautomerization is found to occur via a two-step process over the catalyst. On the other hand, 2-methyl-cyclohexanol (the final product) is produced through two paths. One is direct hydrogenation of the aromatic ring. Another pathway includes partial hydrogenation of the ring, dehydrogenation of -OH group, finally hydrogenation of remaining C atoms and the O atom. Our theoretical results agree well with the experimental observations.

<sup>1</sup>Supported by DOE (DE-SC0004600). This research used the supercomputer resources of NERSC, XSEDE, TACC

#### 4:30PM V47.00011 Multidisciplinary Investigation of the Structural and Electronic Properties of the Pt/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub> interface

, JUDITH YANG, QING ZHU, CECILE BONIFACIO, University of Pittsburgh, JOSH KAS, University of Washington, HENRY AYOOLA, University of Pittsburgh, KIM KISSLINGER, DONG SU, Brookhaven National Laboratory, FERNANDO VILA, University of Washington, STEPHEN HOUSE, University of Pittsburgh, ERIC STACH, Brookhaven National Laboratory, JOHN REHR, University of Washington, WISSAM SAIDI, University of Pittsburgh, UNIVERSITY OF PITTSBURGH TEAM, UNIVERSITY OF WASHINGTON TEAM, BROOKHAVEN NATIONAL LABORATORY TEAM — Pt/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub> is arguably the most important heterogeneous catalyst system. Despite the numerous studies on this system, the detailed structural and electronic properties of this interface remain uncertain. Through controlled oxidation of NiAl (110), we were able to obtain single crystalline Pt/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub> thin films. We also prepared Pt/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub> samples. STEM observations show that use of cryo-electron microscopy techniques prevented electron-beam damage, including direct sample damage, and changes in the EELS oxygen K pre-peak (~532 eV). The oxygen K pre-peak was consistently present in spectra taken at the Pt/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub> interface at cryo-temperatures, but not in those acquired at room temperature. The theoretically calculated EELS oxygen K signals for the Pt on (110) Pt/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub> exhibited a similar pre-peak at 532 eV correlating to the experimental EELS oxygen K data, and we attribute to this feature to the formation of Pt-O complex. This points out an important factor in understanding the reactivity of this catalysis.

#### 4:42PM V47.00012 First Principles Study of a-U<sub>2</sub>N<sub>3</sub> Surfaces and its Anti-oxidant Mechanism

, MENGTING JIN, YANNING ZHANG, Chengdu Green Energy and Green Manufacturing Technology RD Center — With the advantages over oxides as fuel materials for fast nuclear reactors, actinide nitrides have been extensively studied in experiments. In particular, a-U<sub>2</sub>N<sub>3</sub> is also the main composition of surface layer obtained by surface nitriding for the enhancement of oxidation resistance of uranium in ambient conditions.[1-4] However, the anti-oxidant mechanism behind is still unclear, which hinders the further development of surface treatment technologies for uranium. Here we perform extensive *ab initio* studies on the geometric, magnetic and electronic properties of a-U<sub>2</sub>N<sub>3</sub> bulk and (001) surfaces. Then the adsorption and diffusion of O<sub>2</sub> near the stable a-U<sub>2</sub>N<sub>3</sub>(001) surface will be discussed, focusing on the local atomic arrangements of U-N and U-N-O that cannot be observed easily in experiments. Our theoretical results may give some insights in understanding the anti-oxidant mechanism of surface nitriding.

#### 4:54PM V47.00013 Laser driven solid-state diffusional mixing in a Ni-Pt multilayer film probed by hard x-ray diffraction<sup>1</sup>

, AARON LOETHER, BRIAN KELLY, Department of Physics and Astronomy, University of Delaware, ANTHONY DICHARA, ROBERT HENNING, Advanced Photon Source, Argonne National Laboratory, KARL UNRUH, MATTHEW DECAMP, Department of Physics and Astronomy, University of Delaware — Intense optical excitation has been utilized for decades to modify atomic scale structure in the condensed phase. When the optically excited systems are probed by hard x-ray radiation, one can reconstruct the modified atomic structure on a sub-angstrom spatial scale. In this work we utilize sub-picosecond optical radiation to rapidly drive atomic diffusion in a Ni-Pt multilayer film. Transient atomic diffusion was measured using hard x-ray diffraction, thereby directly observing the formation of a new metallic alloy as a function of laser excitation. Our observations demonstrate that the diffusional mixing in the multilayer can be completed in only a few individual laser shots, allowing us to directly probe the dynamics of the atomic scale motion.

<sup>1</sup>This material is based upon work supported by the National Science Foundation under Grant No. 1410076

#### 5:06PM V47.00014 NMR Studies of the Dynamics of HD Adsorbed on MCM-41<sup>1</sup>

, CHAO HUAN, JAHAMAMIDA, NEIL SULLIVAN, University of Florida — We report the results of measurements of the nuclear spin-spin and spin-lattice relaxation times of a monolayer of HD molecules adsorbed on MCM-41 for temperatures  $1.5 < T < 20$  K. Two distinct characteristic relaxation times are observed. A slow diffusion process for  $5 < T < 8.8$  K and a faster rate with a distinctly different activation energy for  $8.9 < T < 12$  K. The behavior is fluid-like above 12 K. We discuss the results in terms of an expected cluster formation at low temperatures followed by the diffusion of single molecules at high temperatures.

<sup>1</sup>Work supported by the National Science Foundation - DMR-1303599 and DMR-1157490 (National High Magnetic Field Laboratory)

**5:18PM V47.00015 Noble gas adsorption in two-dimensional zeolites: a combined experimental and density functional theory study<sup>1</sup>**, MENGGEN WANG, Stony Brook University, JIANQIANG ZHONG, JORGE ANIBAL BOSCOBONIN, DEYU LU, Brookhaven National Laboratory — Zeolites are important industrial catalysts with porous three-dimensional structures. The catalytically active sites are located inside the pores, thus rendering them inaccessible for surface science measurements. We synthesized a two-dimensional (2D) zeolite model system, consisting of an (alumino)silicate bilayer weakly bound to a Ru (0001) surface. The 2D zeolite is suitable for surface science studies; it allows a detailed characterization of the atomic structure of the active site and interrogation of the model system during the catalytic reaction. As an initial step, we use Ar adsorption to obtain a better understanding of the atomic structure of the 2D zeolite. In addition, atomic level studies of rare gas adsorption and separation by zeolite are important for its potential application in nuclear waste sequestration. Experimental studies found that Ar atoms can be trapped inside the 2D-zeolite, raising an interesting question on whether Ar atoms are trapped inside the hexagonal prism nano-cages or at the interface between the (alumino)silicate bilayer and Ru(0001), or both. DFT calculations using van der Waals density functionals were carried out to determine the preferred Ar adsorption sites and the corresponding adsorption energies.

<sup>1</sup>This research used resources of the Center for Functional Nanomaterials, which is a U.S. DOE Office of Science Facility, at Brookhaven National Laboratory under Contract No. DE-SC0012704.

**Thursday, March 17, 2016 2:30PM - 5:30PM –**  
**Session V48 GQI: Readout and Trajectories in Superconducting Circuits** 349 - Kater Murch, Washington University, St. Louis

**2:30PM V48.00001 Probing the Speed Limits of Transmon Dispersive Readout**, THEO WALTER, PHILIPP KURPIERS, MINTU MONDAL, MAREK PECHAL, ANDREAS WALLRAFF, S. GASPARINETTI, ETH Zurich — In circuit QED, faster and more accurate measurement of a qubit's state is necessary to achieve better feedback control, to accomplish more complex quantum algorithms and simulations, and to cross the threshold for fault tolerant quantum computing. In this talk, we discuss our experimental progress to minimize the time needed to readout the state of a dispersively coupled transmon qubit with high fidelity. We outline a signal-to-noise ratio model, illuminate the constraints and find optimal parameters for maximizing measurement speed, while maintaining high readout fidelity. Utilizing a Purcell Filter increases the generality of our results as it becomes possible to reach these speeds with a broader set of system parameters.

**2:42PM V48.00002 Fast Quantum Nondemolition Readout by Parametric Modulation of Longitudinal Qubit-Oscillator Interaction**, JÉRÔME BOURASSA, Cégep de Granby, NICOLAS DIDIER<sup>1</sup>, McGill University and Université de Sherbrooke, ALEXANDRE BLAIS, Université de Sherbrooke and Canadian Institute for Advanced Research — For quantum information processing, qubit readout must be fast, of high-fidelity and ideally quantum non-demolition (QND). To rapidly reuse the measured qubit, fast reset of the measurement pointer states is also needed. Combining these characteristics is essential to meet the stringent requirements of fault-tolerant quantum computation. For superconducting qubits, a common strategy is the dispersive readout where the qubit is coupled to an oscillator acting as pointer. In this talk, we present an alternative strategy based on parametric modulation of longitudinal qubit-oscillator interaction. We show that compared to dispersive readout it leads to a faster, high-fidelity and ideally QND qubit readout with a simple reset mechanism [1]. We moreover show how to exponentially improve the signal-to-noise ratio (SNR) of this measurement with the help of single-mode squeezed input state on the oscillator. We present an implementation of this longitudinal parametric readout in circuit quantum electrodynamics along with results using realistic experimental parameters. [1] N. Didier, J. Bourassa and A. Blais, Phys. Rev. Lett., In Print (2015)

<sup>1</sup>Now at Quantic team, INRIA Paris

**2:54PM V48.00003 Non-QNDness of Dispersive Measurement in Superconducting Qubits, Part I: Theory**, MOSTAFA KHEZRI, University of California, Riverside, DANIEL SANK, Google, ZIJUN CHEN, University of California, Santa Barbara, RAMI BARENDTS, YU CHEN, AUSTIN FOWLER, ROBERT GRAFF, EVAN JEFFREY, JULIAN KELLY, ERIK LUCERO, ANTHONY MEGRANT, JOSH MUTUS, PEDRAM ROUSHAN, TED WHITE, MATTHEW NEELEY, Google, BROOKS CAMPBELL, BENJAMIN CHIARO, ANDREW DUNSWORTH, CHARLES NEILL, PETER O'MALLEY, CHRISTOPHER QUINTANA, AMIT VAINSENER, JAMES WENNER, University of California, Santa Barbara, JOHN M. MARTINIS, Google, University of California, Santa Barbara, ALEXANDER N. KOROTKOV, University of California, Riverside — We theoretically analyze the dispersive measurement of an Xmon qubit in the circuit QED setup at moderately high power, so that the number of photons in the resonator exceeds the so-called critical number by up to an order of magnitude. Our results show an abrupt change of the qubit state when the number of photons reaches a certain threshold, which depends on the detuning between the qubit and the resonator. The simulation results are in agreement with experimental findings for Xmon measurement at moderately high power. We will discuss the physical mechanism causing an abrupt deterioration of the measurement QNDness at the threshold.

**3:06PM V48.00004 Non-QNDness of Dispersive Measurement in Superconducting Qubits, Part II: Experiment**, DANIEL SANK, Google Inc - Santa Barbara, Z. CHEN, UC Santa Barbara, M. KHEZRI, UC Riverside, R. BARENDTS, Google Inc - Santa Barbara, B. CAMPBELL, UC Santa Barbara, Y. CHEN, Google Inc - Santa Barbara, B. CHIARO, A. DUNSWORTH, UC Santa Barbara, A. FOWLER, R. GRAFF, E. JEFFREY, J. KELLY, E. LUCERO, A. MEGRANT, J. MUTUS, M. NEELEY, Google Inc - Santa Barbara, C. NEILL, P. J. J. O'MALLEY, UC Santa Barbara, C. QUINTANA, P. ROUSHAN, Google Inc - Santa Barbara, A. VAINSENER, J. WENNER, UC Santa Barbara, T. WHITE, Google Inc - Santa Barbara, A. KOROTKOV, UC Riverside, J. M. MARTINIS, Google Inc - Santa Barbara — Modern quantum state measurement in transmon qubits uses the interaction between the qubit and a harmonic oscillator. In the dispersive limit of the interaction, the coupling operator  $n\sigma_z$  commutes with the qubit Hamiltonian and should be perfectly QND. However, previous experiments have indicated that sufficiently high resonator drive power causes unwanted qubit state transitions, producing errors. We investigate these errors in detail, connect the results with theory, and comment on the implications for quantum computer design.

**3:18PM V48.00005 Dependence of transmon qubit relaxation rate on readout drive power<sup>1</sup>**, S.O. MUNDHADA, S. SHANKAR, A. NARLA, E. ZALYS-GELLER, S.M. GIRVIN, M.H. DEVORET, Department of Applied Physics, Yale University — In circuit QED experiments, microwave drives are applied to the readout mode for qubit measurement, control and to realize various multi-photon processes. These microwave drives have been observed to detrimentally affect the qubit mode by increasing the qubit relaxation rates for both upward and downward transitions. These transitions demolish the qubit state during a measurement, limiting the maximum measurement strength and thus the readout fidelity and speed. Here, we experimentally investigate this effect for transmon qubits coupled to different realizations of the readout mode: 3-dimensional microwave cavities, strip-line resonators and nonlinear readout modes in a waveguide.

<sup>1</sup>Work supported by: NSF, ARO, AFOSR and YINQE.

**3:30PM V48.00006 A balanced, superconducting multiplier circuit for fast-switching and multiplexed qubit readout: Design and modeling**, ERIC I. ROSENTHAL, BENJAMIN J. CHAPMAN, BRAD A. MOORES, JILA, University of Colorado, Boulder, JOSEPH KERCKHOFF, HRL Laboratories, JILA, University of Colorado, Boulder, K. W. LEHNERT, JILA, University of Colorado, Boulder, National Institute of Standards and Technology, Boulder — Superconducting qubits hold great promise for the development of new quantum-information technology. Coherence times of individual transmon qubits in microwave cavities are consistently improving. While qubits are becoming well developed tools, scaling qubit readout for many-qubit architectures remains prohibitively complex and expensive. Here, we present a concept for a multi-purpose device that enables time or code domain multiplexing of qubit readout. It is a two-port, microwave device that can be switched rapidly between three modes of operation: transmission, reflection and inversion. The design is based on a Wheatstone bridge-like structure of tunable inductors, which we realize with arrays of SQUIDS. A single bias line modulates the flux through the SQUIDS, and hence the imbalance of the bridge, putting the device in one of its three modes of operation. This talk will discuss the theory, design and layout behind the device and its potential use for multiplexing of qubit networks. The device is designed to operate over a broad bandwidth (4-8 GHz), and to have low dissipation, appropriate for integration with superconducting qubit networks.

**3:42PM V48.00007 A balanced, superconducting multiplier circuit for fast-switching and multiplexed qubit readout: Performance and demonstration<sup>1</sup>**, BRAD A. MOORES, BENJAMIN J. CHAPMAN, ERIC I. ROSENTHAL, JILA, University of Colorado, Boulder, JOSEPH KERCKHOFF, HRL Laboratories, JILA, University of Colorado, Boulder, K. W. LEHNERT, JILA, University of Colorado, Boulder — A major challenge of scaling the promising transmon qubits into a quantum information processing machine is the classical hardware burden required to readout many qubits. Within the cavity QED architecture, qubit states are measured by detecting the transmission through microwave cavities. A multiplexing scheme could allow the classical hardware burden of generating and measuring a readout tone to be shared among several cavity-qubit systems. In this talk, we will present measurements of a recently designed superconducting multiplier circuit intended to accomplish time and code domain multiplexed readout. In particular, we characterize three modes of microwave operation: transmission, reflection and inversion. The device can be switched between these modes approximately 100 times faster than typical qubit coherence times. Exploiting this performance, we demonstrate a code domain multiplexing scheme with classical signals created to simulate typical qubit signals. The scheme operates with near unity fidelity at microwave powers comparable to typical qubit tones.

<sup>1</sup>This work is supported by the ARO under the contract W911NF-14-1-0079

**3:54PM V48.00008 Frequency and sensitivity tunable microresonator array for high-speed quantum processor readout**, EMILE HOSKINSON, J. D. WHITTAKER, L. J. SWENSON, M. H. VOLKMANN, P. SPEAR, F. ALTOMARE, A. J. BERKLEY, D-Wave Systems, B. BUMBLE, Jet Propulsion Laboratory, P. BUNYK, D-Wave Systems, P. K. DAY, B. H. EOM, Jet Propulsion Laboratory, R. HARRIS, J. P. HILTON, M. W. JOHNSON, D-Wave Systems, A. KLEINSASSER, Jet Propulsion Laboratory, E. LADIZINSKY, T. LANTING, T. OH, I. PERMINOV, E. TOLKACHEVA, J. YAO, D-Wave Systems — Frequency multiplexed arrays of superconducting microresonators have been used as detectors in a variety of applications. The degree of multiplexing achievable is limited by fabrication variation causing non-uniform shifts in resonator frequencies. We have designed, implemented and characterized a superconducting microresonator readout that incorporates two tunable inductances per detector, allowing independent control of each detector frequency and sensitivity. The tunable inductances are adjusted using on-chip programmable digital-to-analog flux converters, which are programmed with a scalable addressing scheme that requires few external lines.

**4:06PM V48.00009 Simple quantum trajectories for transmon measurement with moderate bandwidth**, ALEXANDER N. KOROTKOV, University of California, Riverside — So far, most experiments on the continuous quantum measurement of superconducting qubits in a circuit QED setup have been well described by the Quantum Bayesian formalism, which assumes the "bad cavity limit": the resonator bandwidth is assumed to be much larger than the measurement-induced dephasing. However, in some experiments this assumption is not applicable, and then the Quantum Bayesian formalism should be extended. We discuss a relatively simple generalization to the case of arbitrary resonator bandwidth, which can be applied when there is no significant qubit evolution due to Rabi oscillations. We also discuss how to include Rabi oscillations and energy relaxation into the simulation of quantum trajectories.

**4:18PM V48.00010 Mapping quantum state dynamics of spontaneous emission**, MAHDI NAGHILOO, NEDA FROUZANI, DIAN TAN, KATER MURCH, Washington University, St. Louis — Controlling the dynamics of spontaneous emission for quantum emitters is relevant to many novel applications in quantum computation and quantum optics. In this work we use homodyne measurements of the spontaneous emission of a superconducting qubit to track its quantum evolution. A resonant pulse is used to prepare the qubit in the excited state and the emission from the system into this environment is monitored with a near-quantum-limited Josephson parametric amplifier acting as a homodyne detector. By an appropriately chosen phase of amplification, we execute weak measurements in the  $\sigma_x$  basis of the qubit. We use the measurement results to track individual quantum trajectories as the qubit evolves from its excited to ground state, revealing rich dynamics that occur in the process of spontaneous emission.

**4:30PM V48.00011 Tracking Multi-State Quantum Jumps in a Superconducting Circuit**, NEDA FOROUZANI, DIAN TAN, MAHDI NAGHILOO, KATER MURCH, Washington University, St. Louis — Quantum measurements are known to be crucial for quantum error-correction and state initialization. Continuous measurements can be used for state tracking and real-time quantum feedback. If the measurements are strong, the state dynamics are described by quantum jumps between states. Using continuous measurements, we track the quantum state of a transmon circuit initially in its lowest energy state. We observe spurious jumps between five observable states of the circuit and use a Bayesian update formalism to estimate state occupation probabilities as well as transition rates over time. Our analysis reveals switching between different quantum jump statistics. Resolving the energy distribution of spurious jumps will help characterize this decoherence process.

**4:42PM V48.00012 Theory and practice of dressed coherent states in circuit QED<sup>1</sup>**, FRANK WILHELM, Saarland University, LUKE C.G. GOVIA, McGill University — In the dispersive regime of qubit-cavity coupling, classical cavity drive populates the cavity, but leaves the qubit state unaffected. However, the dispersive Hamiltonian is derived after both a frame transformation and an approximation. Therefore, to connect to external experimental devices, the inverse frame transformation from the dispersive frame back to the lab frame is necessary. We show that in the lab frame the system is best described by an entangled state known as the dressed coherent state, and thus even in the dispersive regime, entanglement is generated between the qubit and the cavity. Also, we show that further qubit evolution depends on both the amplitude and phase of the dressed coherent state. This provides a limitation to readout in the dispersive regime. We show that only in the limit of infinite measurement time is this protocol QND, as the formation of a dressed coherent state in the qubit-cavity system applies an effective rotation to the qubit state. We show how this rotation can be corrected by a unitary operation, leading to improved qubit initialization by measurement and unitary feedback.] L.C.G. Govia and F.K. Wilhelm Phys. Rev. Applied 4, 054001 (2015) L.C.G. Govia and F.K. Wilhelm, arXiv: 1506.04997

<sup>1</sup>Supported by the ARO under contract W911NF-14-1-0080 and the European Union through ScaleQIT. LCGG acknowledges support from NSERC through an NSERC PGS-D

**4:54PM V48.00013 Design and initial tests of a superconducting circulator for quantum microwave systems<sup>1</sup>**, BENJAMIN J. CHAPMAN, ERIC I. ROSENTHAL, BRAD A. MOORES, JILA, University of Colorado, Boulder, JOSEPH KERCKHOFF, HRL Laboratories, JILA, University of Colorado, Boulder, KEVIN LALUMIÈRE, ALEXANDRE BLAIS, University of Sherbrooke, K.W. LEHNERT, JILA, University of Colorado, Boulder, National Institute of Standards and Technology, Boulder — Microwave circulators enforce a single propagation direction for signals in an electrical network. Unfortunately, commercial circulators are bulky, lossy, and cannot be integrated close to superconducting circuits because they emit large stray magnetic fields. Here we report progress toward the development of a lossless, on-chip, active circulator for superconducting microwave circuits in the 4-8 GHz band. Non-reciprocity is achieved by actively modulating circuit elements on a slow time scale (10 – 100 ns). Our circulator's active components are dynamically tunable inductors constructed with arrays of dc-SQUIDS in series. The array inductance is tuned by varying the magnetic flux through the SQUIDS with fields weaker than 1 Oe. Initial tests show that the device exhibits non-reciprocity, but performance is degraded by trapped magnetic flux in the circuit. Nevertheless, the device meets many design goals including a tunable center frequency between 4-8 GHz and a high (-93 dBm) saturation power. This presentation will describe these tests and a new layout designed to avoid trapped flux.

<sup>1</sup>This work is supported by the ARO under the contract W911NF-14-1-0079.

**5:06PM V48.00014 Squeezing-enhanced superconducting qubit measurement using driven nonlinear resonators**, LUKE C. G. GOVIA, BENJAMIN LEVITAN, AASHISH A. CLERK, McGill University — Dispersive measurement of a superconducting qubit is a key ingredient in many contemporary protocols in circuit quantum electrodynamics, and high measurement fidelity has recently been achieved. However, as the number of qubits on chip and the complexity of protocols increases, so too does the required measurement fidelity. To reach higher fidelity, it has been proposed that squeezed microwave fields injected into the resonator can be used to reduce the noise in the measured field quadrature<sup>1,2</sup>. However, creating, preserving, and injecting a squeezed microwave field is a technologically challenging task. Here, we theoretically analyze the dispersive measurement of a qubit coupled to one or more driven nonlinear resonators, which provide an in situ source of microwave field squeezing. This is potentially a more flexible way of harnessing the physics that leads to the increase in measurement fidelity seen for both single-mode and two-mode squeezed states<sup>1</sup>, without the drawback of having to independently create and inject these states.

<sup>1</sup>Phys. Rev. Lett. 115, 093604 (2015)

<sup>2</sup>Phys. Rev. B 90, 134515 (2014)

**5:18PM V48.00015 Closing a quantum feedback loop for a superconducting qubit inside a cryostat**, CHRISTIAN KRAGLUND ANDERSEN, Aarhus University, JOSEPH KERCKHOFF, KONRAD W LEHNERT, BENJAMIN J CHAPMAN, JILA, University of Colorado, Boulder, KLAUS MLMER, Aarhus University — Several quantum information protocols relies upon efficient feedback (or feed-forward) schemes. Recently, within the field of superconducting qubits, many experiments have shown tremendous progress towards high fidelity quantum feedback scheme. Some experiments work by traditional measurement based schemes where the classical output is processed on a classical "computer" before a signal is fed back to the qubits. Other approaches are working in a continuous coherent manner, where the full quantum description of the system creates an effective bath that relaxes the system into the desired state. This talk will present a different approach that aims to close a measurement based feedback loop inside a cryostat and, thus, the scheme works completely autonomous. This approach sidesteps many of the inefficiencies inherent in two-way communication between temperature stages in typical systems with room temperature controllers, and avoids increasing the cryogenic heat load. This controller may find a broad range of uses in multi-qubit systems, but here I analyze two specific demonstrative cases in single qubit-control and show simulations of the time evolution for the full system dynamics.

## Thursday, March 17, 2016 2:30PM - 5:30PM —

Session V50 DAMOP: Quantum Gases in Optical Lattices Hilton Baltimore Holiday Ballroom 1 - B. Svistunov, University of Massachusetts Amherst

**2:30PM V50.00001 Phase diagram of ferromagnetic spinor bosons in an optical lattice under an external magnetic field<sup>1</sup>**, KOHAKU H. Z. SO, Department of Physics, University of Tokyo, MASAHIITO UEDA, Department of Physics, University of Tokyo, and RIKEN Center for Emergent Matter Science (CEMS) — Recently, cold atoms with spin degrees of freedom have attracted considerable interest because of the possibility they offer of modelling quantum magnetism and exploring the interplay between spatial and spin degrees of freedom. While spinor bosons with antiferromagnetic interaction loaded in optical lattices have been widely studied in this context because of their properties such as an even-odd effect in the superfluid to Mott-insulator transition, those with ferromagnetic interaction has not been studied extensively. However, mean-field analysis in the continuum systems suggests that the competition between an external magnetic field and the ferromagnetic interaction could give rise to new and rich phases. We have studied ferromagnetic spinor bosons in an optical lattice under an external magnetic field. Using the decoupling mean-field approximation, we have obtained a rich ground-state phase diagram, in which, in addition to the well-known Mott-insulator and superfluid phases, polar and broken-axisymmetry superfluid phases arise. We also found that the transition between broken-axisymmetry superfluid phase and other phases is a first-order one across some part of the phase boundary, in remarkable contrast to the case without external magnetic fields.

<sup>1</sup>JSPS KAKENHI (No. 26287088, No. 15H05855), JSPS ALPS

**2:42PM V50.00002 Unconventional Bose-Einstein Condensations of Two-species Bosons in the  $p$ -orbital Bands in Optical Lattice**, JHIH-SHIH YOU, Department of Physics, Harvard University, I-KANG LIU, Department of Physics and Graduate Institute of Photonics, National Changhua University of Education, DAW-WEI WANG, Physics Department and Physics division, National Center for Theoretical Sciences, National Tsing-Hua University, SHIH-CHUAN GOU, Department of Physics and Graduate Institute of Photonics, National Changhua University of Education, CONGJUN WU, Department of Physics, University of California, San Diego — We investigate the unconventional Bose-Einstein condensations of two-species mixture with  $p$ -wave symmetry in the second band of a bipartite optical lattice. Different from the single-species case, the two-species boson mixture exhibits two non-equivalent complex BECs in the intraspecies-interaction-dominating regime, with one breaking time-reversal symmetry while the other not. When the interspecies interaction is tuned across the SU(2) invariant point, the system undergoes a quantum phase transition toward a real-valued checkerboard state characterized by a staggered spin density structure. An experimental scheme for phase measurement is presented. Finally, we will show strong coupling analysis on anti-Hund's rule, Mott-insulating states and the superfluid.

**2:54PM V50.00003 Phase diagram of strongly attractive  $p$ -orbital fermions on optical lattices**, THEJA DE SILVA, Augusta University — We examine a system of doubly degenerate  $p$ -orbital polarized fermions on a two-dimensional square lattice with a strong on-site interaction. For strong attractive interactions at the half filling density limit, a four-site square plaquette interaction term is generated from the directional tunneling dependence of  $p$ -orbitals. By treating both on-site interaction and the four-site square plaquette interaction term in fourth order perturbation theory, we derive an effective Hamiltonian for the system. We then map the resulting effective particle Hamiltonian into an effective spin-Hamiltonian and study the phase diagram of the system by using a variational mean field approach and a linear spin-wave theory. Further, we discuss the experimental signatures of the resulting phases within the context of current cold-atom experimental techniques.

**3:06PM V50.00004 Superfluidity of ultracold atomic gases of Fermi-Fermi mixtures on an optical lattice<sup>1</sup>**, JIBIAO WANG, QIJIN CHEN, Zhejiang University — Superfluidity of ultracold atomic gases of Fermi-Fermi mixtures has been under active investigation recently. Experimentally, mixtures of  $^6\text{Li}$ - $^{40}\text{K}$ ,  $^{171}\text{Yb}$ - $^{173}\text{Yb}$  and  $^6\text{Li}$ - $^{173}\text{Yb}$ , for example, have been prepared and cooled down to the quantum degeneracy regime, making the superfluid phase accessible in the near future. In this talk, we will address the superfluidity of ultracold Fermi-Fermi mixtures on 1D through 3D optical lattices, with varying mass and population imbalances and different densities, as they undergo BCS-BEC crossover, within a pairing fluctuation theory which includes self-consistently the important pseudogap effects at finite temperatures. We will present various phase diagrams and show the dramatic combined effects of mass and population imbalances and lattice periodicity. Implications for future experiment will be discussed. References: [1] Q. J. Chen, I. Kosztin, B. Janko, and K. Levin, Phys. Rev. B 59, 7083 (1999). [2] C. -C. Chien, Y. He, Q. J. Chen, and K. Levin, Phys. Rev. A 77, 011601(R) (2008). [3] C. -C. Chien, Q. J. Chen, and K. Levin, Phys. Rev. A 78, 043612 (2008). [4] Q. J. Chen, Phys. Rev. A 86, 023610 (2012).

<sup>1</sup>Work supported by NSF of China and the National Basic Research Program of China

**3:18PM V50.00005 Magnetic-field-tunable Kondo effect in alkaline-earth cold atoms<sup>1</sup>**, LEONID ISAEV, ANA MARIA REY, JILA, NIST and Department of Physics, University of Colorado Boulder — We study quantum magnetism and emergent Kondo physics in strongly interacting fermionic alkaline-earth atoms in an optical lattice with two Bloch bands: one localized and one itinerant. For a fully filled narrow band (two atoms per lattice site) we demonstrate that an applied magnetic field provides an efficient control of the ground state degeneracy due to the field-induced crossing of singlet and triplet state of the localized atomic pairs. We exploit this singlet-triplet resonance, as well as magnetically tunable interactions of atoms in different electronic states via the recently-discovered inter-orbital Feshbach resonance, and demonstrate that the system exhibits a magnetic field-induced Kondo phase characterized by delocalization of local singlets and a large Fermi surface. We also determine the phase diagram of the system within an effective low-energy model that incorporates the above magnetic-field effect as well as atomic interactions in the two optical lattice bands. Our results can be tested with ultracold  $^{173}\text{Yb}$ , and provide a model for the magnetic field-induced heavy-fermion state in filled skutterudites such as  $\text{PrOs}_4\text{Sb}_{12}$ .

<sup>1</sup>This work was supported by the NSF (PIF-1211914 and PFC-1125844), AFOSR, AFOSR-MURI, NIST and ARO individual investigator awards

**3:30PM V50.00006 Cooling a Band Insulator with a Metal: Fermionic Superfluid in a Dimerized Holographic Lattice<sup>1</sup>**, ARIJIT HALDAR, VIJAY B. SHENOY, Indian Institute of Science Bangalore — A cold atomic realization of a quantum correlated state of many fermions on a lattice, eg. superfluid, has eluded experimental realization due to the entropy problem. Here we propose a route to realize such a state using holographic lattice and confining potentials. The potentials are designed to produce a *band insulating* state (low heat capacity) at the trap center, and a metallic state (high heat capacity) at the periphery. The metal “cools” the central band insulator by extracting out the excess entropy. The central band insulator can be turned into a superfluid by tuning an attractive interaction between the fermions. Crucially, the holographic lattice allows the emergent superfluid to have a *high transition temperature* – even twice that of the effective trap temperature. The scheme provides a promising route to a laboratory realization of a fermionic lattice superfluid, even while being adaptable to simulate other many body states. Reference: Scientific Reports 4, 6665 (2014).

<sup>1</sup>Work supported by CSIR, DST and DAE

**3:42PM V50.00007 Dirac and Weyl Rings in Three Dimensional Cold Atom Optical Lattices.**, YONG XU, CHUANWEI ZHANG, The University of Texas at Dallas — Recently three dimensional topological quantum materials with gapless energy spectra have attracted considerable interests in many branches of physics. Besides the celebrated example, Dirac and Weyl points which possess gapless point structures in the underlying energy dispersion, the topologically protected gapless spectrum can also occur along a ring, named Dirac and Weyl nodal rings. Ultra-cold atomic gases provide an ideal platform for exploring new topological materials with designed symmetries. However, whether Dirac and Weyl rings can exist in the single-particle spectrum of cold atoms remains elusive. Here we propose a realistic model for realizing Dirac and Weyl rings in the single-particle band dispersion of a cold atom optical lattice. Our scheme is based on previously experimentally already implemented Raman coupling setup for realizing spin-orbit coupling. Without the Zeeman field, the model preserves both pseudo-time-reversal and inversion symmetries, allowing Dirac rings. The Dirac rings split into Weyl rings with a Zeeman field that breaks the pseudo-time-reversal symmetry. We examine the superfluidity of attractive Fermi gases in this model and also find Dirac and Weyl rings in the quasiparticle spectrum.

**3:54PM V50.00008 The Detection of Massive Goldenstone (Higgs) Mode in Two-Dimensional Ultra-cold Atomic Lattice Systems**, KUN CHEN, University of Massachusetts, Amherst; University of Science and Technology of China, LONGXIANG LIU, University of Science and Technology of China, YOUJIN DENG, University of Science and Technology of China; University of Massachusetts, Amherst; MANUEL ENDRES, Harvard University; California Institute of Technology, LODÉ POLLET, Ludwig Maximilian University of Munich, NIKOLAY PROKOF'EV, University of Massachusetts, Amherst; Russian Research Center Kurchatov Institute — We discuss how to reveal the massive Goldstone mode, often referred to as the Higgs amplitude mode, near the Superfluid-to-Insulator quantum critical point (QCP) in a system of two-dimensional ultra-cold bosonic atoms in optical lattices. The spectral function of the amplitude response is obtained by analytic continuation of the kinetic energy correlation function calculated by Monte Carlo methods. Our results enable a direct comparison with the recent experiment [M. Endres, T. Fukuhara, D. Pekker, M. Cheneau, P. Schauß, C. Gross, E. Demler, S. Kuhr, and I. Bloch, Nature **487**, 454-458 (2012)], and demonstrate a good agreement for temperature shifts induced by lattice modulation. Based on our numerical analysis, we formulate the necessary conditions in terms of homogeneity, detuning from the QCP and temperature in order to reveal the massive Goldstone resonance peak in spectral functions experimentally. We also propose to apply a local modulation at the trap center to overcome the inhomogeneous broadening caused by the parabolic trap confinement.

**4:06PM V50.00009 Evolution of the Hofstadter butterfly in a tunable optical lattice**, MEHMET O. OKTEL, Bilkent Univ, NUR UNAL, Cornell Univ, FIRAT YILMAZ, Bilkent Univ — Advances in realizing artificial gauge fields on optical lattices promise experimental detection of topologically non-trivial energy spectra. Self-similar fractal energy structures, known as Hofstadter butterflies, depend sensitively on the geometry of the lattice, as well as the applied magnetic field [1]. The recent demonstration of an adjustable lattice geometry [L. Tarruell et al., Nature **483**, 302 (2012)] presents a unique opportunity to study this dependence. We calculate the Hofstadter butterflies that can be obtained in such an adjustable lattice and find three qualitatively different regimes. We show that the existence of Dirac points at zero magnetic field does not imply the topological equivalence of spectra at finite field. As the real-space structure evolves from the checkerboard to the honeycomb lattice, two square lattice Hofstadter butterflies merge to form a honeycomb lattice butterfly in a topologically non-trivial way, as it is accomplished by sequential closing of infinitely many gaps. We discuss the evolution of topological properties with underlying lattice geometry by calculating the Chern numbers and comment on the validity of simulating graphene in such an adjustable lattice. [1] F. Yilmaz, F. Nur Unal, and M. O. Oktel, Phys. Rev. A **91**, 063628 (2015).

**4:18PM V50.00010 Proposals for quantum simulating simple lattice gauge theory models using optical lattices<sup>1</sup>**, JIN ZHANG, University of California, Riverside, JUDAH UNMUTH-YOCKEY, University of Iowa, ALEXEI BAZAVOV, University of California, Riverside, YANNICK MEURICE, University of Iowa, SHAN-WEN TSAI, University of California, Riverside — We derive an effective spin Hamiltonian for the (1+1)-dimensional Abelian Higgs model in the strongly coupled region by integrating out the link variables. With finite spin truncations, the Hamiltonian can be matched with a 1-dimensional two-species Bose Hubbard model in the strong-coupling limit that can be implemented with cold atoms on an optical lattice. We study the phase diagram of the original Abelian Higgs model with Monte Carlo simulation and Tensor Renormalization Group methods. The results show a crossover line which terminates near the Kosterlitz-Thouless transition point. The effective quantum Hamiltonian is also studied with the DMRG method, and we find that they have a similar behavior. We discuss practical experimental implementations for our quantum simulator. Species-dependent optical lattices and ladder systems with double-well potentials are considered. We show how to obtain each of the interaction parameters required in the Bose-Hubbard model that we obtained, and confirm the possibility of tuning these interactions to the region in which our mapping is valid. We emphasize that this proposal for quantum simulating a gauge theory uses a manifestly gauge-invariant formulation and Gauss's Law is therefore automatically satisfied.

<sup>1</sup>Supported by DoD ARO under Grant No. W911NF-13-1-0119 and by the NSF under Grants No. DMR-1411345

**4:30PM V50.00011 Topological Nodal-Line Superfluid in Spin-Orbit Coupled Cold Atomic Systems**, WEN-YU HE, DONG-HUI XU, TONG ZHOU, K. T. LAW, Hong Kong University of Science and Technology, HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY COLLABORATION — Topological nodal line superconductivity or superfluidity is a fascinating topological gapless phase which hosts bulk Weyl ring degeneracy in the quasiparticle excitation spectrum and supports Majorana zero bound modes with a large density of states at the edge. In this work, based on the experimentally realized 1D spin orbit coupling, we show the emergence of topological nodal line superfluid phase in Fermionic atoms trapped in 3D cubic optical lattice when the s wave pairing field is introduced through Feshbach resonance between the two atomic hyperfine spin states. The nodal line degeneracy is further found to evolve into Weyl nodes once another component of spin orbit coupling field enters to break the chiral symmetry. The momentum resolved radio frequency spectroscopy is suggested to manifest the topological nodal line superfluid phase.

**4:42PM V50.00012 Vacancy dynamics in the paramagnetic environment**, JOHAN CARLSTROM, BORIS SVISTUNOV, NIKOLAY PROKOFIEV, University of Massachusetts — We consider the motion of a single vacancy in a magnetic spin-1/2 lattice. Examples of realisations of this model include vacancies in a He3 solid or holes in the t-J model with J=0. This motion is ballistic when spins exhibit ferromagnetic order, with  $\langle |r(t)| \rangle$  growing linearly with time. However in the disordered paramagnet, the motion of the vacancy becomes highly nontrivial, and no exact solution to this outstanding problem is known. This scenario is known as the Brinkman-Rice problem. We report here numerical results for the spatial probability distribution of the vacancy obtained by integrating the time evolution operator through Monte Carlo and averaging over a large number of random spin realisations. We find highly counterintuitive results, with the probability of finding the vacancy at a given site oscillating in time. These results can be verified in experiments with ultra-cold fermions in optical lattice at a temperature high enough that the spins are disordered.

**4:54PM V50.00013 Scratched-XY Universality and Phase Diagram of Disordered 1D Bosons in Optical Lattice**, ZHIYUAN YAO, Department of Physics, University of Massachusetts, Amherst, MA 01003, USA, LODE POLLET, Department of Physics, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, University of Munich, Theresienstrasse 37, 80333 M, NIKOLAY PROKOF'EV, BORIS SVISTUNOV, Department of Physics, University of Massachusetts, Amherst, MA 01003, USA — The superfluid-insulator quantum phase transition in a 1D system with weak links belongs to the so-called scratched-XY universality class, provided the irrenormalizable exponent  $\zeta$  characterizing the distribution of weak links is smaller than 2/3. With a combination of worm-algorithm Monte Carlo simulations and asymptotically exact analytics, we accurately trace the position of the scratched-XY critical line on the ground-state phase diagram of bosonic Hubbard model at unity filling. In particular, we reveal the location of the tricritical point separating the scratched-XY criticality from the Giamarchi-Schulz one.

**5:06PM V50.00014 Application of the DMRG in two dimensions: a parallel tempering algorithm<sup>1</sup>**, SHIJIE HU, Department of Physics and Research Center Optimas, Technical University Kaiserslautern, 67663 Kaiserslautern, Germany, JIZE ZHAO, Institute of Applied Physics and Computational Mathematics, Beijing 100088, China, XUEFENG ZHANG, SEBASTIAN EGGERT, Department of Physics and Research Center Optimas, Technical University Kaiserslautern, 67663 Kaiserslautern, Germany — The Density Matrix Renormalization Group (DMRG) is known to be a powerful algorithm for treating one-dimensional systems. When the DMRG is applied in two dimensions, however, the convergence becomes much less reliable and typically "metastable states" may appear, which are unfortunately quite robust even when keeping a very high number of DMRG states. To overcome this problem we have now successfully developed a parallel tempering DMRG algorithm. Similar to parallel tempering in quantum Monte Carlo, this algorithm allows the systematic switching of DMRG states between different model parameters, which is very efficient for solving convergence problems. Using this method we have figured out the phase diagram of the xxz model on the anisotropic triangular lattice which can be realized by hardcore bosons in optical lattices.

<sup>1</sup>SFB Transregio 49 of the Deutsche Forschungsgemeinschaft (DFG) and the Allianz für Hochleistungsrechnen Rheinland-Pfalz (AHRP)

**5:18PM V50.00015 Many-body physics of ultracold doublet sigma molecules in optical lattices<sup>1</sup>**, GAVRIIL SHCHEDRIN, DANIEL JASCHKE, WEI HAN, LINCOLN CARR, Colorado School of Mines, Golden, Colorado, USA, DERMOT G. GREEN, Durham University, Durham, UK, JESUS ALDEGUNDE, Universidad de Salamanca, Salamanca, Spain, JEREMY M. HUTSON, Durham University, Durham, UK — The creation of ultracold polar molecules provides a unique opportunity to discover and explore new regimes in strongly interacting many-body quantum systems. Polar molecules have strong long-range dipole-dipole interactions that allow one to realize exotic phenomena such as topological phases and quantum magnetism. We explore quantum many-body systems formed by molecules in doublet sigma ( $^2\Sigma$ ) states, with both electric dipole moments and electron spin  $S = 1/2$ , but without electronic orbital momentum. The Hamiltonian for doublet sigma molecules includes molecular rotation terms, spin-rotation interaction, hyperfine terms including both spin-spin and nuclear electric quadrupole interactions, and molecular dipole-dipole interactions. The complete control of the molecular quantum states can be accomplished by applying electric and magnetic fields to molecules trapped in optical lattices. We provide the complete theoretical treatment for experimentally relevant doublet sigma molecules such as SrF and CaF and discuss the associated single-body and many-body physics.

<sup>1</sup>Funded by AFOSR and NSF

**Thursday, March 17, 2016 2:30PM - 5:30PM —**  
**Session V51 FIAP: Semiconductors (Theory)** Hilton Baltimore Holiday Ballroom 2 - Gerhard Klimeck, Purdue University

**2:30PM V51.00001 Accurate Electronic, Transport, and Bulk Properties of Wurtzite Beryllium Oxide (BeO)** , CHEICK OUMAR BAMBA, YURIY MALOZOVSKY, LASHOUNDA FRANKLIN, DIOLA BAGAYOKO, Department of Physics, Southern University and AM College, Baton Rouge, LA 70813 — We present *ab-initio*, self-consistent density functional theory (DFT) description of electronic, transport, and bulk properties of wurtzite Beryllium oxide (w-BeO). We used a local density approximation potential (LDA) and the linear combination of atomic orbitals (LCAO) formalism. Our implementation of the Bagayoko, Zhao, and Williams (BZW) method, as enhanced by Ekuma and Franklin (BZW-EF), ensures the full, physical content of our local density approximation (LDA) calculations – as per the derivation of DFT [AIP Advances, 4, 127104 (2014)] We report the band gap, density of states, partial density of state, effective masses, and the bulk modulus. Our calculated band gap of 10.29 eV, using an experimental, room temperature lattice constant of 2.6979 Å at room temperature is in agreement with the experimental value of 10.6 eV. Acknowledgments: This work was funded in part the US National Science Foundation [NSF, Award Nos. EPS-1003897, NSF (2010-2015)-RII-SUBR, and HRD-1002541], the US Department of Energy, National Nuclear Security Administration (NNSA, Award No. DE-NA0002630), LaSPACE, and LONI-SUBR.

**2:42PM V51.00002 First principles studies of the stability and Schottky barriers of metal/CdTe(111) interfaces** , ZHEN LIU, Department of Physics, California State University Northridge, MASOEHNG MIAO, Department of Chemistry and Biochemistry, California State University Northridge, NICHOLAS KIOUSSIS, Department of Physics, California State University Northridge, FIKRI AQARIDEN, Y. CHANG, CHRISTOPH GREIN, Sivananthan Laboratories, 590 Territorial Dr, Unit H Bolingbrook — CdZnTe and CdTe based semiconductor X-Ray and Gamma-Ray detectors have been intensively studied recently due to their promising potentials for achieving high-resolution, high signal-to-noise ratios and low leakage current, all are desirable features in applications ranging from medical diagnostics to homeland security. Using density functional calculations, we systematically studied the stability, the atomic and electronic structures of the interfaces between CdTe (111) surfaces (Cd- and Te-terminated) and the selected metals (Cu, Al Ni, Pd and Pt). We also calculated the Schottky barrier height (SBH) by aligning the electrostatic potentials in semiconductor and metal regions. Our calculations revealed significant differences between the Cd- and Te- terminated interfaces. While metals tend to deposit directly on reconstructed Te-terminated surfaces, they form a Te-metal alloy layer at the Cd-Terminated metal/CdTe interface. For both Te- and Cd- terminated interfaces, the Schottky barrier heights do not depend much on the choice of metals despite the large variation of the work functions. On the other hand, the interface structure is found to have large effect on the SBH, which is attributed to the metal induced states in the gap.

**2:54PM V51.00003 Ab-initio Electronic, Transport and Related Properties of Zinc Blende Boron Arsenide (zb-BAs)** , IFEANYI H. NWIGBOJI, Department of Computational Science, University of Texas at El Paso, El-Paso, TX 79968 USA., YURIY MALOZOVSKY, DIOLA BAGAYOKO, Department of Physics, Southern University and AM College, Baton Rouge, LA 70813 — We present results from *ab-initio*, self-consistent density functional theory (DFT) calculations of electronic, transport, and bulk properties of *zinc blende* boron arsenide (zb-BAs). We utilized a local density approximation (LDA) potential and the linear combination of atomic orbital (LCAO) formalism. Our computational technique follows the Bagayoko, Zhao, and Williams method, as enhanced by Ekuma and Franklin. Our results include electronic energy bands, densities of states, and effective masses. We explain the agreement between these findings, including the indirect band gap, and available, corresponding, experimental ones. This work confirms the capability of DFT to describe accurately properties of materials, provided the computations adhere to the conditions of validity of DFT [AIP Advances, 4, 127104 (2014)]. Acknowledgments: This work was funded in part by the National Science Foundation (NSF) and the Louisiana Board of Regents, through LASiGMA [Award Nos. EPS- 1003897, NSF (2010-15)-RII-SUBR] and NSF HRD-1002541, the US Department of Energy – National, Nuclear Security Administration (NNSA) (Award No. DE- NA0002630), LaSPACE, and LONI-SUBR.

**3:06PM V51.00004 Ab-initio Density Functional Theory (DFT) Studies of Electronic, Transport, and Bulk Properties of Sodium Oxide (Na<sub>2</sub>O).** , DANIEL POLIN, Department of Physics New York University, New York, NY 10003, USA, JOSHUA ZIEGLER, Department of Physics Case Western Reserve University, Cleveland, OH 44106, USA., YURIY MALOZOVSKY, DIOLA BAGAYOKO, Department of Physics Southern University and AM College, Baton Rouge, LA 70813, USA. — We present the findings of *ab-initio* calculations of electronic, transport, and structural properties of cubic sodium oxide (Na<sub>2</sub>O). These results were obtained using density functional theory (DFT), specifically a local density approximation (LDA) potential, and the linear combination of Gaussian orbitals (LCAO). Our implementation of LCAO followed the Bagayoko, Zhao, and Williams method as enhanced by the work of Ekuma and Franklin (BZW-EF). We describe the electronic band structure of Na<sub>2</sub>O with a direct band gap of 2.22 eV. Our results include predicted values for the electronic band structure and associated energy eigenvalues, the total and partial density of states (DOS and pDOS), the equilibrium lattice constant of Na<sub>2</sub>O, and the bulk modulus. We have also calculated the electron and holes effective masses in the  $\Gamma$  to L,  $\Gamma$  to X, and  $\Gamma$  to K directions. Acknowledgments: This work was funded in part by the National Science Foundation (NSF) and the Louisiana Board of Regents, through LASiGMA [Award Nos. EPS- 1003897, NSF (2010-15)-RII-SUBR] and NSF HRD-1002541, the US Department of Energy – National, Nuclear Security Administration (NNSA) (Award No. DE- NA0002630), LaSPACE, and LONI-SUBR.

**3:18PM V51.00005 Hybrid DFT calculations of the band structure of alpha-Sn** , ERIN DUPAY<sup>1</sup>, LUCAS DOMULEVICZ<sup>2</sup>, HENRY CASTEJON<sup>3</sup>, AMJAD NAZZAL<sup>4</sup>, Wilkes Univ — The electronic properties of bulk alpha-tin were revisited using first principles. The band structure, in addition to other properties, such as the absorption spectrum and density of states, were calculated using Density Functional Theory and the HSE06 hybrid functional. The direct and indirect band gaps obtained from these calculations are in better agreement with experimental results than previously reported calculations.

<sup>1</sup>Graduate Student

<sup>2</sup>Undergraduate Student

<sup>3</sup>Faculty

<sup>4</sup>faculty

**3:30PM V51.00006 Ab-initio Calculation of Optoelectronic and Structural Properties of Cubic Lithium Oxide (Li<sub>2</sub>O).** , JOSHUA ZIEGLER, Department of Physics, Case Western Reserve University, Cleveland, OH 44106, USA, DANIEL POLIN, Department of Physics, New York University, New York City, NY 10003, USA, YURIY MALOZOVSKY, DIOLA BAGAYOKO, Department of Physics, Southern University and AM College, Baton Rouge, LA 70813, USA — Using the Bagayoko, Zhao, and Williams (BZW) method, as enhanced by Ekuma and Franklin (BZW-EF), we performed *ab-initio*, density functional theory (DFT) calculations of optoelectronic, transport, and bulk properties of Li<sub>2</sub>S. In so doing, we avoid “band gap” and problems plaguing many DET calculations [AIP Advances 4, 127104 (2014)]. We employed a local density approximation (LDA) potential and the linear combination of atomic orbitals (LCAO). With the BZW-EF method, our results possess the full, physical content of DFT and agree with available, corresponding experimental ones. In particular, we found a room temperature indirect band gap of 6.659 eV that compares favorably with experimental values ranging from 5 to 7.99 eV. We also calculated total and partial density of states (DOS and PDOS), effective masses of charge carriers, the equilibrium lattice constant, and the bulk modulus. Acknowledgments: This work was funded in part by the National Science Foundation (NSF) and the Louisiana Board of Regents, through LASiGMA [Award Nos. EPS- 1003897, NSF (2010-15)-RII-SUBR] and NSF HRD-1002541, the US Department of Energy – National, Nuclear Security Administration (NNSA) (Award Nos. DE-NA0001861 and DE- NA0002630), LaSPACE, and LONI-SUBR.

**3:42PM V51.00007 Comparisons of Accurate Electronic, Transport, and Bulk Properties of XP (X=B, Al, Ga, In).** , YURIY MALOZOVSKY, JOHN EJEMBI, Department of Physics Southern, University and AM College, Baton Rouge, LA 70813, USA, AZIZJON SALIEV, Department of Electrical and Computer Engineering, Binghamton University, NY 13902, USA, LASHOUNDA FRANKLIN, DIOLA BAGAYOKO, Department of Physics Southern, University and AM College, Baton Rouge, LA 70813, USA — We present comparisons of results from *ab-initio*, self-consistent local density approximation (LDA) calculations of accurate, electronic and related properties of zinc blende XP (X=B, Al, Ga, In) phosphides. We implemented the linear combination of atomic orbitals following the Bagayoko, Zhao, and Williams (BZW) method as enhanced by Ekuma and Franklin (BZW-EF). Consequently, our results have the full physical content of DFT and agree very well with corresponding experimental ones [AIP Advances, 4, 127104 (2014)]. Our calculated, indirect band gap of 2.02 eV for BP, 2.56 eV for AIP, and of 2.29 eV for GaP, from  $\Gamma$  to X-point, are in excellent agreement with experimental values. Our calculated direct band gap of 1.43 eV, at  $\Gamma$ , for InP is also in an excellent agreement with experimental value. We discuss calculated electron and hole effective masses, total (DOS) and partial (pDOS) densities of states, and the bulk modulus of these phosphides. Acknowledgments: NSF and the Louisiana Board of Regents, LASIGMA [Award Nos. EPS- 1003897, NSF (2010-15)-RII-SUBR] and NSF HRD-1002541, DOE – National, Nuclear Security Administration (NNSA) (Award Nos. DE-NA0001861 and DE- NA0002630), LaSPACE, and LONI-SUBR.

**3:54PM V51.00008 *Ab-initio* Calculations of Electronic Properties of Calcium Fluoride (CaF<sub>2</sub>)** , BIR BOHARA, LASHOUNDA FRANKLIN, YURIY MALOZOVSKY, DIOLA BAGAYOKO, Department of Physics, Southern University and AM College, Baton Rouge, LA 70813, USA — We have performed first principle, local density approximation (LDA) calculations of electronic and related properties of cubic calcium fluoride (CaF<sub>2</sub>). Our non-relativistic computations employed the Ceperley and Alder LDA potential and the linear combination of atomic orbitals (LCAO) formalism. The implementation of the LCAO formalism followed the Bagayoko, Zhao, and Williams (BZW) method, as enhanced by Ekuma and Franklin (BZW-EF). We discuss the electronic energy bands, including the large band gap, total and partial density of states, electron and hole effective masses, and the bulk modulus. Our calculated, indirect (X- $\Gamma$ ) band gap is 12.98 eV; it is 1 eV above an experimental value of 11.8 eV. The calculated bulk modulus (82.89 GPa) is excellent agreement with the experimental result of 82.0  $\pm$  0.7. Our predicted equilibrium lattice constant is 5.42Å. Acknowledgments: This work is funded in part by the National Science Foundation (NSF) and the Louisiana Board of Regents, through LASIGMA [Award Nos. EPS- 1003897, NSF (2010-15)-RII-SUBR], and NSF HRD-1002541, the US Department of Energy, National, Nuclear Security Administration (NNSA) (Award No. DE-NA-0002630), LaSPACE, and LONI-SUBR.

**4:06PM V51.00009 Direct detection of dark matter via single-electron excitations in semiconductors** , ROUVEN ESSIG, MARIVI FERNANDEZ-SERRA, Stony Brook University, JEREMY MARDON, Stanford University, ADRIAN SOTO, Stony Brook University, TOMER VOLANSKY, Tel Aviv University, TIEN-TIEN YU, Stony Brook University — Over the last several decades, there has been an enormous experimental effort to search for dark matter (DM). Traditionally, semiconductors have been used to detect DM via scattering with nuclei and the subsequent relaxation of the crystal. However, if DM has mass below order 10 GeV these methods lose detection sensitivity. This is because the DM is lighter than a typical nucleus and, since DM particles move at non-relativistic speeds, they cannot transfer enough energy and momentum to the crystal to produce observable signals. In our work [arXiv:1509.01598], we demonstrate that DM-electron scattering in semiconductors increases the sensitivity of DM detection in this mass regime by several orders of magnitude and is a viable avenue for the direct detection of sub-GeV DM. We use density functional theory (DFT) to calculate the crystal wavefunctions and the band energies, which we correct with an empirical scissor operator. These wavefunctions are used to do perturbation theory, which allows us to calculate the DM-electron scattering rates. In this talk we will focus on the computational and theoretical challenges, discuss future directions and present new expected limits for DM-electron scattering.

**4:18PM V51.00010 Raman spectra calculations for Si-Ge core-shell nanocrystals using *ab initio* real-space methods**<sup>1</sup> , N. SCOTT BOBBITT, JAMES R. CHELIKOWSKY, Univ of Texas, Austin — We use a real-space pseudopotential method within density functional theory to calculate Raman spectra for Si-Ge core-shell nanocrystals. We examine the lattice strain induced by the interface of the core and the shell. We calculate how this strain affects the vibrational modes and Raman spectra. We also find that the relative size of the Si and Ge peaks in the Raman spectrum is proportional to the size of the Si core and Ge shell regions, which suggests that Raman spectroscopy can be used to experimentally determine the relative size of the core and the outer shell in these nanocrystals.

<sup>1</sup>This work is supported by the DOE under grant number DE-FG02-06ER46286. Computations were performed on machines at TACC and NERSC.

**4:30PM V51.00011 *k.p* Parameters with Accuracy Control from Preexistent First-Principles Band Structure Calculations**<sup>1</sup> , GUILHERME SIPAHI, CARLOS M. O. BASTOS, FERNANDO P. SABINO, PAULO E. FARIA JUNIOR, TIAGO DE CAMPOS, JUAREZ L. F. DA SILVA, Universidade de So Paulo — The *k.p* method is a successful approach to obtain band structure, optical and transport properties of semiconductors. It overtakes the *ab initio* methods in confined systems due to its low computational cost since it is a continuum method that does not require all the atoms' orbital information. From an effective one-electron Hamiltonian, the *k.p* matrix representation can be calculated using perturbation theory and the parameters identified by symmetry arguments. The parameters determination, however, needs a complementary approach. In this paper, we developed a general method to extract the *k.p* parameters from preexistent band structures of bulk materials that is not limited by the crystal symmetry or by the model. To demonstrate our approach, we applied it to zinc blende GaAs band structure calculated by hybrid density functional theory within the Heyd-Scuseria-Ernzerhof functional (DFT-HSE), for the usual 8×8 *k.p* Hamiltonian. Our parameters reproduced the DFT-HSE band structure with great accuracy up to 20% of the first Brillouin zone (FBZ). Furthermore, for fitting regions ranging from 7-20% of FBZ, the parameters lie inside the range of values reported by the most reliable studies in the literature.

<sup>1</sup>The authors acknowledge financial support from the Brazilian agencies CNPq (grant #246549/2012-2) and FAPESP (grants #2011/19333-4, #2012/05618-0 and #2013/23393-8).

**4:42PM V51.00012 Transferable tight binding model for strained group IV and III-V heterostructures** , YAOHUA TAN, Dr, MICHEAL POVOLOTSKYI, TILLMANN KUBIS, TIMOTHY BOYKIN, GERHARD KLIMECK, Prof — Modern semiconductor devices have reached critical device dimensions in the range of several nanometers. For reliable prediction of device performance, it is critical to have a numerical efficient model that are transferable to material interfaces. In this work, we present an empirical tight binding (ETB) model with transferable parameters for strained IV and III-V group semiconductors. The ETB model is numerically highly efficient as it make use of an orthogonal sp<sup>3</sup>d<sup>5</sup>s\* basis set with nearest neighbor inter-atomic interactions. The ETB parameters are generated from HSE06 hybrid functional calculations. Band structures of strained group IV and III-V materials by ETB model are in good agreement with corresponding HSE06 calculations. Furthermore, the ETB model is applied to strained superlattices which consist of group IV and III-V elements. The ETB model turns out to be transferable to nano-scale hetero-structure. The ETB band structures agree with the corresponding HSE06 results in the whole Brillouin zone. The ETB band gaps of superlattices with common cations or common anions have discrepancies within 0.05eV.

**4:54PM V51.00013 Valley Physics in Tin (II) Sulfide**, ALEKSANDR RODIN, LIDIA GOMES, ALEXANDRA CARVALHO, ANTONIO CASTRO NETO, Natl Univ of Singapore — The field of 2D physics has experienced a rapid growth in recent years. Improved manipulation and growth techniques have resulted in isolation and characterization of novel materials with fascinating properties. A family of compounds that was described recently is transition metal monochalcogenides. Due to their non-trivial crystal structure, studying these materials is a challenging task. Using a combination of density functional theory (DFT) and analytical methods, we investigate the band structure of tin (II) sulfide, a naturally occurring material, to discover that SnS has two pairs of valleys positioned in perpendicular orientation to each other. DFT is employed to construct  $\mathbf{k} \cdot \mathbf{p}$  Hamiltonians around each of the valleys. Finally, we show that these individual valley pairs can be separated using linearly polarized light or by utilizing the nonlinear current response, making SnS a candidate for valleytronic applications.

**5:06PM V51.00014 Reduced-Density-Matrix Description of Single-Photon and Multi-Photon Processes in Quantized Many-Electron Systems<sup>1</sup>**, VERNE JACOBS, Naval Research Laboratory, ALEX KUTANA, Rice University — The frequency-dependent transition rates for single-photon and multi-photon processes in quantized many-electron systems are evaluated using a reduced-density-matrix approach. We provide a fundamental quantum-mechanical foundation for systematic spectral simulations. A perturbation expansion of the frequency-domain Liouville-space self-energy operator is introduced for detailed evaluations of the spectral-line shapes. In the diagonal-resolvent (isolated-line) and short-memory-time (Markov) approximations, the lowest-order contributions to the spectral-line widths and shifts associated with environmental electron-photon and electron-phonon interactions are systematically evaluated. Our description is directly applicable to electromagnetic processes in a wide variety of many-electron systems, without premature approximations. In particular, our approach can be applied to investigate quantum optical phenomena involving electrons in both bulk and nanoscale semiconductor materials entirely from first principles, using a single-electron basis set obtained from density functional theory as a starting point for a many-electron description.

<sup>1</sup>Work supported by the Office of Naval Research through the Basic Research Program at The Naval Research Laboratory. A portion of this work was performed under the ASEE post doc program at NRL.

**5:18PM V51.00015 Lifshitz Transitions in Bias-Resonant Twisted Bilayer Graphene**, STEVE CARTER, HRIDIS PAL, MARKUS KINDERMANN, Georgia Institute of Technology — Topological transitions of the Fermi surface (Lifshitz transitions) have been shown to cause discontinuities in materials properties. One such transition has been predicted to occur in AB-stacked bilayer graphene.<sup>[1]</sup> In this talk we discuss incommensurately twisted bilayer graphene with an interlayer bias energy.<sup>[2]</sup> New physics emerges when the bias energy is tuned into resonance with the kinetic energy cost of interlayer hopping due to the mismatch between the Dirac points of the twisted layers. We show that the system near resonance is described by relatively simple low-energy theories that nevertheless produce a vast number of Lifshitz transitions. An exhaustive description of the topological transitions in a universal regime at weak interlayer coupling will be presented. [1] Y. Lemonik et al. Phys. Rev. B, 82:201408 (2010). [2] H.K. Pal et al. arXiv:1409.1971 (2014).

## Thursday, March 17, 2016 2:30PM - 4:18PM – Session V53 DFD: Fluid Mechanics - General Hilton Baltimore Holiday Ballroom 4 -

**2:30PM V53.00001 Equivalence of Non-Equilibrium Ensembles and Representation of Friction in Turbulent Flows: The Lorenz '96 Model**, VALERIO LUCARINI, University of Hamburg, Hamburg, Germany, GIOVANNI GALLAVOTTI, Sapienza University of Roma — We construct different equivalent non-equilibrium ensembles in the Lorenz '96 model of atmospheric turbulence. The vector field can be decomposed into an energy-conserving, time-reversible part, plus a non-time reversible part, including forcing and dissipation. We construct a modified version of the model where viscosity varies with time, so that energy is conserved, and the dynamics is time-reversible. The statistical properties of the irreversible and reversible model are in excellent agreement, if in the latter the energy is kept constant at a value equal to the time-average realized with the irreversible model. The average contraction rate of the phase space of the time-reversible model agrees with that of the irreversible model, where it is constant by construction. We show that the phase space contraction rate obeys the fluctuation relation, and we interpret its finite time corrections. A local version of the fluctuation relation is explored and successfully checked. The equivalence between the two ensembles extends to the Lyapunov exponents. These results have relevance in motivating the importance of the chaotic hypothesis. In explaining that we have the freedom to model non-equilibrium systems using different but equivalent approaches.

**2:42PM V53.00002 Optimum design of vortex generator elements using Kriging surrogate modelling and genetic algorithm**, RITHWIK NEELAKANTAN, RAMAN BALU, ABHINAV SAJI, Ace College of Engineering — Vortex Generators (VGs) are small angled plates located in a span wise fashion aft of the leading edge of an aircraft wing. They control airflow over the upper surface of the wing by creating vortices which energise the boundary layer. The parameters considered for the optimisation study of the VGs are its height, orientation angle and location along the chord in a low subsonic flow over a NACA0012 airfoil. The objective function to be maximised is the L/D ratio of the airfoil. The design data are generated using the commercially available ANSYS FLUENT software and are modelled using a Kriging based interpolator. This surrogate model is used along with a Generic Algorithm software to arrive at the optimum shape of the VGs. The results of this study will be confirmed with actual wind tunnel tests on scaled models.

**2:54PM V53.00003 Predicting the Noise of High Power Fluid Targets Using Computational Fluid Dynamics**, MICHAEL MOORE, Jefferson Lab, Old Dominion University, SILVIU COVRIG DUSA, Jefferson Lab — The 2.5 kW liquid hydrogen (LH2) target used in the  $Q_{weak}$  parity violation experiment is the highest power LH2 target in the world and the first to be designed with Computational Fluid Dynamics (CFD) at Jefferson Lab. The  $Q_{weak}$  experiment determined the weak charge of the proton by measuring the parity-violating elastic scattering asymmetry of longitudinally polarized electrons from unpolarized liquid hydrogen at small momentum transfer ( $Q^2 = 0.025 \text{ GeV}^2$ ). This target satisfied the design goals of  $< 1\%$  luminosity reduction and  $< 5\%$  contribution to the total asymmetry width (the  $Q_{weak}$  target achieved  $2\%$  or 55ppm). State of the art time dependent CFD simulations are being developed to improve the predictions of target noise on the time scale of the electron beam helicity period. These predictions will be bench-marked with the  $Q_{weak}$  target data. This work is an essential component in future designs of very high power low noise targets like MOLLER (5 kW, target noise asymmetry contribution  $< 25 \text{ ppm}$ ) and MESA (4.5 kW).

### 3:06PM V53.00004 Fluid Dynamical Consequences of Current and Stress-Energy Conservation

, DILLON SCOFIELD, Dept Physics, Oklahoma State University, PABLO HUQ, College of Earth, Ocean, and Environment, Univ. Delaware — The dynamical consequences of fluid current conservation combined with the conservation of fluid stress-energy are used to develop the geometrodynamical theory of fluid flow (GTF). In the derivation of the GTF, we highlight the fact the continuity equation, equivalently the conservation of current density, implies the existence of the fluid dynamical vortex field. The vortex field transports part of the stress-energy; the other part of the stress-energy is transported by the fluid inertia field. Two channels of energy dissipation are determined by the GTF. One is an analog of the Joule heating found in electrodynamics. This follows from the conservation of stress-energy. The other dissipation channel arises from mechanisms leading to complex-valued constitutive parameters described in the electrodynamical analogy as due to a lossy medium. The dynamical consequences of the continuity equation, combined with the conservation of total stress-energy, then lead to a causal, covariant, theory of fluid flow, consistent with thermodynamics for all physically possible flow rates.

### 3:18PM V53.00005 The Geometry and Dynamics of a Propagating Front in a Chaotic Flow

Field, MARK PAUL, Virginia Tech — There are many important problems regarding transport in complex fluid flows with implications in science, nature, and technology. Examples include the combustion of pre-mixed gases in a turbulent flow, the complex patterns of reagents in a chemical system, the spread of a forest fire, and the outbreak of an epidemic. This talk explores the transport and dynamics of a reacting species in a chaotic fluid flow field. Large-scale parallel numerical simulations are used to explore the dynamics of propagating fronts in complex three-dimensional time-dependent fluid flows for the precise conditions of the laboratory. It is shown that a chaotic flow field enhances the front propagation when compared with a purely cellular flow field. This enhancement is quantified by computing measures of the spreading rate of the products and by quantifying the complexity of the three-dimensional front geometry for a range of chaotic flow conditions.

### 3:30PM V53.00006 Surface Acoustic Wave Transport and Mixing in Fluids in an Enclosed

Nanoslit, MORTEZA MIANSARIGAVZAN, JAMES FRIEND, University of California, San Diego — Non-laminar fluid flow was generated in a nanoslit using 20 MHz surface acoustic waves. A novel acoustic nanofluidic device was fabricated by a unique room-temperature, high-strength bonding method combining a 128-YX lithium niobate (LN) substrate with a second LN substrate containing a 1-cm long, 50–300-nm thick, 400  $\mu\text{m}$ -wide planar nanoslit. The nanoslit was verified to be extremely smooth (roughness  $< 5$  nm) and possess a uniformly rectangular shape. Despite an exceptionally low ( $\sim 10^{-5}$ ) hydrodynamic Reynolds number within the nanoslit, acoustic streaming induced by the SAW is found to drive filling of the *hydrophilic* nanoslit greatly in excess of the typical Washburn capillary filling rate, a unique ability to completely *drain* the hydrophilic nanoslit of fluid, induce rapid mixing of fluid within, and drive nanoparticle and early evidence of molecular separation from the fluid at the nanoslit exit as the fluid passes through. The unique physical phenomena may prove to be useful across a broad range of applications where it facilitates the use of nanofluidics in chemistry and medicine. It illuminates an extraordinary ability to use sound at ever smaller scales to manipulate fluids and particles within in unexpected ways.

### 3:42PM V53.00007 Electroosmotic Entry Flow with Joule Heating Effects.

, RAMA PRABHAKARAN, AKSHAY KALE, XIANGCHUN XUAN, Clemson University — Electrokinetic flow, which transports liquids by electroosmosis and samples by electrophoresis, is the transport method of choice in microfluidic chips over traditional pressure-driven flows. Studies on electrokinetic flows have so far been almost entirely limited to inside microchannels. Very little work has been done on the electroosmotic fluid entry from a reservoir to a microchannel, which is the origin of all fluid and sample motions in microchips. We demonstrate in this talk that strong vortices of opposite circulating directions can be generated in electroosmotic entry flows. We also develop a two-dimensional depth-averaged numerical model of the entire microchip to predict and understand the fluid temperature and flow fields at the reservoir-microchannel junction.

### 3:54PM V53.00008 Accounting for anomalous energy-dissipation in guided flows

, PABLO HUQ, College Earth, Ocean, and Environment, Univ. Delaware, DILLON SCOFIELD, Dept. of Physics, Oklahoma State University — The Navier-Stokes theory significantly underestimates energy-dissipation in time-dependent flows through flow guides such as ones with helical geometry. We show the geometrodynamical theory of fluids (GTF) accounts for this anomalous energy-dissipation by predicting the excitation of transverse modes of flow leading to such dissipation. According to the GTF, the transverse modes are composed of vorticity and swirl fields which together constitute a vortex field  $F$  which is a function of the swirl and vorticity fields. Analysis shows the energy-dissipation depends on the wave energy, the dot product of the swirl and the vorticity, as well as their cross product. These lead to heating of the fluid at a rate proportional to the work the current does against the swirl field. For the constitutive parameters of the theory we find the values for water to be  $\lambda = 0.01/(\text{cm/s})$ , and  $\kappa = 1$  [unitless]. A lower bound for the effective value of the speed of the first transverse modes is found to be 90 cm/sec. We determine that a dimensionless vortex number,  $R_v$ , usefully delineates the excitation of the transverse mode flow regime.

### 4:06PM V53.00009 Effect of Curvature Parameter on Non-Darcy Mixed Convective Flow in a Vertical Annulus: A LTNE Approach

, MOUMITA BHOWMIK, PREMANANDA BERA, Indian Institute of Technology Roorkee — The influence of curvature parameter on fully developed mixed convective flow in a vertical annulus filled with porous medium under local thermal non-equilibrium (LTNE) state has been addressed here. Since the curvature parameter ( $C$ ) describes the size of the enclosure, therefore the main emphasize is given to understand its impact on other controlling parameters. Based on computational results,  $C$  has a significant impact on both heat transfer rate as well as flow profiles for stably stratified flow. It has a tendency to reduce the magnitude of the maximum velocity. It is also observed that depending on other parameters, increment in  $C$  may have tendency to make the velocity profile free from back flow. The heat transfer rate is obtained maximum at a small value of  $C$  which is independent of media permeability and converges asymptotically on increasing  $C$ . At the end, the linear stability analysis based on normal mode technique has been used to verify the results obtained from basic flow study. Overall, from both basic flow as well as linear stability results, it is found that increment in  $C$  makes the flow profile smooth which means  $C$  has tendency to stabilize the flow.

**Thursday, March 17, 2016 2:30PM - 5:30PM –**

Session V55 DBIO GSNP DPOLY: DNA Physics and Chromatin Organization Hilton Baltimore Holiday Ballroom 6 - Alexandre V. Morozov, Rutgers University

## 2:30PM V55.00001 Micromechanical study of protein-DNA interactions and chromosomes<sup>1</sup>

JOHN MARKO<sup>2</sup>, Northwestern University — I will discuss micromechanics experiments that our group has used to analyze protein-DNA interactions and chromosome organization. In single-DNA experiments we have found that a feature of protein-DNA complexes is that their dissociation rates can depend strikingly on bulk solution concentrations of other proteins and DNA segments; I will describe experiments which demonstrate this effect, which can involve tens-fold changes in off-rates with submicromolar changes in solution concentrations. Second, I will discuss experiments aimed at analyzing large-scale human chromosome structure; we isolate metaphase chromosomes, which in their native form behave as remarkably elastic networks of chromatin. Exposure to DNA-cutting restriction enzymes completely eliminates this elasticity, indicating that there is not a mechanically contiguous protein "scaffold" from which the chromosome gains its stability. I will show results of siRNA experiments indicating that depletion of condensin proteins leads to destabilization of chromosome mechanics, indicating condensin's role as the major chromatin "cross-linker" in metaphase chromosomes. Finally I will discuss similar experiments on human G1 nuclei, where we use genetic and chemical modifications to separate the contributions of the nuclear lamina and chromatin to the mechanical stiffness of the nucleus as a whole.

<sup>1</sup>Supported by the NSF (DMR-1206868, MCB-1022117) and the NIH (GM105847, CA193419).

<sup>2</sup>I'd like to present my talk from my laptop (movies)

## 3:06PM V55.00002 Polymer models of chromosome (re)organization, LEONID MIRNY, MIT — Chromosome

Conformation Capture technique (Hi-C) provides comprehensive information about frequencies of spatial interactions between genomic loci. Inferring 3D organization of chromosomes from these data is a challenging biophysical problem. We develop a top-down approach to biophysical modeling of chromosomes. Starting with a minimal set of biologically motivated interactions we build ensembles of polymer conformations that can reproduce major features observed in Hi-C experiments. I will present our work on modeling organization of human metaphase and interphase chromosomes. Our works suggests that active processes of loop extrusion can be a universal mechanism responsible for formation of domains in interphase and chromosome compaction in metaphase.

## 3:42PM V55.00003 Action at a Distance in the Cell's Nucleus<sup>1</sup>, JANE KONDEV, Brandeis University — Various

functions performed by chromosomes involve long-range communication between DNA sequences that are tens of thousands of bases apart along the genome, and microns apart in the nucleus. In this talk I will discuss experiments and theory relating to two distinct modes of long-range communication in the nucleus, chromosome looping and protein hopping along the chromosome, both in the context of DNA-break repair in yeast. Yeast is an excellent model system for studies that link chromosome conformations to their function as there is ample experimental evidence that yeast chromosome conformations are well described by a simple, random-walk polymer model. Using a combination of polymer physics theory and experiments on yeast cells, I will demonstrate that loss of polymer entropy due to chromosome looping is the driving force for homology search during repair of broken DNA by homologous recombination. I will also discuss the spread of histone modifications along the chromosome and away from the DNA break point in the context of simple physics models based on chromosome looping and kinase hopping, and show how combining physics theory and cell-biology experiment can be used to dissect the molecular mechanism of the spreading process. These examples demonstrate how combined theoretical and experimental studies can reveal physical principles of long-range communication in the nucleus, which play important roles in regulation of gene expression, DNA recombination, and chromatin modification.

<sup>1</sup>This work was supported by the NSF DMR-1206146

## 4:18PM V55.00004 How, when, and where in pattern formation: Spying on embryonic development one molecule at a time., HERNAN GARCIA, Univ of California - Berkeley — An abiding mystery in the study of living matter

is how a single cell develops into a multicellular organism. As this cell divides, its progeny read the program encoded on their DNA and adopt different fates becoming familiar cell types such as those found in muscle, liver and our brains. We now know that the decisions that cells make during development are not so much based on which genes to express, but rather on when, where and how to express them. Despite advances in determining the identities of the molecules that mediate these decisions we are still incapable of predicting how simple physical parameters such as the number, position and affinity of binding sites for these molecules on the DNA determine developmental fates. Using the fruit fly, one of the classic model systems for embryonic development, I will show how a combination of new technologies, quantitative experiments, and statistical mechanics is providing new insights about cellular decision making during development. In particular, I will describe how the specification of macroscopic body parts in an organism is linked to the non-equilibrium molecular-scale processes inside single cells. The goal of this interdisciplinary research is to produce a predictive understanding of developmental programs which will enable the rational control of biological size, shape and function.

## 4:54PM V55.00005 Energy Landscapes of Folding Chromosomes, BIN ZHANG, Rice University — The genome,

the blueprint of life, contains nearly all the information needed to build and maintain an entire organism. A comprehensive understanding of the genome is of paramount interest to human health and will advance progress in many areas, including life sciences, medicine, and biotechnology. The overarching goal of my research is to understand the structure-dynamics-function relationships of the human genome. In this talk, I will be presenting our efforts in moving towards that goal, with a particular emphasis on studying the three-dimensional organization, the structure of the genome with multi-scale approaches. Specifically, I will discuss the reconstruction of genome structures at both interphase and metaphase by making use of data from chromosome conformation capture experiments. Computationally modeling of chromatin fiber at atomistic level from first principles will also be presented as our effort for studying the genome structure from bottom up.

## Friday, March 18, 2016 8:00AM - 10:24AM —

Session X1 DCMP GMAG: Complex Oxide Interfaces at the Nanoscale: Electronic, Magnetic and Superconducting Properties Ballroom I - Chang-Beom Eom, University of Wisconsin-Madison

## 8:00AM X1.00001 Electron pairing without superconductivity<sup>1</sup>, JEREMY LEVY, University of Pittsburgh —

Strontium titanate (SrTiO<sub>3</sub>) is the first and best known superconducting semiconductor. It exhibits an extremely low carrier density threshold for superconductivity, and possesses a phase diagram similar to that of high-temperature superconductors—two factors that suggest an unconventional pairing mechanism. Despite sustained interest for 50 years, direct experimental insight into the nature of electron pairing in SrTiO<sub>3</sub> has remained elusive. Here we perform transport experiments with nanowire-based single-electron transistors at the interface between SrTiO<sub>3</sub> and a thin layer of lanthanum aluminate, LaAlO<sub>3</sub>. Electrostatic gating reveals a series of two-electron conductance resonances—paired electron states—that bifurcate above a critical pairing field  $B_p$  of about 1–4 tesla, an order of magnitude larger than the superconducting critical magnetic field. For magnetic fields below  $B_p$ , these resonances are insensitive to the applied magnetic field; for fields in excess of  $B_p$ , the resonances exhibit a linear Zeeman-like energy splitting. Electron pairing is stable at temperatures as high as 900 millikelvin, well above the superconducting transition temperature (about 300 millikelvin). These experiments demonstrate the existence of a robust electronic phase in which electrons pair without forming a superconducting state. Key experimental signatures are captured by a model involving an attractive Hubbard interaction that describes real-space electron pairing as a precursor to superconductivity.

<sup>1</sup>Support from AFOSR, ONR, ARO, NSF, DOE and NSSEFF is gratefully acknowledged.

**8:36AM X1.00002 Magnetic coupling through lanthanum nickelate in non-metallic (111)  $\text{LaMnO}_3/\text{LaNiO}_3$  superlattices**, JEAN-MARC TRISCON, DQMP, University of Geneva — Perovskite nickelates ( $\text{RNiO}_3$ , RE = Rare Earth) are fascinating materials, well known for their metal to insulator transition (MIT) and unique antiferromagnetic (AFM) ground state [1]. In this presentation, I will first discuss how one can control the MIT and the magnetic properties of high quality epitaxial nickelate films through a variety of techniques [2-6]. I will then describe our work on heterostructures containing  $\text{LaNiO}_3$  – the only member of the family that is metallic and paramagnetic in the bulk down to low temperature – and ferromagnetic  $\text{LaMnO}_3$ . In this system we observed an unusual exchange bias in [111] oriented  $(\text{LaNiO}_3)/(\text{LaMnO}_3)$  superlattices [7] and an antiferromagnetic interlayer exchange coupling above the blocking temperature of the exchange biased state specifically in 7 unit cells  $\text{LaNiO}_3$ / 7 unit cells  $\text{LaMnO}_3$  superlattices. The antiferromagnetic coupling is attributed to the presence of a  $(1/4, 1/4, 1/4)$  wavelength AFM structure in  $\text{LaNiO}_3$ . The complex exchange bias observed in this  $(\text{LaNiO}_3)/(\text{LaMnO}_3)$  system is explained in this context also considering the presence of two types of interfaces [8]. [1] M.L. Medarde, Journal of Physics: Condensed Matter, 9, 1679 (1997). [2] R. Scherwitzl et al., Advanced Materials 22, 5517 (2010). [3] S. Catalano et al., Appl. Phys. Lett. Mat. 2, 116110 (2014). [4] S. Catalano et al., Appl. Phys. Lett. Mat. 3, 062506 (2015). [5] A. Caviglia et al., Phys. Rev. Lett. 108, 136801 (2012). [6] M. Först et al., Nat. Mat. 14, 883 (2015). [7] M. Gibert et al., Nat. Mat. 11, 195 (2012). [8] M. Gibert et al., Nanoletters in press (2015).

**9:12AM X1.00003 Emergent nanoscale superparamagnetism at oxide interfaces**, ELI ZELDOV, Weizmann Institute of Science — Atomically sharp oxide heterostructures exhibit a range of novel physical phenomena that do not occur in the parent bulk compounds. The most prominent example is the appearance of highly conducting and superconducting states at the interface between the band insulators  $\text{LaAlO}_3$  and  $\text{SrTiO}_3$ . We present a new emergent phenomenon at the  $\text{LaMnO}_3/\text{SrTiO}_3$  interface in which an antiferromagnetic insulator abruptly transforms into a superparamagnetic state. Above a critical thickness of  $\text{LaMnO}_3$  of five unit cells, our scanning nanoSQUID-on-tip microscopy [1] shows spontaneous formation of isolated magnetic islands with in-plane moment of  $10^4$  to  $10^5 \mu_B$  with characteristic diameter of 10 to 50 nm [2]. The nanoscale islands display superparamagnetic dynamics of random moment reversals by thermal activation or in response to an in-plane magnetic field [1]. We propose a charge reconstruction model of the polar  $\text{LaMnO}_3/\text{SrTiO}_3$  heterostructure which describes a sharp emergence of thermodynamic phase separation leading to nucleation of metallic ferromagnetic islands in an insulating antiferromagnetic matrix. The model suggests that a gate tunable superparamagnetic-ferromagnetic transition can be induced, holding potential for applications in magnetic storage and spintronics. [1] D. Vasyukov et al., Nature Nanotechnology 8, 639 (2013). [2] Y. Anahory, L. Embon, C. J. Li, S. Banerjee, A. Meltzer, H. R. Naren, A. Yakovenko, J. Cuppens, Y. Myasoedov, M. L. Rappaport, M. E. Huber, K. Michaeli, T. Venkatesan, and E. Zeldov, arXiv:1509.01895

**9:48AM X1.00004 Spatially resolved ultrafast magnetic dynamics initiated at a complex oxide heterointerface.**, ANDREA CAVIGLIA, Kavli Institute of Nanoscience TU Delft — Static strain in complex oxide heterostructures has been extensively used to engineer electronic and magnetic properties at equilibrium. In the same spirit, deformations of the crystal lattice with light may be used to achieve functional control across heterointerfaces dynamically. Here, by exciting large-amplitude infrared-active vibrations in a  $\text{LaAlO}_3$  substrate we induce magnetic order melting in a  $\text{NdNiO}_3$  film across a heterointerface. Femtosecond resonant soft X-ray diffraction is used to determine the spatiotemporal evolution of the magnetic disordering. We observe a magnetic melt front that propagates from the substrate interface into the film, at a speed that suggests electronically driven motion. Light control and ultrafast phase front propagation at heterointerfaces may lead to new opportunities in optomagnetism.

**Friday, March 18, 2016 8:00AM - 11:00AM –**

**Session X2 DCMP DAMOP: Recent Advances in Many Body Localization** Ballroom II - Christopher Laumann, University of Washington

**8:00AM X2.00001 A rigorous result on many-body localization**, JOHN IMBRIE, University of Virginia — The mathematical theory of many-body localization is in its infancy. Lack of thermalization is associated with the existence of a complete set of quasi-local integrals of motion. I will discuss a proof that a particular one-dimensional spin chain with random local interactions exhibits many-body localization. The proof depends on a physically reasonable assumption that limits the amount of level attraction in the system. In a KAM-style construction, a sequence of local unitary transformations is used to diagonalize the Hamiltonian and connect the exact many-body eigenfunctions to the original basis vectors. This provides an explicit construction of integrals of motion via convergent expansions.

**8:36AM X2.00002 Many-body localization: Entanglement and efficient numerical simulations**, FRANK POLLMANN, Max Planck Institute for the Physics of Complex Systems — Many-body localization (MBL) occurs in isolated quantum systems when Anderson localization persists in the presence of finite interactions. To understand this phenomenon, the development of new efficient numerical methods to find highly excited many-body eigenstates is essential. In this talk, we will discuss two complementary approaches to simulate MBL systems: First, we introduce a variant of the density-matrix renormalization group (DMRG) method that obtains individual highly excited eigenstates of MBL systems to machine precision accuracy at moderate to large disorder. This method explicitly takes advantage of the local spatial structure and the low entanglement which is characteristic for MBL eigenstates. Second, we propose an approach to directly find an approximate compact representation of the diagonalizing unitary by using a variational unitary matrix-product operator.

**9:12AM X2.00003 Dynamical Response of Many-Body Localized Systems**, VEDIKA KHEMANI, Princeton University — Many-body localization (MBL) is the long sought-after generalization of Anderson localization to interacting systems. Many-body localized systems fail to thermalize, and display a variety of novel properties and phases that have no equilibrium analog. In this talk, I will review our rapidly evolving understanding of the MBL phase before describing the eigenstate properties and dynamical response of these phases in some detail. In particular, I will show how a slow local perturbation surprisingly induces a highly non-local charge response despite the localized nature of the phase. This effect lies beyond linear response theory and has implications for numerous fields, including topological quantum computation in quantum Hall systems and quantum control in disordered environments. I will also discuss the low-frequency Kubo conductivity of MBL systems, and discuss the crossover from the linear to the non-linear response regime with an emphasis on the time-scales and amplitudes of the drive.

**9:48AM X2.00004 Universal dynamics across many-body localization phase transition** , MAKSYM SERBYN, Univ of California - Berkeley — Many body localization allows quantum systems to evade thermalization owing to the emergence of extensive number of local conserved quantities [1,2]. Many-body localized (MBL) systems exhibit universal dynamics, qualitatively distinct from dynamics in ergodic systems. In this talk I will survey recent progress in understanding the properties of the MBL phase, which follow from the picture of local conserved quantities. In particular, I will discuss the power-law relaxation of local observables [3], which gives an experimentally observable signatures of the MBL phase. In the second part of my talk, I will demonstrate how the delocalization transition can be probed by characterizing the breakdown of local conservation laws. Using statistics of matrix elements of local operators, I will introduce an analogue of many-body Thouless conductance which probes the response of the system to local perturbations [4]. Its scaling allows one to locate the MBL transition, and predicts the onset of logarithmically slow transport at the MBL transition, consistent with results from the renormalization group [5,6]. In addition, I will demonstrate how the properties of matrix elements govern the crossover of the level statistics across the MBL transition, and relate to the dynamics in the ergodic phase. I will conclude by discussing experimental implications and open challenges in understanding the MBL transition.

[1] M. Serbyn, Z. Papic, D. A. Abanin, Phys. Rev. Lett. 110, 260601 (2013); Phys. Rev. Lett. 111, 127201 (2013).

[2] D. A. Huse, V. Oganesyan, Phys. Rev. B 90, 174202 (2014).

[3] M. Serbyn, Z. Papic, D. A. Abanin, Phys. Rev. B 90, 174302 (2014).

[4] M. Serbyn, Z. Papic, D. A. Abanin, arXiv: 1507.01635.

[5] R. Vosk, D. A. Huse, E. Altman, Phys. Rev. X 5, 031032 (2015).

[6] A. C. Potter, R. Vasseur, S. A. Parameswaran, Phys. Rev. X 5, 031033 (2015).

**10:24AM X2.00005 Many-body localisation of interacting fermions in a quasi-random optical lattice** , IMMANUEL BLOCH, Max Planck Institute of Quantum Optics — We experimentally observe many-body localization (MBL) of interacting fermions in a one-dimensional quasi-random optical lattice. We identify the many-body localization transition through the relaxation dynamics of an initially-prepared charge density wave. For sufficiently weak disorder the time evolution appears ergodic and thermalizing, erasing all remnants of the initial order. In contrast, above a critical disorder strength a significant portion of the initial ordering persists, thereby serving as an effective order parameter for localization. The stationary density wave order and the critical disorder value show a distinctive dependence on the interaction strength, in agreement with numerical simulations. I will also present recent results on the fate of an MBL system upon coupling to the environment through photon scattering or by coupling identical 1d systems. Finally, progress to observe MBL in a 2d setting of interacting bosons will be presented that can provide a new route for identifying and characterizing the MBL phase transition

**Friday, March 18, 2016 8:00AM - 11:00AM –**

**Session X3 DCMP GSOF: Design, Characterization and Assembly of Hyperuniform Materials**

Ballroom III - Dreyfus Remi, CNRS

**8:00AM X3.00001 Ensemble Theory for Stealthy Hyperuniform Disordered Ground States** , SALVATORE TORQUATO, Princeton University — Disordered hyperuniform many-particle systems [1] have been receiving recent attention because they are distinguishable exotic states of matter poised between a crystal and liquid that are endowed with novel thermodynamic and physical properties. It has been shown numerically that systems of particles interacting with “stealthy” bounded, long-ranged pair potentials (similar to Friedel oscillations) have classical ground states that are, counterintuitively, disordered, hyperuniform and highly degenerate. The task of formulating an ensemble theory that yields analytical predictions for the structural characteristics and other properties of stealthy degenerate ground states in d-dimensional Euclidean space is highly nontrivial because the dimensionality of the configuration space depends on the number density and there is a multitude of ways of sampling the ground-state manifold, each with its own probability measure for finding a particular ground-state configuration. A new type of statistical-mechanical theory had to be invented to characterize these exotic states of matter. I report on some initial progress that we have made in this direction [2]. We show that stealthy disordered ground states behave like “pseudo”-equilibrium hard-sphere systems in Fourier space. Our theoretical predictions for the structure and thermodynamic properties of the stealthy disordered ground states and associated excited states are in excellent agreement with computer simulations across dimensions. [1] Torquato and F. H. Stillinger, Local Density Fluctuations, Hyperuniform Systems, and Order Metrics, Physical Review E, 68, 041113 (2003); [2] S. Torquato, G. Zhang, and F. H. Stillinger, Ensemble Theory for Stealthy Hyperuniform Disordered Ground States, Physical Review X, 5, 021020 (2015).

**8:36AM X3.00002 Hyperuniformity Disorder Length Spectroscopy - Method and Applications** , DOUGLAS DURIAN, University of Pennsylvania — The original idea is that fluctuations in a hyperuniform system are controlled by particles on the surface of the measuring windows [Torquato and Stillinger, PRE 2003]. But particles live in a volume; therefore, we introduce a “hyperuniformity disorder length”  $h(L)$  such that the relevant particles are within a distance  $h(L)$  of the  $L^d$  measuring window boundaries. Then the asymptotic volume fraction variance scaling becomes dimensionally correct as  $\sigma_\phi^2(L) \propto \langle v \rangle h(L)/L^{d+1}$  where  $\langle v \rangle$  is the average particle volume. After giving the technical definition of  $h(L)$ , I'll discuss two bounds, and I'll show simulation results for crystal vacancy and Einstein patterns to help build intuition for scaling of  $h(L) \sim L$  in systems with liquid-like fluctuations and as  $h(L) = \text{constant}$  in strongly hyperuniform systems. Then, in terms of the real-space spectrum of  $h(L)$  versus  $L$ , I'll show how different kinds of packings become increasingly uniform on approach to jamming and reach hyperuniformity at jamming. An important theme is to bring meaning to the value, as well as the scaling, of density fluctuations. Various parts of this work are in collaboration with A. Chieco, R. Dreyfus, C. Goodrich, A.J. Liu, and S. Torquato.

**9:12AM X3.00003 Unusual Fluctuations in Absorbing State Models** , HEXNER DANIEL, Technion — No abstract available.

**9:48AM X3.00004 Emergent Hyperuniformity in Periodically Driven Emulsions** , DENIS BARTOLO, ENS Lyon — I will discuss the self-organization of microfluidic emulsions into anomalously homogeneous structures. Upon periodic driving confined emulsions undergo a first-order transition from a reversible to an irreversible dynamics. We evidence that this dynamical transition is accompanied by structural changes at all scales yielding macroscopic yet finite hyperuniform structures. Numerical simulations are performed to single out the very ingredients responsible for the suppression of density fluctuations. We show that, as opposed to equilibrium systems, the long-range nature of the hydrodynamic interactions are not required for the formation of hyperuniform patterns, thereby suggesting a robust relation between reversibility and hyperuniformity which should hold in a broad class of periodically driven materials.

**10:24AM X3.00005 Hyperuniform disordered photonic bandgap materials, from microwave to infrared wavelength regime.**<sup>1</sup> , WEINING MAN, SFSU — Recently, we have introduced a new class of hyperuniform disordered (HUD) photonic bandgap (PBG) materials enabled by a novel constrained optimization method for engineering the material's Fourier transform to be continuous, isotropic and stealthy. Their structure factor  $S(k)$  is equal to zero for small  $k$  and exhibits a broad ring of maximum values around a characteristic wave-length range. Experimentally, an isotropic complete PBG (at all angles and for all polarizations) in an alumina-based HUD structure and single-polarized PBGs for plastic-based HUD structure have been demonstrated. Using measured and simulated transmission and phase delay information through these HUD structures, we also unfolded their band structures and reconstructed the effective dispersion relations of propagating electromagnetic modes in them. The intrinsic isotropy in these disordered structures is an inherent advantage associated with the lack of crystalline order, offering unprecedented freedom for functional defect design impossible to achieve in photonic crystals. In the microwave regime, we have shown the creation of freeform waveguides, which can channel photons robustly along arbitrarily curved paths and around sharp bends, and be decorated with defects to produce sharply resonant structures useful for filtering and frequency splitting. Recent simulation and experimental results for waveguides and modulators based on submicron-scale planar hyperuniform disordered PBG structures further highlight their ability to serve as highly compact, flexible and energy-efficient platforms for photonic integrated circuits.

<sup>1</sup>NSF DMR-1308084, EPSRC (UK) DTG Grant KD5050, EPSRC (UK) Strategic Equipment Grant EP/M008576/1, NSF SBIR-1345168, NSF MRI-1040444

**Friday, March 18, 2016 8:00AM - 11:00AM –**

**Session X4 DPOLY: From Polymer Topology to Performance Materials** Ballroom IV - Chinedum Osuji, Yale University

**8:00AM X4.00001 Continuous Liquid Interface Production (CLIP)** , JOHN TUMBLESTON, Carbon3D, Inc. —

Continuous liquid interface production (CLIP) can rapidly produce 3D parts using a range of polymeric materials. A DLP-based form of additive manufacturing, CLIP proceeds via projecting a sequence of UV images through an oxygen-permeable, UV-transparent window below a liquid resin bath. A thin uncured liquid layer, or dead zone, is created above the window and maintains a liquid interface below the advancing part. Above the dead zone, the curing part is drawn out of the resin bath creating suction forces that renew reactive liquid resin. The dead zone is created due to oxygen inhibition of photopolymerization, a process that is traditionally a nuisance in other photopolymerization applications. However, for CLIP oxygen inhibition and creation of the dead zone allows for a continuous mode of printing where UV exposure, resin renewal, and part elevation are conducted simultaneously. This continual process is fundamentally different from traditional bottom-up stereolithography printers where these steps must be conducted in separate and discrete steps. Furthermore, the relatively gentle nature of CLIP due to the established dead zone enables the use of unique materials with a wide range of mechanical properties. This presentation will showcase the CLIP technology and provide a detailed picture of interactions between different resin and process parameters. New applications for 3D printing that span the micro- to macro-scale enabled by CLIP's combination of unique materials and part production speed will also be presented.

**8:36AM X4.00002 Polymer Grafted Nanoparticle Assemblies: From Optical to Mechanical Performance through Clusters, Monolayers and Monoliths**<sup>1</sup> , RICHARD VAIA, Air Force Research Laboratory — Solution or melt-based fabrication of large area, matrix-free, ordered assemblies of polymer grafted nanoparticles (PGN) will enable additive manufacturing of novel membrane, electronic, and photonic elements. Due to the single component nature of these hybrids, aggregation and phase separation common in blended polymer nanocomposites are avoided. Architecturally, PGNs combine characteristics of colloids, brushes and high molecular weight polymers. Thus the processing-structure-property relationship of the entangled PGN assembly is unique from analogous condensed nano-structures, such as ligand stabilized nanoparticles, hard-sphere colloids, star macromolecules and linear chain – nanoparticle blends. Here in, we will discuss the intermediate character of PGNs with respect to deformability, physical aging, and rapid fabrication of stable, large-area, ordered PGN monolayers. For example, processing via flow coating follows that of classic colloids; however local structure and order within the PGN assembly is determined by the canopy architecture and substrate interactions. From this insight, large-area (cm<sup>2</sup>), highly-ordered, monolayer polystyrene-Au nanoparticle films that are resistant to de-wetting can be fabricated on substrates with high interface energy (80 mN/m) within seconds using flow-coating and a volatile solvent (THF). Overall these findings imply intriguing parallels between PGN assemblies and other mesoscale ordered polymeric systems including hard-soft block copolymers and semi-crystalline polymers. With the appropriate corona architecture, PGNs afford opportunities to design high inorganic fraction hybrids that retain processibility and enable the creation of films and fibers for next generation optoelectronic applications.

<sup>1</sup>Aknowledgement: Justin Che, Christopher A. Grabowski, Yang Jiao, Ming-Siao Hsiao, Kyoungweon Park, Lawrence Drummy

**9:12AM X4.00003 Translating polymer physics from the lab to the field** , JAN GENZER, North Carolina State Univ — Recent years witnessed increased activity in the application of fundamental principles of polymer physics and polymer chemistry in helping solve pressing environmental issues using eco-friendly approaches. We will describe examples of two polymer material platforms, i.e., surface-anchored polymer grafts and silicone elastomers, and their utilization in 1) minimizing non-specific bioadsorption, and 2) removal of metals/toxins and volatile organic compounds (VOCs) from contaminated waters. Optimal performance of such materials requires detailed knowledge and tunability of their chemical composition and topology. We will demonstrate that non-specific bioadsorption is heavily reduced on substrates made of PEG-ylated or zwitterionic chemistries whose topologies comprise either gels or polymeric grafts with high areal densities. We will also present an effective method utilizing organic mimics of metalloproteins, high cysteine containing peptides, for removing heavy metals and toxins from contaminated waters. Finally, we will discuss a simple, yet powerful, method of removing VOCs from waters by utilizing silicone elastomers that act as effective “sponges”.

**9:48AM X4.00004 Using Polymer Confinement for Stem Cell Differentiation: 3D Printed vs Molded Scaffolds.**<sup>1</sup> , MIRIAM RAFAILOVICH, Stony Brook University — Additive manufacturing technologies are increasingly being used to replace standard extrusion or molding methods in engineering polymeric biomedical implants, which can be further seeded with cells for tissue regeneration. The principal advantage of this new technology is the ability to print directly from a scan and hence produce parts which are an ideal fit for an individual, eliminating much of the sizing and fitting associated with standard manufacturing methods. The question though arises whether devices which may be macroscopically similar, serve identical functions and are produced from the same material, interact in the same manner with cells and living tissue. Here we show that fundamental differences can exist between 3-D printed and extruded scaffolds which can impact stem cell differentiation and lineage selection. We will show how polymer confinement inherent in these methods affect the printed features on multiple length scales. We will also and how the differentiation of stem cells is affected by substrate heterogeneity in both morphological and mechanical features.

<sup>1</sup>NSF-Inspire award 1344267

**10:24AM X4.00005 Directed self-assembly of performance materials**, PAUL NEALEY, University of Chicago — Directed self-assembly (DSA) is a promising strategy for high-volume cost-effective manufacturing at the nanoscale. Over the past decades, manufacturing techniques have been developed with such remarkable efficiency that it is now possible to engineer complex systems of heterogeneous materials at the scale of a few tens of nanometers. Further evolution of these techniques, however, is faced with difficult challenges not only in feasibility of implementation at scales of 10 nm and below, but also in prohibitively high capital equipment costs. Materials that self-assemble, on the other hand, spontaneously form structures at the mesoscale, but the micrometer areas or volumes over which the materials self-assemble with adequate perfection in structure is incommensurate with the macroscopic dimensions of working devices and systems of devices of industrial relevance. Directed Self-Assembly (DSA) refers to the integration of self-assembling materials with traditional manufacturing processes. Here we will discuss DSA of block copolymers to revolutionize sub 10 nm lithography and the manufacture of integrated circuits and storage media, DSA of ex-situ synthesized nanoparticles for applications in nanophotonics, and DSA of liquid crystals for advanced optics.

**Friday, March 18, 2016 8:00AM - 11:00AM –**  
**Session X5 GMAG DMP: Frustrated Magnetism: Kagome Lattice** 301 - Oleg Tchernyshyov, Johns Hopkins University

**8:00AM X5.00001 A Dichotomy of the Spin Liquid and the Correlated Impurities in Herbertsmithite**, TIANHENG HAN, University of Chicago — It is debatable whether RVB spin liquids exist in kagome systems. Enthusiasm in spin-1/2 kagome antiferromagnets gained extra momentum from the observation of a spinon continuum in  $\text{ZnCu}_3(\text{OD})_6\text{Cl}_2$  (herbertsmithite). In low-energy limit, where insightful many-body theories exist, impurities complicate experimental interpretations. Two important progresses were made in the past year. Single-crystalline  $^{170}\text{Yb}$  NMR experiment provided evidence for pristine kagome layers and a spin gap. Below the spinon continuum's energies, neutron scattering measurements revealed 3 dimensional spin correlations, which likely originate from the impurities. I will present the intrinsic-extrinsic dichotomy in  $\text{ZnCu}_3(\text{OD})_6\text{Cl}_2$  as well as my thoughts on future directions.

**8:36AM X5.00002 Fractionalized spin-wave continuum in kagome spin liquids**, JIA-WEI MEI, Perimeter Institute for Theoretical Physics, XIAO-GANG WEN, Department of Physics, Massachusetts Institute of Technology and Perimeter Institute for Theoretical Physics — Motivated by spin-wave continuum (SWC) observed in recent neutron scattering experiments in Herbertsmithite, we use Gutzwiller-projected wave functions to study dynamic spin structure factor  $S(\mathbf{q}, \omega)$  of spin liquid states on the kagome lattice. Spin-1 excited states in spin liquids are represented by Gutzwiller-projected two-spinon excited wave functions. We investigate three different spin liquid candidates, spinon Fermi-surface spin liquid (FSL), Dirac spin liquid (DSL) and random-flux spin liquid (RSL). FSL and RSL have low energy peaks in  $S(\mathbf{q}, \omega)$  at  $K$  points in the extended magnetic Brillouin zone, in contrast to experiments where low energy peaks are found at  $M$  points. There is no obvious contradiction between DSL and neutron scattering measurements. Besides a fractionalized spin (*i.e.* spin-1/2), spinons in DSL carry a fractionalized crystal momentum which is potentially detectable in SWC in the neutron scattering measurements.

**8:48AM X5.00003 A mean-field study of the Hubbard model on the kagome lattice<sup>1</sup>**, MATTHEW ENJALRAN, Southern Connecticut State University — The experimental work on the herbertsmithite compound,  $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$ , almost a decade ago ignited intense interest in the field of frustrated magnetism because it represented the best material realization of a spin-1/2 Heisenberg antiferromagnet (AFM) on the kagome lattice and its ground state was a gapless spin liquid. Many theoretical and numerical studies of the quantum Heisenberg AFM on the kagome lattice have been performed since and have coalesced around the general consensus of a small gapped spin liquid ground state for the model. Although there is not currently a metallic kagome material system, the work on  $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$  has motivated theoretical and numerical investigations of itinerant electrons on the kagome lattice. We contribute to this pursuit by studying the single band Hubbard model on the kagome lattice, where the frustration can be tuned by adjusting the hopping along different bonds,  $t_1$  and  $t_2$ ; however, we are mainly interested in the isotropic limit,  $t_1 = t_2 = t$ . We report preliminary results on the low temperature correlations in the half filled model as a function of frustration and interaction strength in the mean-field, Hartree-Fock, limit.

<sup>1</sup>CSU Research Grant

**9:00AM X5.00004 Structure and Physical Properties of  $\text{SrNiRu}_5\text{O}_{11}$  Single Crystals: A New Frustrated R-type Ferrite Based on Ordered Kagome Nets<sup>1</sup>**, LANCE DE LONG, University of Kentucky, Department of Physics and Astronomy, LARYSA SHLYK, RAINER NIEWA, Universitt Stuttgart, Institut für Anorganische Chemie — Single crystals of the R-type ferrite  $\text{SrNiRu}_5\text{O}_{11}$  were grown from a chloride flux. The hexagonal crystal structure contains ruthenium located on Kagome nets, distorted due to formation of Ru–Ru dumbbells via metal-metal bonding.  $\text{SrNiRu}_5\text{O}_{11}$  does not show long-range magnetic order down to 4.5 K. The low-temperature magnetic susceptibilities,  $\chi_\perp$  and  $\chi_\parallel$  c-axis, diverge as  $T^{-0.3}$ , and the electric resistivity varies as  $T^{1.6}$  below 40 K, which is typical of non-Fermi liquid materials. This anomalous behavior might originate from the competition between residual magnetic interactions among  $\text{Ni}^{2+}$  ( $S = 1$ ) spins and geometrical frustration on the two-dimensional Kagome lattice of  $\text{Ru}^{3+}$  ( $S = 1/2$ ) spins. The transverse magnetoresistivity  $\rho_{xy}$ , of a  $\text{SrNiRu}_5\text{O}_{11}$  single crystal at constant temperature  $T = 5$  K for current-magnetic-field configurations,  $\mathbf{J} \perp \mathbf{H} \parallel \text{c-axis}$  and  $\mathbf{J} \parallel \mathbf{H} \perp \text{c-axis}$ , reveals no anomalous contribution, which is typical for non-magnetic materials. Fits of the heat capacity data below 10 K require a dominant, but unusual electronic term of the form  $C_{el} = \gamma T^{1.2}$ , which is expected for massless Dirac fermion states in topological insulators or spin liquid phases.

<sup>1</sup>Research at University of Kentucky supported by U.S. Department of Energy grant no. DE-FG02-97ER-45653.

**9:12AM X5.00005 Local probe study of Sr-Vesignieite**, AIM VERRIER, JEFFREY QUILLIAM, Universit de Sherbrooke, FABRICE BERT, PHILIPPE MENDELS, Laboratoire de physique des solides, Universit Paris-Sud XI, DAVID BOLDRIN, ANDREW WILLS, University College London — We discuss the results of local probe measurements (NMR and  $\mu\text{SR}$ ) on a powder sample of  $\text{SrCu}_3\text{V}_2\text{O}_8(\text{OH})_2$  (Sr-Vesignieite)[D. Boldrin and A. S. Wills, J. Mat. Chem. C 3, 4308(2015)], a spin-1/2 kagome lattice with antiferromagnetic interactions.<sup>63,65</sup>  $^{63,65}\text{Cu}$  zero-field NMR and  $^{51}\text{V}$  NMR (in-field) reveal static magnetism at low temperatures and allow us to measure the intrinsic local susceptibility of the kagome lattice. Muon spin rotation ( $\mu\text{SR}$ ) experiments also demonstrate static magnetism at low  $T$ . We discuss the possible role of the Dzyaloshinsky-Moriya interaction and the proximity of this material to a quantum critical point between ordered and quantum spin liquid phases.

**9:24AM X5.00006 Hidden Order in Spin-Liquid  $\text{Gd}_3\text{Ga}_5\text{O}_{12}$**  , JOSEPH PADDISON, School of Physics, Georgia Institute of Technology, USA, and Department of Chemistry, University of Oxford, UK, and STFC-ISIS, UK, HENRIK JACOBSEN, Nanoscience Center, University of Copenhagen, Denmark, and European Spallation Source, Sweden, OLEG PETRENKO, Department of Physics, University of Warwick, UK, MARIA TERESA FERNÁNDEZ-DÍAZ, Institut Max von Laue - Paul Langevin, France, PASCALE DEEN, Nanoscience Center, University of Copenhagen, Denmark, and European Spallation Source, Sweden, ANDREW GOODWIN, Department of Chemistry, University of Oxford, UK — Frustrated magnetic materials are promising candidates for new states of matter because lattice geometry suppresses conventional magnetic dipole order, potentially allowing non-dipole ("hidden") order to emerge in its place. However, an atomic-scale model of a hidden-order state has been difficult to obtain because microscopic probes are not directly sensitive to hidden order. We use a combination of neutron-scattering experiments and reverse Monte Carlo refinements to develop a model of the spin-liquid state in the canonical frustrated magnet  $\text{Gd}_3\text{Ga}_5\text{O}_{12}$ . We show that this state exhibits a hidden order which has three unusual properties. First, it is a collective phenomenon, in which multipoles are formed from ten-spin loops. Second, it is long-range, with a diverging correlation length. Third, it is a consequence of the interplay between antiferromagnetic spin correlations and local planar magnetic anisotropy, which allows it to be indirectly observed in our neutron-scattering experiments.

**9:36AM X5.00007 Topologically non-trivial electronic and magnetic states in doped copper Kagome lattices<sup>1</sup>** , DANIEL GUTERDING, HARALD O. JESCHKE, ROSER VALENTI, Institute for Theoretical Physics, University of Frankfurt, Frankfurt a.M., Germany — We present a theoretical investigation of doped copper kagome materials based on natural minerals Herbertsmithite  $[\text{ZnCu}_3(\text{OH})_6\text{Cl}_2]$  and Barlowite  $[\text{Cu}_4(\text{OH})_6\text{FBr}]$ . Using ab-initio density functional theory calculations we estimate the stability of the hypothetical compounds against structural distortions and analyze their electronic and magnetic properties. We find that materials based on Herbertsmithite present an ideal playground for investigating the interplay of non-trivial band-topology and strong electronic correlation effects. In particular, we propose candidates for the Quantum Spin Hall effect at filling 4/3 and the Quantum Anomalous Hall effect at filling 2/3. For the Barlowite system we point out a route to realize a Quantum Spin Liquid.

<sup>1</sup>This work was supported by Deutsche Forschungsgemeinschaft under Grant No. SFB/TR 49 and the National Science Foundation under Grant No. PHY11-25915.

**9:48AM X5.00008 DMRG studies of the frustrated kagome antiferromagnets and the application to volborthite<sup>1</sup>** , SHOU-SHU GONG, National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32310, USA, D. N. SHENG, Department of Physics and Astronomy, California State University, Northridge, California 91330, USA, KUN YANG, Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32306, USA — Motivated by the recent magnetization measurements on the high-quality single crystals of the kagome antiferromagnet volborthite, we study the ground state and magnetization properties of two kagome models proposed from the electronic structure simulations, which treat the volborthite as either the coupled trimers or the coupled frustrated chains on the kagome lattice. We study the models using density-matrix renormalization group on the cylinder geometry with the system width up to 4 legs. We find a quantum phase diagram of the models with changing couplings, and identify the magnetic properties of each phase. In the antiferromagnetic phases, we also study the magnetization curve and the different phases in the magnetic field. Finally, we compare the magnetization properties of the models with the experimental observations of volborthite.

<sup>1</sup>NSF DMR-1157490, DMR-1408560, and the State of Florida

**10:00AM X5.00009 Spin-wave analysis of a broad magnetization plateau in volborthite** , EDWARD PARKER, LEON BALENTS, Univ of California - Santa Barbara — Volborthite  $(\text{Cu}_3\text{V}_2\text{O}_7(\text{OH})_2 \cdot 2\text{H}_2\text{O})$  is a system comprised of spin-1/2 ions forming quasi-2D layers of Kagomé lattices. It displays two striking experimental features: strong geometric frustration (with a magnetic ordering temperature more than two orders of magnitude below its Curie temperature), and an extremely broad  $m = \frac{1}{3}m_{\text{sat}}$  magnetization plateau extending over a range of more than 100 T. Density functional theory calculations suggest that it has a complicated anisotropic spin coupling structure with both ferromagnetic and antiferromagnetic first- and second-nearest-neighbor bonds. We present results for the classical phase diagram for this system, focusing on how the upper and lower critical fields of the magnetization plateau depend on the exchange couplings. We also present a semiclassical large- $S$  expansion, and show how including the leading quantum corrections in  $1/S$  gives a magnon self-energy that shifts the classical values for the plateau's critical fields.

**10:12AM X5.00010 Changing the Electron Count in Spin Liquids<sup>1</sup>** , ZACHARY KELLY, TYREL MCQUEEN, Johns Hopkins Univ — Materials which possess the resonating valence bond (RVB) "spin-liquid" state have been long sought after by scientists due to their predicted exotic properties. Several materials have been identified as potential spin liquid candidates and laboratory studies have only just begun to provide insight into the properties of these materials and their theoretical description. Recently theoretical calculations predict doping of a spin liquid could lead to a rich and unique phase diagram including complex magnetic states, Dirac metal behavior, and superconductivity. We report the results of structural and physical property characterizations of newly synthesized doped candidate spin liquids.

<sup>1</sup>This work was supported by a Cottrell Scholar Award

**10:24AM X5.00011 A Kagome Map of Spin Liquids<sup>1</sup>** , KARIM ESSAFI, OWEN BENTON, LUDOVIC D. C. JAUBERT, Okinawa Inst of Sci & Tech — Competing interactions in frustrated magnets prevent ordering down to very low temperatures and stabilize exotic highly degenerate phases where strong correlations coexist with fluctuations. We study a very general nearest-neighbour Heisenberg spin model Hamiltonian on the kagome lattice which consist of Dzyaloshinskii-Moriya, ferro- and antiferromagnetic interactions. We present a three-fold mapping which transforms the well-known Heisenberg antiferromagnet (HAF) and XXZ model onto two lines of time-reversal Hamiltonians. The mapping is exact for both classical and quantum spins, *i.e.* preserves the energy spectrums of the HAF and XXZ model. As a consequence, our three-fold mapping gives rise to a connected network of quantum spin liquids centered around the Ising antiferromagnet. We show that this quantum disorder spreads over an extended region of the phase diagram at linear order in spin wave theory, which overlaps with the parameter region of Herbertsmithite  $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$ . At the classical level, all the phases have an extensively degenerate ground-state which present a variety of properties such as ferromagnetically induced pinch points in the structure factor and spontaneous scalar chirality which was absent in the original HAF and XXZ models.

<sup>1</sup>This work was supported by the Okinawa Institute of Science and Technology Graduate University.

**10:36AM X5.00012 Nature of Possible  $Z_6$  symmetry breaking magnetic phases in frustrated hyperkagome iridate**, RYUICHI SHINDOU, School of Physics, Peking University — To obtain a comprehensive understanding of classical magnetism possible in frustrated hyperkagome iridate  $\text{Na}_4\text{Ir}_3\text{O}_8$  (Na-438), we postulated additional lattice symmetries other than an exact crystal symmetry, and introduced a relatively simpler effective spin model for Na-438. Using Monte Carlo simulation and Luttinger-Tisza analysis, we derived a classical magnetic phase diagram for Na-438. We show that a  $Z_6$  symmetry breaking magnetic phase is stabilized by the thermal order by disorder. Our finite-size scaling analysis reveals that the criticality of the ordering temperature of the  $Z_6$  phase is characterized by the 3D XY universality class, where the system acquires effectively a higher symmetry than high- $T$  disorder phase (dubbed as emergent U(1) symmetry). For a finite size system, an intermediate temperature regime appears below the ordering temperature, where the spin anisotropy term becomes effectively irrelevant and spin ordering develops in the U(1) symmetric way. We showed that this crossover phenomena can be well accounted for in terms of the 3-d ferromagnetic  $Z_6$  Potts model. Based on this crossover behavior, we introduced a possible phenomenology of low-temperature magnetic behaviors of polycrystalline Na-438. Reference: arXiv.1509.01002

**10:48AM X5.00013 Competing phases of  $S=1$  XXZ model on Kagome lattice<sup>1</sup>**, ZHENYUE ZHU, STEVEN WHITE, UC Irvine — We numerically study the  $S=1$  XXZ model on the kagome lattice with the Density matrix renormalization group. We focus on the two types of expected magnetic order,  $Q = 0$  and  $\sqrt{3} \times \sqrt{3}$ . As a function of the coupling  $\Delta$  for the  $S_z S_z$  terms, we find two possible phase transitions. For  $\Delta < \Delta_1$ , we find that the  $Q = 0$  state has lower energy, but the difference between these two magnetic ordered phase is very small. For  $\Delta_1 < \Delta < \Delta_2$ ,  $\sqrt{3} \times \sqrt{3}$  magnetic ordered state is the ground state. For  $\Delta > \Delta_2$ , we find that the magnetic ordered phases disappears, entering a magnetic disordered phase. We find a close competition between a trimerized phase and a hexagon singlet phase, which is consistent with recent numerical studies of  $S=1$  Heisenberg model on the Kagome lattice.

<sup>1</sup>We acknowledge support from the NSF under grant DMR-1505406 and from the Simons Foundation through the Many Electron collaboration.

## Friday, March 18, 2016 8:00AM - 11:00AM –

Session X6 GMAG DMP: Nanoparticles, Nanowires, and Clusters 302 - Deepak Singh, Univ. of Missouri

**8:00AM X6.00001 Using Magnetic Proximity Effects to Stabilize Magnetic Nanoparticles<sup>1</sup>**, JOSE A. DE TORO, Instituto Regional de Investigacin Cientfica Aplicada (IRICA) and Departamento de Fsica Aplicada, Universidad de Castilla-La Mancha — The current miniaturization trend in magnetic applications has led to a quest to suppress spontaneous thermal fluctuations (superparamagnetism) in ever-smaller nanostructures, which constitutes a clear example of the fundamental efforts of condensed matter physics to meet technological challenges (e.g., the continued growth of magnetic recording density). We have demonstrated that ferromagnetic (FM) Co nanoparticles with blocking temperature below 70 K become magnetically stable above 400 K when embedded in a high Neel temperature antiferromagnetic (AFM) NiO matrix [1]. This remarkable stabilization is due to a magnetic proximity effect between a thin CoO shell (with low Neel temperature and high anisotropy) surrounding the Co nanoparticles and the NiO matrix (with high Neel temperature but low anisotropy). This proximity effect yields an effective antiferromagnet with an apparent ordering temperature beyond that of bulk CoO, and an enhanced anisotropy compared to NiO. In turn, the Co core FM moment is stabilized against thermal fluctuations via core-shell exchange-bias coupling, leading to the observed increase in blocking temperature. A mean-field model, corrected for thermal activation effects, closely reproduces the experimental exchange-bias data, corroborating the above interpretation and providing a semi-quantitative understanding of the nature of the proposed proximity effect. The results presented in this study constitute a striking illustration of how a subtle combination of interactions may permit the occurrence of unique magnetic properties by exploiting proximity effects in magnetism. 1. J. A. De Toro, D. P. Marques, P. Muniz, V. Skumryev, J. Sort, D. Givord, and J. Nogues, Phys. Rev. Lett. 115, 057201 (2015).

<sup>1</sup>This work has been supported by projects from the Junta de Comunidades de Castilla-La Mancha [PEII11-0226-8769] and from the Generalitat de Catalunya (2014-SGR-1015)

**8:36AM X6.00002 Emergent  $1/f$  noise in collections of individually oscillating magnetic dots<sup>1</sup>**, BARRY COSTANZI, E DAN DAHLBERG, Univ of Minnesota - Twin Cities — We experimentally demonstrate an emergent  $1/f$  spectrum from a superposition of the noise from random telegraph noise (RTN) oscillators. The system consists of individual square magnetic permalloy dots with dimensions on the order of  $200\text{nm} \times 200\text{nm} \times 10\text{nm}$  that exhibit RTN in their magnetization at appropriate applied fields. The magnetization fluctuations are measured by the anisotropic magnetoresistance (AMR). AMR is used to find applied fields necessary to exhibit RTN, which result in Lorentzian spectra in the power spectral density of the measurement. A composite AMR measurement of multiple oscillating dots at once, however, shows an emergent  $1/f$  spectrum in the power spectral density. This agrees with the prediction of Van Der Ziel [1] that, for an appropriate distribution of oscillators showing Lorentzian spectra, the composite spectrum will have a  $1/f$  character. This experimental demonstration of  $1/f$  noise from a system of two-state oscillators indicates a possible mechanism for the origin of  $1/f$  spectra observed in both other magnetic systems, and potentially in other, more disparate systems. [1] A. van der Ziel, Physica 16, 359 (1950).

<sup>1</sup>This work was supported by ONR Grant N00014-11-1-0850. Samples were fabricated in the Minnesota Nano Center, which receives funding from the NSF through the NNIN program.

**8:48AM X6.00003 Magnetic and Structural Properties of  $\text{Mn}_5\text{Ge}_3$  Nanoparticles<sup>1</sup>**, ONUR TOSUN, MOHAMMAD SALEHI-FASHAMI, GEORGE C. HADJIPANAYIS, Univ of Delaware, DAVID J. SELLMYER, BALAMURUGAN BALASUBRAMANIAN, Univ of Nebraska-Lincoln, UNIV OF DELAWARE TEAM, UNIV OF NEBRASKA-LINCOLN COLLABORATION — Magnetic nanoparticles have unique and interesting properties which are scientifically important and attractive for numerous advanced technologies. In this work, we have used the cluster-beam deposition technique to synthesize  $\text{Mn}_5\text{Ge}_3$  nanoparticles with different size. The composition, crystal structure and magnetic properties of the nanoparticles have been characterized by energy dispersive x-ray spectroscopy (EDS), X-ray diffraction, high-resolution transmission electron microscopy (HR-TEM) and magnetometry, respectively. Particles made with 1.7 Torr Argon pressure, and power of 80 W had an average size of 14 nm. Selected area electron diffraction showed that the particles had a hexagonal  $\text{Mn}_5\text{Si}_3$ -type structure with space group  $P63/mcm$  which is the same as in bulk. Magnetic measurements showed that the nanoparticles are ferromagnetic with a Curie temperature near room temperature. The effects of particle size and temperature on the magnetic properties are currently being studied and the results will be reported and discussed.

<sup>1</sup>DOE-BES-DE-FG02-04ER4612 and DE-FG02-04ER46152

**9:00AM X6.00004 Computational Atomistic Modeling of Bi-Magnetic Core-Shell Nanoparticles<sup>1</sup>**, RAHUL SAHAY, Sacred Heart Academy and Department of Physics, Central Michigan University, Mount Pleasant, MI, JUAN PERALTA, Department of Physics, Central Michigan University, Mount Pleasant, MI, 48859, GABRIEL CARUNTU, Department of Chemistry, Central Michigan University, Mount Pleasant, MI, 48859 — Since its discovery, there has been an increasing interest in the modeling of magnetic phenomena found in materials that present exchange bias. In particular, ferro-antiferromagnetic core-shell nanoparticles are an interesting case in which the magnetic properties of the nanostructure can be altered by adjusting their size, shape, and composition. Here we present a computational scheme that efficiently models the magnetic behavior of bi-magnetic core-shell nanostructures. Using a Heisenberg-Dirac-van Vleck Hamiltonian in combination with a continuous spin model, we simulate a wide range of hysteresis diagrams displaying exchange bias. Furthermore, we will demonstrate our efforts towards improving the efficiency of the simulation algorithms, aiming to afford magnetic atomistic simulations of large nanostructures by using a method based on a tessellated unit sphere to account for spin orientations. Our results allow for further semi-quantitative comparisons with existing experimental data and provide a means to discover new phenomena associated with these core-shell nanoparticles and other nanostructures.

<sup>1</sup>NSF DMR-1206920

**9:12AM X6.00005 Angular dependence of magnetization in single crystalline cobalt nanowires**, KINJAL GANDHA, KEVIN ELKINS, NARAYAN POUDYAL, J. PING LIU, University of Texas at Arlington — In this work, the magnetization behavior of Co nanowires has been investigated by applying the Stoner-Wohlfarth model. The single crystalline cobalt nanowires with a diameter of about 15 nm and a mean length of 200 nm were synthesized via a solvothermal chemical process that have high coercivity up to 12.5 kOe. It is found that the c-axis (002) or the easy magnetization direction of the single-crystalline wires is along the long axis of the nanowires. Particular attention has been paid to the angular dependence of magnetic properties on the applied magnetic field orientation with respect to the c-axis. The angular dependence of coercivity has been modeled and it was revealed that the coherent mode rotation gives the best fitting with the experimental observations. In addition, surface oxidized Co nanowires have also been studied that provided us a unique opportunity to understand the exchange bias in the aligned Co/CoO core-shell nanostructures. Ferromagnetic nanowires of this type are ideal building blocks for future bonded, consolidated and thin film magnets with high energy density and high thermal stability.

**9:24AM X6.00006 Chalcogenide Cobalt telluride nanotubes<sup>1</sup>**, BISHNU DAHAL, RAJENDRA DULAL, IAN L. PEGG, JOHN PHILIP, The Catholic University of America — Cobalt telluride nanotubes are grown using wet chemical and hydrothermal syntheses. Wet chemical synthesized nanotubes display nearly 1: 1 Co to Te ratio. On the other hand, CoTe nanotubes synthesized using hydrothermal method show excess Co content leading to the compound Co<sub>58</sub>Te<sub>42</sub>. Both CoTe and Co<sub>58</sub>Te<sub>42</sub> display magnetic properties, but with totally different characteristics. The Curie temperature of CoTe is higher than 400 K. However, the T<sub>c</sub> of Co<sub>58</sub>Te<sub>42</sub> is below 50 K. Transport properties of cobalt telluride (CoTe) nanotube devices show that they exhibit p-type semiconducting behavior. The magnetoresistance measured at 10 K show a magnetoresistance of 54%.

<sup>1</sup>National Science Foundation under ECCS-0845501 and NSF-MRI, DMR-0922997

**9:36AM X6.00007 Effect of Bi Substitution on the FCC to L1<sub>0</sub> Phase Transformation in CoPt(Bi) Nanoparticles**, FRANK ABEL, Physics and Astronomy, University of Delaware, VASILIS TZITZIOS, Institute of Nanoscience and Nanotechnology, NCSR, DAVID SELLMYER, Physics and Astronomy and NCMN, University of Nebraska, GEORGE HADJIPANAYIS, Physics and Astronomy, University of Delaware — The transformation from the fcc to fct structure L1<sub>0</sub> in CoPt requires annealing at temperatures over 600<sup>0</sup> C, as compared to FePt which can occur at 550<sup>0</sup> C. In the past, similar attempts to lower the transformation temperature in CoPt have been unsuccessful. In this work, we report for the first time a decrease in the phase transformation temperature of chemically synthesized CoPt nanoparticles by the addition of a small amount of bismuth. Our studies have shown that the phase transformation occurs in as-made CoPt(Bi) nanoparticles at refluxing temperatures as low as 330<sup>0</sup> C, which is significantly lower than previously reported values in CoPt nanoparticles and thin films. The as-made CoPt nanoparticles with 5% atomic weight Bi show partial L1<sub>0</sub> ordering with an average size of 11.7 nm, as shown by TEM imaging, and have a coercivity of 1 kOe and saturation magnetization of 32 emu/g. Annealing of the CoPt(Bi) nanoparticles produced maximum coercivities of 12.4 kOe when annealed at 700<sup>0</sup> C for 1 hour. The effect of amount of Bi addition on the formation and ordering of L1<sub>0</sub> structure will be discussed.

**9:48AM X6.00008 Magnetic and Structural Properties of Co<sub>5</sub>Ge<sub>3</sub> Nanoparticles.<sup>1</sup>**, MOHAMMAD SALEHI-FASHAMI, VIMAL DEEPCHAND, University of Delaware, RALPH SKOMSKI, DAVID J. SELLMYER, University of NebraskaLincoln, GEORGE C. HADJIPANAYIS, University of Delaware — Magnetic semiconductor alloy nanostructures play a crucial role in advanced technologies due to their tunable band gaps and electronic properties. Among these magnetic semiconductor alloys, Co-Ge is important both scientifically and technologically. In this work, we studied the magnetic and transport properties of Co<sub>5</sub>Ge<sub>3</sub> nanoparticles(NPs) fabricated by cluster-beam deposition. The NPs were characterized by X-ray powder diffraction and the results demonstrated that they had the same hexagonal structure P6<sub>3</sub>/mm-type as in bulk. Transmission-electron-microscope observations revealed that the particles have a single crystalline structure with an average size of 8nm. Selected-area electron diffraction(SAED) confirmed the XRD data, showing clearly that the particles have the hexagonal structure mentioned above. High-resolution electron microscopy images show lattice fringes with spacing of 1.99Å and 2.02Å which correspond to the (102) and (110) superlattice reflections of the hexagonal ordered Co<sub>5</sub>Ge<sub>3</sub> structure. Magnetic properties showed that these nanoparticles are ferromagnetic at room temperature as-compared to bulk samples that are paramagnetic at all temperatures. This magnetic behavior in Co-Ge nanoparticles indicates new size-controlled spin structures in confined nanosize systems.

<sup>1</sup>Work supported by DOE DE-FG02-04ERU4612and DE-FG02-04ER46152.

**10:00AM X6.00009 Evolution of Magnetic Moments in Cobalt and Nickel Clusters<sup>1</sup>**, MASAHIRO SAKURAI, JAIME SOUTO-CASARES, JAMES CHELIKOWSKY, University of Texas at Austin — Ferromagnetism in transition-metal clusters has attracted much interest owing to their enhanced magnetic moments as compared to those of bulk phases. Here, we investigate the stability and the magnetism of Co and Ni clusters with various structures using a real-space formalism of pseudopotentials within the spin-polarized density-functional theory, i.e., the PARSEC code. We will discuss how the calculated magnetic moments evolve as a function of cluster size and compare them to experiment.

<sup>1</sup>We acknowledge support by the National Science Foundation Grant No. DMR 14-35219.

**10:12AM X6.00010 Spin Moments and Stability of VCun+ Clusters: The curious case of VCu<sub>4</sub><sup>+</sup>, VCu<sub>8</sub><sup>+</sup>, and VCu<sub>12</sub><sup>+</sup>**, WILLIAM BLADES, ARTHUR REBER, SHIV KHANNA, VCU, LUIS SOSA, PATRIZIA CALAMINICI, ANDREAS KOSTER, Civestav — The atomic structures, bonding characteristics, magnetic spin moments, and stability of VCu<sub>n</sub><sup>+</sup> clusters have been examined within density functional theory. Our studies show that at small sizes, the spin moments of the vanadium atom (3d<sup>3</sup> 4s<sup>2</sup>) due to 3d electrons are unquenched as the bonding is primarily through 4s electrons. As the cluster grows, the 3d orbitals of the vanadium atom start to participate in hybridized bonding with the copper atoms, resulting in a quenching of the magnetic moment. Upon closer examination of the electronic structures, we observe shell closure at VCu<sub>5</sub><sup>+</sup>, VCu<sub>7</sub><sup>+</sup>, and VCu<sub>14</sub><sup>+</sup>. However, the observed abundances in the photofragmentation profile do not correspond to these shell closures and the subsequent electronic stability they provide. Instead, the enhanced abundances of VCu<sub>4</sub><sup>+</sup>, VCu<sub>8</sub><sup>+</sup>, and VCu<sub>12</sub><sup>+</sup> seen in the mass spectrum are justified through geometric means and a cluster growth mechanism is proposed. Through synergetic theoretical and experimental efforts, the unusual enhanced stability of VCu<sub>4</sub><sup>+</sup>, VCu<sub>8</sub><sup>+</sup>, VCu<sub>12</sub><sup>+</sup>, and their magnetic properties are probed and explained.

<sup>1</sup>We gratefully acknowledge support from Department of Energy under award number DE-SC0006420

**10:24AM X6.00011 Model for ferromagnetic behavior of metal cluster-fullerene superatomic solids.**, PALLABI SUTRADHAR, VIKAS CHAUHAN, SHIV KHANNA, JAYASIMHA ATULASIMHA, Virginia Commonwealth Univ — Recent work has explored the precise assembly of binary superatomic solids from metal clusters and fullerene [1] as well as experimentally demonstrated ferromagnetic behavior in such assemblies at low temperatures (less than 10K). However, the origin of this behavior is not yet completely understood and modeled rigorously. We report theoretical analyses and simulations that explain the origin of ferromagnetic behavior from super exchange mechanism and model the temperature dependent magnetic behavior of these superatomic solids. [1] X. Roy et al., Science, 341, 157, 2013. [2] C.H. Lee et al., J. Am. Chem. Soc. 136, 16926, 2014.

**10:36AM X6.00012 Transition metal doped semiconductor quantum dots: Optical and magnetic properties**, YURI DAHNOVSKY, VITALY PROSHCHENKO, ARTEM PIMACHEV, Department of Physics & Astronomy, University of Wyoming — We study optical and magnetic properties of CdSe and Cd-Mn-Se quantum dots (QD). We find that there are two luminescence lines, one is fast and another is slow (~1ms). With the increase of a QD diameter the slow luminescence disappears at some critical QD size, thus only one line (fast) remains. Using the SAC SI computational method we find that D = 3.2 nm and D = 2.7 nm if the Mn impurity is located inside a QD or on a QD surface, respectively. For two or four Mn atoms in the quantum dot, now absorption takes place because the transition is spin-allowed. The DFT calculations of the magnetic state reveal that it is an antiferromagnet. We also study other quantum dots such as Cd-Mn-Se, Zn-Mn-S, and Zn-Mn-Se, doped and undoped. We find the slow luminescence energies for low concentrations of Mn impurities for each QD type. The calculations indicate that two luminescence lines, fast and slow, should always take place. However for Pb-Mn-S quantum dots there are now Mn levels inside a HOMO-LUMO gap, i.e., the Mn-levels are located in a PbS conduction band. The presence of Mn dopants increases the band gap and also removes the exciton peak. This effect is different to the other quantum dots.

**10:48AM X6.00013 Anomalous Hall Effect and Electron Transport in Co<sub>2</sub>Si Nanocluster Films**, BALAMURUGAN BALASUBRAMANIAN, TOM GEORGE, BHASKAR DAS, RALPH SKOMSKI, DAVID SELLMYER, Nebraska Center for Materials and Nanoscience and Department of Physics and Astronomy, University of Nebraska — Magnetic nanoparticles or clusters are of fundamental and technological importance, since they exhibit entirely different and/or improved magnetic and electronic properties as compared to bulk alloys. Our recent research shows large average magnetic moments of up to 0.70μ<sub>B</sub>/Co at 10K and 0.49μ<sub>B</sub>/Co at 300K for cluster-deposited Co<sub>2</sub>Si nanoparticles, in sharp contrast to the nearly vanishing bulk magnetization. In this talk, we present interesting electron-transport properties in Co<sub>2</sub>Si nanoparticle films. The film shows a room-temperature negative magnetoresistance (MR) of 0.14% at kOe, which become as high as 1.8% at low temperatures. We also observed anomalous field-dependent Hall resistivities (ρ<sub>xy</sub>) in the nanoparticle film, which corroborate the magnetic hysteresis loops. Interestingly, the longitudinal metallic resistivity (ρ<sub>xx</sub>) shows a resistivity minimum at around 10K, similar to Kondo effects observed in the case of non-magnetic metals due to dilute magnetic impurities. The transport properties will be discussed in terms of the underlying spin correlations in the Co<sub>2</sub>Si nanoparticle films. This work is supported by the U.S. DOE-BES-DMSE (Grant No. DE-FG02-04ER46152) and NCMN.

**Friday, March 18, 2016 8:00AM - 10:24AM –**

**Session X7 DMP FIAP: Dopants and Defects in Semiconductors: Compound Semiconductors**

303 - Christophe Boehme, University of Utah

**8:00AM X7.00001 Electronic structure and scattering property of 4H-SiC(0001)/SiO<sub>2</sub> interface**, TOMOYA ONO, CHRISTOPHER KIRKHAM, Center for Computational Sciences, University of Tsukuba, Japan, SHIGERU IWASE, Department of Precision Science and Technology, Osaka University, Japan — SiC is attracted much attention as a promising material for the high-power electronics devices. We carried out a first-principles calculations to reveal the relationship between the electronic structure and the interface defects appearing in the thermal oxidation. We found interlayer states along the SiC conduction band edge (CBE), whose location changes depending on which of two possible lattice sites, *h* or *k*, is at the interface. Excess O atoms at the interface lead to defect structures which alter the electronic structure. Changes to the valence band edge are the same whether *h* or *k* sites are at the interface. On the other hand, defects remove the interlayer state of the CBE between the first and second SiC bilayers if an *h* site is at the interface, but have no effect when there is a *k* site. The scattering property of the defects was also examined by electron-transport calculations. Carriers at the CBE of the *h*-type interface are easily scattered by the defects because of the absence of the interlayer states while those at the *k*-type interface is not. Since recent SiC-MOSFETs mainly use the conduction band as a channel, the behavior of these interlayer states at the CBE might play an important role in the performance of these devices.

**8:12AM X7.00002 Measurements of depth dependent modification of optical constants arising from H<sup>+</sup> implantation in n-type 4H-SiC using coherent acoustic phonons<sup>1</sup>**, ANDREY BAYDIN, HALINA KRZYZANOWSKA, Vanderbilt University, M. DHANUNJAYA, S.V.S. NAGESWARA RAO, University of Hyderabad, JIMMY L. DAVIDSON, Vanderbilt University, LEONARD C. FELDMAN, Rutgers University, NORMAN H. TOLK, Vanderbilt University — Silicon carbide (SiC) is an ideal material for new electronics, such as high power/high temperature devices, and a candidate for advanced optical applications such as room temperature spintronics and quantum computing. Both types of applications may require the control of defects created by ion bombardment. In this work, we examine depth dependent modification of optical constants of 4H-SiC due to hydrogen implantation at 180keV and low doses ranging from 10<sup>14</sup> to 10<sup>16</sup> cm<sup>-2</sup> probed by coherent acoustic phonon (CAP) spectroscopy. For our studies, we used Si-face 10μm epilayers of n-type 4H-SiC grown by CVD on 4H-SiC substrate. A comprehensive analysis of the reference and implanted spectra shows a strong dependence of 4H-SiC complex refractive index shape versus depth on the H<sup>+</sup> fluence. We extract the complex refractive index as a function of depth and ion beam dose. Our results demonstrate that the implantation-modified refractive index is distributed over a greater depth range than Monte Carlo calculation predictions of the implantation induced structural damage. These studies provide insight into the application of hydrogen ion implantation to the fabrication of SiC-based photonic and optoelectronic devices.

<sup>1</sup>Work is supported by ARO under contract No. W911NF-14-1-0290

**8:24AM X7.00003 Revealing Hidden Interfacial States in NO Passivated 4H-SiC/SiO<sub>2</sub> Structures using TEM-EELS and XPS<sup>1</sup>**, JOSHUA TAILLON, University of Maryland, College Park, SARIT DHAR, Auburn University, GANG LIU, LEONARD FELDMAN, Rutgers University, TSVETANKA ZHELEVA, AIVARS LELIS, US Army Research Laboratory, LOURDES SALAMANCA-RIBA, University of Maryland, College Park — The interface between 4H-SiC and SiO<sub>2</sub> in metal oxide semiconductor (MOS) devices contains a high density of electrically active defects, which adversely affect SiC microelectronic devices. Various treatments and altering the substrate's crystallographic orientation can improve electronic performance. We have previously shown an inverse relationship between nitric oxide (NO) anneal time and the width of the transition layer at this interface ( $w_{TL}$ ).<sup>2</sup> More recent work analyzing  $w_{TL}$  has revealed much narrower interfaces that do not appear to narrow when subjected to an NO post-oxidation anneal, contradicting expectations. To further explore these interfaces, high resolution transmission electron microscopy and spatially resolved electron energy-loss spectroscopy (EELS) have been used. In addition, X-ray photoemission spectroscopy measurements were taken at the interface. Advanced EELS analysis via machine learning techniques has revealed interfacial bonding states for different post-oxidation annealing processes. The nature of these interfacial states is compared for devices made on substrates with different orientations and for NO post-oxidation annealing. <sup>2</sup>J. Taillon *et al.*, *J. Appl. Phys.* **113**, 044517 (2013).

<sup>1</sup>Supported by ARL Grant W911NF-11-2-0044 and NSF GRFP Grant DGE1322106

**8:36AM X7.00004 Generalization of the van der Pauw Method: Analyzing Longitudinal Magnetoresistance Asymmetry to Quantify Doping Gradients<sup>1</sup>**, M. GRAYSON, WANG ZHOU, HEUN-MO YOO, S. PRABHU-GAUNKAR, Northwestern University, L. TIEMANN, C. REICHL, W. WEGSCHEIDER, ETH Zurich, Switzerland — A longitudinal magnetoresistance asymmetry (LMA) between a positive and negative magnetic field is known to occur in both the extreme quantum limit and the classical Drude limit in samples with a nonuniform doping density. By analyzing the current stream function in van der Pauw measurement geometry, it is shown that the electron density gradient can be quantitatively deduced from this LMA in the Drude regime [1]. Results agree with gradients interpolated from local densities calibrated across an entire wafer, establishing a generalization of the van der Pauw method to quantify density gradients. Results will be shown of various semiconductor systems where this method is applied, from bulk doped semiconductors, to exfoliated 2D materials. [1] W. Zhou, H.M. Yoo, S. Prabhu-Gaunkar, L. Tiemann, C. Reichl, W. Wegscheider, and M. Grayson, *Phys. Rev. Lett.* **115**, 186804 (2015).

<sup>1</sup>McCormick Catalyst Award from Northwestern University, EECS Bridge Funding, and AFOSR FA9550-15-1-0247.

**8:48AM X7.00005 First principles modeling of grain boundaries in CdTe<sup>1</sup>**, MARIA K.Y. CHAN, FATIH SEN, Argonne National Laboratory, CHRISTOPHER BUURMA, EPIR, TADÁS PAULASKAS, University of Illinois Chicago, CE SUN, MOON KIM, University of Texas at Dallas, ROBERT KLIE, University of Illinois Chicago — The role of extended defects is of significant interest for semiconductors, especially photovoltaics since energy conversion efficiencies are often affected by such defects. In particular, grain boundaries in CdTe photovoltaics are enigmatic since the achievable efficiencies of CdTe photovoltaics are higher in polycrystalline devices as compared to single crystalline devices. Yet, despite recent advances, the efficiency of poly-CdTe devices are still substantially below the theoretical maximum. We carry out an atomistic-level study using Scanning Transmission Electron Microscopy (STEM), together with first principles density functional theory (DFT) modeling, in order to understand the properties of specific bicrystals, i.e. artificial grain boundaries, constructed using wafer bonding. We discuss examples of bicrystals, including some involving large scale DFT calculations, and trends in defect and electronic properties.

<sup>1</sup>This work was funded by DOE SunShot BRIDGE program.

**9:00AM X7.00006 Origin of High Electronic Quality in Solar Cell Absorber CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>**, WANJIAN YIN, Soochow University, TINGTING SHI, University of Toledo, SUHUA WEI, Beijing Computational Science Research Center, YANFA YAN, University of Toledo — Thin-film solar cells based on CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> halide perovskites have recently shown remarkable performance. First-principle calculations and molecular dynamic simulations show that the structure of pristine CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> is much more disordered than the inorganic archetypal thin-film semiconductor CdTe. However, the structural disorders from thermal fluctuation, point defects and grain boundaries introduce rare deep defect states within the bandgaps; therefore, the material has high electronic quality. We have further shown that this unusually high electronic quality is attributed to the unique electronic structures of halide perovskite: the strong coupling between cation lone-pair Pb *s* orbitals and anion *p* orbitals and the large atomic size of constitute cation atoms. We further found that although CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> GBs do not introduce a deep gap state, the defect level close to the VBM can still act as a shallow hole trap state. Cl and O can spontaneously segregate into GBs and passivate those defect levels and deactivate the trap state.

**9:12AM X7.00007 Mn Doping Effects on the Electronic Band Structure of PbS Quantum Dot Thin Films: A Scanning Tunneling Microscopy Analysis<sup>1</sup>**, ANDREW J. YOST, GAURAB RIMAL, JINKE TANG, TEYU CHIEN, University of Wyoming — A thorough understanding of the phenomena associated with doping of transition metals in semiconductors is important for the development of semiconducting electronic technologies such as semiconducting quantum dot sensitized solar cells (QDSSC). Manganese doping is of particular interest in a PbS QD as it is potentially capable of increasing overall QDSSC performance [1]. Here we present scanning tunneling microscopy and spectroscopy studies about the effects of Manganese doping on the energy band structures of PbS semiconducting QD thin films, grown using pulsed laser deposition. As a result of Manganese doping in the PbS QD thin films, a widening of the electronic band gap was observed, which is responsible for the observed increase in resistivity. Furthermore, a loss of long range periodicity observed by XRD, upon incorporation of Manganese, indicates that the Manganese dopants also induce a large amount of grain boundaries. [1] Qilin Dai *et al.*, *APL* **104**, 183901 (2014).

<sup>1</sup>This work was supported by the following: U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Science and Engineering, DEFG02-10ER46728 and the National Science Foundation Grant 0948027

**9:24AM X7.00008 Electronic structure and defect properties of selenophosphate Pb<sub>2</sub>P<sub>2</sub>Se<sub>6</sub> for  $\gamma$ -ray detection<sup>1</sup>**, OLEG Y. KONTSEVOI, JINO IM, BRUCE W. WESSELS, MERCOURI G. KANATZIDIS, ARTHUR J. FREEMAN, Northwestern University — Heavy metal chalcophosphate Pb<sub>2</sub>P<sub>2</sub>Se<sub>6</sub> has shown a significant promise as an X-ray and  $\gamma$ -ray detector material. To assess the fundamental physical properties important for its performance as detector, theoretical calculations were performed for the electronic structure, band gaps, electron and hole effective masses, and static dielectric constants. The calculations were based on first-principles density functional theory (DFT) and employ the highly precise full potential linearized augmented plane wave method and the projector augmented wave method and include nonlocal exchange-correlation functionals to overcome the band gap underestimation in DFT calculations. The calculations show that Pb<sub>2</sub>P<sub>2</sub>Se<sub>6</sub> is an indirect band gap material with the calculated band gap of 2.0 eV, has small effective masses, which could result in a good carrier mobility-lifetime product  $\mu\tau$ , and a very high static dielectric constant, which could lead to high mobility of carriers by screening of charged scattering centers. We further investigated a large set of native defects in Pb<sub>2</sub>P<sub>2</sub>Se<sub>6</sub> to determine the optimal growth conditions for application as  $\gamma$ -ray detectors. The results suggest that the prevalent intrinsic defects are selenium vacancies, followed by lead vacancies, then phosphorus vacancies and antisite defects. The effect of various chemical environments on defect properties was examined and the optimal conditions for material synthesis were suggested. <sup>1</sup>Supported by DHS (Grant No. 2014-DN-077-ARI086-01).

**9:36AM X7.00009 Challenges in p-type Doping of CdTe**, JEDIDIAH MCCOY, SANTOSH SWAIN, KELVIN LYNN, Center for Materials Research at Washington State University — We have made progress in defect identification of arsenic and phosphorous doped CdTe to understand the self-compensation mechanism which will help improve minority bulk carrier lifetime and net acceptor density. Combining previous measurements of un-doped CdTe, we performed a systematic comparison of defects between different types of crystals and confirmed the defects impacting the doping efficiency. CdTe bulk crystals have been grown via vertical Bridgman based melt growth technique with varying arsenic and phosphorous dopant schemes to attain p-type material. Furnace temperature profiles were varied to influence dopant solubility. Large carrier densities have been reproducibly obtained from these boules indicating successful incorporation of dopants into the lattice. However, these values are orders of magnitude lower than theoretical solubility values. Infrared Microscopy has revealed a plethora of geometrically abnormal second phase defects and X-ray Fluorescence has been used to identify the elemental composition of these defects. We believe that dopants become incorporated into these second phase defects as Cd compounds which act to inhibit dopant solubility in the lattice.

**9:48AM X7.00010 Diversity of surface conduction in pyrite FeS<sub>2</sub> single crystals**, CHRIS LEIGHTON, JEFF WALTER, XIN ZHANG, FRAZIER MORK, RYAN HOOL, MIKE MANNO, ERAY AYDIL, University of Minnesota — Pyrite FeS<sub>2</sub> has long been recognized as an attractive material for solar cells because of its high absorptivity, potential low cost, high abundance, and low toxicity. Despite having appropriate band gap (0.95 eV) and minority carrier diffusion length (100-1000 nm), low open circuit voltages ( $V_{oc} \leq 0.1$  V) have plagued FeS<sub>2</sub>-based cells. Surface conduction has been proposed as a contributing factor for the low  $V_{oc}$ , particularly a p-type surface inversion layer on n-type crystals [1]. Here we report a detailed electronic transport study of a large number of well-characterized CVT-grown n-FeS<sub>2</sub> single crystals. Abundant evidence of surface conduction is found from the  $T$  dependence of resistivity, resistance anisotropy, low  $T$  behavior at the 2D quantum resistance, thickness dependence, and the influence of contact metal work function. However, striking diversity in this surface conduction is found, even in nominally identical crystals at similar doping. The results cannot be understood by surface inversion alone, pointing to as yet uncontrolled surface factors. [1] Limpinsel *et al.* Energy Environ. Sci. (2014). Work supported by NSF.

**10:00AM X7.00011 Grain boundaries and surfaces in polycrystalline photovoltaics**, PAUL HANEY, National Institute of Standards and Technology, HEAYOUNG YOON, The University of Utah, NIKOLAI ZHITENEV, National Institute of Standards and Technology — Despite the fact that polycrystalline photovoltaics materials such as CdTe and CIGS are an established commercial technology, the precise role of grain boundaries in their performance remains poorly understood. The high defect density at grain boundaries is generally detrimental to carrier lifetime, however the electric fields surrounding charged grain boundaries may separate electrons and holes, effectively passivating the grain boundary. One difficulty in ascertaining the properties of grain boundaries is that high spatial resolution experimental techniques needed to probe individual grain boundaries are generally surface sensitive. For this reason, extracting quantitative grain boundary and other material properties from this data requires a quantitatively accurate model of the exposed surface. Motivated by these considerations, we present a theoretical analysis of the response of a polycrystalline semiconductor to a localized excitation near a grain boundary, and near the surface. We use our analytical results to interpret electron beam induced current (EBIC) data on polycrystalline CdTe solar cells.

**10:12AM X7.00012 Individual iso-electronic N and Bi centers in GaAs studied by Scanning Tunneling Microscopy.**, PAUL KOENRAAD, CHRISTIAN KRAMMEL, RIANNE PLANTENGA, Eindhoven University of Technology, VICTORIA KORTAN, MICHAEL FLATT, University of Iowa, FREDDY TILLEY, MERVIN ROY, PETER MAKSYM, University of Leicester, TAKASHI KITA, Kobe University — Nitrogen and bismuth iso-electronic doping centers in GaAs have received considerable interest in the last few years due to their peculiar behaviour in dilute nitrides and bismides. In these materials effects such as a strong band bowing and the formation of resonant states in respectively the conduction and valence band have been reported. In this contribution we will report our exploration of individual nitrogen and bismuth atoms in the outermost layers of a freshly cleaved (110) GaAs surface by STM. Depending on the tunnel conditions we are able to either visualise the lattice distortion or image the charge distribution of the resonant state. We clearly observe that nitrogen pulls its neighbouring atoms inwards whereas bismuth pushes its neighbouring atoms away. A straightforward geometrical model based on the covalent radii of the dopants and substrate atoms is used to interpret the observed crystal deformation seen in our STM images of nitrogen and bismuth under the appropriate tunnel conditions. At small positive voltages we could observe the charge distribution of the resonant state induced by iso-electronic nitrogen atoms in GaAs. Tight Binding Modelling (TBM) was used to explain the observed strongly anisotropic charge distribution.

**Friday, March 18, 2016 8:00AM - 10:48AM –**

**Session X8 DMP GMAG: Organic Inorganic Perovskite Spintronics** 304 - Oana Jurchescu, Wake Forest University

**8:00AM X8.00001 Organometal Trihalide Perovskite Spintronics<sup>1</sup>**, DALI SUN, University of Utah — The family of organometal trihalide perovskite (OTP), CH<sub>3</sub>NH<sub>3</sub>PbX<sub>3</sub> (where X is halogen) has recently revolutionized the photovoltaics field, and shows promise in applications such as solar energy harnessing, light emitting diodes, field effect transistors and laser action. The OTP spin characteristic properties are influenced by the large spin-orbit-coupling of the Pb atoms, and thus may offer a new class of semiconductors for spin-based applications. In this talk we will summarize the 'magnetic field effect' on photocurrent and electroluminescence in OTP optoelectronic devices, and photoluminescence from OTP films [1]; and report more recent studies of pure spin-current and spin-aligned carrier injection in OTP spintronics devices using 'spin-pumping' and 'spin-injection', respectively. We measured relatively large inverse-spin-Hall effect using pulsed microwave excitation in OTP devices at resonance with a ferromagnetic (FM) layer, and giant magnetoresistance in OTP-based spin-valves. Our studies launch the field of OTP spintronics. [1] C. Zhang *et al.* Nat. Phys. 11, 427-434 (2015)

<sup>1</sup>Research sponsored by the DOE, Office of Science, grant DE-SC0014579. Work done in collaboration with Chuang Zhang, Marzieh Kavand, Kipp J. van Schooten, Hans Malissa, Matthew Groesbeck, Ryan McLaughlin, Christoph Boehme, and Z. Vally Vardeny.

**8:36AM X8.00002 Magneto-optical properties of hybrid organic-inorganic perovskites**, ZHI-GANG YU, Washington State University — In semiconductors the k.p Hamiltonian played a central role in understanding material properties because the model parameters are directly related to experimental measurable properties. Here we construct a 8-band k.p Hamiltonian for tetragonal perovskites from both perturbation and group theories and determine the parameters from first-principles band-structure calculations and experiments. This Hamiltonian is then used to study conduction- and valence-band states as well as excitons under an arbitrary magnetic field. The calculated electron and hole g-factors can explain the exciton g-factors measured by magneto-absorption and magneto-luminescence and the field-dependent exciton energies are consistent with the high-field magneto-absorption experiment, which has been used to accurately determine the exciton binding energy.

**8:48AM X8.00003 Studies of Gilbert magnetization damping in NiFe/organometallic trihalide perovskite bilayers investigated by broadband ferromagnetic resonance<sup>1</sup>**, MATTHEW GROESBECK, DALI SUN, RYAN MCLAUGHLIN, CHUANG ZHANG, HAOLIANG LIU, ZEEV VALY VARDENY, University of Utah Dept. of Physics and Astronomy — Organo-metallic trihalide perovskites (OTP) have recently been suggested as promising candidates for spintronics applications, motivated by the presence of strong spin-orbit coupling, and recent studies of spin dynamics in  $\text{CH}_3\text{NH}_3\text{PbI}_3$ . To help elucidate the spin transport properties in these materials, we have studied the Gilbert magnetization damping parameter in NiFe ferromagnetic films related to spin-pumping into adjacent OTP layers under ferromagnetic resonance (FMR) excitation conditions, using a broadband FMR detection system. We found an increase of the damping parameter associated with spin-pumping into the OTP. The obtained thickness-dependent results are compared to those of NiFe/Cu and NiFe/Pt bilayer structures, where spin transport characteristics are well-known.

<sup>1</sup>Research sponsored by the DOE, Office of Science, grant DE-SC0014579

**9:00AM X8.00004 Optical Generation of Ballistic and Diffusive Spin Currents in Organic-Inorganic Lead Halide Perovskites**, JUNWEN LI, PAUL HANEY, National Institute of Standards and Technology — Organic-inorganic halide perovskite solar cells have attracted enormous attention in recent years due to their remarkable photovoltaic power conversion efficiency. These materials should exhibit interesting spin-dependent properties as well, owing to the strong spin-orbit coupling and the broken inversion symmetry present at room temperature. In this work, we consider the spin-dependent optical response of  $\text{CH}_3\text{NH}_3\text{PbI}_3$  on two distinct time scales. We first use density functional theory to compute the ballistic spin current injected by absorption of linearly polarized light. This spin current persists on a time scale of the momentum relaxation time. We then consider diffusive transport of photogenerated charge and spin for a thin perovskite layer with a passivated surface and an Ohmic, non-selective back contact. The spin densities and spin currents are evaluated by solving the drift-diffusion equations for a 3-dimensional Rashba model. We comment on the applications of optically excited spin densities and spin currents in these materials.

**9:12AM X8.00005 Exciton spin dynamics in  $\text{MAPbI}_3$  measured by Hanle effect**, WILLIAM TALMADGE, University of Utah Department of Physics and Astronomy, RUIZHI WANG, University of Utah Department of Physics and Astronomy, Nanjing University of Science and Technology, PATRICK ODENTHAL, NATHAN GUNDLACH, CHUANG ZHANG, DALI SUN, ZEEV VALY VARDENY, YAN (SARAH) LI, University of Utah Department of Physics and Astronomy — The organic-inorganic hybrid perovskites have emerged as a highly promising class of semiconductors for photovoltaic applications. The properties responsible for the high photoconversion efficiency are under extensive investigation. There have, however, been fewer investigations of spin-dependent effects in this class of materials. We present energy dependent photoinduced Faraday rotation in polycrystalline thin film  $\text{CH}_3\text{NH}_3\text{PbI}_3$ , which benefit from the band structure and optical selection rules. The Faraday rotation spectrum follows the exciton absorption band at low temperatures, indicating its excitonic origin. Through the Hanle effect, based on Faraday rotation, we found the coexistence of two spin components at 4 K, which was confirmed through time resolved measurements.

**9:24AM X8.00006 Photoexcited carrier spin dynamics in  $\text{CH}_3\text{NH}_3\text{PbI}_3$ <sup>1</sup>**, PATRICK ODENTHAL, NATHAN GUNDLACH, WILLIAM TALMADGE, University of Utah, RUIZHI WANG, Nanjing University of Science and Technology, CHUANG ZHANG, DALI SUN, ZEEV VALY VARDENY, YAN (SARAH) LI, University of Utah — Metal halide perovskites have shown great promise for the field of spintronics due to their large tunable spin-orbit coupling, spin dependent optical selection rules and predicted electrically tunable Rashba band. The spin sensitive optical transitions allow optical spin orientation of carriers using circularly polarized light, and detection of the spin polarization via optical Faraday rotation measurement. We study carrier spin dynamics on solution-processed polycrystalline  $\text{CH}_3\text{NH}_3\text{PbI}_3$  films using time-resolved Faraday rotation (TRFR). TRFR reveals unexpected long spin lifetimes exceeding 1ns at 4K. This is significant given that Pb and I exhibit large spin-orbit coupling, which usually lead to fast spin relaxation.

<sup>1</sup>Research supported by the NSF-MRSEC (DMR 1121252) at the University of Utah.

**9:36AM X8.00007 Composition, Temperature, and Electric Field Dependence of Magneto-Optical Properties of Lead Halide Perovskites<sup>1</sup>**, RYAN MCLAUGHLIN, CHUANG ZHANG, DALI SUN, Z. VALY VARDENY, University of Utah — Organometallic Perovskites have received much attention in recent years due to their remarkable efficiency in photovoltaic cells, along with their highly tunable optical and electrical properties. It is an important goal to quantify and understand the effects of Spin-Orbit Coupling in Perovskite-based optoelectronic devices, which can be characterized by magneto-optical properties such as Kerr rotation and Faraday rotation. Here we use the Verdet constant to investigate the tunability of the Spin-Orbit coupling parameters of Organometallic Perovskites as a function of chemical composition, temperature, and electric field.

<sup>1</sup>Research sponsored by the NSF (Grant No. DMR-1104495) and NSF-MRSEC (DMR 1121252).

**9:48AM X8.00008 ABSTRACT WITHDRAWN —**

**10:00AM X8.00009 Neutron and X-Ray Scattering Studies of Hybrid Perovskites for Photovoltaic Applications**, MICHAEL CRAWFORD, DuPont Company, PAMELA WHITFIELD, NIINA JALARVO, GEORG EHLERS, SNS, Oak Ridge National Laboratory, MADHUSUDAN TYAGI, NIST Center for Neutron Research, NORMAN HERRON, LYNDIA JOHNSON, DuPont Company, WILLIAM GUISE, DuPont Company and APS, Argonne National Laboratory, IVAN MILAS, DuPont Company, YONGQIANG CHENG, LUKE DAEMEN, ANIBAL RAMIREZ-CUESTA, KATHARINE PAGE, XIAOPING WANG, FENG YE, SNS, Oak Ridge National Laboratory — Hybrid perovskites ( $\text{ABX}_3$ ) have attracted a great deal of attention recently as light absorbers for photovoltaics. In these materials the A site is occupied by organic cations, for example methyl ammonium (MA) or formamidinium (FA) cations, the B site is occupied by metals, for example Pb or Sn, and the X anions are halogens (I, Br, or Cl). Typical of perovskites, these materials exhibit a series of structural phase transitions involving rotations or tilts of the  $\text{BX}_6$  octahedra, but with the added complexity that the inorganic framework is coupled to order-disorder transitions of the organic cations. We have used neutron scattering techniques to characterize the structures and dynamics of several of these compounds as a function of temperature. In addition, high resolution synchrotron x-ray diffraction measurements have been performed to investigate the structural phase transitions. These studies yield a detailed picture of the structures, dynamics, and structural phase transitions of these compounds, and provide a firm basis for understanding their excellent photovoltaic properties.

**10:12AM X8.00010 Electric Field Effects on Photoconductivity and Photoluminescence in  $\text{MAPbI}_3$  Perovskite<sup>1</sup>**, CHUANG ZHANG, DALI SUN, ZEEV VALY VARDENY, Department of Physics & Astronomy, University of Utah — The origin of “hysteresis behavior” in I-V response of  $\text{MAPbI}_3$  perovskite devices is still under debate. We characterized this electric field induced hysteresis by monitoring the changes of photoconductivity (E-PC) and photoluminescence (E-PL) from the  $\text{MAPbI}_3$  film deposited on inter-digital electrodes. Interestingly, we observed a “sign change” in both E-PC and E-PL effects, depending on the applied field and temperature. The E-PC/E-PL could be “frozen” when cooling the device under external field to lower temperature. These results reveal multiple possible reasons for the intrinsic hysteresis behavior in  $\text{MAPbI}_3$  perovskite devices. This work was supported by the Utah NSF-MRSEC program DMR 1121252.

<sup>1</sup>Electric Field Effects on Photoconductivity and Photoluminescence in  $\text{MAPbI}_3$  Perovskite

**10:24AM X8.00011 Nanoimprinting Perovskite by Hot Stamping for Improved Crystallinity and Morphology**, BALASUBRAMANIAM BALACHANDRAN, ROSS HAROLDSON, YIXIN REN, ANVAR ZAKHIDOV, WENCHUANG HU, JULIA CHAN, Univ of Texas - Dallas, UTD NANOIMPRINT TEAM — We present an innovative approach of using thermal nanoimprinting lithography (NIL by hot embossing) to pattern hybrid perovskites into ordered micro and nanostructures with improved crystallinity and morphology. The spin-coated thin films of organic-inorganic perovskite CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> have been embossed by large area stamps of highly periodic nanopatterns at the scale of 200 to 600 nm. XRD shows the larger and aligned grains, while SEM reveals much improved film morphology with no pin-holes and much less grain boundaries. The obtained ordered periodic micro- and nanostructures show iridescent coloration due to Bragg scattering in planar perovskite photonic crystals.

**10:36AM X8.00012 Spatially resolved optoelectronic characterization of perovskite lead iodide nanostructures**, RUI XIAO, XINGYU PENG, YASEN HOU, DONG YU, Univ of California - Davis — The high power conversion efficiency of organo-lead halide perovskite-based solar cells has attracted world-wide attention over the past few years. The high efficiency was believed to originate from the unusual properties including long carrier lifetimes and consequent long carrier diffusion lengths in these materials. Ion drift, ferroelectricity, and charge traps have been proposed to account for the efficient charge separation and photocurrent hysteresis. However, it remains unclear which mechanism is dominating. We fabricate field effect transistors (FETs) incorporating single nanoplates/nanowires of organic perovskite and perform scanning photocurrent microscopic (SPCM) measurements to extract carrier diffusion lengths as a function of gate voltage, source-drain bias. Spatially resolved optoelectronic investigations of single crystalline perovskite nanostructures provide valuable information and key evidence on distinguishing the dominating charge transport/separation mechanism.

**Friday, March 18, 2016 8:00AM - 11:00AM —**

**Session X11 DMP: New Fe-based Superconductors and Related Materials II** 307 - Xianhui Chen, University of Science and Technology of China

**8:00AM X11.00001 Interplay of structure, magnetism and superconductivity in the 112 Fe based superconducting family**, NI NI, Univ of California - Los Angeles — Both cuprates and Fe-based superconductors, the two known high T<sub>c</sub> superconducting families, show rich emergent phenomena near the superconductivity (SC). To understand the mechanism of unconventional SC, it is crucial to unravel the nature of these emergent orders. The 112 Fe pnictide superconductor (FPS), Ca<sub>1-x</sub>RE<sub>x</sub>FeAs<sub>2</sub> (CaRE112), shows SC up to 42 K, the highest bulk T<sub>c</sub> among all nonoxide FPS [2]. Being an exceptional FPS where the global C<sub>4</sub> rotational symmetry is broken even at room temperature, it is important to extract the similarities and differences between 112 and other FPS so that critical ingredients in inducing SC in FPS can be filtered. In this talk, I will review current progress in the study of 112. The comparison between Co doped CaLa112 and Co doped 10-3-8 will be made and the importance of interlayer coupling will be discussed. The work on 112 is supported by NSF while the work on 10-3-8 is supported by DOE.

**8:36AM X11.00002 Structural symmetries of the 112-type iron-based superconductor (Ca<sub>1-x</sub>La<sub>x</sub>)FeAs<sub>2</sub> studied using nonlinear and ultrafast optics**, JOHN HARTER, HAO CHU, Institute for Quantum Information and Matter, California Institute of Technology, SHAN JIANG, NI NI, Department of Physics & Astronomy, University of California, Los Angeles, DAVID HSIEH, Institute for Quantum Information and Matter, California Institute of Technology — The crystal structure of the newly discovered 112-type iron-based superconductors contains symmetry-breaking arsenic chains, avoiding the need for local probes or uniaxial strain in order to study the ubiquitous electronic nematic state that exists in the vicinity of magnetic order in the iron pnictides. In addition, the 112-type materials are the first known high-temperature superconductors without a center of inversion, with interesting ramifications for Cooper pairing in the superconducting state. We present details of the structure of 112-type (Ca<sub>1-x</sub>La<sub>x</sub>)FeAs<sub>2</sub> using rotational anisotropy second harmonic generation and pump-probe transient reflectivity experiments. These all-optical techniques are complimentary to conventional diffraction measurements and enable a precise determination of crystallographic symmetries. Our measurements highlight the novel structural properties of the 112-type materials.

**8:48AM X11.00003 ABSTRACT WITHDRAWN —**

**9:00AM X11.00004 The Interplay of Fe and Ce Magnetism in Ca<sub>0.71</sub> Ce<sub>0.29</sub>(Fe<sub>1-x</sub>Co<sub>x</sub>)As<sub>2</sub> single crystals<sup>1</sup>**, SHAN JIANG, Univ of California - Los Angeles, LIAN LIU, Columbia University, HUIBO CAO, WEI TIAN, Oak Ridge National Lab, EVE EMMANUELIDU, AOSHUANG SHI, Univ of California - Los Angeles, YASUTOMO UEMURA, Columbia University, NI NI, Univ of California - Los Angeles — In this talk, we will present the synthesis and characterization of the Ca<sub>0.71</sub> Ce<sub>0.29</sub>(Fe<sub>1-x</sub>Co<sub>x</sub>)As<sub>2</sub> single crystals. Elastic neutron scattering complemented by resistivity, susceptibility and heat capacity measurements has revealed a paramagnetic-to-antiferromagnetic phase transition of the Fe sublattice at 69K and a monoclinic-to-triclinic structural phase transition at 73 K in Ca<sub>0.71</sub> Ce<sub>0.29</sub>FeAs<sub>2</sub>. In addition, Fe spin reorientation and Ce ordering at lower temperatures, reminiscent of the one in REFeAsO (RE=Ce, Pr, Nd) materials, exist. The Co substitution on the Fe sites completely suppresses the ordering of Fe sublattice at x=0.032. However, it only slightly affects the Ce ordering, which prevents the formation of superconductivity in Ca<sub>0.71</sub> Ce<sub>0.29</sub>(Fe<sub>1-x</sub>Co<sub>x</sub>)As<sub>2</sub>.

<sup>1</sup>Work at UCLA was supported by the NSF DMREF DMR-1435672. Work at Columbia and TRIUMF was supported by the NSF DMREF DMR-1436095, PIRE project IIA 0968226 and DMR-1105961. Work at ORNL's High Flux Isotope Reactor was sponsored by DOE

**9:12AM X11.00005 Thallium-doped BaFe<sub>2</sub>As<sub>2</sub> crystals: The unusual competition between magneto-elastic coupling and charge doping<sup>1</sup>**, ATHENA SEFAT, LI LI, HUIBO CAO, BRIAN SALES, MICHAEL MCGUIRE, RADU CUSTELCEAN, DAVID PARKER, Oak Ridge National Lab — We partially substitute thallium for barium and report the effects of interlayer coupling in Ba<sub>1-x</sub>Tl<sub>x</sub>Fe<sub>2</sub>As<sub>2</sub> crystals. We demonstrate the unusual competition between magneto-elastic coupling and charge doping in an iron-arsenide material, whereby T<sub>N</sub> temperature rises in BaFe<sub>2</sub>As<sub>2</sub>, and then falls with additional TI-doping. Evidence from temperature-dependent bulk thermodynamic and transport properties, and neutron diffraction results will be presented. Using LDA, we illustrate that small changes related to 3d transition-metal state can have profound effects on magnetism.

<sup>1</sup>The work is supported by the U.S. DOE, Office of Science, BES, Materials Sciences and Engineering Division, and Chemical Sciences, Geosciences, and Biosciences Division. The work at ORNLs HFIR is sponsored by the Scientific User Facilities Division.

**9:24AM X11.00006 Structural and antiferromagnetic properties of  $\text{Ba}(\text{Fe}_{1-x-y}\text{Co}_x\text{Rh}_y)_2\text{As}_2$  compounds**<sup>1</sup>, MIN GYU KIM, Lawrence Berkeley National Laboratory, T. W. HEITMANN, The Missouri Research Reactor, S. R. MULCAHY, University of California, Berkeley, E. D. BOURRET-COURCHESNE, Lawrence Berkeley National Laboratory, R. J. BIRGENEAU, University of California, Berkeley — We present a systematic investigation of the electrical, structural, and antiferromagnetic properties for the series of  $\text{Ba}(\text{Fe}_{1-x-y}\text{Co}_x\text{Rh}_y)_2\text{As}_2$  compounds with fixed  $x = 0.027$  and  $0 < y < 0.035$ . We compare our results for the Co-Rh doped  $\text{Ba}(\text{Fe}_{1-x-y}\text{Co}_x\text{Rh}_y)_2\text{As}_2$  compounds with  $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$  compounds. We demonstrate that the electrical, structural, antiferromagnetic, and superconducting properties of the Co-Rh doped compounds are similar to the properties of the Co doped compounds. We find that the overall behaviors of  $\text{Ba}(\text{Fe}_{1-x-y}\text{Co}_x\text{Rh}_y)_2\text{As}_2$  and  $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$  compounds are very similar when the total number of the extra electrons per Fe/*TM* (*TM* = transition metal) site is considered, which is consistent with the rigid band model. Despite the similarity, we find that the details of the transitions are different in between  $\text{Ba}(\text{Fe}_{1-x-y}\text{Co}_x\text{Rh}_y)_2\text{As}_2$  and  $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$  compounds.

<sup>1</sup>The work at the Lawrence Berkeley National Laboratory was supported by the U.S. Department of Energy (DOE), Office of Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract No. DE-AC02-05CH11231.

**9:36AM X11.00007 Search for New Superconductors: An Electro-Magnetic Phase Transition in an Iron Meteorite Inclusion at 117 K**, STEFAN GUÉNON, PIT, Nano Atomoptics, University of Tuebingen, Germany, JUAN GABRIEL RAMIREZ, Department of Physics, Universidad de los Andes, Bogota, Colombia, ALI C. BASARAN, Department of Physics, Gebze Technical University, Turkey, JAMIE WAMPLER, Department of Physics and Center for Advanced Nanoscience, University of California San Diego, MARK THIEMENS, Department of Chemistry and Biochemistry, University of California San Diego, IVAN K. SCHULLER, Department of Physics and Center for Advanced Nanoscience, University of California San Diego — We investigated a natural iron sulfide based materials (Troilite) inclusion with its associated minerals in the iron meteorite Tlacotepec. The search for superconductivity in these heterogeneous materials requires a technique capable of detecting minute amounts of a superconducting phase embedded in a non-superconducting matrix. We used Magnetic Field Modulated Microwave Spectroscopy (MFMMS), a very sensitive, selective, and non-destructive technique, to search for superconductivity in heterogeneous systems. Here, we report the observation of an electro-magnetic phase transition at 117 K that causes a MFMMS-response typical of a superconductor. A pronounced and reproducible peak together with isothermal magnetic field sweeps proves the appearance of an electromagnetic phase below 117 K. This is very similar to the characteristic response due to flux trapping in a granular superconductor with a short coherence length. This work was supported by the AFOSR under the grant number AFOSR-MURI FA9550-14-1-0202.

**9:48AM X11.00008 Heisenberg Model Analysis on Inelastic Powder Neutron Scattering Data Using Pure and K doped  $\text{BaMn}_2\text{As}_2$  samples**<sup>1</sup>, MEHMET RAMAZANOGLU, Istanbul Technical University, A. SAPKOTA, A. PANDEY, D. JOHNSTON, ALAN GOLDMAN, A. KREYSSIG, Ames Lab. & Iowa State Univ., Ames, IA, 50011, D. ABERNATHY, J. NIEDZIELA, M. STONE, Oak Ridge National Lab., TN, 37831, R.J. MCQUEENEY, Ames Lab. & Iowa State Univ., Ames, IA, 50011 — Low temperature powder inelastic neutron scattering measurements (INS) were performed on powders of  $\text{Ba}(1-x)\text{KxMn}_2\text{As}_2$  with  $x=0$ (BMA), 0.125 and 0.25. BMA is a G type antiferromagnet (AFM) which has local magnetic modulations bridging between the pnictide and cuprate superconductors. Hole doping (K) introduces more metallic behavior. The magnetic contribution to the intensities were retrieved by subtracting the estimated phonon background obtained at high momentum transfers from the raw. The resultant estimated magnetic intensities were analyzed by using damped harmonic oscillator model. The K doping effects create a broadening in the magnetic peak profiles consistent with expected weak FM fluctuations. We also analyzed the INS data using a powder integration routine which is based on J1-J2-Jz Heisenberg Model. The Monte Carlo integration technique is used to obtain the powder-averaged  $S(\mathbf{Q}, E)$  for a series of Js. The representative values (with lowest chi-squared) obtained for BMA are in agreement with previous results. The values obtained for K doped samples were found in the close proximity to the parent ones. Overall we conclude that the original AFM structure seen in BMA retained its character even in the K doped samples with minimal differences.

<sup>1</sup>Work at Ames Laboratory is supported by USDOE under Contract No. DE-AC02-07CH11358 and Work at ITU is supported by TUBITAK 2232

**10:00AM X11.00009 A new class of half-metallic ferromagnets based on the pnictide superconductors from first principles.**<sup>1</sup>, SINEAD GRIFFIN, JEFFREY NEATON, Lawrence Berkeley Natl Lab/UC Berkeley — Most theoretical and experimental efforts in the Fe-pnictide class of superconductors aim to optimize the superconducting  $T_c$ . Significant substitution with other transition-metal ions is detrimental to superconductivity, however recent experiments on doped  $\text{BaMn}_2\text{As}_2$  point to its potential as a half-metallic ferromagnet. Using ab initio calculations we investigate Mn-based structures as a new family of half-metallic ferromagnets, and discuss tuning the chemical composition and physical parameters for optimal device performance.

<sup>1</sup>Support from Swiss National Science Foundation

**10:12AM X11.00010 Antiferromagnetism in  $\text{CaAl}_2\text{Si}_2$ -type  $\text{CaMn}_2\text{As}_2$  and  $\text{SrMn}_2\text{As}_2$  single crystals**<sup>\*</sup>, N. S. SANGEETHA, ABHISHEK PANDEY, ZACKERY A. BENSON, D. C. JOHNSTON, Ames Laboratory, Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011 — Magnetic susceptibility versus temperature  $\chi(T)$  measurements of  $\text{CaMn}_2\text{As}_2$  and  $\text{SrMn}_2\text{As}_2$  crystals show clear antiferromagnetic (AFM) transitions at  $T_N \approx 65$  K and 120 K,<sup>1</sup> respectively. The anisotropic behaviors in  $\chi(T \leq T_N)$  suggest that both compounds are noncollinear antiferromagnets which may result either from an intrinsic noncollinear structure or from multiple collinear AFM domains that are not aligned collinearly.<sup>2</sup> The  $\chi(T)$  data at  $T > T_N$  reveal that both compounds exhibit strong short-range AFM ordering, evidently associated with quasi-two-dimensional spin lattices. The electrical resistivities show insulating ground states with activation energies of  $\approx 63$  meV in  $\text{CaMn}_2\text{As}_2$  and 44 meV in  $\text{SrMn}_2\text{As}_2$ . The experimental results thus reveal that both (Ca, Sr) $\text{Mn}_2\text{As}_2$  materials are AFM insulators at low temperatures and in analogy with the high  $T_c$  cuprates, may be potential parent compounds for  $\text{CaAl}_2\text{Si}_2$ -type superconductors.

<sup>\*</sup>Work was supported by the USDOE under Contract No. DE-AC02-07CH11358.

<sup>1</sup>Z.W. Wang et. al, J. Phys. Chem. Solids **72**, 457 (2011).

<sup>2</sup>D. C. Johnston, PRL **109**, 077201 (2012); PRB **91**, 064427 (2015).

**10:24AM X11.00011 Resistivity Anisotropy in Single Crystals of  $\text{CaCo}_{1.86}\text{As}_2$** <sup>1</sup>, M. A. TANATAR, V. K. ANAND, A. PANDEY, N. S. SANGEETHA, D.C. JOHNSTON, R. PROZOROV, Ames Laboratory and Iowa State University — In-plane and inter-plane resistivity was measured in single crystals of type A antiferromagnet  $\text{CaCo}_{2-x}\text{As}_2$  ( $x = 0.14$ ). Clear anomalies in the temperature dependent resistivity are observed at the magnetic ordering at  $T_N \approx 50$  K. The transition shifts to lower temperatures upon application of 9 T magnetic field both along tetragonal (001) axis,  $H \parallel c$ , and transverse to it,  $H \perp c$ . The temperature - magnetic field phase diagrams determined from the resistivity measurements are in good agreement with magnetization measurements [1]. No additional anomalies are found at the spin-flip transition in the compound, suggesting that the direction of the spin does not play an appreciable role in the spin-disorder scattering in this compound. [1] V. K. Anand *et al.* Phys. Rev B **89**, 214409 (2014).

<sup>1</sup>This work was supported by the U.S. Department of Energy, Office of Basic Energy Science, Materials Science and Engineering Division and was performed at the Ames Laboratory, Iowa State University under contract DE-AC02-07CH11358.

**10:36AM X11.00012 Wall-like spin excitations in A-type antiferromagnetic  $\text{CaCo}_2\text{As}_2$** <sup>1</sup>, A. SAPKOTA, B. G. UELAND, ABHISHEK PANDEY, D. C. JOHNSTON, A. KREYSSIG, R. J. MCQUEENEY, A. I. GOLDMAN, Ames Laboratory, Dept. of Physics and Astronomy, Iowa State University, V. K. ANAND, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, J. L. NIEDZIELA, D. L. ABERNATHY, Oak Ridge National Laboratory — The  $\text{ACo}_2\text{As}_2$  ( $A = \text{Ca, Sr, Ba}$ ) compounds are structurally and chemically similar to  $\text{AFe}_2\text{As}_2$  and possess some interesting similarities and differences in their magnetism. We recently discovered that  $\text{SrCo}_2\text{As}_2$  has stripe antiferromagnetic (AFM) spin correlations similar to stripe-ordered  $\text{AFe}_2\text{As}_2$ . On the other hand,  $\text{CaCo}_2\text{As}_2$  orders in an A-type AFM structure with ferromagnetic correlation of the spins in the square-lattice Co-layer and AFM correlations between layers. Despite the A-type order, our recent inelastic neutron scattering measurements show that spin excitations in  $\text{CaCo}_2\text{As}_2$  are not associated with either the A-type or stripe-type order. Instead, we observe broad excitations that extend longitudinally (along (1,1,0) in reciprocal space), but remain sharply defined in the transverse direction. These excitations seem to be best characterized as a “wall” of scattering and suggest that  $\text{CaCo}_2\text{As}_2$  has quasi-one-dimensional spin dynamics very different than in  $\text{AFe}_2\text{As}_2$  and  $\text{SrCo}_2\text{As}_2$ .

<sup>1</sup>Work at Ames Laboratory was supported by US DOE, Basic Energy Sciences, Division of Materials Sciences and Engineering, under Contract No. DE-AC02-07CH11358. Work at ORNL was supported by US DOE, Office of Basic Energy Sciences, Scientific User Facilities Division.

**10:48AM X11.00013 Pressure-induced collapsed-tetragonal phase in  $\text{SrCo}_2\text{As}_2$  at ambient temperature**, W. T. JAYASEKARA, U. S. KALUARACHCHI, B. G. UELAND, A. PANDEY, Y. B. LEE, V. TAUFOR, A. SAPKOTA, K. KOTHAPALLI, N. S. SANGEETHA, S. L. BUD'KO, B. N. HARMON, P. C. CANFIELD, D. C. JOHNSTON, A. KREYSSIG, A. I. GOLDMAN, Ames Lab., Dept. of Physics and Astronomy, Iowa State Univ., G. FABBRIS, Y. FENG, L. S. I. VEIGA, Argonne Natl. Lab., A. M. DOS SANTOS, Oak Ridge Natl. Lab. — Our recent high-energy (HE) high-pressure (HP) x-ray powder diffraction measurements on tetragonal (T)  $\text{SrCo}_2\text{As}_2$  have revealed a first-order pressure-induced structural phase transition to a collapsed tetragonal (cT) phase with a reduction in  $c$  by -7.9% and the  $c/a$  ratio by -9.9%. The T and cT phases coexist for applied pressures 6 GPa to 18 GPa at 7 K. Resistance measurements up to 5.9 GPa and down to 1.8 K signatures likely associated with the cT phase above 5.5 GPa and found no evidence for superconductivity. Neutron diffraction data show no evidence of magnetic order up to 1.1 GPa. Here, we show that the T to cT transition occurs around 6.8 GPa at ambient temperature, and that the transition is nearly temperature-independent from 300 K down to 7 K, which indicates a steep  $p - T$  phase line.

Work at Ames Lab. was supported by US DOE, BES, DMSE under DE-AC02-07CH11358. This research used resources at the APS and ORNL, US DOE, SC, User Facilities.

## Friday, March 18, 2016 8:00AM - 11:00AM – Session X12 DCMP DMP: Topological Materials: Theory and Experiment 308 -

**8:00AM X12.00001 Phase diagram of disordered, time reversal invariant topological superconductors in two and three dimensions**, SUDIP CHAKRAVARTY, UCLA, PALLAB GOSWAMI, University of Maryland — In the absence of spin rotational invariance, time reversal symmetric topological superconducting states (belonging to the class DIII) can be realized in all three spatial dimensions. We construct the global phase diagrams of disordered, class DIII superconductors in two and three dimensions. In both spatial dimensions the Bogoliubov de Gennes quasiparticles can exhibit two topologically distinct localized (gapped) phases, in addition to a diffusive (gapless) phase that possesses metallic thermal conductivity. We also obtain exact localization length exponents and approximate crossover scaling functions for the relevant topological quantum phase transitions. For sufficiently weak disorder, we show that the direct topological transition between two gapped states is described by a four component, massless Dirac fermion with a dynamical exponent  $z = 1$  and a correlation/localization length exponent  $\nu_M = 1$ . For stronger disorder, we demonstrate how two topologically distinct localized states and the delocalized diffusive phase meet at a line of disorder controlled fixed points, which governs the nature of the localization-delocalization transitions. We show the existence of a universal localization length exponent  $\nu_M = 2/d$  and a nonuniversal dynamical exponent for the localization

**8:12AM X12.00002 Converting a topologically trivial superconductor into a chiral topological superconductor via diluted magnetic doping**<sup>1</sup>, WEI QIN, University of Science and Technology of China, DI XIAO, Carnegie Mellon University, KAI CHANG, Chinese Academy of Sciences, SHUN-QING SHEN, University of Hong Kong, ZHENYU ZHANG, University of Science and Technology of China — We employ two complementary theoretical approaches to explore the feasibility of altering the topological properties of two-dimensional Rashba spin-orbit coupled superconductors by proper introduction of magnetic disorders. First, using the self-consistent Born approximation, we show that a topologically trivial superconductor can be driven into a chiral topological superconductor upon diluted doping of isolated magnetic disorders, which gradually narrow, close, and reopen the quasi-particle gap of the paired electrons in a nontrivial manner. Such a topological phase transition is further characterized by the change in the corresponding topological invariant. The central predictions made here are then confirmed using the complementary numerical approach by solving the Bogoliubov-de Gennes equations self-consistently within a tight-binding model. We also discuss the validity of the present model studies in connection with existing experimental findings. Collectively, the present study offers appealing new schemes for potential experimental realization of topological superconductors.

<sup>1</sup>Supported by NSF of China

**8:24AM X12.00003 Quantum Monte Carlo study of strange correlator in interacting topological insulators**, HAN-QING WU, YUAN-YAO HE, Renmin Univ of China, YI-ZHUANG YOU, CENKE XU, Department of Physics, University of California, Santa Barbara, California, ZI YANG MENG, Institute of Physics, Chinese Academy of Sciences, ZHONG-YI LU, Renmin Univ of China — Distinguishing the nontrivial symmetry-protected topological (SPT) phase from the trivial insulator phase in the presence of electron-electron interaction is an urgent question to the study of topological insulators. In this work, we demonstrate that the strange correlator is a sensitive diagnosis to detect SPT states in interacting systems. Employing large-scale quantum Monte Carlo (QMC) simulations, we investigate the interaction-driven quantum phase transition in the Kane-Mele-Hubbard model. The transition from the quantum spin Hall insulator at weak interaction to an antiferromagnetic Mott insulator at strong interaction can be readily detected by the momentum space behavior of the strange correlator in single-particle, spin, and pairing sectors. The interaction effects on the symmetry-protected edge states in various sectors are well captured in the QMC measurements of strange correlators. Moreover, we demonstrate that the strange correlator is technically easier to implement in QMC and more robust in performance than other proposed numerical diagnoses for interacting topological states, as only static correlations are needed. The attempt in this work paves the way for using the strange correlator to study interaction-driven topological phase transitions.

**8:36AM X12.00004 Avoided quantum criticality in disordered three-dimensional Dirac semi-metals**, JEDEDIAH PIXLEY, Condensed Matter Theory Center and Joint Quantum Institute, Department of Physics, University of Maryland, DAVID HUSE, Princeton University — We study the effects of short-range random potential disorder on three-dimensional Dirac semi-metals. We focus on the proposed quantum critical point (QCP) separating a semi-metal and diffusive metal phase driven by disorder. We will briefly review the existing evidence of such a QCP. We will then explore the non-perturbative effects of rare regions using Lanczos and the kernel polynomial method, from which we establish the existence of two distinct types of excitations in the weak disorder regime. The first are perturbatively renormalized dispersive Dirac states and the second are weakly dispersive quasi-localized “rare” eigenstates. We establish that these rare eigenstates contribute an exponentially small but non-zero density of states at zero energy, thus converting the semi-metal to diffusive metal transition into an avoided quantum critical point.

**8:48AM X12.00005 Explicit derivation of duality between a free Dirac cone and quantum electrodynamics in  $(2+1)$  dimensions**, DAVID F. MROSS, JASON ALICEA, OLEXEI I. MOTRUNICH, Caltech — A single Dirac cone of (free) electrons famously arises on the surface of a 3D topological insulator. Recent work proposed that these metallic surfaces can alternatively be described by quantum electrodynamics in  $(2+1)$  dimensions (QED<sub>3</sub>), where charge-neutral ‘dual fermions’ strongly couple to an emergent photon. We explicitly derive this duality via an exact, non-local mapping from electrons to dual fermions on the level of path integrals. This mapping allows us to construct Hamiltonians for exotic topological-insulator surface phases, and to derive the particle-hole-symmetric field theory of a half-filled Landau level. By running the duality ‘in reverse’ we can constrain scaling dimensions for operators in QED<sub>3</sub> and establish duality between bosonic topological insulator surfaces and QED<sub>3</sub> with two fermion flavors.

**9:00AM X12.00006 Correlation effects in 3D triple-Weyl semimetals**, SHI-XIN ZHANG, Tsinghua University, SHAO-KAI JIAN, HONG YAO, Institute for Advanced Study, Tsinghua University — We study interaction effects, including short-range interactions and long-range Coulomb interactions, in three-dimensional topological triple-Weyl semimetals whose triple-Weyl points are protected by crystalline symmetries. In the low-energy effective field theory of triple-Weyl semimetals, by considering symmetries and utilizing Fierz identity, we find that there are only four independent short-range interaction terms. We then perform Wilsonian renormalization group analysis to determine the effect of short-range interactions at low energy and long distance by finding fixed points as well as stable strong-coupling limits. For those strong-coupling limits due to short-range interactions, spontaneous symmetry-breaking ordering is expected and is analyzed by self-consistent mean-field calculations combined with RG flow. For long-range Coulomb interactions, we find anisotropic screening effect, similar with the one in double-Weyl semimetals, and hence a qualitatively different fixed point from the Gaussian one.

**9:12AM X12.00007 First-Principles Design of a Half-Filled Flat Band of the Kagome Lattice in Two-Dimensional Metal-Organic Frameworks**, MASAHIKO G. YAMADA, Institute for Solid State Physics, University of Tokyo, TOMOHIRO SOEJIMA, Department of Chemistry, Massachusetts Institute of Technology, NAOTO TSUJI, RIKEN Center for Emergent Matter Science (CEMS), DAISUKE HIRAI, Department of Physics, University of Tokyo, MIRCEA DINCĂ, Department of Chemistry, Massachusetts Institute of Technology, HIDEO AOKI, Department of Physics, University of Tokyo — Metal-organic frameworks (MOFs) are crystalline materials composed of metal ions and bridging organic molecules, which have been the subject of numerous investigations in inorganic and materials chemistry. Owing to their typically trivial electronic states, MOFs have not attracted much attentions from condensed-matter physicists. However, recent experimental success in fabricating two-dimensional (2D) MOFs with kagome lattice structures is bridging the gap between condensed-matter physics and chemistry. Then, we design from first principles a new type of 2D MOFs with phenalenyl-based ligands to realize a half-filled flat band of the kagome lattice, which belongs to the lattice family that shows Lieb-Mielke-Tasaki’s flat-band ferromagnetism. We find that *trans*-Au-THTAP(trihydroxytriaminophenalenyl) has an ideal band structure, where the Fermi energy is adjusted right at the nearly flat band. The spin-orbit coupling opens a band gap and gives a non-zero Chern number to the nearly flat band. This is a novel and realistic example of a system in which a nearly flat band is both ferromagnetic and topologically non-trivial. See arXiv:1510.00164.

**9:24AM X12.00008 Nernst and magneto-thermal conductivity in a lattice model of Weyl fermions<sup>1</sup>**, GIRISH SHARMA, Clemson University, PALLAB GOSWAMI, University of Maryland, College Park, MD, SUMANTA TEWARI, Clemson University — Weyl semimetals (WSM) are topologically protected three dimensional materials whose low energy excitations are linearly dispersing massless Dirac fermions, possessing a non-trivial Berry curvature. Using semi-classical Boltzmann dynamics in the relaxation time approximation for a lattice model of time reversal (TR) symmetry broken WSM, we compute both magnetic field dependent and anomalous contributions to the Nernst coefficient. In addition to the magnetic field dependent Nernst response, which is present in both Dirac and Weyl semimetals, we show that, contrary to previous reports, the TR-broken WSM also has an anomalous Nernst response due to a non-vanishing Berry curvature. We also compute the thermal conductivities of a WSM in the Nernst ( $\nabla T \perp \mathbf{B}$ ) and the longitudinal ( $\nabla T \parallel \mathbf{B}$ ) set-up and confirm from our lattice model that in the parallel set-up, the Wiedemann-Franz law is violated between the longitudinal thermal and electrical conductivities due to chiral anomaly.

<sup>1</sup>G.S and S.T are supported by AFOSR (FA9550-13-1-0045). P.G was supported by NSF-JQI-PFC and and LPS-CMTC.

**9:36AM X12.00009 Topological edge states in pnictides<sup>1</sup>**, CODY YOUMANS, City College of New York; The Graduate Center, CUNY, POUYAN GHAEMI, City College of New York, MEHDI KARGARIAN, University of Maryland — In some members of the ferro-pnictides, non-trivial topology in the bulk band-structure is related to potentially observable gapless edge states. We study these states numerically and analytically for a range of parameters, with and without superconductivity and antiferromagnetic SDW ordering, and their relation to the symmetries and topologically non-trivial aspects of our model Hamiltonian.

<sup>1</sup>Support was provided by the Doctoral Student Research Grant program at the Graduate Center, CUNY.

**9:48AM X12.00010 Symmetry-enriched topological invariants from tensor network representations**, BRAYDEN WARE, Univ of California - Santa Barbara, MENG CHENG, BELA BAUER, Microsoft Station Q — We examine topologically ordered quantum phases in  $2+1$  dimensions where in the presence of symmetries the topological phase splits into multiple symmetry enriched topological (SET) phases. These SET phases become adiabatically connected when the symmetry is broken, but are separated by phase transitions when symmetry is enforced. Using tensor network representations of representative wavefunctions for certain SET phases, we demonstrate the calculation of the extended modular matrices, a generalization of the well-known modular matrices that have been used to robustly characterize topological phases in numerical calculations. Here, the crucial extension is to systems with symmetry defects. The extended modular matrices are used to form symmetry-enriched topological invariants which distinguish different SET phases.

**10:00AM X12.00011 Electronic structure studies of topological materials**, SHUYUN ZHOU, Department of Physics, Tsinghua University — Three-dimensional (3D) Dirac fermions are a new class of topological quantum materials. In 3D Dirac semimetals, the conduction and valence bands touch each other at discrete points in the momentum space and show linear dispersions along all momentum directions, forming 3D Dirac cones which are protected by the crystal symmetry. Here I will present our recent studies of the electronic structures of novel materials which host 3D Dirac fermions by using angle-resolved photoemission spectroscopy.

**10:12AM X12.00012 Propagation of Surface Plasmon Polaritons in Thin Films of Topological Insulators<sup>1</sup>**, YURY DESHKO, ZHIYI CHEN, LIA KRUSIN-ELBAUM, VINOD MENON, City College of New York – CUNY, JACOB TREVINO, Advanced Science Research Center – CUNY, ALEXANDER KHANIKAEV, Queens College – CUNY — Surface Plasmon Polaritons (SPP) are coupled collective oscillations of surface charges and electromagnetic waves confined to the interface between a metal and a dielectric. Three dimensional topological insulators (TI), such as Bi<sub>2</sub>Se<sub>3</sub>, Bi<sub>2</sub>Te<sub>3</sub>, and Sb<sub>2</sub>Te<sub>3</sub> are narrow band-gap semiconductors in the bulk while having conducting surface with the linear energy dispersion for the surface electronics states. Similar to double-layered graphene a thin single film of TI supports two SPP modes in the far-infrared range. We study the propagation of these modes in thin films of Bi<sub>2</sub>Se<sub>3</sub>, Bi<sub>2</sub>Te<sub>3</sub>, and Sb<sub>2</sub>Te<sub>3</sub>. The dispersion curves and the propagation lengths are estimated for all three materials. The explanation of the discrepancy between the theory [1] and the first experimental observation of standing wave SPPs in Bi<sub>2</sub>Se<sub>3</sub> [2] is proposed. Finally, the possibilities of tuning the SPP dispersion relations in thin films of TI are discussed.

[1] T. Stauber, G. Gomez-Santos, and L. Brey, Phys. Rev. B 88, 205427 (2013).

[2] P. Di Pietro, M. Ortolani, O. Limaj, A. Di Gaspare, V. Giliberti, F.

Giorgianni, M. Brahlek, N. Bansal, N. Koirala, S. Oh, P. Calvani, and S. Lupi, Nature Nanotechnology 8, 556 (2013).

<sup>1</sup>Supported by NSF DMR-1420634 and DOD-W911NF-13-1-0159

**10:24AM X12.00013 Observation of a topologically non-trivial surface state in half-Heusler PtLuSb (001) thin films**, JOHN LOGAN, SAHIL PATEL, SEAN HARRINGTON, Univ of California - Santa Barbara, CRAIG POLLEY, Max IV Laboratory, BRIAN SCHULTZ, Univ of California - Santa Barbara, T. BALASUBRAMANIAN, Max IV Laboratory, ANDERSON JANOTTI, University of Delaware, ANDERS MIKKELSEN, Lund University, CHRIS PALMSTRM, Univ of California - Santa Barbara — Topological insulators are a recently discovered new quantum state of matter that has a bulk band gap but also possesses cross-gap surface states which are protected by time-reversal symmetry. The experimental realization of topologically non-trivial surface states (TSSs) in materials such as Bi<sub>2</sub>Se<sub>3</sub> has generated widespread interest in identifying other material systems that exhibit TSSs due to their many uses including spintronic devices. In particular, recent theory calculations suggest that TSSs may be found in certain half-Heusler ternary compounds. If experimentally realizable, this would provide an opportunity for the creation of entirely new heterostructure spintronic devices that make use of the structurally-identical but electronically-varied nature of Heusler compounds. Here, we show the presence of a TSS in the half-Heusler compound PtLuSb. Spin and angle-resolved photoemission spectroscopy reveals a surface state with linear dispersion and a helical tangential spin texture consistent with theoretical predictions and the expectation for a topological insulator.

**10:36AM X12.00014 Predicted Growth of Two-Dimensional Topological Insulators Consisting of Hydrogenated III-V Thin films on Si(111) Substrate**, FENG-CHUAN CHUANG, CHRISTIAN CRISOSTOMO, LIANG-ZI YAO, CHUN-CHEN YEH, SHU-MING LAI, ZHI-QUAN HUANG, CHIA-HSIU HSU, Natl. Sun Yat-sen U., HSIN LIN, Natl. U. of Singapore, MARVIN ALBAO, U. of the Philippines Los Baos College, ARUN BANSIL, Northeastern U. — We have carried out systematic first-principles electronic structure calculations of growth of ultrathin films of compounds of group III (B, Al, In, Ga and Tl) with group V (N, P, As, Sb and Bi) elements on Si(111) substrate, including effects of hydrogenation. A total of six compounds (GaBi, InBi, TlBi, TIAs, TISb and TIN) are identified to be nontrivial in unhydrogenated case; whereas for hydrogenated case, only four (GaBi, InBi, TlBi and TISb) remains nontrivial. The band gap is found to be as large as 855 meV for the hydrogenated TlBi film, making this class of III-V materials suitable for room temperature applications. TlBi remains topologically nontrivial with a large band gap at various hydrogen coverages, indicating the robustness of its band topology against bonding effects of substrates. Two bilayers (BLs) of AlBi, InBi, GaBi, TIAs and TISb are found to support a topological phase over a wide range of strains, in addition to BBi, TIN and TlBi which can be driven into the nontrivial phase via strain. One and two BL films of GaBi and 2 BL films of InBi and TIAs on Si(111) surface possess nontrivial phases with a band gap as large as 121 meV in the case of 2 BL film of GaBi. Persistence of the nontrivial phase upon hydrogenations in the III-V thin films suggests that these films are suitable for growing on various substrates.

**10:48AM X12.00015 Transport properties of superconducting high indium-doped SnTe single crystals**, CHENG ZHANG, RUIDAN ZHONG, GENDA GU, QIANG LI, Brookhaven National Laboratory — The discovery of topological crystalline insulator SnTe has ignited a search for the predicted topological superconductors. Recently, we performed the transport measurement on a series of indium-doped SnTe single crystals (Sn<sub>1-x</sub>In<sub>x</sub>Te). Hall measurement shows that carrier type changes when indium doping level is between  $x = 0.2$  and  $0.3$ . Weak anti-localization effect and Shubnikov-de Hass oscillations was found in  $x = 0.45$  samples, which have the highest superconducting transition temperature at 4.5 K. Both superconducting and normal state properties of high indium-doped SnTe will be discussed.

**Friday, March 18, 2016 8:00AM - 11:00AM –**

**Session X13 GMAG DMP: Hall-Bar Structure for the Detection of Spin/Valley Hall Effect** 309  
- Wei Han, Peking University

**8:00AM X13.00001 Topological Superconductivity in HgTe-based Devices**, LAURENS MOLENKAMP, Wuerzburg University — Suitably structured HgTe has been shown to be a topological insulator in both 2- (a quantum well wider than some 6.3 nm) and 3 (an epilayer grown under tensile strain) dimensions with favorable properties for quantum transport studies, i.e. a good mobility and a complete absence of bulk carriers. In this talk I will summarize the results of our efforts (in collaboration with colleagues all over the globe) to induce superconductivity in the topological surface states of these materials. Special emphasis will be given to recent results on the ac Josephson effect. We will present data on Shapiro step behavior that is a very strong indication for the presence of a gapless Andreev mode in our Josephson junctions.

**8:36AM X13.00002 Origins of Nonlocality Near the Neutrality Point in Graphene**, JOSHUA FOLK, University of British Columbia — Nonlocal measurements are an effective experimental tool for probing non-charge characteristics of carriers using a (charge) transport measurement. For example, nonlocal signals in a Hall bar geometry can indicate spin currents, or valley currents, or heat currents flowing through a sample without an accompanying charge current. We present an experimental study of nonlocal electrical signals near the Dirac point in graphene, with the goal of disentangling the various types of current that might give rise to nonlocality. The in-plane magnetic field dependence of the nonlocal signal confirms the role of spin in this effect, as expected from predictions of the Zeeman spin Hall effect in graphene, but our experiments show that thermo-magneto-electric effects also contribute to nonlocality, and the effect is sometimes stronger than that due to spin.

## 9:12AM X13.00003 Spin Hall effect and spin transport in graphene and 2D heterostructures

, BARBAROS OEZYILMAZ<sup>1</sup>, National University of Singapore — Semiconducting 2D materials offer new opportunities in both alternative technologies and fundamental discoveries by using the spin degree freedom of electrons. One of the main challenges in this field is to identify new materials which allow the control of spin currents by means of the electric field effect. This requires either a sizeable spin-orbit coupling strength or a sizeable bandgap or both. Unfortunately, pristine graphene has a negligibly small spin-orbit coupling strength. Recently we have addressed this problem in three distinct ways. First we have used chemical functionalization to introduce locally sp<sup>3</sup> type bonding. Next we used metal ad-atoms to increase spin-orbit coupling via local enhancement of the spin-orbit coupling strength due to resonant scattering. Finally, I will show that the proximity of graphene on transition metal dichalcogenides can also lead to a significant enhancement of the spin-orbit coupling strength. I will complete my talk with a brief discussion on the possibility of all electrical spin injection into complementary 2D crystals such as WS<sub>2</sub>, MoS<sub>2</sub> or black phosphorus.

<sup>1</sup>Membership Pending in the abstract Special Instructions field

## 9:48AM X13.00004 Electron transport nonlocality in monolayer graphene modified with hydrogen silsesquioxane polymerization<sup>1</sup>

, ALEXEY KAVERZIN, Univ of Groningen — Physical properties of electrons in graphene offer not only functionality in terms of conventional charge transport, but also allow to explore spin and valley degrees of freedom. The presence of internal coupling between the nontrivial current states and normal charge current provides the effective mechanism for studying these properties. At the same time a nonlocal geometry of the transport experiments allows to separate the useful signal associated with either spin or valley degree of freedom from trivial charge contribution. In this work using the nonlocal geometry we study the transport properties of hydrogenated graphene Hall bar devices. The observed nonlocal signal is seen to substantially exceed the background ohmic contribution and, therefore, has to be understood in terms of nontrivial mediative current. The channel length dependence of the useful signal falls into direct/inverse spin Hall effect description, however, the absence of the modulation of the measured effect with the applied in plane magnetic field discredits the spin nature of the observed phenomenon. Our findings cannot be explained with the existing models suggesting that further investigation is required.

<sup>1</sup>European Unions Seventh Framework Programme grant 604391 Graphene Flagship, FOM, NWO

## 10:24AM X13.00005 Spin Hall Angle in Gold thin films: large or small?

, XIAOFENG JIN, Fudan University — Most of the methods so far adopted to determine the spin Hall angle are involved with the interface between a ferromagnetic (FM) and a nonmagnetic (NM) material, which would inevitably produce some complications in the analysis. Here, we report a new method using simply nanoscale H-pattern of gold, which is free from any interface between FM/NM, to obtain the spin Hall angle in gold thin films. A spin Hall angle around 0.1 is obtained for 10nm gold film but negligibly small for 60 nm gold. This result has not only clarified the controversy about the spin hall angle in gold thin film, but also proved the feasibility of using H-pattern to measure SHE in metallic system.

## Friday, March 18, 2016 8:00AM - 11:00AM –

Session X14 DMP: Transition Metal Dichalcogenides: Growth and Synthesis 310 - Manish Chhowalla, Rutgers University

## 8:00AM X14.00001 van der Waals Heterostructures Grown by MBE

, CHRISTOPHER HINKLE, University of Texas at Dallas — In this work, we demonstrate the high-quality MBE heterostructure growth of various layered 2D materials by van der Waals epitaxy (VDWE). The coupling of different types of van der Waals materials including transition metal dichalcogenide thin films (e.g., WSe<sub>2</sub>, WTe<sub>2</sub>, HfSe<sub>2</sub>), insulating hexagonal boron nitride (h-BN), and topological insulators (e.g., Bi<sub>2</sub>Se<sub>3</sub>) allows for the fabrication of novel electronic devices that take advantage of unique quantum confinement and spin-based characteristics. The relaxed lattice-matching criteria of van der Waals epitaxy has allowed for high-quality heterostructure growth with atomically abrupt interfaces, allowing us to couple these materials based primarily on their band alignment and electronic properties. We will discuss the impact of sample preparation, surface reactivity, and lattice mismatch of various substrates (sapphire, graphene, TMDs, Bi<sub>2</sub>Se<sub>3</sub>) on the growth mode and quality of the films and will discuss our studies of substrate temperature and flux rates on the resultant growth and grain size. Structural and chemical characterization was conducted via reflection high energy electron diffraction (RHEED), X-ray diffraction (XRD), transmission electron microscopy (TEM), scanning tunneling microscopy/spectroscopy (STM/S), atomic force microscopy (AFM), X-ray photoelectron spectroscopy (XPS), and Raman spectroscopy. Experimentally determined band alignments have been determined and compared with first-principles calculations allowing the design of novel low-power logic and magnetic memory devices. Initial results from the electrical characterization of these grown thin films and some simple devices will also be presented. These VDWE grown layered 2D materials show significant potential for fabricating novel heterostructures with tunable band alignments and magnetic properties for a variety of nanoelectronic and optoelectronic applications.

## 8:36AM X14.00002 Direct growth of single- and few-layer MoS<sub>2</sub> on h-BN by CVD method<sup>1</sup>

, AIMING YAN, JAIRO VELASCO, JR., SALMAN KAHN, Univ of California - Berkeley, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Japan, FENG WANG, MICHAEL CROMMIE, Univ of California - Berkeley, ALEX ZETTL, Univ of California - Berkeley; Materials Sciences Division, LBNL; Kavli Energy NanoSciences Institute at the Univ of California, Berkeley and LBNL — As a promising candidate for the next-generation electronics, large-scale single- and few-layer molybdenum disulfide (MoS<sub>2</sub>) grown by CVD method is an important advancement towards technological implementation of this material. However, the choice of substrate can significantly affect the performance of MoS<sub>2</sub> based devices. An attractive insulating substrate or mate for MoS<sub>2</sub> (and related materials such as graphene) is hexagonal boron nitride (h-BN). Stacked heterostructures of MoS<sub>2</sub> and h-BN have been produced by manual transfer methods, but a more efficient and scalable assembly method is needed. Here we demonstrate the direct growth of single- and few-layer MoS<sub>2</sub> on h-BN by chemical vapor deposition (CVD) method. The growth mechanisms for single- and few-layer samples are found to be distinct, and for single-layer samples low relative rotation angles (<5°) between the MoS<sub>2</sub> and h-BN lattices prevail. In addition, MoS<sub>2</sub> directly grown on h-BN maintains its intrinsic 1.89 eV bandgap. Our CVD synthesis method presents a viable path towards high-quality MoS<sub>2</sub> based field effect transistors in a controllable and scalable fashion.

<sup>1</sup>Acknowledgement: the U.S. Department of Energy under Contract DE-AC02-05CH11231; NSF grant DMR-1206512

## 8:48AM X14.00003 Spiral Growth of Few-Layer MoS<sub>2</sub> by Chemical Vapor Deposition<sup>1</sup>

, XI DONG, DUSHYANT TOMER, LIAN LI, Univ of Wisconsin, Milwaukee — Monolayer and few-layer transition metal dichalcogenide MoS<sub>2</sub> are grown by chemical vapor deposition on SiO<sub>2</sub>/Si substrates using MoO<sub>3</sub> and S powder as precursors. Before growth, the substrates are pretreated with perylene-3, 4, 9, 10-tetracarboxylic acid tetrapotassium salt to promote nucleation. Monolayer MoS<sub>2</sub> islands are triangularly shaped with sizes ranging from a few to tens of micrometers, which also exhibits the characteristic Raman bands at 403.36 and 385.05 cm<sup>-1</sup> corresponding to the A<sub>1g</sub> and E<sub>2g</sub> modes, respectively. Atomic force microscopy imaging further confirms the monolayer thickness to be 0.8 nm. For few-layer MoS<sub>2</sub> films, triangular spirals are observed with both left- and right-handed chirality. Raman spectra showed interesting features of these growth spirals, the details of which will be presented at the meeting.

<sup>1</sup>NSF DMR-1508560.

**9:00AM X14.00004 Controlled synthesis of single-layer MoSe<sub>2</sub> nanostructures**, YUXUAN CHEN, CHEN-DONG ZHANG, Univ of Texas, Austin, PING CUI, ZHENYU ZHANG, Univ. of Science and Technology of China, CHIH-KANG SHIH<sup>1</sup>, Univ of Texas, Austin — Group VIB transition metal dichalcogenides (TMD), such as MoSe<sub>2</sub>, WS<sub>2</sub>, etc., are a family of layered materials with weak van der Waals (vdW) interaction between neighboring layers. A transition from indirect to direct bandgap semiconductor takes place for most of these materials when they become single layer (SL), and the values of these direct band gap are comparable to visible light. This makes SL TMDs attractive candidates for 2D electronic and optoelectronic devices. Though epitaxial SL TMDs have been successfully prepared, there is controversy in their growth conditions and in their edge structures. Moreover, some intriguing theoretical predictions about the finite-size effect on SL TMDs are still awaiting experimental proof. Here we report systematic studies of the thermodynamics/ kinetics of SL MoSe<sub>2</sub> formation on a vdW surface (namely, highly oriented pyrolytic graphite) using molecular beam epitaxy (MBE). We also report the controlled creation of various nanostructures of MBE SL MoSe<sub>2</sub>. The edge properties and the influence of the in-plane confinement on the electronic structure are addressed by in-situ STM and STS. Theoretical calculations have been carried out to help understanding the experimental discoveries.

<sup>1</sup>corresponding author

**9:12AM X14.00005 Large Area Synthesis of 2D Materials**, ERIC VOGEL, Georgia Inst of Tech — Transition metal dichalcogenides (TMDs) have generated significant interest for numerous applications including sensors, flexible electronics, heterostructures and optoelectronics due to their interesting, thickness-dependent properties. Despite recent progress, the synthesis of high-quality and highly uniform TMDs on a large scale is still a challenge. In this talk, synthesis routes for WSe<sub>2</sub> and MoS<sub>2</sub> that achieve monolayer thickness uniformity across large area substrates with electrical properties equivalent to geological crystals will be described. Controlled doping of 2D semiconductors is also critically required. However, methods established for conventional semiconductors, such as ion implantation, are not easily applicable to 2D materials because of their atomically thin structure. Redox-active molecular dopants will be demonstrated which provide large changes in carrier density and workfunction through the choice of dopant, treatment time, and the solution concentration. Finally, several applications of these large-area, uniform 2D materials will be described including heterostructures, biosensors and strain sensors.

**9:48AM X14.00006 Thermal stability of MBE-grown epitaxial MoSe<sub>2</sub> and WSe<sub>2</sub> thin films<sup>1</sup>**, YOUNG JUN CHANG, BYOUNG KI CHOY, Department of Physics, University of Seoul, Seoul, 130-743, Korea, SOO-HYON PHARK, Center for Nanometrology, Korea Research Institute of Standards & Science, Korea, MINU KIM, Center for Correlated Electron Systems, Institute for Basic Science (IBS), Seoul 151-747, Republic of Korea — Layered transition metal dichalcogenides (TMDs) draw much attention, because of its unique optical properties and band structures depending on the layer thicknesses. However, MBE growth of epitaxial films demands information about thermal stability of stoichiometry and related electronic structure for high temperature range. We grow epitaxial MoSe<sub>2</sub> and WSe<sub>2</sub> ultrathin films by using molecular beam epitaxy (MBE). We characterize stoichiometry of films grown at various growth temperature by using various methods, XPS, EDX, and TOF-MEIS. We further test high temperature stability of electronic structure for those films by utilizing in-situ ellipsometry attached to UHV chamber. We discuss threshold temperatures up to 700~1000°C, at which electronic phases changes from semiconductor to metal due to selenium deficiency. This information can be useful for potential application of TMDs for fabrication of Van der Waals multilayers and related devices.

<sup>1</sup>This research was supported by NanoMaterial Technology Development Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Science, ICT and Future Planning.(2009-0082580), NRF-2014R1A1A1002868

**10:00AM X14.00007 Synthesis and Optical Control of Circular Polarization in monolayer Tungsten Disulfide.<sup>1</sup>**, KATHLEEN MCCREARY, AUBREY HANBICKI, BEREND JONKER, MARC CURRIE, Naval Research Laboratory, GEORGE KIOSEOGLOU, University of Crete, Greece — The unique electronic band structure in single layer WS<sub>2</sub> provides the ability to selectively populate a desired valley by exciting with circularly polarized light. The valley population is reflected through the circular polarization of photoluminescence (PL). We investigate the circularly polarized PL in WS<sub>2</sub> monolayers synthesized using chemical vapor deposition (CVD). The resulting polarization is strongly dependent on the sample preparation. As-grown CVD WS<sub>2</sub> (still on the growth substrate) exhibits low polarized emission, regardless of laser excitation or laser power. Removing WS<sub>2</sub> from the growth substrate and repositioning on the same substrate significantly impacts the optical properties. In transferred films, the excitonic state is optically controlled via high-powered laser exposure such that subsequent PL is solely from either the charged exciton state or the neutral exciton state. Neutral excitonic emission exhibits zero polarization whereas the trion polarization can exceed 25% at room temperature. The removal process may modify the strain, sample-to-substrate distance, and chemical doping in the WS<sub>2</sub> monolayer, and work is underway to determine how these factors influence the valley populations. These results demonstrate a new method to control the excitonic state and PL polarization in monolayer WS<sub>2</sub>.

<sup>1</sup>Supported by core programs at NRL and the NRL Nanoscience Institute, and by the Air Force Office of Scientific Research AOARD 14IOA018-134141.

**10:12AM X14.00008 Atomically flat Ge buffer layers and alternating shutter growth of CaGe<sub>2</sub> for large area germanane<sup>1</sup>**, JINSONG XU, JYOTI KATOCH, ADAM AHMED, IGOR PINCHUK, ROBERT WILLIAMS, DAVID MCCOMB, ROLAND KAWAKAMI, Ohio State University — Germanane (GeH), which is converted from CaGe<sub>2</sub> by soaking in HCl acid, has recently attracted interest because of its novel properties, such as large band gap (1.56eV), spin orbit coupling and predictions of high mobility (18000 cm<sup>2</sup>/Vs). Previously CaGe<sub>2</sub> was successfully grown on Ge(111) substrates by molecular beam epitaxy (MBE) growth. But there were cracks between m-sized islands, which is not desirable for scientific study and application, and limits the material quality. By growing atomically flat Ge buffer layers and using alternating shutter MBE growth, we are able to grow crack-free, large area films of CaGe<sub>2</sub> films. Reflection high energy electron diffraction (RHEED) patterns of Ge buffer layer and CaGe<sub>2</sub> indicates high quality two dimensional surfaces, which is further confirmed by atomic force microscopy (AFM), showing atomically flat and uniform Ge buffer layer and CaGe<sub>2</sub>. The appearance of Laue oscillation in X-ray diffraction (XRD) and Kiessig fringes in X-ray reflectivity (XRR) proves the uniformity of CaGe<sub>2</sub> film and the smoothness of the interface. The high quality of CaGe<sub>2</sub> film makes it promising to explore novel properties of GeH.

<sup>1</sup>Funded by NSF MRSEC DMR-1420451

**10:24AM X14.00009 Synthesis and Properties of Group IV Graphane Analogues**, JOSHUA GOLDBERGER, The Ohio State University — Similar to how carbon networks can be sculpted into low-dimensional allotropes such as fullerenes, nanotubes, and graphene with fundamentally different properties, it is possible to create similar ligand terminated sp<sup>3</sup>-hybridized honeycomb graphane derivatives containing Ge or Sn that feature unique and tunable properties. Here, we will describe our recent success in the creation of hydrogen and organic-terminated group IV graphane analogues, from the topochemical deintercalation of precursor Zintl phases, such as CaGe<sub>2</sub>. We will discuss how the optical, electronic, and thermal properties of these materials can be systematically controlled by substituting either the surface ligand or via alloying with other Group IV elements. Additionally, we have also developed an epitopotaxial approach for integrating precise thicknesses of germanane layers onto Ge wafers that combines the epitaxial deposition of CaGe<sub>2</sub> precursor phases with the topotactic interconversion into the 2D material. Finally, we will describe our recent efforts on the synthesis and crystal structures of Sn-containing graphane alloys in order to access novel topological phenomena predicted to occur in these graphanes.

# Friday, March 18, 2016 8:00AM - 11:00AM –

Session X15 DMP: Unconventional Two Dimensional Materials. 314 - Luis Jauregui, Harvard University

## 8:00AM X15.00001 Electrons and phonons in layered and monolayer vanadium pentoxide.<sup>1</sup>

WALTER R. L. LAMBRECHT, Case Western Reserve University — Vanadium pentoxide ( $V_2O_5$ ) is a layered material with the potential for interesting new properties when made in 2D mono- or few-layer form. Its band structure is characterized by a split-off conduction band. The lowest conduction band is separated from the rest of the conduction bands by about 1 eV and consists of  $V-d_{xy}$  orbitals, non-bonding to the oxygens by symmetry. This narrow band has dispersion essentially along the direction of chains occurring in the layer. When this band becomes half-filled by doping, spin-splitting occurs accompanied by an antiferromagnetic coupling between nearest neighbors along the chain direction. This situation is well known to occur in the so-called ladder compound  $NaV_2O_5$ , which was extensively studied in the late 90s as a potential spin-Peierls or charge ordering compound. However, the monolayer form of  $V_2O_5$  may allow for other ways to control the doping by gating, removing vanadyl oxygens, adsorption of alkali metals, nanoribbon formation, etc. Our calculations predict a switch from antiferromagnetic to ferromagnetic coupling for doping slightly less than half filling of the split-off band. In this talk we will discuss our recent work on the electronic band structure of both bulk and monolayer  $V_2O_5$  as well as the phonons. We find that the quasi-particle self-consistent  $GW$  method strongly overestimates the band gap. Lattice polarization corrections of the screening are required because of the large LO/TO phonon frequency ratios. Excitonic effects may also be expected to be fairly large. We find that some of the vibrational modes, notably the vanadyl-oxygen bond stretch perpendicular to the layer, unexpectedly shows a strong blue shift. This is explained in terms of reduced screening affecting the long-range dipole components of the force constants.

<sup>1</sup>Supported by AFOSR and DOE. Work done with Churna Bhandari, Mark van Schilfgaarde and Andre Schleiffe.

## 8:36AM X15.00002 Doping effects on the electronic and magnetic properties of $V_2O_5$ <sup>1</sup>

CHURNA BHANDARI, WALTER R.L. LAMBRECHT, Case Western Reserve University — We study doping of the  $V_2O_5$  split-off conduction band using different methods: by adding electrons compensated by an artificial homogeneous background, a virtual crystal approximation (VCA), by changing the atomic number  $Z_v$ , and explicitly by intercalating Na as a dopant. The former two are mathematical models to simulate injected charge by gating, the latter occurs in the vanadium bronze  $NaV_2O_5$ . We also study  $Na_{1-x}V_2O_5$  using the VCA by changing  $10 \leq Z_{Na} \leq 11$ . We discuss the electronic band structure and the optical conductivity using the quasiparticle self-consistent QSGW method including a lattice polarization effect and the local density functional method with Hubbard- $U$  correction (LSDA+ $U$ ) for all these models. We show that the ground state prefers anti-ferromagnetic order along the chain (crystallographic  $b$ ) direction and extract various near neighbor exchange interactions from total energy differences of different spin configurations. We find that the coupling between the nearest V-neighbors changes from anti-ferromagnetic to ferromagnetic when the electron concentration is reduced from half filling of the band (1e/V atom) to about 0.88 e/V atom. The magnetic moment gradually decreases with decreasing electron concentration.

<sup>1</sup>This work was supported by AFSOR Grant No: FA 9550-12-1-0441(CB) and US DOE Grant No: ER -46874-SC0008933(WL)

## 8:48AM X15.00003 ABSTRACT WITHDRAWN —

## 9:00AM X15.00004 Two-dimensional, ordered, double transition metals carbides (MXenes)

PAUL KENT, Oak Ridge National Lab, BABAK ANASORI, Drexel University, YU XIE, Oak Ridge National Lab, MAJID BEIDAGHI, Drexel University, JUN LU, Linköping University, Sweden, BRIAN HOSLER, Drexel University, LARS HULTMAN, Linköping University, Sweden, YURY GOGOTSI, MICHEL BARSQUM, Drexel University — We use [1] density functional theory to predict the existence of two new families of 2D ordered carbides (MXenes),  $M'_2M''C_2$  and  $M'_2M''C_3$ , where each M is a different early transition metal. Synthesizing  $Mo_2TiC_2T_x$ ,  $Mo_2Ti_2C_3T_x$ , and  $Cr_2TiC_2T_x$  (where T is a surface termination), we validated the DFT predictions. Since the Mo and Cr atoms are on the outside, they control the 2D flakes' chemical and electrochemical properties. The latter was proven by showing quite different electrochemical behavior of  $Mo_2TiC_2T_x$  and  $Ti_3C_2T_x$ . This work further expands the family of 2D materials, offering additional choices of structures, chemistries, and ultimately useful properties. [1] B. Anasori et al. ACS Nano 9 9507 (2015). DOI: 10.1021/acsnano.5b03591

## 9:12AM X15.00005 Unusual electronic and magnetic responses from sulfur-decorated graphene.

CHOONGYU HWANG, Materials Sciences Division, Lawrence Berkeley Natl. Lab. and Department of Physics, Pusan National University, South Korea, S. A. CYBART, S. M. WU, R. C. DYNES, Materials Sciences Division, Lawrence Berkeley Natl. Lab. and Department of Physics, University of California, San Diego, CA, S. J. SHIN, E. E. HALLER, Department of Materials Science and Engineering, University of California, Berkeley, CA and Materials Sciences Division, Lawrence Berkeley Natl. Lab., S. KIM, K. KIM, B. I. MIN, Department of Physics, Pohang University of Science and Technology, South Korea, T. G. RAPPOPORT, Instituto de Física, Universidade Federal do Rio de Janeiro, Brazil, C. JOZWIAK, A. V. FEDOROV, S. -K. MO, Advanced Light Source, Lawrence Berkeley Natl. Lab., A. H. CASTRO NETO, Graphene Research Centre, National University of Singapore, D. -H. LEE, A. LANZARA, Department of Physics, University of California, Berkeley, CA, and Materials Sciences Division, Lawrence Berkeley Natl. Lab. — Interactions between two different materials can produce strong electronic correlations that do not exist when each material stands alone. We search for such correlations from graphene, a non-magnetic semi-metal, decorated by sulfur, a diamagnetic insulator, using angle-resolved photoemission spectroscopy and magneto-transport measurements. Sulfur-decorated graphene exhibits unusual electronic and magnetic responses that are clearly distinguished from clean graphene. Our findings provide intriguing insights on the search for novel quantum phases in graphene-based compounds.

## 9:24AM X15.00006 Electronic correlations in monolayer $VS_2$

ERIC B. ISAACS, CHRIS A. MARIANETTI, Department of Applied Physics and Applied Mathematics, Columbia University — The layered transition metal dichalcogenide vanadium disulfide ( $VS_2$ ), which nominally has 1 electron in the  $3d$  shell, is potent for strong correlation physics and is possibly another realization of the one-band Hubbard model beyond the cuprates. Here we investigate the octahedral (OCT) and trigonal prismatic (TP) phases of monolayer  $VS_2$  using density functional theory plus Hubbard  $U$  calculations. Unlike the OCT phase, the TP phase has an isolated low-energy band due to the crystal field splitting and the nearest-neighbor V-V hopping. Within DFT, ferromagnetism spin splits this band leading to a low-band-gap  $S = 1/2$  ferromagnetic insulating TP phase, which is lower in energy than the OCT phase. The on-site interaction  $U$ , which we find to be approximately 4 eV via linear response, increases the band gap, leads to Mott insulating behavior, and for sufficiently high values stabilizes the ferromagnetic OCT phase. We explore the impact of charge density waves in monolayer  $VS_2$  and discuss the possibility to experimentally realize the TP phase.

## 9:36AM X15.00007 Competing antiferromagnetism in a quasi-2D itinerant ferromagnet:

$Fe_3GeTe_2$ , ZHENG GAI, JIEYU YI, HOULONG ZHUANG, S.A. CALDER, P.R.C. KENT, Oak Ridge National Laboratory, DAVID MANDRUS, University of Tennessee, Knoxville, TN, OAK RIDGE NATIONAL LABORATORY COLLABORATION, UNIVERSITY OF TENNESSEE, KNOXVILLE, TN COLLABORATION —  $Fe_3GeTe_2$  is known as an air-stable layered metal with itinerant ferromagnetism with a transition temperature of about 220 K. From extensive dc and ac magnetic measurements, we have determined that the ferromagnetic layers of  $Fe_3GeTe_2$  order antiferromagnetically along the  $c$ -axis below 152 K. The antiferromagnetic state was further substantiated by theoretical calculation to be the ground state. A magnetic structure model was proposed to describe the antiferromagnetic ground state as well as competition between antiferromagnetic and ferromagnetic states.  $Fe_3GeTe_2$  shares many common features with pnictide superconductors and may be a promising system in which to search for unconventional superconductivity.

**9:48AM X15.00008 Many-body effects in doped graphene on a piezoelectric substrate.<sup>1</sup>** , F. SOLS, D. G. GONZALEZ, I. ZAPATA, Universidad Complutense de Madrid (Spain), J. SCHIEFELE, IMDEA Nanociencia (Madrid, Spain) , F. GUINEA, IMDEA Nanociencia (Madrid, Spain) and University of Manchester (UK) — We study theoretically the role of piezoelectric acoustic phonons in the context of piezoelectric substrates covered by graphene. They are responsible for effective, substrate dependent electron-electron interactions which can be strong and give rise to novel many-body effects. We present a new derivation of the electron-phonon interaction matrix element which generalizes previous calculations made within the simpler and not always justified isotropic approximation. We study several many-body effects, including the temperature-dependent phonon renormalization due to the electron cloud surrounding the lattice vibration, as well as the electron self-energies arising from the effective electron-electron interactions in the perturbative  $G_0W$  approximation. We also perform calculations of the graphene electron mobility on substrates with various levels of piezoelectricity. Finally, we discuss how these piezoelectric phonons can influence the superconducting instability. For completeness, we compare our results with the situation found for the two-dimensional electron gas and for conventional three-dimensional BCS superconductors.

<sup>1</sup>Work supported by MINECO (Spain), CEI Moncloa UCM-UPM, ERC (EU), and the European Commission Graphene Flagship.

**10:00AM X15.00009 Electrochemical intercalation of lithium ions into NbSe<sub>2</sub> nanosheets** , EMILY HITZ, JIAYU WAN, (UMD), ANAND PATEL, (NIST), YUE XU, (UMD), LOUISA MESHI, (NIST), JIAQI DAI, YANAN CHEN, (UMD), ALBERT DAVYDOV, Materials Science and Engineering Division, National Institute of Standards and Technology, Gaithersburg, Maryland 20878, USA, LIANGBING HU, Department of Materials Science and Engineering, University of Maryland, College Park, MD 20742, USA — Transition metal dichalcogenides (TMDCs) have been known for decades to have unique properties and recently attracted broad attention for their two-dimensional (2D) characteristics. One TMDC that has been studied for its charge density wave transition behavior and superconductivity is metallic NbSe<sub>2</sub>, yet it is still largely unexplored for device applications in electronics, optics, and batteries. Through this work, we demonstrate successful electrochemical intercalation of lithium ions into layered NbSe<sub>2</sub>. We present evidence of lithium intercalation as a technique capable of modifying the material properties of hexagonal NbSe<sub>2</sub> for further study. We confirm our result through X-ray diffraction, showing a unit cell size increase in NbSe<sub>2</sub> after intercalation from 12.57 Å to 13.57 Å in the “c” lattice dimension. Additionally, planar half-cell micro-battery devices are fabricated using ultra-thin NbSe<sub>2</sub> from platelets to observe Li-ion intercalation through an increase in the optical transmittance of the material in the visible range. At 550 nm wavelength light, we observed an increase in the optical transmittance of the material by 26% due to electrochemical intercalation.

**10:12AM X15.00010 Electronic and magnetic properties of nanoribbons<sup>1</sup>** , GAYANATH FERNANDO, ZHIWEI ZHANG, Univ of Connecticut - Storrs, ARMEN KOCHARIAN, California State Univ - Los Angeles — We have performed tight-binding calculations with open boundary conditions on a set of twisted nanoribbons (4x100), monitoring the band structure as a function of the twist angle  $\theta$ . When this angle is zero, the ribbon is rectangular and when it is 60 degrees, the ribbon is cut from a honeycomb lattice. Depending on the parameters of the tight-binding model and the filling factor, semi-metallic or insulating behavior is observed. We have also studied the electronic structure of such ribbons due to the adsorption of small atoms such as nitrogen, a magnetic field and the Rashba spin-orbit interaction. The role of the adsorbed atoms and the Rashba term with regard to the conducting properties and the symmetry breaking of the ribbons will be discussed in some detail. In addition, the effects of electronic correlations on selected small ribbons will be examined.

<sup>1</sup>The authors acknowledge the computing facilities provided by the Center for Functional Nanomaterials, Brookhaven National Laboratory supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No.DE-AC02-98CH10886.

**10:24AM X15.00011 SU(4) quantum spin liquids in critical Coulomb impurity lattices on MoS<sub>2</sub>** , X. DOU, University of Oklahoma, V. N. KOTOV, University of Vermont, BRUNO UCHOA, University of Oklahoma — In the critical regime, massive Dirac fermions are known to form a bound state in the vicinity of a Coulomb impurity. We find that in the presence of electron-electron interactions, the electrons in this bound state will valley and spin polarize. We show that the interaction of the spin and valley polarized electrons bounded to two different Coulomb impurities naturally maps into a Heisenberg model with SU(4) symmetry. We propose that quantum spin-orbital liquids with that symmetry can be engineered in artificial Coulomb impurity lattices on the surface of MoS<sub>2</sub> monolayer. We discuss possible experiments to detect those states.

**10:36AM X15.00012 Crystalline topological insulators in ultrashort optical pulse<sup>1</sup>** , SEYYEDEL AZAR OLIAEIMOTLAGH, VADYM APALKOV, MARK STOCKMAN, Georgia State University — We study theoretically interaction of ultrashort and ultrashort optical pulse with crystalline topological insulators, which have quadratic band degeneracy at the surface. Coherent electron surface dynamics in such optical pulse is determined by interband dipole coupling, which is highly anisotropic in these materials. Within two-band  $k \cdot p$  model of the surface states of topological insulator the electron dynamics is described in terms of the mixing of two (valence and conduction) bands. Such mixing is characterized by residual, i.e., after the pulse, conduction band population. Residual electron momentum distribution in the conduction band is highly anisotropic and follows the profile of the interband dipole coupling. Depending on polarization of the optical pulse, the residual conduction band population has one or two strong peaks in the momentum space, where the shapes of the peaks change with the amplitude of the pulse. The conduction band population is almost one at these peaks.

<sup>1</sup>Crystalline topological insulators in ultrashort optical pulse

**10:48AM X15.00013 Gate tunable magneto-optical effects in layered antiferromagnets<sup>1</sup>** , NIKHIL SIVADAS, Department of Physics, Carnegie Mellon University, SATOSHI OKAMOTO, Materials Science and Technology Division, Oak Ridge National Laboratory, DI XIAO, Department of Physics, Carnegie Mellon University — It has long been believed that the Faraday and the magneto-optic Kerr effects are absent in collinear antiferromagnets due to their vanishing net magnetic moment. To the contrary, using first-principles calculations we demonstrate that these effects can be controlled by a perpendicular voltage in bilayer MnPSe<sub>3</sub>, which has a collinear AF-Néel spin texture. The Kerr rotation can be as high as 10 mrad, and is reversed on the reversal of the polarity of gate voltage. The tunable nature of the magneto-optic effects can result in novel optoelectronic device applications. It also provides a nondestructive way to characterize the magnetic ground state of 2D materials.

<sup>1</sup>This work is supported by AFOSR No. FA9550-12-1-0479 and FA9550-14-1-0277

**Friday, March 18, 2016 8:00AM - 10:48AM –**  
**Session X16 DCMP DMP: Two-Dimensional Material Heterostructures** 315 - Masa Ishigami, University of Central Florida

**8:00AM X16.00001 Interlayer Hybridization in van der Waals Heterostructures.** , NAM LE, University of South Florida, Department of Physics, HUAN TRAN, University of Connecticut, Institute of Materials Science, LILIA WOODS, University of South Florida, Department of Physics — Van der Waals heterostructures composed of chemically inert dissimilar layers are of great interest for fundamental science and applications. The weak interplanar interactions and orbital overlap are expected to bring modifications to the constituent materials. By using first principles simulations, we investigate the properties of several heterostructures, including graphene/silicene, graphene/MoS<sub>2</sub>, and silicene/MoS<sub>2</sub>. The calculations reveal superlattice characteristic points in the Brillouin zone associated with the different stacking patterns. Band structures projected on each of the constituents show hybridization features related to specific orbital overlap for each heterostructure. Phonon dispersion spectra for the considered heterostructures are also investigated.

**8:12AM X16.00002 Vertically Stacked Graphene/Transition-Metal-Dichalcogenides/Graphene Heterojunction Devices for High Performance Photodetectors** , JINSEONG HEO, HEEJEONG JEONG, JAEHO LEE, KIYOUNG LEE, EUN-KYU LEE, SANGYEON LEE, YEONCHOO CHO, KYUNG-EUN BYUN, CHANG-WON LEE, SEONGJUN PARK, SUNGWOO HWANG, Samsung Advanced Institute of Technology — Photodetectors based on vertically stacked graphene heterojunctions have advantages of short transit length for photo-generated carriers and large sensing area, thus implying fast response time and high responsivity. Previously, vertically stacked Graphene (Gr)/Transition-Metal-Dichalcogenide (TMDC)/Gr junctions were introduced for optoelectronic devices, showing high current on and off ratio as well as photoresponsivity. But for high performance photodetectors, both thorough and comparative study in terms of the figures of merit such as photoresponse time and photoresponsivity depending on different TMDC materials is crucial. Here, we report fast response time (28 us) and high responsivity (20 A/W) from Gr/WS<sub>2</sub> and MoS<sub>2</sub>/Gr, respectively. At the same time, those devices operate as p- and n-type barrier-variable transistors, respectively, being a potential building block for optoelectronic system on a chip.

**8:24AM X16.00003 Ab initio Mapping of Interlayer Coupling in Transition Metal Dichalcogenides and Graphene<sup>1</sup>** , SHIANG FANG, EFTHIMIOS KAXIRAS, Harvard University — Two-dimensional layered materials cover a wide variety of physics phenomena, such as topological phases, superconductivity, magnetism and charge density waves. Owing to the layered geometry and the van der Waals interactions in between, stacks of these van der Waals layered materials provide a venue to create a heterostructure with various physics properties. The interaction between different physics properties is particularly interesting to engineer the material with the desired properties. One of the crucial ingredients in understanding the heterostructure is the interlayer coupling in between. In the literature, such kind of coupling has been proposed in various empirical forms. However, a true ab initio coupling model is still lacking. For the first time, here we have derived such interlayer coupling model from the first principle calculations based on the Wannier transformation of graphene stacks. We further investigate the Fermi velocity renormalization, van Hove singularities and the moiré pattern for electron localization. Such microscopic understanding of the interlayer coupling would shed light on orbital hybridization and transport in multilayer stacks.

<sup>1</sup>This work was supported by the STC Center for Integrated Quantum Materials, NSF Grant No. DMR-1231319, and by ARO MURI Award No. W911NF-14-0247.

**8:36AM X16.00004 The Interlayer Resistance of a Misoriented Bilayer MoS<sub>2</sub> Interface** , KUAN ZHOU, UC Riverside, DARSHANA WICKRAMARATNE, UC Santa Barbara, SUPENG GE, ROGER LAKE, UC Riverside — The performance of electrical and opto-electronic devices with vertically stacked transition metal dichalcogenides (TMDCs) has been found to be degraded by the rotated interface between bilayer system. The band properties and interlayer coupling have been researched experimentally and computationally, however, the dependence of the interlayer resistance on the disorientation angle of the two layers forming bilayer MoS<sub>2</sub> remains unknown. Ab-initio methods combined with non-equilibrium Greens functions are used to calculate the transport properties of the misoriented bilayer MoS<sub>2</sub> system. The energy and angle dependence of the interlayer resistivity is determined. The difference between the electron and hole transmission properties is analyzed. The influence of spin polarization in the K valleys of the TMDC system is also been discussed.

**8:48AM X16.00005 Probing in-plane anisotropy and interlayer interactions in ReS<sub>2</sub> and ReSe<sub>2</sub> by Raman spectroscopy** , ETIENNE LORCHAT, GUILLAUME FROELICHER, STÉPHANE BERCAUD, IPCMS (CNRS - Université de Strasbourg) — We address the intriguing Raman response of rhenium disulfide (ReS<sub>2</sub>) and rhenium diselenide (ReSe<sub>2</sub>). These layered semiconductors belong to the family of transition metal dichalcogenides and exhibit significant in-plane anisotropy and can be represented as a distorted 1T-phase (octahedral), with considerably lower symmetry than the more extensively studied 2H-phase (trigonal prismatic) compounds based on molybdenum or tungsten. Nevertheless, we will demonstrate that the low-frequency rigid layer vibrational modes of *N*-layer ReS<sub>2</sub> and ReSe<sub>2</sub> can, on the one hand, be described using a linear chain model but, on the other hand, make it possible to directly probe the in-plane anisotropy and to determine the crystal orientation. Since in-plane anisotropy also has a direct impact on the optical and electron transport properties, our work opens avenues for engineering novel optoelectronic devices relying on ReS<sub>2</sub> and ReSe<sub>2</sub>.

**9:00AM X16.00006 Twisted Van der Waals Systems<sup>1</sup>** , SATRIO GANI, ENRICO ROSSI, William and Mary College — Van der Waals systems formed by two-dimensional (2D) crystals and nanostructures possess electronic properties that make them extremely interesting for basic science and for possible technological applications. By tuning the relative angle (the twist angle) between the layers, or nanostructures, forming the Van der Waals systems experimentalists have been able to control the stacking configuration of such systems. We study the dependence on the twist angle of the electronic properties of two classes of Van der Waals systems: double layers formed by two, one-atom thick, layers of a metal dichalcogenide such as molybdenum disulfide (MoS<sub>2</sub>), and graphene nanoribbons on a hexagonal boron nitride substrate. We present results that show how, for both classes of systems, the electronic properties can be strongly tuned via the twist angle.

<sup>1</sup>Work supported by ACS-PRF-53581-DNI5 and NSF-DMR-1455233

**9:12AM X16.00007 Epitaxial MoS<sub>2</sub>/GaN structures to enable vertical 2D/3D semiconductor heterostructure devices** , D. RUZMETOV, US Army Research Laboratory, K. ZHANG, Pennsylvania State University, G. STAN, B. KALANYAN, NIST, S. EICHFELD, PSU, R. BURKE, P. SHAH, T. O'REGAN, F. CROWNE, A.G. BIRDWELL, ARL, J. ROBINSON, PSU, A. DAVYDOV, NIST, T. IVANOV, ARL — MoS<sub>2</sub>/GaN structures are investigated as a building block for vertical 2D/3D semiconductor heterostructure devices that utilize a 3D substrate (GaN) as an active component of the semiconductor device without the need of mechanical transfer of the 2D layer. Our CVD-grown monolayer MoS<sub>2</sub> has been shown to be epitaxially aligned to the GaN lattice which is a pre-requisite for high quality 2D/3D interfaces desired for efficient vertical transport and large area growth. The MoS<sub>2</sub> coverage is nearly 50 % including isolated triangles and monolayer islands. The GaN template is a double-layer grown by MOCVD on sapphire and allows for measurement of transport perpendicular to the 2D layer. Photoluminescence, Raman, XPS, Kelvin force probe microscopy, and SEM analysis identified high quality monolayer MoS<sub>2</sub>. The MoS<sub>2</sub>/GaN structures electrically conduct in the out-of-plane direction and across the van der Waals gap, as measured with conducting AFM (CAFM). The CAFM current maps and I-V characteristics are analyzed to estimate the MoS<sub>2</sub>/GaN contact resistivity to be less than 4 Ω-cm<sup>2</sup> and current spreading in the MoS<sub>2</sub> monolayer to be approx. 1 μm in diameter. Epitaxial MoS<sub>2</sub>/GaN heterostructures present a promising platform for the design of energy-efficient, high-speed vertical devices incorporating 2D layered materials with 3D semiconductors.

**9:24AM X16.00008 ABSTRACT WITHDRAWN —**

**9:36AM X16.00009 Raman spectrum of MoS<sub>2</sub>/WS<sub>2</sub> heterostructure from first-principles calculation of phonon electron coupling<sup>1</sup>**, JUN JIANG, XIAO GUANG ZHANG, Univ of Florida - Gainesville, LIANGBO LIANG, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, GEORGIOS D. BARMPPARIS, Crete Center for Quantum Complexity and Nanotechnology, Department of Physics, University of Crete, Heraklion 71003, Greece, YEVGENIY S. PUZYREV, SOKRATES T. PANTELIDES, Department of Physics and Astronomy, Vanderbilt University, Nashville, TN 37235, USA — We present a first-principles method to calculate Raman spectrum of MoS<sub>2</sub>/WS<sub>2</sub> heterostructure due to electron excitation. The first step is to calculate the ground state phonon modes and the displacements of the atoms from the ground state to the excited states. In the next step, inelastic multi-phonon relaxation for the excited electron is considered to produce the Raman spectrum quantitatively. The relative Raman intensity, peak width and shape are obtained directly from a sum over trillions of configurations of multiple phonon modes using a Monte Carlo scheme. Alternatively, we also calculate the overlap between the ground state phonon mode eigenvectors and the excited state atomic displacements, which provides a quick and qualitative description for the Raman shifting due to electron excitation.

<sup>1</sup>This work is supported by NSF grant 1508898.

**9:48AM X16.00010 Optical properties of few-layer MoS<sub>2</sub>-based heterostructures**, ASMA ALKABSH, HASSANA SAMASSEKOU, ANDREW WALKER, DIPANJAN MAZUMDAR, SAIKAT TALAPATRA, Southern IL Univ-Carbondale — 2D materials such as Transition metal dichalcogenides (TMDs) are promising for a number of electronic/optoelectronic applications. In particular, semiconducting MoS<sub>2</sub>, is considered as one of the most interesting 2D material due to its direct band gap at the monolayer level [1]. For device applications, such desirable properties have to translate when MoS<sub>2</sub> is layered with other materials and substrates. In this research, the optical properties of select MoS<sub>2</sub>-based heterostructures are investigated. In particular, the effect of various insulating underlayers such as BN, SiO<sub>2</sub> on few-layer MoS<sub>2</sub> are examined using spectroscopic ellipsometry. The angles  $\Psi$  and  $\Delta$ , as well as layer specific optical constants such as extinction coefficient (k) and refractive index (n) shall be extracted using Tauc-Lorentz oscillator model and as a function of MoS<sub>2</sub> layer thickness and underlayer structure. The band gap properties of few-layer MoS<sub>2</sub> will be analyzed using optical spectroscopy

**10:00AM X16.00011 The vertical transport properties of misoriented graphene/hexagonal-boron-nitride/graphene heterostructure devices<sup>1</sup>**, SUPENG GE, MASUM HABIB, ROGER LAKE, Univ of California - Riverside, LATTE TEAM — Hexagonal boron nitride (hBN) has an atomically smooth surface free of dangling bonds, minimal lattice mismatch with graphene and a wide band gap, which makes it an ideal insulator material for graphene devices. Recently, transistor devices made with the few layers of hBN sandwiched between two layers of graphene has attracted attention since interesting phenomenon such as negative differential resistance has been observed. In experiment, the device fabrication usually gives rise to random orientation of interfaces. To have a better understanding of the effect of misorientation, we employed non-equilibrium Greens function (NEGF) method to calculate transmission across graphene/hBN/graphene heterostructures devices. We find that the rotation can cause the transmission to change by more than one order of magnitude. The resistance and current as functions of h-BN layer thickness, commensurate rotation angles, gating voltage, and bias voltage are described.

<sup>1</sup>Acknowledgement: This work is supported in part by FAME, one of six centers of STARnet, a Semiconductor Research Corporation program sponsored by MARCO and DARPA.

**10:12AM X16.00012 Characterization of Graphene Transferred onto Hydrated "Soft" Substrates<sup>1</sup>**, M. BLADES, P. VENDOLA, W. PIERRE, S. JEDLICKA, S.V. ROTKIN, Lehigh University — Graphene's unique properties have recently found application in the fields of biosensing and bioimaging. Substrate selection is an important step in the use of graphene for this purpose; however, choices are usually limited to hard, dry surfaces such as silicon dioxide. Here we demonstrate a modified procedure, based on the H<sub>2</sub> bubbling method, for transferring graphene to the soft hydrogel polyacrylamide. Widefield imaging and confocal Raman mapping were performed to characterize the quality of the transfer.

<sup>1</sup>NSF ECCS-1509786

**10:24AM X16.00013 The effects of quenched disorder on high-order sideband generation in GaAs/AlGaAs quantum wells<sup>1</sup>**, HUNTER BANKS, DARREN VALOVICIN, Physics Department, UCSB, SHAWN MACK, Naval Research Lab, ARTHUR GOSSARD, Materials Department, UCSB, LOREN PFEIFFER, Department of Electrical Engineering, Princeton University, MARK SHERWIN, Physics Department, UCSB — When a near-IR laser resonantly pumps excitons into a strong terahertz field, individual excitons tunnel ionize and the resulting electrons and holes are driven apart and then back together by the terahertz field. Resulting recollisions create a large number of sidebands around the pump frequency, in the process of high-order sideband generation (HSG) [1]. The high kinetic energy of the electron-hole recollisions yields substantial information about the underlying structure of the individual excitons as well as the interaction of energetic single electrons and holes with each other, the lattice, and quenched disorder at sub-micron length scales. We present a comparison of smooth-walled GaAs quantum wells with 5[1] B. Zaks, et al., Nature 483 (7391), 580 (2012) and H. Banks, et al., Physical Review Letters 111, 267402 (2013)

<sup>1</sup>This work is supported by NSF-DMR 1405964

**10:36AM X16.00014 Passivation of CdSe Quantum Dots by Graphene and MoS<sub>2</sub> Monolayer Encapsulation**, DATONG ZHANG, DENNIS ZI-REN WANG, RICHARD C. CRESWELL, Columbia University, CHENGUANG LU, National Center for Nanoscience and Technology, IRVING P. HERMAN, Columbia University — The encapsulation of a monolayer of CdSe quantum dots (QDs) by one-to-three layer graphene and MoS<sub>2</sub> sheets protects the QDs from oxidation. Photoluminescence (PL) from the QD cores shows a much slower decrease in core diameter over time due to slower oxidation in regions where the QDs are covered by van der Waals (vdW) layers than in those where they are not, for chips stored both in the dark and in the presence of light. PL mapping shows that the CdSe QDs under the central part of the vdW sheet age slower than those near its edges, because oxidation of the covered QDs is limited by transport of oxygen from the edges of the vdW sheets and not transport across the vdW layers. This encapsulation effect is also tested with other environments. Preliminary results show that vdW materials could be promising candidates for nano-coating materials for devices operating in extreme environments.

**Friday, March 18, 2016 8:00AM - 11:00AM –**

**Session X17 DMP: 2D Semiconductor Physics III** 316 - Yu Ye, University of California, Berkeley

**8:00AM X17.00001 Enhanced Valley Zeeman Splitting in MoS<sub>2</sub>/EuS due to interfacial exchange field**, CHUAN ZHAO, THOMAS SCRACE, PAYAM TAHERI, PEIYAO ZHANG, TENZIN NORDEN, BRETT BLIZZARD, ATHOS PETROU, HAO ZENG, Department of Physics, University at Buffalo, SUNY, PUQIN ZHAO, Nanjing Tech University, GEORGE KIOSEOGLOU, University of Crete, Greece — A monolayer transition metal dichalcogenides such as MoS<sub>2</sub> with broken inversion symmetry possesses two degenerate yet inequivalent valleys that can be selectively excited by circularly polarized light. The ability to manipulate valley degrees of freedom with light or external magnetic field makes them attractive for optoelectronic and spintronic applications. On the other hand, it has been demonstrated recently that a magnetic insulator such as EuS can induce magnetic exchange field (MEF) on graphene through proximity effect. Thus, construction of a magnetic insulator/TMDC heterostructure may induce large MEF on TMDC, which may lead to giant valley Zeeman splitting. In this work, we report the observation of valley Zeeman splitting in monolayer MoS<sub>2</sub> and other TMDCs due to the MEF from EuS substrates. Using magneto-reflectivity, we measured a Zeeman splitting of valley exciton of 2 meV at 7 tesla and 4 K, for monolayer MoS<sub>2</sub> on a SiO<sub>2</sub> substrate. This is consistent with values reported in monolayer WSe<sub>2</sub>. However, when EuS is used as the substrate, we observed an increase of valley splitting from 2 to 10 meV. We attribute this enhanced valley splitting to the MEF from the EuS substrate. Utilizing MEF of a magnetic insulator can induce magnetic ordering and giant Zeeman splitting in 2D TMDCs, which might enable novel spintronics applications.

**8:12AM X17.00002 Exciton diamagnetic shifts and valley Zeeman effect in monolayer WS<sub>2</sub> and MoS<sub>2</sub> to 65Tesla**, A. V. STIER, NHMFL, Los Alamos, K. A. MCCREARY, B. T. JONKER, Naval Research Laboratory, J. KONO, Rice University, S. A. CROOKER, NHMFL, Los Alamos — We report circularly-polarized optical reflection spectroscopy of monolayer WS<sub>2</sub> and MoS<sub>2</sub> at low temperatures (4 K) and in high magnetic fields to 65 T [1]. Both the A and the B exciton transitions exhibit a clear and very similar Zeeman splitting of approximately  $-230 \mu\text{eV/T}$  ( $g \simeq -4$ ), providing the first measurements of the valley Zeeman effect and associated g-factors in monolayer transition-metal disulphides. These results complement and are compared with recent low-field photoluminescence measurements of valley degeneracy breaking in the monolayer diselenides MoSe<sub>2</sub> and WSe<sub>2</sub>. Further, the very large magnetic fields used in our studies allows us to observe the small quadratic diamagnetic shifts of the A and B excitons in monolayer WS<sub>2</sub> (0.32 and 0.11  $\mu\text{eV/T}^2$ , respectively), from which we calculate exciton radii of 1.53 nm and 1.16 nm. When analyzed within a model of non-local dielectric screening in monolayer semiconductors, these diamagnetic shifts also constrain and provide estimates of the exciton binding energies (410 meV and 470 meV for the A and B excitons, respectively), further highlighting the utility of high magnetic fields for understanding new 2D materials. [1] A. V. Stier et al., submitted, arxiv:1510.07022 (2015)

**8:24AM X17.00003 Valley selective high field magneto-spectroscopy of monolayer MoSe<sub>2</sub>**, JONATHAN LUDWIG, Florida State University and National High Magnetic Field Lab, Y. LI, Stanford University and SLAC National Accelerator Lab, Z. LU, Florida State University and National High Magnetic Field Lab, X.X. ZHANG, Stanford University and SLAC National Accelerator Lab, X. CUI, J. HONE, Columbia University, T.F. HEINZ, Stanford University and SLAC National Accelerator Lab, D. SMIRNOV, National High Magnetic Field Lab — Monolayer transition metal dichalcogenides (TMDs) have recently emerged as a new class of direct bandgap 2D semiconductors with valleys at the  $\pm K$  points in the Brillouin zone. Due to the broken inversion symmetry in monolayer TMDs, this valley degree of freedom can be selectively addressed by optical helicity. We report on circularly polarized resolved photoluminescence on gated monolayer MoSe<sub>2</sub> in perpendicular and parallel magnetic fields up to 30T. In a perpendicular field at low carrier density, the PL energies of both the trion and exciton experience a linear shift with a slope of  $\approx \pm 2\mu_B/T$  for the  $\pm K$  valleys, demonstrating valley degeneracy lifting. This is in contrast to the measurements in parallel field, where no such linear splitting occurs. In addition, we report quadratic corrections to the linear magnetic field dependence of the trion and exciton energy in the perpendicular configuration.

**8:36AM X17.00004 Valley-selective optical Stark effect in monolayer WS<sub>2</sub>**, NUH GEDIK, MIT — Monolayer semiconducting transition-metal dichalcogenides (TMDs) have a pair of valleys that, by time-reversal symmetry, are energetically degenerate. Lifting the valley degeneracy in these materials is of great interest because it would allow for valley specific band engineering and offer additional control in valleytronic applications. In this talk, I will show that circularly polarized light, which breaks time-reversal symmetry, can be used to lift the valley degeneracy by means of the optical Stark effect [1]. We demonstrate that this effect is capable of raising the exciton level in monolayer TMD WS<sub>2</sub> by as much as 18 meV in a controllable valley-selective manner. The resulting energy shift is extremely large, comparable to the shift that would be obtained using a very high magnetic field (approximately 100 Tesla). These results offer a novel way to control valley degree of freedom, and may provide a means to realize new valley-selective Floquet topological state of matter. [1] E J Sie, J W McIver, Y H Lee, L Fu, J Kong and N Gedik, Nature Materials 14, 290 (2015)

**9:12AM X17.00005 Valley-Polarized Interlayer Excitons in 2D Semiconductor Heterostructures**, PASQUAL RIVERA, KYLE SEYLER, Univ of Washington, HONGYI YU, University of Hong Kong, JOHN SCHAIBLEY, Univ of Washington, JIAQIANG YAN, DAVID MANDRUS, University of Tennessee, XIAODONG XU, Univ of Washington — Vertically stacked monolayers of MoSe<sub>2</sub> and WSe<sub>2</sub> feature a type-II band alignment causing the formation of interlayer excitons, where the Coulomb bound hole and electron reside in different layers. This species of exciton has lifetime many orders of magnitude longer than intralayer valley excitons, providing a unique and advantageous system for investigating valley exciton physics. Here, we optically pump the MoSe<sub>2</sub>-WSe<sub>2</sub> heterostructure with circularly polarized light, creating interlayer valley excitons with gate-tunable spin-valley polarization lifetime up to 40 ns. This long valley lifetime enables the diffusion of the interlayer valley exciton gas to be visualized. Under increasing excitation power we observe the formation of a ring in the spatial distribution of the valley polarization, a manifestation of significant valley-selective exchange interactions at high exciton densities. The combination of long valley polarization and spatial diffusion makes the interlayer exciton in semiconductor heterostructures an exciting platform for studies of valley exciton physics.

**9:24AM X17.00006 Valley-Polarized Exciton-Polaritons in a Monolayer Semiconductor Embedded in a Microcavity**<sup>1</sup>, YEN-J. CHEN, TEODOR K. STANEV, NATHANIEL P. STERN, Department of Physics and Astronomy, Northwestern University, JEFFREY D. CAIN, VINAYAK P. DRAVID, Department of Materials Science and Engineering, Northwestern University — Two-dimensional transition metal dichalcogenides (TMDs) are semiconductors that exhibit degenerate, but inequivalent, valleys at their  $K$ -point band gaps which selectively couple to circularly-polarized light fields. Coherent hybrid states of light and matter, exciton-polaritons, have been observed when monolayer TMDs strongly interact with photon fields in a microcavity<sup>2</sup>. The degree of polarization is determined by the relative rates of exciton and intervalley relaxation, which can be modified for microcavity exciton-polaritons. Preservation of valley-polarization in a microcavity at room temperature is compared to the nearly zero polarization for bare monolayer MoS<sub>2</sub> on SiO<sub>2</sub>, demonstrating cavity-modified relaxation dynamics of the coherent valley-specific exciton-polaritons. These results suggest promising opto-electronic applications for valley-based polaritonic and photonic devices integrating monolayer TMDs.

<sup>1</sup>This work is supported by the U.S. Department of Energy (BES DE-SC0012130) and the National Science Foundation MRSEC program (DMR-1121262). N.P.S. is an Alfred P. Sloan Research Fellow.

<sup>2</sup>X. Liu, T. Galfsky, Z. Sun, F. Xia, E.-C. Lin, Y.-H. Lee, S. Kena-Cohen, and V. M. Menon. *Nature. Photon.* **9**, 30 (2015)

**9:36AM X17.00007 Valley Polarization in Size-Tunable Monolayer Semiconductor Quantum Dots<sup>1</sup>**, GUOHUA WEI, Applied Physics Program, Northwestern University, DAVID A. CZAPLEWSKI, IL WOONG JUNG, Center for Nanoscale Materials, Argonne National Lab, ERIK J. LENFERINK, TEODOR K. STANEV, NATHANIEL P. STERN, Department of Physics, Northwestern University — Controlling the size of semiconductor nanostructures allows manipulation of the optical and electrical properties of band carriers. We show that laterally-confined monolayer MoS<sub>2</sub> quantum dots can be created through top-down nanopatterning of an atomically-thin two-dimensional semiconductor. Semiconductor-compatible nanofabrication processing allows for these low-dimensional materials to be integrated into complex systems that harness their controllable optical properties. Size-dependent exciton energy shifts and linewidths are observed, demonstrating the influence of quantum confinement. The patterned dots exhibit the same valley polarization characteristics as in a continuous MoS<sub>2</sub> sheet, suggesting that monolayer semiconductor quantum dots could have potential for advancing quantum information applications.

<sup>1</sup>This work is supported by ISEN, the DOE-BES (DE-SC0012130), the NSF MRSEC program (DMR-1121262), and the Center for Nanoscale Materials, DOE-BES (DE-AC02-06CH11357). N.P.S. is an Alfred P. Sloan Research Fellow.

**9:48AM X17.00008 Valley-selective harmonic generations in transition metal dichalcogenide monolayers**, JINGXIN CHENG, TAO JIANG, YUWEI SHAN, YINGGUO LI, Fudan University, XIANHUI CHEN, University of Science and Technology of China, Y.R. SHEN, Fudan University; University of California, Berkeley, WEITAO LIU, SHIWEI WU, Fudan University — Transition metal dichalcogenide monolayer has emerged as another star in the family of atomically thin two dimensional materials. Different from graphene, the two sublattices in its honeycomb-like structure are occupied by different atoms, leading to the reduced rotational symmetry from six fold to three fold. The reduced symmetry and dimension not only result in many intriguing physics such as valley and excitons, but also lead to rich nonlinear optical phenomena such as strong second harmonic generation. In this talk, we will present a systematic study on linearly and circularly polarized harmonic generations in this wonder material. We show that both the second and third harmonic generations follow the conservation of angular momentum and are valley-selective. Furthermore, these nonlinear optical processes could be used as a powerful imaging tool for studying transition metal dichalcogenide monolayers and other similar 2D materials.

**10:00AM X17.00009 Efficient evaluation of epitaxial MoS<sub>2</sub> on sapphire by direct band structure imaging<sup>1</sup>**, HOKWON KIM, DUMITRU DUMCENCO, MATHIEU FREGNAUX, Ecole Polytechnique Federale de Lausanne, ANASS BENAYAD, CEA, LETI, YEN-CHENG KUNG, ANDRAS KIS, Ecole Polytechnique Federale de Lausanne, OLIVIER RENAULT, CEA, LETI, LANES GROUP, EPFL TEAM, LETI, CEA TEAM — The electronic band structure evaluation of two-dimensional metal dichalcogenides is critical as the band structure can be greatly influenced by the film thickness, strain, and substrate. Here, we performed a direct measurement of the band structure of as-grown monolayer MoS<sub>2</sub> on single crystalline sapphire by reciprocal-space photoelectron emission microscopy with a conventional laboratory ultra-violet He I light source. Arrays of gold electrodes were deposited onto the sample in order to avoid charging effects due to the insulating substrate. This allowed the high resolution mapping ( $\Delta E = 0.2$  eV;  $\Delta k = 0.05$  Å<sup>-1</sup>) of the valence states in momentum space down to 7 eV below the Fermi level. The high degree of the epitaxial alignment of the single crystalline MoS<sub>2</sub> nuclei was verified by the direct momentum space imaging over a large area containing multiple nuclei. The derived values of the hole effective mass were 2.41 0.05 m<sub>0</sub> and 0.81 0.05 m<sub>0</sub>, respectively at  $\Gamma$  and K points, consistent with the theoretical values of the freestanding monolayer MoS<sub>2</sub> reported in the literature.

<sup>1</sup>HK acknowledges the french CEA Basic Technological Research program (RTB) for funding.

**10:12AM X17.00010 ABSTRACT WITHDRAWN —**

**10:24AM X17.00011 Nanoscale Photoconductivity Imaging of Thin-film Semiconductors by Laser-assisted Microwave Impedance Microscopy<sup>1</sup>**, ZHAODONG CHU, DI WU, YUAN REN, SEUNGCHEOL YANG, LIUYANG SUN, XIAOQIN LI, KEJI LAI, University of Texas at Austin — The photo-response of semiconductors is usually studied by detecting the photocurrent across source-drain electrodes under light illumination. By integrating the microwave impedance microscopy (MIM) technique with focused-laser stimulation, we are able to perform the real-space photoconductivity mapping of photo-sensitive materials without the need of patterning contact electrodes. Here, we report the MIM results of various thin-film materials, such as In<sub>2</sub>Se<sub>3</sub> nano-sheets and transition metal dichalcogenides (TMD) flakes, illuminated by laser beams of different wavelengths in the ambient condition. With no or below-gap illumination, the samples were highly resistive, as indicated by the low MIM signals. The MIM contrast emerges under above-gap light and increases as increasing laser intensity, which clearly demonstrates the local imaging of photoconductivity rather than the transport photocurrent. Interestingly, clear domain structures with mesoscopic length scales were seen in the data due to the coexistence of multiple phases in In<sub>2</sub>Se<sub>3</sub>. The unique combination of MIM and laser stimulation thus provides a new direction to explore the microscopic origin of various light-driven phenomena in complex systems.

<sup>1</sup>We gratefully acknowledge financial support from NSF.

**10:36AM X17.00012 High-harmonic generation from an atomically thin semiconductor**, HANZHE LIU, YILEI LI, Stanford Univ./SLAC national accelerator laboratory, SHAMBHU GHIMIRE, SLAC national accelerator laboratory, TONY HEINZ, DAVID REIS, Stanford Univ./SLAC national accelerator laboratory — The process of high-harmonic generation (HHG) from ultrashort laser pulses has recently been observed in bulk solids, complementing the well-established process in the gas phase. HHG is of interest both as a source of ultrashort pulses in the attosecond regime that has photon energies extending up to the soft x-ray region and as a method of probing material response outside the regime of perturbative nonlinear optics. In this paper, we present the observation of HHG from a single atomic layer of MoS<sub>2</sub> driven by a strong infrared pulse of 100 fs duration and 0.3 eV photon energy. We observe distinct harmonics up to the 13<sup>th</sup> order of the infrared excitation. The non-perturbative nature of the HHG process is demonstrated by the weak power dependence of the harmonic intensities. To gain further insight into the process, we have investigated the variation of the HHG signal with sample orientation and the ellipticity of pump excitation. We compare and contrast the process with that from the bulk MoS<sub>2</sub> crystal. We find significant differences in the response for the monolayer and bulk crystal, which can be understood in terms of the distinct crystallographic symmetries in the two cases.

**10:48AM X17.00013 Optical spectroscopy and imaging of the higher energy excitons and bandgap of monolayer MoS<sub>2</sub>**, NICHOLAS BORYS, WEI BAO, EDWARD BARNARD, Molecular Foundry, Lawrence Berkeley National Lab, CHANGHYUN KO, University of California Berkeley, SEFAATIN TONGAY, Arizona State University, JUNQIAO WU, University of California Berkeley, LI YANG, Washington University in St. Louis, P. JAMES SCHUCK, Molecular Foundry, Lawrence Berkeley National Lab — Monolayer MoS<sub>2</sub> (ML-MoS<sub>2</sub>) exhibits a rich manifold of excitons that dictate optoelectronic performance and functionality. Disentangling these states, which include the quasi-particle bandgap, is critical for developing 2D optoelectronic devices that operate beyond the optical bandgap. Whereas photoluminescence (PL) spectroscopy only probes the lowest-energy radiative state and absorption spectroscopy fails to discriminate energetically degenerate states, photoluminescence excitation (PLE) spectroscopy selectively probes only the excited states that thermalize to the emissive ground state exciton. Using PLE spectroscopy of ML-MoS<sub>2</sub>, we identify the Rydberg series of the exciton A and exciton B states as well as signatures of the quasi-particle bandgap and coupling between the indirect C exciton and the lowest-energy A exciton, which have eluded previous PLE studies. The assignment of these states is confirmed with density functional theory. Mapping the PLE spectrum reveals spatial variations of the higher-energy exciton manifold and quasi-particle bandgap which mirror the heterogeneity in the PL but also indicate variations in local exciton thermalization processes and chemical potentials.

# Friday, March 18, 2016 8:00AM - 11:00AM –

Session X18 GMAG DMP: Bulk and Artificial Skyrmions 317 - Gong Chen, Berkeley National Laboratory

**8:00AM X18.00001 Emergence of skyrmions from rich parent phases in the molybdenum nitrides**, JIADONG ZANG, Univ of New Hampshire, WEI LI, Shanghai Institute of Microsystem and Information Technology, CAS, CHIMING JIN, High Magnetic Field Laboratory, CAS, RENCHAO CHE, Fudan University, WENSEN WEI, LANGSHENG LIN, LEI ZHANG, HAIFENG DU, MINGLIANG TIAN, High Magnetic Field Laboratory, CAS — We report a new family of skyrmion materials originated from the antisymmetric Dzyaloshinskii-Moriya (DM) interactions. Based on the symmetric tensor technique, the molybdenum nitrides with the  $\beta$ -manganese structure,  $A_2Mo_3N$  with  $A=Fe, Co, Rh$ , are predicted to support the skyrmion phase. This predication is directly proved in doped  $Fe_xCo_{1-x}Rh_{0.5}Mo_3N$  components by high resolution Lorentz transmission electron imaging. Interestingly, the parent compounds  $Fe_2Mo_3N$ ,  $Co_2Mo_3N$ , and  $Rh_2Mo_3N$  exhibit ferromagnetic, anti-ferromagnetic, and even superconducting orderings respectively. Magnetism in these parent phases is theoretically clarified by the first principle calculations, where the corrected nature of the magnetism is revealed..

**8:12AM X18.00002 Magnetic phase diagram of doped MnSi**, CHETAN DHITAL, MOJAMMEL KAHN, ADAM P. PHELAN, DAVID P. YOUNG, RONGYING JIN, JOHN DITUSA, Louisiana State University — The noncentrosymmetric chiral structure of cubic  $B20$  compound MnSi favors Dzyaloshinskii-Moria (DM) interaction ( $D$ ) where the broken inversion symmetry determines direction of  $D$  and the strength of spin-orbit coupling determines the magnitude of  $D$ . This relatively weak DM interaction  $D$  competes against the exchange interaction ( $J$ ) resulting in rather unusual long wavelength helimagnetism with the period set by the ratio  $(J/D)$ . Previous work has shown that both helimagnetic period ( $\lambda$ ) and the transition temperature ( $T_C$ ) are reduced as a result of either Fe or Co substitutions on Mn site [1, and references therein]. Recently we have started to investigate the effect on the helimagnetic/Skyrmion structure and the transition temperature by chemical substitutions on the Si site. I will present our preliminary magnetization and neutron scattering results where we have found clear evidence of increase in both  $T_C$  and helimagnetic period as a result of doping. The possible connection between carrier doping and the strength of DM interaction strength will be discussed.

1. Bauer, A., et al. "Quantum phase transitions in single-crystal  $Mn_{1-x}Fe_xSi$  and  $Mn_{1-x}Co_xSi$ : Crystal growth, magnetization, ac susceptibility, and specific heat." *Physical Review B* 82.6 (2010) .

**8:24AM X18.00003 First-principles simulation and low-energy effective modeling of three-dimensional skyrmion in MnGe**<sup>1</sup>, HONGCHUL CHOI, YUAN-YEN TAI, JIAN-XIN ZHU, Los Alamos National Laboratory, T-4 TEAM — The skyrmion spin textures are mostly observed in two-dimensional (2D) space, which can be topologically mapped onto the surface of the sphere with an integer multiple of topological winding number. Recently, MnGe has been reported as a candidate of 3D skyrmion crystal, showing the variation of the skyrmion size along the z-direction [1,2]. We have performed the first-principles simulation and constructed a tight-binding model with calculated electronic-structure information to investigate the 3D skyrmion phase in MnGe. Our first-principles study within density functional theory shows that the calculated magnetic moment is larger than that for MnSi (with different lattice constant), implying the possibility of a multiple magnetic transition under pressure [3]. We have also found that the small-sized skyrmion could be stabilized in a 2D structure. Such a high density of the skyrmion is in good agreement with the experimental finding of large topological Hall effect [1]. Finally, we will extend our study to consider the 3D skyrmion structure based on the constructed tight-binding model. [1] Y. Shiomi et al., Phys. Rev. B 88, 064409 (2013); [2] T. Tanigaki et al., Nano Lett. 15, 5438 (2015); [3] M. Deutsch et al., Phys. Rev. B 89, 180407 (2014).

<sup>1</sup>This work was carried out under the auspices of the National Nuclear Security Administration of the U.S. Department of Energy at Los Alamos National Laboratory (LANL) under Contract No. DE-AC52-06NA25396, and was supported by the LANL LDRD Program.

**8:36AM X18.00004 Study of topological spin texture in B20 crystalline FeGe films**, EMRAH TURGUT, ALBERT PARK, KAYLA NGUYEN, ROBERT HOVDEN, School of Applied and Engineering Physics, Cornell University, Ithaca, NY 14853 USA, LENA KOURKOUTIS, DAVID MULLER, GREGORY FUCHS, School of Applied and Engineering Physics & Kavli Institute at Cornell in Nanoscale Science, Cornell University, Ithaca, NY 14853 USA — The possibility of efficient and robust information storage in B20-hellimagnet systems has been attracted significant interest. Although there have been promising transmission electron microscopy (TEM) and transport studies on bulk B20 crystalline materials, the development of applications motivates study of thin-film samples grown with scalable techniques such as magnetron sputtering. Here we report transport and characterization measurements of FeGe thin films grown on Si  $\langle 111 \rangle$  by magnetron co-sputtering. We obtain well-oriented but polycrystalline FeGe films with the B20 crystalline phase after post-growth annealing. Low temperature TEM imaging reveals that the lattice mismatch between the Si substrate and FeGe film introduces disordered helical magnetic phases. In addition, bulk susceptibility measurements of a continuous film and AMR measurements of micron-size wires indicate helical, conical, and ferromagnetic phases, but not an obvious skyrmion phase. Similar to recent reports, our measurements confirm that the observations of additional contributions to Hall effect measurements in B20 materials are not necessarily proof of magnetic skyrmion phase, and that more careful experimental studies are needed to understand thin film properties of B20 materials.

**8:48AM X18.00005 Skyrmion domains in Cu<sub>2</sub>OSeO<sub>3</sub>: Short-Range Order and Domain Wall Formation**, SHILEI ZHANG, Department of Physics, University of Oxford, ANDREAS BAUER, Physik Department, Technische Universität München, HELMUTH BERGER, Ecole Polytechnique Fédérale de Lausanne (EPFL), STAVROS KOMINEAS, Department of Mathematics and Applied Mathematics, University of Crete, DAVID BURN, Diamond Light Source, CHRISTIAN PFLEIDERER, Physik Department, Technische Universität München, GERRIT VANDER LAAN, Diamond Light Source, THORSTEN HESJEDAL, Department of Physics, University of Oxford — Cu<sub>2</sub>OSeO<sub>3</sub> is a chiral ferrimagnetic insulator carrying a long-range order magnetic skyrmion phase. Here, we report a short-range ordered equilibrium skyrmion state on the surface of Cu<sub>2</sub>OSeO<sub>3</sub> single crystal, studied by resonant soft x-ray scattering. Soft x-ray scattering at the  $L_{2,3}$  edge of  $3d$  compounds is an ideal tool to probe the magnetic order, and is only sensitive to 60-70 unit cells in depth of Cu<sub>2</sub>OSeO<sub>3</sub>. Our results show that under the arbitrary magnetic field directions that deviate from the cubic main axes, the six-fold-symmetric skyrmion order breaks into domains, and the initial, anisotropy-governed pinning of propagation directions is completely unwound. We show that uniform 360° Bloch domain walls form between the skyrmion domains. Our findings provide a new way to manipulate and engineer the skyrmion state locally, or even individually, on the surface which will enable applications in the future.

**9:00AM X18.00006 Transverse field muon-spin rotation in skyrmion-hosting materials**, TOM LANCASTER, FAN XIAO, ROBERT WILLIAMS, Durham University, ZAHER SALMAN, Paul Scherrer Institut, STEPHEN BLUNDELL, University of Oxford, FRANCIS PRATT, STFC ISIS Facility, IORWERTH THOMAS, Durham University, MONICA CIOMAGA HATNEAN, GEETHA BALAKRISHNAN, University of Warwick, SHILEI ZHANG, THORSTEN HESJEDAL, University of Oxford — We present the results of transverse field (TF) muon-spin rotation ( $\mu^+SR$ ) measurements on examples of materials that host a skyrmion lattice (SL) phase. In measurements on bulk Cu<sub>2</sub>OSeO<sub>3</sub>, we measure the response of the TF  $\mu^+SR$  signal in the SL phase along with the surrounding ones, and suggest how the phases might be distinguished using the results of these measurements. Dipole field simulations support the conclusion that the muon is sensitive to the SL via the TF lineshape and, based on this interpretation, our measurements suggest that the SL is quasistatic on a timescale  $\tau > 100$  ns. We also discuss TF  $\mu^+SR$  measurements on an epitaxially grown 40 nm-thick film of MnSi on Si(111) in the region of the field-temperature phase diagram where a skyrmion phase has been observed in the bulk. We identify changes in the quasistatic magnetic field distribution sampled by the muon, along with evidence for magnetic transitions around  $T \approx 40$  K and 30 K. Our results suggest that the cone phase is not the only magnetic texture realized in film samples for out-of-plane fields.

### 9:12AM X18.00007 Antiferromagnetic skyrmions<sup>1</sup> , OLEG TRETIAKOV, JOSEPH BARKER, IMR, Tohoku University —

Skyrmions are topologically protected entities in magnetic materials which have the potential to be used in spintronics for information storage and processing. However, skyrmions in ferromagnets have some intrinsic difficulties which must be overcome to use them for spintronic applications, such as the inability to move straight along current. We show that skyrmions can also be stabilized and manipulated in antiferromagnetic materials. An antiferromagnetic skyrmion is a compound topological object with a similar but of opposite sign spin texture on each sublattice, which e.g. results in a complete cancelation of the Magnus force. We find that the composite nature of antiferromagnetic skyrmions gives rise to different dynamical behavior, both due to an applied current and temperature effects.

<sup>1</sup>O.A.T. and J.B. acknowledge support by the Grants-in-Aid for Scientific Research (Nos. 25800184, 25247056, 25220910 and 15H01009) from the Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan and SpinNet.

### 9:24AM X18.00008 Creating Skyrmions Using Spin Transfer Torque , JENNIFER GRAB, ALISON RUGAR, DAVID MACNEILL, Cornell University, GIOVANNI FINOCCHIO, University of Messina, ROBERT BUHRMAN, DANIEL RALPH, Cornell University —

Finding efficient methods to read and write individual skyrmions under ambient conditions is an important first step toward realizing skyrmion-based applications, such as high density information storage and racetrack memory. Of recent interest experimentally are heavy metal /ferromagnet bilayers with a strong interfacial Dzyaloshinskii-Moriya Interaction and perpendicular magnetic anisotropy (PMA), which favor the formation of helical spin textures. Micromagnetic simulations of these materials suggest that an out of plane spin polarized current could be used to write isolated skyrmions and excite skyrmion breathing modes. In this project, we attempt to create skyrmions using a spin valve like device. Our devices consist of a PMA nanopillar on top of a bulk Co/Pt bilayer. The nanopillar generates a spin polarized current, which is expected to locally reverse the magnetization of the film underneath the pillar via spin transfer torque. We report measurements of the DC current and field dependence of the pillar resistance. By monitoring the magnetization state of the bilayer independently, these measurements can be used to isolate the resistive signatures of skyrmion formation.

### 9:36AM X18.00009 Generation of magnetic skyrmion bubbles by inhomogeneous spin-Hall currents<sup>1</sup> , OLLE HEINONEN, WANJUN JIANG, HAMOUD SOMAILY, SUZANNE G.E. TE VELTHUIS, AXEL HOFFMANN, Argonne Natl Lab —

Recent experiments have shown that magnetic skyrmion bubbles can be generated and injected at room temperature in thin films<sup>1</sup>. Here, we demonstrate, using micromagnetic modeling, that such skyrmions can be generated by an inhomogeneous spin Hall torque in the presence of Dzyaloshinskii-Moriya interactions (DMIs). In the experimental Ta-Co<sub>20</sub>Fe<sub>60</sub>B<sub>20</sub> thin films, the DMI is rather small; nevertheless, the skyrmion bubbles are stable, or at least metastable on observational time scales. We identify two different mechanisms, one in a low-current regime and the other in a high current regime, that destabilize a domain wall injected from a narrow region into an expanding region with inhomogeneous spin-Hall torque. In the first, asymmetric torques on the domain wall lead to a cascade of bubble formation and subsequent fragmentation. In the second, an approximately steady-state texture is injected into the wide region. When the current is turned off, the inhomogeneous spin texture relaxes and regions can coalesce into bubbles that attain a definite chirality because of the DMI. [1] W. Jiang *et al.*, Science **349**, 283 (2015).

<sup>1</sup>This work was funded by the Department of Energy Office of Science, Materials Science and Engineering Division.

### 9:48AM X18.00010 Tailoring the chiral magnetic interaction between two individual atoms<sup>1</sup> , J. WIEBE, Institute for Nanostructure and Solid State Research, Hamburg University, A. A. KHAJETOORIANS, Institute for Molecules and Materials, Radboud University, Nijmegen, M. STEINBRECHER, Institute for Nanostructure and Solid State Research, Hamburg University, M. TERNES, Max Planck Institute for Solid State Research, Stuttgart, M. BOUHASSOUNE, M. DOS SANTOS DIAS, S. LOUNIS, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, R. WIESENDANGER, Institute for Nanostructure and Solid State Research, Hamburg University —

Chiral magnets are a promising route toward dense magnetic storage technology due to their inherent nano-scale dimensions and energy efficient properties. Engineering chiral magnets requires atomic-level control of the magnetic exchange interactions, including the Dzyaloshinskii-Moriya interaction, which defines a rotational sense for the magnetization of two coupled magnetic moments. Here we show that the indirect conduction electron mediated Dzyaloshinskii-Moriya interaction between two individual magnetic atoms on a metallic surface can be manipulated by changing the interatomic distance with the tip of a scanning tunneling microscope. We quantify this interaction by comparing our measurements to a quantum magnetic model and ab-initio calculations yielding a map of the chiral ground states of pairs of atoms depending on the interatomic separation. The map enables tailoring the chirality of the magnetization in dilute atomic-scale magnets.

<sup>1</sup>Acknowledgements: SFB668, GrK1286, SFB767, LO 1659 5-1, Emmy Noether Program of the DFG, FOM of NWO, VH-NG-717

### 10:00AM X18.00011 Collapse and control of the MnAu<sub>2</sub> spin spiral state through pressure and dopin , JAMES GLASBRENNER, National Research Council/Naval Research Lab —

MnAu<sub>2</sub> is a spin spiral material with ferromagnetic Mn layers that rotate from plane to plane. The spiral angle  $\theta$  decreases with pressure and collapses to a ferromagnetic state above a critical threshold, although different experiments do not agree on whether the collapse is first or second order. To resolve this contradiction, we employ density functional theory to calculate magnetic energies in the spiral state under both pressure and charge doping and fit the results to the  $J_1 - J_2 - J_3 - J_4$  Heisenberg model, which predicts either first or second order phase transitions depending on the set of exchange parameters. At ambient pressure, MnAu<sub>2</sub> sits very close to a dividing line separating first and second order transitions, and applying either pressure or electron doping shifts the system towards the second order region of parameter space. Our findings show how variations in material quality can impact how the spiral state collapses, which resolves the contradiction in pressure experiments. Our results also suggest that MnAu<sub>2</sub> is amenable to engineering via chemical doping and to controlling  $\theta$  using pressure and gate voltages, which holds potential for integration in spintronic devices.

### 10:12AM X18.00012 Neutron Study of Spiral Magnetism in Au<sub>2</sub>Mn , I-LIN LIU, MARIA PASCALE, University of Maryland, College Park, NICHOLAS BUTCH, NIST - Natl Inst of Stds & Tech —

The binary compound Au<sub>2</sub>Mn is known to order magnetically with a spiral structure. The pitch of the spiral has been previously shown to be dependent upon temperature and pressure. We will discuss the results of neutron diffraction measurements, in which we study the low temperature behavior of the spiral to higher pressure.

### 10:24AM X18.00013 Chiral Magnets Under a Tilted Magnetic Field: Noncircular Skyrmions , AVADH SAXENA, SHI-ZENG LIN, Los Alamos National Lab —

The equilibrium and dynamical properties of skyrmions in thin films of chiral magnets are studied in the presence of oblique magnetic fields. The shape of an individual skyrmion is found to be noncircular and the skyrmion density decreases with the tilt angle (from the normal of the film). Consequently, the interaction between two skyrmions depends on the relative angle between them besides their separation. Under a perpendicular magnetic field a triangular lattice of skyrmions is formed which is distorted into a centered rectangular lattice when the magnetic field is tilted. For low skyrmion densities a chainlike structure of skyrmions is formed. The dynamical response (including the Hall angle of motion) of the noncircular skyrmions is found to depend on the direction of external currents.

**10:36AM X18.00014 Anisotropy of Skyrmion Lattice in  $\text{Mn}_{0.9}\text{Fe}_{0.1}\text{Si}$  probed by magnetic field orientation dependence of the topological Hall effect and magnetoresistance**<sup>1</sup>, PETER SIEGFRIED, ANDREW TREGLIA, ALEXANDER BORNSTEIN, University of Colorado Boulder, THOMAS WOLF, Karlsruhe Institute of Technology, MINHUEA LEE, University of Colorado Boulder — We report the magnetic field orientation dependence of the topological Hall effect (THE) and magnetoresistance (MR) of  $\text{Mn}_{0.9}\text{Fe}_{0.1}\text{Si}$  in the *A*-phase within the applied magnetic field (*H*) temperature (*T*) phase diagram. In the *A*-phase a two dimensional Skyrmion lattice is formed in the plane perpendicular to the direction of *H*, which is responsible for the observed THE signal. At a given *T* within the *A*-phase, we investigated the angular dependence of THE and MR at a fixed *H* to probe the boundaries of the *A*-phase region. We find the MR signal exhibits a unique *H*-direction dependence at the entering and exiting of the *A*-phase, whereas, in the middle *H* range, i.e. in the core of *A*-phase, the angular dependence is consistent with what is expected from a perfect 2D Skyrmion lattice. However, THE signals show extreme sensitivity upon entering the *A*-phase and unexpected angular dependence, yet did not leave any trace through exiting. The discrepancy between the angular dependence of MR and THE signals at the *A*-phase boundaries indicates a crucial role of Fe impurities as pinning centers for the Skyrmions. We will discuss further our *H*-orientation dependence of the THE, compared to sweeping *H* at a fixed angle in Fe doped MnSi.

<sup>1</sup>Work at the University of Colorado was supported by the US DOE Basic Energy Sciences under Award No. DE-SC0006888.

**10:48AM X18.00015 Critical phenomena of emergent monopoles in a chiral magnet**, XIAO-XIAO ZHANG, Univ. of Tokyo, NAOTO NAGAO, Univ. of Tokyo and RIKEN CEMS — A three-dimensional cubic Skyrmion crystal in the bulk, which is simultaneously a lattice of monopole-antimonopole pairs predicted theoretically, has been recently identified experimentally in MnGe. Adopting appropriate temperature Green's function technique for optical conductivity and devising a solvable phonon-magnon interaction, we systematically developed the theory of coupling spin-waves to both itinerant electrons and mechanical degrees of freedom in this chiral magnet, describing the latest experimental observations including anomalies and critical phenomena in magnetotransport and magnetoelasticity, which are identified as hallmarks of fluctuations of the emergent monopolar fields upon the nontrivial monopole dynamics and especially a topological phase transition signifying strong correlation. As a whole, they speak for a crucial role played by the monopole defects and hence the real-space spin topology in this material.

**Friday, March 18, 2016 8:00AM - 11:00AM –**  
**Session X19 GMAG DMP: Magnetic Oxide Thin Films and Heterostructures: Electrostatic, Ionic, and Magnetoelectric Coupling** 318 - Philip Ryan, Argonne National Laboratory

**8:00AM X19.00001 Electric-Field Coupling to Spin Waves in a Centrosymmetric Ferrite**, TIANYU LIU, Optical Science and Technology Center and Department of Physics and Astronomy, University of Iowa, Iowa City, Iowa 52242, USA — A systematic control of spin waves via external electric fields has been a long standing issue for the design of magnonic devices, and is of fundamental interest. One way to attain such control is to use multiferroics [1], whose electric and magnetic polarizations are inherently coupled. The lack of electric polarization in a centrosymmetric ferrite, however, makes direct coupling of its magnetization to external electric fields a challenge. Indirect electric control of spin waves has been accomplished by hybridizing yttrium iron garnet (YIG), a centrosymmetric ferrite, with a piezoelectric material [2]. Here, we predict direct control of spin waves in YIG by a *flexoelectric interaction*, which couples an electric field to the spatial gradient of the magnetization, and thus the spin waves [3]. Based on a superexchange model, which describes the antiferromagnetic coupling between two nearest neighbor iron ions through an oxygen ion, including spin-orbit coupling, we estimate the coupling constant and predict a phase shift linear in the applied electric fields [4]. The theory is then confirmed by experimental measurement of the electric-field-induced phase shift in a YIG waveguide [5]. In addition to the flexoelectric effect, another electric effect is observed, which couples the electric field directly with the magnetization of YIG. We call this a magnetoelectric effect. By adjusting the direction of the electric field, the two effects can be well separated. Experimental results agree quantitatively with the theoretical prediction. A phenomenological coupling constant for the magnetoelectric effect is also obtained. Our findings point to an important avenue for manipulating spin waves and developing electrically tunable magnonic devices. [1] P. Rovillain *et al.*, Nat. Mater. 9, 975 (2010). [2] M. Bao *et al.*, Appl. Phys. Lett. 101, 022409 (2012). [3] T. Liu and G. Vignale, J. Appl. Phys. 111, 083907 (2012). [4] T. Liu and G. Vignale, Phys. Rev. Lett. 106, 247203 (2011). [5] X. Zhang *et al.*, Phys. Rev. Lett. 113, 037202 (2014). [6] The author gratefully acknowledges collaborations with G. Vignale, M.E. Flatté, X. Zhang and H. X. Tang. This work is supported by DARPA MESO and an ARO MURI.

**8:36AM X19.00002 Enhanced magneto-ionic switching of interface anisotropy in Pt/Co/GdOx films**, AIK JUN TAN, MAX MANN, UWE BAUER, GEOFFREY BEACH, MIT — Voltage control of magnetic anisotropy is of great interest for reducing the switching energy barrier in spintronic devices. It has recently been shown that electric field-driven oxygen ion migration near the interface of ferromagnet/oxide bilayers can lead to very large changes in magnetic anisotropy at elevated temperature. Here, we examine magneto-ionic switching in ultrathin Pt(3nm)/Co(0.9nm)/GdOx(*t<sub>ox</sub>*)/Au(*t<sub>Au</sub>*) films with perpendicular anisotropy, in which the GdOx layer and gate structure are optimized for efficient room-temperature oxygen conduction. We study voltage-induced switching dynamics as a function of the GdOx stoichiometry and the thickness of the Au gate layer. We find that for optimally oxidized GdOx, a positive bias voltage applied to the Au electrode results in a transition from PMA to in-plane magnetization, and at zero bias, the PMA spontaneously returns. The rate of this transition depends on the thickness of the Au gate which suggests that the rate-limiting step is removal and reintroduction of oxygen by gate voltage. This toggling of PMA under positive bias does not require oxidation of the Co layer, in contrast to earlier work by Uwe *et al.* We demonstrate that by optimizing the electrode materials, extremely fast room-temperature switching can be achieved in these devices.

**8:48AM X19.00003 Giant enhancement of magnetocrystalline anisotropy in ultrathin manganese films via nanoscale 1D periodic depth modulation**, ANIL RAJAPITAMAHUNI, LE ZHANG, VIJAY SINGH, JOHN BURTON, MAK KOTEN, JEFFREY SHIELD, EVGENY TSYMBAL, XIA HONG, University of Nebraska-Lincoln — We report a unusual giant enhancement of in-plane magnetocrystalline anisotropy (MCA) in ultrathin colossal magnetoresistive oxide films due to 1D nanoscale periodic depth modulation. High quality epitaxial thin films of  $\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$  (LSMO) of thickness 6 nm were grown on (001)  $\text{SrTiO}_3$  substrates via off-axis radio frequency magnetron sputtering. The top 2 nm of LSMO films are patterned into periodic nano-strips using e-beam lithography and reactive ion etching. The resulting structure consists of nano-strips of 2 nm height and 100-200 nm width on top of a 4 nm thick continuous base layer. We employed planar Hall effect measurements to study the in-plane magnetic anisotropy of the unpatterned and nanopatterned films. The unpatterned films show a biaxial anisotropy with easy axis along [110]. The extracted anisotropy energy density is  $\sim 1.1 \times 10^5$  erg/cm<sup>3</sup>, comparable to previously reported values. In the nanopatterned films, a strong uniaxial anisotropy is developed along one of the biaxial easy axes. The corresponding anisotropy energy density is  $\sim 5.6 \times 10^6$  erg/cm<sup>3</sup> within the nano-striped volume, comparable to that of Co. We attribute the observed uniaxial MCA to  $\text{MnO}_6$  octahedral rotations/tilts and the enhancement in the anisotropy energy density to the strain gradient within the nano-strips.

**9:00AM X19.00004 Magnetoelectric Dead Layer and Uncompensated Spins in Magnetic/Ferroelectric Heterostructures**, MIKEL HOLCOMB, CHIH-YEH HUANG, JINLING ZHOU, ROBBYN TRAPPEN, GUERAU CABRERA, West Virginia University, YING-HAO CHU, National Chiao Tung University, WEST VIRGINIA UNIVERSITY TEAM, NATIONAL CHIAO TUNG UNIVERSITY TEAM — Interfacial magnetoelectricity across a multilayer system is known to sometimes result in much larger coupling between electric and magnetism than in single phase systems. We compared the magnetic domains in  $\text{LaSrMnO}_3$  thin films, ferroelectric domains in  $\text{PbZrTiO}_3$  and observed uncompensated spin at the interface. Several techniques to quantify image contrast switching between left and right circularly polarized x-ray absorption spectra of magnetic domains and uncompensated spin were developed and gave similar results. Not surprisingly, the magnetic domain switching increased with magnetic film thickness, but the uncompensated spin did as well. This results suggests that there may be an effective magnetoelectric dead layer at the interface between coupled magnetic and ferroelectric layers, which is likely linked to at least the magnetic dead layer in the magnetic film. These measurements were taken by L-edge spectromicroscopy at the PEEM3 beamline of the Advanced Light Source.

**9:12AM X19.00005 Magnetoelectric Coupling Characteristics of the  $\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3/\text{PbZr}_{0.2}\text{Ti}_{0.8}\text{O}_3(001)$  Interface<sup>1</sup>**, MAHMOUD HAMMOURI, DMITRY KARPOV, New Mexico State University, EDWIN FOHTUNG, New Mexico State University and Los Alamos National Laboratory, IGOR VASILIEV, New Mexico State University — Multiferroic heterostructures composed of thin layers of ferromagnetic and ferroelectric perovskites have attracted considerable attention in recent years. We apply *ab initio* computational methods based on density functional theory to study the characteristics of the magnetoelectric coupling at the (001) interface between  $\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$  (LSMO) and  $\text{PbZr}_{0.2}\text{Ti}_{0.8}\text{O}_3$  (PZT). The calculations are carried out using the Quantum ESPRESSO electronic structure code combined with Vanderbilt ultrasoft pseudopotentials. Our study shows that the interfacial interaction between LSMO and PZT and the polarization of PZT have a strong influence on the distribution of magnetization within the LSMO layer. A significant change in the magnetization of the LSMO layer adjacent to PZT is observed after reversal of the direction of polarization of PZT.

<sup>1</sup>Supported by NMSU GREG award. EF is funded by the DoD-AFOSR under award No FA9550-14-1-0363.

**9:24AM X19.00006 Large enhancement of magnetic anisotropy and laser induced resistive switching effect in  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$  films due to strain from  $\text{BaTiO}_3$  substrates<sup>1</sup>**, V KALAPPATTIL, R DAS, H SRIKANTH, M.H PHAN, Department of Physics, University of South Florida, X MOYA, Department of Materials Science, University of Cambridge, UK — Multifunctional oxide materials are interesting for their fundamental physical properties and technological applications. Epitaxial films of  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$  (LSMO) on  $\text{BaTiO}_3$  (BTO) show intriguing properties such as a giant magnetoelectric effect due to strain from BTO substrate. The LSMO film shows sharp jumps in magnetization  $M(T)$  and resistance  $R(T)$  at first-order structural phase transitions of BTO ( $T_{R-O}$  200K and  $T_{O-T}$  270 K) due to strain coupling from BTO. A temperature evolution of effective in-plane anisotropy field ( $H_K$ ) measured using the radio-frequency transverse susceptibility (TS) shows a sharp increase in  $H_K$  around  $T_{R-O}$ , which vanishes around  $T_{O-T}$ . The in-plane magnetic anisotropy plays an important role in changing the magnetic and resistive states around  $T_{O-T}$ . A switchable laser-induced resistive change of up to 300 %, which is about 10 times greater than those of conventional oxide systems, has been achieved in LSMO films using a 0.5 W violet laser just below the  $T_{O-T}$ . The repeatability and stability of the laser-induced resistive switching effect reveal potential applications of LSMO/BTO heterostructures in developing new type of temperature sensors and memory devices.

<sup>1</sup>Work at USF supported by ARO Grant No. W911NF-15-1-0626

**9:36AM X19.00007 Reversible Control of Magnetism in  $\text{La}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$  through Chemically-Induced Oxygen Migration**, ALEXANDER GRUTTER, DUSTIN GILBERT, BRIAN MARANVILLE, JULIE BORCHERS, BRIAN KIRBY, National Institute of Standards and Technology, ELKE ARENHOLZ, Lawrence Berkeley National Lab, URUSA ALAAN, YURI SUZUKI, Stanford University, KAI LIU, University of California, Davis — There has been a surge of interest in controlling magnetism through oxygen migration for applications in hybrid ionic/magnetoelectric device architectures. With a rich magnetic and electronic phase diagram, the colossal magnetoresistive perovskite  $(\text{La,Sr})\text{MnO}_3$  (LSMO) is an ideal candidate for achieving large modulations in magnetic properties with small changes in oxygen content. We demonstrate reversible control of magnetism in LSMO films through interfacial oxygen migration. Gd metal capping layers deposited onto LSMO leach oxygen from the film to form porous  $\text{Gd}_2\text{O}_3$ . X-ray absorption and polarized neutron reflectometry measurements show Mn valence alterations consistent with high oxygen vacancy concentrations, resulting in suppressed magnetization and increased coercive fields. Oxygen migration is observed both at the interface and also throughout the majority of a 40 nm thick film, suggesting extensive oxygen vacancy diffusion. After Gd-capped LSMO is exposed to atmospheric oxygen for a prolonged period of time, oxygen diffuses through the  $\text{Gd}_2\text{O}_3$  layer and the magnetization of the LSMO returns to the uncapped value. These findings showcase perovskite heterostructures as ideal candidates for developing functional interfaces through chemically-induced oxygen migration.

**9:48AM X19.00008 Detecting interfacial defects at magnetic/non-magnetic junctions<sup>1</sup>**, NICHOLAS HARMON, MICHAEL FLATTÉ, University of Iowa — Recent three terminal (3T) measurements in  $\text{Co/LaAlO}_3/\text{SrTiO}_3$  show that spin-dependent transport through an interfacial defect is occurring instead of Hanle dephasing [1]. We propose extending 3T measurements into a coherent regime where single defects are detected by their local fields. The setup involves defects being situated between biased non-magnetic (NM) and ferromagnetic (FM) contacts. Spin torque on the FM drives an AC magnetization. Due to the large exchange interaction, the ability for charge to enter the FM depends on its spin and FM's relative orientation. As the FM precesses, the spin is dynamically filtered and a precessing spin accumulation remains at the defect. Local fields also precess the defect spin and interfere with the dynamic spin filtering. If the AC and local field are resonant, the spin accumulation is locked anti-parallel to the FM and leads to a dip in current. By adjusting the AC frequency, information on the local field is ascertained which, for hyperfine local fields, tells which nuclei are present at the defect and aids in identifying the defect. In the DC limit, defect spin accumulation leads to modifications in Hanle signals. [1] H. Inoue, A.G. Swartz, N.J. Harmon, M.E. Flatté, T. Tachikawa, Y. Hikita, and H.Y. Hwang. In press at Phys. Rev. X.

<sup>1</sup>This material is based on work supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Award Number DE-SC0014336.

**10:00AM X19.00009 Electronic and Magnetic Properties of Transition-Metal Oxide Nanocomposites: A Tight-Binding Modeling at Mesoscale.**<sup>1</sup>, YUAN-YEN TAI, Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA, JIAN-XIN ZHU, Theoretical Division and Center for Integrated Nanotechnologies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — Transition metal oxides (TMOs) exhibit many emergent phenomena ranging from high-temperature superconductivity and giant magnetoresistance to magnetism and ferroelectricity. In addition, when TMOs are interfaced with each other, new functionalities can arise, which are absent in individual components. In this talk, I will present an overview on our recent efforts in theoretical understanding of the electronic and magnetic properties TMO nanocomposites. In particular, I will introduce our recently developed tight-binding modeling of these properties arising from the interplay of competing interactions at the interfaces of planar and pillar nanocomposites. Our theoretical tool package will provide a unique capability to address the emergent phenomena in TMO nanocomposites and their mesoscale response to such effects like strain and microstructures at the interfaces, and ultimately help establish design principles of new multifunctionality with TMOs.

<sup>1</sup>This work was carried out under the auspices of the National Nuclear Security Administration of the U.S. Department of Energy at LANL under Contract No. DE-AC52-06NA25396, and was supported by the LANL LDRD Program.

**10:12AM X19.00010 Direct measurement of voltage-controlled reversal of the antiferromagnetic spin structure in magnetoelectric Cr<sub>2</sub>O<sub>3</sub>**<sup>1</sup>, JUNLEI WANG, CHRISTIAN BINEK, University of Nebraska-Lincoln — The frequency dependence of the electric field induced magneto-optical Faraday effect is investigated in the magnetoelectric antiferromagnet chromia. Two electrically induced Faraday signals superimpose in proportion to the linear magnetoelectric susceptibility and the antiferromagnetic order parameter. The relative strength of these contributions is determined by the frequency of the probing light beam. It allows tuning the Faraday signal between extreme characteristics which follow the temperature dependence of the magnetoelectric susceptibility or solely that of the antiferromagnetic order parameter. The frequency dependence is analyzed in terms of electric dipole transitions of perturbed Cr<sup>3+</sup> crystal-field states. The results lead to a table-top set-up allowing to measure voltage-controlled selection and temperature dependence of the antiferromagnetic order parameter. The Faraday rotation per applied voltage is independent of the sample thickness making the method scalable and versatile for thin film investigations. Scalability, compactness, and simplicity of the data analysis combined with low photon flux requirements make the Faraday approach advantageous for the investigation of the otherwise difficult to access voltage-controlled switching of antiferromagnetic domain states in magnetoelectric thin films.

<sup>1</sup>This project is supported by NRI via CNFD through tasks SRC 2398.001 and 2587.001, by C-SPIN, a SRC program, sponsored by MARCO and DARPA, and by NSF through Nebraska MRSEC DMR-1420645.

**10:24AM X19.00011 Voltage Control of Exchange Bias in a Chromium Oxide Based Thin Film Heterostructure**<sup>1</sup>, WILL ECHTENKAMP, MIKE STREET, ATHER MAHMOOD, CHRISTIAN BINEK, Univ of Nebraska - Lincoln — Controlling magnetism by electrical means is a key challenge in the field of spintronics, and electric control of exchange bias is one of the most promising routes to address this challenge. Isothermal electric control of exchange bias has been achieved near room temperature using bulk, single crystal, magnetoelectric Cr<sub>2</sub>O<sub>3</sub> [1,2]. In this study the electrically-controlled exchange bias is investigated in an all thin film Cr<sub>2</sub>O<sub>3</sub>/PdCo exchange bias heterosystem where an MBE grown ferromagnetic and perpendicular anisotropic Pd/Co multilayer has been deposited on a PLD grown (0001) Cr<sub>2</sub>O<sub>3</sub> thin film. Prototype devices are fabricated using lithography techniques. Using a process of magnetoelectric annealing, voltage control of exchange bias in Cr<sub>2</sub>O<sub>3</sub> heterostructures is demonstrated with significant implications for scalability of ultra-low power memory and logical devices. In addition, the dependence of the exchange bias on the applied electric and magnetic fields are independently studied at 300K and isothermal voltage-controlled switching is investigated. [1] Xi He, et. al., Nature Mater.9, 579585 (2010). [2] W. Echtenkamp and Ch. Binek, Phys. Rev. Lett. 111, 187204 (2013).

<sup>1</sup>This project was supported by SRC through CNFD, an SRC-NRI Center, by C-SPIN, part of STARnet, and by the NSF through MRSEC DMR-0820521

**10:36AM X19.00012 Eliminating leakage current in voltage-controlled exchange-bias devices**<sup>1</sup>, ATHER MAHMOOD, WILL ECHTENKAMP, MICHAEL STREET, CHRISTIAN BINEK, Univ of Nebraska - Lincoln, MAGNETIC HETEROSTRUCTURES TEAM — Manipulation of magnetism by electric field has drawn much attention due to the technological importance for low-power devices, and for understanding fundamental magnetoelectric phenomena. A manifestation of electrically controlled magnetism is voltage control of exchange bias (EB). Robust isothermal voltage control of EB was demonstrated near room temperature using a heterostructure of Co/Pd thin film and an exchange coupled single crystal of the antiferromagnetic Cr<sub>2</sub>O<sub>3</sub> (Chromia) [1,2]. A major obstacle for EB in lithographically patterned Chromia based thin-film devices is to minimize the leakage currents at high electric fields (>10 kV/mm). By combining electrical measurements on patterned devices and conductive Atomic Force Microscopy of Chromia thin-films, we investigate the defects which form conducting paths impeding the application of sufficient voltage for demonstrating the isothermal EB switching in thin film heterostructures. Technological challenges in the device fabrication will be discussed. [1] Xi He, et.al, Nat. Mater. 9, 579-585 (2010) [2] W. Echtenkamp, Ch. Binek, Phys. Rev. Lett. 111, 187204 (2013)

<sup>1</sup>This project was supported by SRC through CNFD, an SRC-NRI Center, by C-SPIN, part of STARnet, and by the NSF through MRSEC Abstract DMR-0820521

**10:48AM X19.00013 Electrostatic doping limits and control of magnetism in electrolyte gated LaAlO<sub>3</sub>(001)/La<sub>0.5</sub>Sr<sub>0.5</sub>CoO<sub>3-δ</sub> thin films**, JEFF WALTER, HELIN WANG, CHRIS LEIGHTON, University of Minnesota — Recently developed ionic liquid/gel gating techniques have proven remarkably expedient in the study of charge density effects in a variety of conductors, ranging from organics to complex oxides. Here we present electrolyte gate control of magnetism in ultrathin (8 u.c.) La<sub>0.5</sub>Sr<sub>0.5</sub>CoO<sub>3-δ</sub> (LSCO) films, using ion gels in electric double layer transistors. The LSCO films are initially metallic and ferromagnetic ( $T_c \approx 170$  K), with anomalous Hall conductivity up to 40 S/cm, and strong perpendicular magnetic anisotropy. Based on extensive temperature and gate voltage dependences we first determined the limits for electrostatic vs. electrochemical operation, concluding that negative bias enables reversible hole accumulation, whereas positive bias irreversibly induces oxygen vacancies. Following this we demonstrated clear voltage-control of resistivity, magnetoresistance, and  $T_c$ . Utilizing the anomalous Hall conductivity as an exceptional probe of the magnetic order parameter in the gated surface region, a 12 K shift in  $T_c$  is obtained. This compares favorably to the state-of-the-art and exhibits potential for much larger modulation in films of lower Sr content. Work supported by NSF MRSEC.

**Friday, March 18, 2016 8:00AM - 10:12AM —**

Session X20 DMP: Van der Waals Bonding in Advanced Materials: Carbon Allotropes and Boron Nitride 319 - John Singleton, Los Alamos National Laboratory

**8:00AM X20.00001 Growth systematics for the controlled generation of nanostructured materials**, NICOLE GROBERT, University of Oxford — Whilst nanomaterials are well established in the research arena they are yet to be exploited at the industrial scale due to their limited availability. A series of bottlenecks must still be overcome before their outstanding properties can be fully unlocked. This fact applies to nanomaterials across the board including tailored 0D, 1D, 2D structures and combinations thereof. This talk addresses the challenges that need to be overcome related to up-scaling the production of novel nanomaterials, possible solutions and the necessity for the development of dedicated nanomaterials for end- user applications will also be discussed.

**8:36AM X20.00002 Investigation of intermolecular interactions between single walled nanotubes and conjugated oligomers using the dispersion-corrected DFT methods<sup>1</sup>**, JOLANTA B LAGOWSKI, SUAD ALJOHANI, M. ZAHIDUL H. KHAN, YUMING ZHAO, Memorial University — The area of carbon nanotubes (CNT)-polymer composites has been progressing rapidly in recent years. Pure CNT and CNT-polymer composites have many useful (industry related) properties: ranging from electronic electrical conductivity to superior strength. However the full potential of using CNTs as reinforcements (in say a polymer matrix) has been severely limited because of complications associated with the dispersion of CNTs. CNTs tend to entangle with each other forming materials that have properties that fall short of the expectations. The goal of this work is to identify the type of conjugated oligomers that are best suited for the dispersion of single walled CNT (SWCNT). For this purpose, various methods of dispersion corrected density functional theory (DFT-D/B97D, /WB97XD, /CAM-B3LYP) have been used to investigate the interaction between the SWCNT and the organic conjugated oligomers with different end groups (aldehyde (ALD) and dithiafulvenyl (DTF)). We investigate the effect of intermolecular interactions on the structure, polarity and energetics of the oligomers and SWCNT combinations. The comparison of results obtained using different DFT approximations is made. Our results show that DFT-endcapped oligomer interact more strongly with CNT than ALD-endcapped oligomer.

<sup>1</sup>The financial support from NSERC, SACBC and Memorial University and the computational resources from Compute Canada were received.

**8:48AM X20.00003 Probing moiré physics in low angle twisted bilayer graphene**, YUAN CAO, JASON LUO, Massachusetts Inst of Tech-MIT, JAVIER D. SANCHEZ-YAMAGISHI, Harvard University, KENJI WATANABE, TAKASHI TANIGUCHI, NIMS, Japan, PABLO JARILLO-HERRERO, Massachusetts Inst of Tech-MIT — When two sheets of honeycomb structured graphene are stacked together, a moiré pattern that depend on the twist angle forms. A gapped superlattice band structure is resulted when this angle is small enough so that the energy of moiré modulated hybridization between wave functions on the two sheets that are separated by only 0.34nm is low enough. Apart from the energy gaps, the superlattice band structure also manifests reduced Fermi velocity which implies comparatively higher density of states, multiple van Hove singularities below and above the gaps, and Hofstadter butterfly physics when magnetic field is applied. We show electronic transport measurements of high-quality low-angle twist bilayer graphene devices fabricated by a novel tear-and-stack technique, at zero, low and high magnetic fields. We also present angle dependence of the electronic structure along with magneto-transport features that possibly imply electron-electron interactions. A brief discussion about the transition between the low-twist and high-twist bilayer graphene, the physics of the latter of which is believed to be essentially based on decoupled monolayer graphene according to our previous work, is included.

**9:00AM X20.00004 Moire pattern interlayer potentials in van der Waals materials from high level ab initio calculations**, JEIL JUNG, NICOLAS LECONTE, University of Seoul, Korea, SEBASTIEN LEBEGUE, Université de Lorraine, France, TIMOTHY GOULD, Griffith University, Australia — Stacking-dependent interlayer interactions are important for understanding the structural and electronic properties in incommensurable two dimensional material assemblies where long-range moiré patterns arise due to small lattice constant mismatch or twist angles. We study the stacking-dependent interlayer coupling energies between graphene (G) and hexagonal boron nitride (BN) single layers for different possible combinations such as G/G, G/BN and BN/BN using high-level EXX+RPA *ab initio* calculations. The total energies differ substantially when compared with conventional LDA, but for stacking-dependent total energy differences we find that the dominance of short-range covalent-type binding over the longer-ranged van der Waals tails near equilibrium geometries renders the LDA as a reasonable starting point for ab initio calculation based analyses for the systems we have studied. Our calculations are useful input for study of strains originated by interlayer interactions in incommensurable 2D van der Waals crystals.

**9:12AM X20.00005 Near-field study in graphene/hBN moiré superlattices.**, GUANGXIN NI, University of California, San Diego, HAOMIN WANG, Shanghai Institute of Microsystem and Information Technology, JIHI-SHENG WU, ZHE FEI, MICHAEL GOLDFLAM, FRITZ KEILMANN, University of California, San Diego, BARBAROS ZYLMAZ, ANTONIO CASTRO NETO, National University of Singapore, XIAOMING XIE, Shanghai Institute of Microsystem and Information Technology, MICHAEL FOGLER, DIMITRI BASOV, University of California, San Diego — Moiré patterns are periodic superlattice structures that appear when two crystals with a minor lattice mismatch are superimposed. A prominent recent example is that of monolayer graphene placed on a crystal of hexagonal boron nitride (hBN). As a result of the moiré pattern superlattice created by this stacking, the electronic band structure of graphene is radically altered, acquiring satellite sub-Dirac cones at the superlattice zone boundaries. To probe dynamical response of the moiré graphene, we use infrared (IR) nano-imaging to explore propagation of surface plasmons, collective oscillations of electrons coupled to IR light. We show that interband transitions associated with the superlattice minibands in concert with free electrons in the Dirac bands produce two additive contributions to composite IR plasmons in graphene moiré superstructures. This novel form of collective modes is likely to be generic to other forms of moiré-forming superlattices, including van der Waals heterostructures.

**9:24AM X20.00006 Optical control of inter-layer distance of hBN: a TDDFT study**, YOSHIYUKI MIYAMOTO, AIST, HONG ZHANG, Sichuan University, TAKEHIDE MIYAZAKI, AIST, ANGEL RUBIO, Max Planck Institute for the Structure and Dynamics of Matter — In this presentation, we introduce an idea to modify inter-layer distance of hBN by shining IR laser in resonance with the frequency of the optical phonon ( $A_{2u}$  mode). By performing the TDDFT-MD simulation under the IR laser, significant grow in an amplitude of the  $A_{2u}$  phonon mode was observed and inter-layer contraction over 11 % of the original distance was achieved. The source of the stronger attraction of hBN sheets was attributed with increase of dipole moment of each layer coming from the motions of boron (B) and nitrogen (N) atoms in opposite directions. Since the dipole moments of these layers remain as parallel throughout the  $A_{2u}$  phonon vibration, the increase of attractive force occurs between the two hBN sheets in analogy of the London force. In this talk, we will further discuss proper intensity of IR laser and potential applications of this phenomenon. This work was published in Phys. Rev. Lett **114**, 116102 (2015).

**9:36AM X20.00007 Using quantum Monte Carlo for the interaction of water with carbon and BN based substrates and assessing exchange-correlation functionals**, YASMINE AL-HAMDANI, Department of Chemistry, University College London and Thomas Young Centre, DARIO ALFE, Department of Earth Sciences, University College London and Thomas Young Centre, O. ANATOLE VON LILIENFELD, Argonne National Laboratories, Argonne, and Institute of Physical Chemistry, Chemistry Department, University of Basel, ANGELOS MICHAELIDES, Department of Physics, University College London and Thomas Young Centre — The interaction of water with the pure surfaces, graphene and hexagonal boron nitride (h- BN), has received a lot of attention because of interesting phenomena exhibited by these systems and their promising potential applications in clean energy, water purification, hydrogen storage, and bio-sensing. BN doped graphene can also now be made, opening the way to carefully designed hybrid materials. However, much of the fundamental mechanisms regarding the interaction between these surfaces and water is still not well understood. We use quantum Monte Carlo to establish accurate benchmarks for water on a number of carbonaceous and BN based substrates, including 2-dimensional periodic surfaces, for which van der Waals interactions play a key role. The benchmarks are then used to test and understand various exchange-correlation functionals in density functional theory. We find that the physisorption of water is poorly described in terms of the adsorption site and the interaction energy by a range of different classes of exchange- correlation functionals, including some that account for dispersion, and we show where these inadequacies might come from.

**9:48AM X20.00008 'Guanigma': the revised structure of biogenic anhydrous guanine**, ANNA HIRSCH, DVIR GUR, Weizmann Institute of Science, Israel, IRYNA POLISHCHUK, DAVIDE LEVY, BOAZ POKROY, Technion, Israel, AURORA J. CRUZ-CABEZA, University of Manchester, United Kingdom, LIA ADDADI, LEEOR KRONIK, LESLIE LEISEROWITZ, Weizmann Institute of Science, Israel — Living organisms display a spectrum of colors, produced by pigmentation, structural coloration, or both. A relatively well-studied system, which produces colors via an array of alternating anhydrous guanine crystals and cytoplasm, is responsible for the metallic luster of many fish. The structure of biogenic anhydrous guanine was believed to be the same as that of the synthetic one - a monoclinic polymorph. Here we re-examine the structure of biogenic guanine, using experimental X-ray and electron diffraction (ED) data exposing troublesome inconsistencies - namely, a 'guanigma'. To address this, we sought alternative candidate polymorphs using symmetry and packing considerations, then used first principles calculations to determine whether the selected candidates could be energetically stable. We identified theoretically a different monoclinic polymorph, were able to synthesize it, and to confirm using X-ray diffraction that it is this polymorph that occurs in biogenic samples. However, the ED data were still not consistent with this polymorph, but rather with a theoretically generated orthorhombic polymorph. This apparent inconsistency was resolved by showing how the ED pattern could be affected by crystal structural faults composed of offset molecular layers.

**10:00AM X20.00009 Sorption Properties of Halogen Containing Graphene Oxide Frameworks.**, JACOB BURRESS, ELIZABETH BAKER, DONALD BETHEA, KATHERINE FRANGOS, Univ of South Alabama — Physisorption of gases has applications in gas storage (e.g. methane, hydrogen for vehicles) and gas separation (carbon dioxide from flue gas). The van der Waals force in narrow pores is strong enough to condense even supercritical gases to much higher densities. Additionally, differences in the binding energy between different gases and the sorbent surface are sufficient to for gas separations. Beyond adsorption interactions, simple steric (size, shape) effects also play a role in gas separations. One class of materials currently being investigated for numerous gas storage/separation applications is graphene oxide frameworks (GOFs). GOFs consist of layers of graphene/graphene oxide separated by chemical linkers covalently bonded on both sides. This presentation will give results from boronic acid-based GOFs that contain halogen group elements. Effects of different linkers on pore shape will be presented. Physical behavior of the gases investigated (hydrogen, methane, carbon dioxide, nitrogen), including binding energies and steric effects for gas separation will also be presented. The physics mechanism behind pore breathing (expansion and contraction of pore volume) in these materials will be discussed.

## Friday, March 18, 2016 8:00AM - 11:12AM –

**Session X21 GSCCM DCOMP DMP: Materials in Extremes: Metals at High Strain Rates** 320

- Tim Germann, Los Alamos National Laboratory

**8:00AM X21.00001 Elastic-plastic structure of shock waves in single crystal copper<sup>1</sup>**, R. RAVELO, Univ of Texas, El Paso, B.L. HOLIAN, T.C. GERMANN, Los Alamos National Laboratory — Large-scale atomistic simulations of shock wave propagation in defect-free copper single crystals exhibit an orientation dependent elastic limit and elastic-plastic two-wave regimes for shock propagation along the (110) and (111) low-index directions but not along (100). By contrast, no orientational difference in the Us-Up profiles of single crystals compared with polycrystalline samples has been reported in shock experiments. The elastic-plastic response of copper shocked along (111) was examined via large-scale non-equilibrium molecular dynamics (NEMD) simulations employing samples of up to 3.5 microns in length and particle velocities between 0.5 and 2.5 km/s (20- 130 GPa). The longer time and length scales allow for a more accurate determination of the elastic limit, longitudinal and plastic wave speeds. Results show a steady elastic precursor for particle velocities below 1.6 km/s, which does not decay in time. The NEMD data for the plastic wave velocity in the split-wave regime extrapolates linearly in particle velocity to the shear-wave speed at zero pressure.

<sup>1</sup>This work supported by the Department of Energy under contract DE-AC52-06NA25396 and the Air Force Office of Scientific Research under AFOSR Award FA9550-12-1-0476

**8:12AM X21.00002 Tantalum strength model incorporating temperature, strain rate and pressure**, HOJUN LIM, CORBETT BATTAILE, JUSTIN BROWN, MATT LANE, Sandia National Laboratories — Tantalum is a body-centered-cubic (BCC) refractory metal that is widely used in many applications in high temperature, strain rate and pressure environments. In this work, we propose a physically-based strength model for tantalum that incorporates effects of temperature, strain rate and pressure. A constitutive model for single crystal tantalum is developed based on dislocation kink-pair theory, and calibrated to measurements on single crystal specimens. The model is then used to predict deformations of single- and polycrystalline tantalum. In addition, the proposed strength model is implemented into Sandia's ALEGRA solid dynamics code to predict plastic deformations of tantalum in engineering-scale applications at extreme conditions, e.g. Taylor impact tests and Z machine's high pressure ramp compression tests, and the results are compared with available experimental data. Sandia National Laboratories is a multi program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

**8:24AM X21.00003 Molecular simulation of dislocation motion in magnesium alloys under high strain rates**, PENG YI, ROBERT CAMMARATA, MICHAEL FALK, Johns Hopkins University — Dislocation motion of  $\langle a \rangle$ -dislocations on the basal and the prismatic planes under simple shear was studied using molecular simulations in Mg/Al and Mg/Y alloys. The critical resolved shear stress (CRSS) was calculated at temperature from 0K to 500K with solute concentrations from 0 to 7 at.%. The strain rates of  $10^6$ - $10^8$  s<sup>-1</sup> used in the simulation correspond to experimental strain rates of  $10^1$ - $10^5$  s<sup>-1</sup> based on Orowan's equation. Basal slip is dominated by the  $\langle a \rangle$ -edge dislocations. Solute hardening to the CRSS follows a power law,  $c^n$ , where  $c$  is the solute concentration. The exponent  $n$  transitions from close to 2/3 at low temperature to close to 1 at high temperature. Temperature and strain rate effects on the CRSS are captured by Kocks model based on thermally activated events. Prismatic slip is controlled by the  $\langle a \rangle$ -screw dislocation that cross-slips between the basal and the prismatic planes, in a locking-unlocking pattern. Temperature affects the slip kinetics through the diffusion of the screw dislocation on the basal plane, which leads to vacancy and loop generation. Solute softening was observed for both Mg/Al and Mg/Y alloys. The softening on prismatic slip is due to the solute pinning effect on the basal plane, and Al is more effective in softening.

**8:36AM X21.00004 Simulating the dynamic response of magnesium alloys**, JEFFREY LLOYD, RICHARD BECKER, US Army Research Laboratory — Unlike several conventional metals, the mechanical response of magnesium is severely anisotropic for quasistatic and dynamic loading conditions. In this work we present a crystal-based strength model that is the same order of magnitude in computational cost as rate-dependent isotropic strength models, yet is able to capture essential features exhibited by textured magnesium polycrystals. The model demarcates plastic deformation into contributions from basal slip, extension twinning, and non-basal slip mechanisms. Comparisons are made between model predictions and experiments for two magnesium alloys with differing processing histories. The model is then used to explore and quantify the dependence of metallurgical and processing variations for several dynamic experiments that probe propensity for localization and failure under complex loading conditions.

**8:48AM X21.00005 Deformation twinning in a polycrystalline magnesium alloy during dynamic compression**, CALEB HUSTEDT, Johns Hopkins University, JEFFREY LLOYD, Army Research Laboratory, PAUL LAMBERT, VIGNESH KANNAN, Johns Hopkins University, DANIEL CASEM, Army Research Laboratory, K.T. RAMESH, Johns Hopkins University, NICHOLAS SINCLAIR, Washington State University, RICHARD BECKER, Army Research Laboratory, TODD HUFNAGEL, Johns Hopkins University — We report the results of combined in situ x-ray diffraction studies and crystal plasticity modeling of deformation twinning in polycrystalline magnesium during dynamic compression. Diffraction experiments were conducted at the Dynamic Compression Sector (DCS) of the Advanced Photon Source, on magnesium alloy (AZ31B) specimens (with various crystallographic textures) loaded at strain rates of  $\sim 1000 \text{ s}^{-1}$  in a compression Kolsky bar. The diffraction patterns, recorded with temporal resolution of 5-10 microseconds, provide information about the evolution of crystallographic texture during deformation, which we interpret in terms of the twinning mechanism (so-called “extension” or “tensile” twinning). We compare our observations quantitatively with predictions of the evolution of crystallographic texture from an efficient reduced crystal plasticity model. This model explicitly accounts for basal slip and extension twinning on a rate-independent basis, but treats other mechanisms (pyramidal and prismatic slip) as isotropic, rate-dependent functions. This combination yields substantial improvements in efficiency over full crystal-plasticity models while retaining key aspects of the most important deformation mechanisms.

**9:00AM X21.00006 Deformation twinning activated  $\alpha \rightarrow \omega$  transformation in titanium under shock compression.**, HONGXIANG ZONG, TURAB LOOKMAN, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA — Materials dynamics, especially the behavior of solids under extreme compression, is a topic of broad scientific and technological interest. However, less is known of the role of grain boundary structures on the shock response of hexagonal-close-packed metals. We use molecular dynamics simulations to study deformation mechanisms in shock compressed Ti bicrystals containing three types of grain boundary (GB) microstructures, i.e., coherent twin boundaries (CTBs), symmetric incoherent twin boundaries (ITB) and  $\{1\text{-}210\}$  asymmetric tilt grain boundaries. Our results show that both dislocation activity and the  $\alpha \rightarrow \omega$  phase transformation in Ti are sensitive to the GB characteristics. In particular, we find that the elastic shock wave can readily trigger the  $\alpha \rightarrow \omega$  transformation at CTBs but not at the other two GBs, and the activation of the  $\alpha \rightarrow \omega$  transformation at CTBs leads to considerable wave attenuation (i.e., the elastic precursor decay). Combined with first principle calculations, we find that CTBs can facilitate the overcoming of the energy barrier for the  $\alpha \rightarrow \omega$  transformation. Our findings have potential implications for interface engineering and materials design under extreme conditions.

**9:12AM X21.00007 Microstructural Effects on Materials under Extreme Dynamic Environments**, CYRIL WILLIAMS, U.S. Army Research Laboratory — Studies have shown that microstructure and microstructure evolution can play a major role on the shock response of metals and metallic alloys. When metals and metallic alloys are deformed during shock compression, large numbers of lattice defects such as dislocations can be introduced in the material. These dislocations can lead to strengthening effects such as hardening and/or softening such as dynamic recovery which may consequently change the material behavior. Therefore, to better understand the effects of microstructure and microstructure evolution on the spall response of metals, both in-situ and end-state gas gun plate impact experiments were employed to study 1100-O aluminum. The results show a sharp increase in pullback velocity for 1100-O aluminum with increase in peak shock stress between 4.0 and 8.3 GPa due to shock hardening, followed by a decrease for peak shock stresses up to 12.0 GPa due to softening induced by dynamic recovery. In addition, the effects of microstructure on the spall properties of two magnesium alloys fabricated via ECAE (AZ31B-4E) and SWAP (AMX602) were also investigated. The pullback velocities were found to decrease by approximately 15% for AZ31B-4E between 1.7 GPa to 4.6 GPa shock stress. On the contrary, the pullback velocities for AMX602 were found to be random for the same shock stress range studied. Residual microstructure of the post-shocked AZ31B-4E magnesium shows that aluminum-manganese intermetallic inclusions were perhaps responsible for the reduction in pullback velocity. Also, the post-shocked residual microstructure of the AMX602 magnesium revealed features that may have been responsible for its random response.

**9:24AM X21.00008 Damage Tolerant Microstructures for Shock Environments**, ELLEN CERRETA, DARCIE DENNIS-KOLLER, LANL, JUAN PABLO ESCOBEDO, University of New South Wales, SARYU FENSIN, STEVE VALONE, CARL TRUJILLO, CURT BRONKHORST, RICARDO LEBENSOHN, LANL — While dynamic failure, due to shock loading, has been studied for many years, our current ability to predict and simulate evolving damage during dynamic loading remains limited. One reason for this is due to the lack of understanding for the linkages between process-induced as well as evolved microstructure and damage. To this end, the role of microstructure on the early stages of dynamic damage has been studied in high purity Ta and Cu. This work, which utilizes plate-impact experiments to interrogate these effects, has recently been extended to a subset to Cu-alloys (Cu-Pb, Cu-Nb, and Cu-Ag). These multi-length scale studies, have identified a number of linkages between damage nucleation and growth and microstructural features such as: grain boundary types, grain boundary orientation with respect to loading direction, grain orientation, and bi-metal interfaces. A combination of modeling and simulation techniques along with experimental observation has been utilized to examine the mechanisms for the ductile damage processes such as nucleation, growth and coalescence. This work has identified differing features of importance for damage nucleation in high purity and alloyed materials, lending insight into features of concern for mitigating shock induced damage in more complicated alloy systems.

**9:36AM X21.00009 Rate-dependent scaling laws for spall failure**, JUSTIN WILKERSON, University of Texas at San Antonio, KT RAMESH, Hopkins Extreme Materials Institute — Here we derive simple bounds on the growth rate of voids considering the combined retarding effects of micro-inertia and dislocation kinetics. We make use of these bounds to derive simple scaling laws capable of predicting the strong rate-dependence of spall strength. We show that the rate-sensitivity exponent for spall strength is bounded to below  $6/7$  when micro-inertia is the dominant retarding effect on void growth. However, under conditions in which the void growth is predominately governed by dislocation kinetics the rate-sensitivity exponent may rise to a maximum value of 1. With these scaling laws in hand, we go on to further explore the role of microstructure on spall strength. Though simple, the derived scaling laws compare well with experimental measurements and prove useful in shedding light on some of the more perplexing observations associated with spall failure. In particular, the scaling laws are helpful in understanding the somewhat anomalous dependence of spall strength on pre-existing microstructure, e.g. grain size and purity content.

**9:48AM X21.00010 Diffusion of Dissipative Correlation in the Dynamic Failure of Solids**, DENNIS GRADY, Applied Research Associates — A property identified as the dissipative action has found application as a unifying attribute underlying the dynamic failure of solid materials. Failure modes include tensile spall, impact-induced dynamic shear, shock compaction and steady shock-wave compression. The present work explores the possible application of Langevin dynamics and related statistical mechanical implications as underlying the extreme dynamic failure of solids.

**10:00AM X21.00011 A model for ductile metal friction at high velocities<sup>1</sup>** , J. E. HAMMERBERG, Los Alamos National Laboratory, R.J. RAVELO, Univ. of Texas - El Paso, T.C. GERMANN, Los Alamos National Laboratory — We describe a meso-macro scale model for the frictional force at ductile metal interfaces for high velocities and large compressions. The model incorporates the micro-mesoscopic growth and refinement of material microstructure in a highly strained region at the sliding interface and incorporates both rate dependent plasticity and thermal conduction. The model compares favorably with recent large scale (1.8 billion atom) simulations to 50 ns of 3-dimensional polycrystalline 13-50 nm grain size Al-Al interfaces at pressures of 15 GPa using the SPaSM NonEquilibrium Molecular Dynamics (NEMD) simulation code.

<sup>1</sup>This work was performed under the auspices of the U.S. Dept. of Energy under contract DE-AC52-06NA25396. The support of the LANL ASC-PEM program is gratefully acknowledged.

**10:12AM X21.00012 Novel Feed-through Richtmyer-Meshkov Instability (RMI) Experiment for Characterization of Dynamic Material Response<sup>1</sup>** , SAUL OPIE, SUDRISHTI GAUTAM, ELIZABETH FORTIN, JENNA LYNCH, Arizona State University, ERIC LOOMIS, Los Alamos National University, PEDRO PERALTA, Arizona State University — Hydrodynamic instabilities occur often in applications where forces act across a bimaterial interface. In Rayleigh-Taylor (RT) instabilities, surface perturbations grow exponentially under opposing pressure and density gradients. In the closely related Richtmyer-Meshkov (RM) instability, the same perturbations grow linearly due to an impulsive acceleration, e.g., a passing shock wave. These effects are often analyzed with linear fluid theory, but it is well known that for materials possessing shear strength the perturbation evolution can be significantly affected. A challenge in modeling these effects is that existing knowledge of the interplay between strength and hydrodynamic instabilities in solids is limited for the loads and strain rates that are typically used to study them. We have developed novel feed-through RM instability experiments that are useful to understand and model this interplay. We will describe the experimental setup and show simulations that agree well with experimental results in two materials, one-phase copper, and iron loaded above and below the alpha-epsilon phase boundary, where modeling used a phase-aware strength model. In copper, the growth of surface perturbations is quite sensitive to strength model parameters, and so is the amplitude of the shock front perturbations. This is also observed in iron, along with an additional sensitivity in the modeling results to the parameters used to describe phase change kinetics.

<sup>1</sup>Work supported by Department of Energy (DOE) [grant number DE-SC0008683] from the Office of Fusion Energy Science.

**10:24AM X21.00013 A method using the surface perturbation to determine the strength of materials** , JIANWEI YIN, HAO PAN, ZIHUI WU, XIAOMIAN HU, Institute of Applied Physics and Computational Mathematics, Beijing — The determination of the dynamic strength of materials at high pressure and strain rate has been focused by the shock dynamics community for many years. This paper simulated the surface perturbation problems under high pressure and strain rate loading. By adjusting the characteristic geometric variables as wave number, amplitude of initial perturbation at the free surface, we studied the growth of the perturbations in the improved forms of the theoretical results given by Piriz et al. (Phys. Rev. E 78, 056401, 2008). The critical condition that the surface perturbation was restrained from unstable growth was also deduced. In the stable region of perturbation growth, the relationship among the relative velocities, displacements of the key positions at the perturbed surface and the material strength was studied. The experimental feasibility of using the improved relationship to determine the strength of materials was also discussed.

**10:36AM X21.00014 Dynamic Failure Mode Transitions in 7075Al Expanding rings driven by Electromagnetic loading** , MINGTAO LIU, TIEGANG TANG, ZHAOLIANG GUO, CHENG FAN, Institute of Fluid Physics, China Academy of Engineering Physics, Mianyang 621900, Sichuan, China — Dynamic failure mode transitions are observed in 7075Al electromagnetic expanding rings with a typical size of 3mm in thickness and 0.5mm in height. The rings are driven to maximum expanding velocities ranged from 60m/s to 180m/s, corresponding to strain rates of about 3000 to 9000 per second. At lower strain rates, the fractures of the rings are dominated by the hoop tensile stress, and the cracks are along the radial direction. At higher strain rates, the fractures of the rings are dominated by the maximum shear stress, and the cracks are lie along with an angle of about 45 degree with the radial direction. While the rings deform at medium strain rates, a mixed failure mode is observed, which simultaneously consists of tensile fracture and shear fracture. The failure strains of the specimen and the numbers of the fragmentations were measured after testing. The failure strains show a maximum value as the strain rate increasing, but the numbers of the fragmentations increase firstly, then decrease and then increase again. These phenomena were found to have a close relationship with the dynamic failure mode transitions.

**10:48AM X21.00015 Study of expanding fracture behavior of a copper cylinder under hollow explosive loading.<sup>1</sup>** , CHENG FAN, ZHAOLIANG GUO, MINGTAO LIU, TIEGANG TANG, None — We study the expanding fracture behavior of a copper cylinder under hollow explosive loading. Besides the tensile fracture along the circumferential direction, spall fracture along radial direction occurs, which is evidenced by the step-like behavior with three velocity jumps in the free surface velocity curves and microstructure study of the soft recovered fragments. After considering the spall fracture mechanism, a numerical simulation is carried out and the result shows good agreement with the experiment data.

<sup>1</sup>This work was supported by the National Natural Science Foundation of China (Grants No. 11172279)

**11:00AM X21.00016 Compressible Heating in the Condense Phase due to Pore Collapse in HMX<sup>1</sup>** , JU ZHANG, Florida Institute of Technology, THOMAS JACKSON, University of Florida — Axisymmetric pore collapse in HMX is studied numerically by solving multi-phase reactive Euler equations. The generation of hot spots in the condense phase due to compressible heating is examined. The motivation is to improve the understanding of the role of embedded cavities in the initiation of reaction in explosives, and to investigate the effect of hot spots in the condense phase due to compressible heating alone, complementing previous study on hot spots due to the reaction in the gas phase and at the interface. It is found that the shock-cavity interaction results in pressures and thus temperatures that are substantially higher than the post-shock values in the condense phase. However, these hot spots in the condense phase due to compressible heating alone do not seem to be sufficiently hot to lead to ignition at shock pressures of 1-3 GPa. Thus, compressible heating in the condense phase may be excluded as a mechanism for initiation of explosives. It should be pointed out that the ignition threshold for the temperature, the so-called "switch-on" temperature, of hot spots depend on chemistry kinetics parameters. Switch-on temperature is lower for faster reaction rate. The current chemistry kinetics parameters are based on previous experimental work.

<sup>1</sup>This work was supported in part by the Defense Threat Reduction Agency and by the U.S. Department of Energy

**Friday, March 18, 2016 8:00AM - 10:48AM –  
Session X22 DCMF: Mott Physics Model Calculations 321 -**

**8:00AM X22.00001 Dimensional reduction in spin dynamics at Mott quantum criticality**, JAE-HO HAN, YONG-HEUM CHO, KI-SEOK KIM, Department of Physics, POSTECH, Pohang, Gyeongbuk 790-784, Korea — One physical picture in describing metal-insulator transitions driven by strong interactions starts from a UV fixed point. Here, localized magnetic moments play the role of a source of strong inelastic scattering in Mott quantum criticality, which seems quite successful description at high temperature (e.g. anomalous scaling in electric resistivity). However, it has somewhat fundamental difficulty in explaining the low energy physics of a particular class of Mott insulators such as organic salts, where emergent localized magnetic moments are believed to form a spin liquid state. Here, starting from this spin-liquid IR fixed point, we investigate the Mott quantum criticality in (2+1) dimension (D). Our renormalization group analysis suggests that (2+1) D critical spin dynamics turns into (1+1) D dynamics, which originates from gauge invariance at Mott quantum criticality. Applying the bosonization framework, we find that critical spin dynamics is described by SU(2)  $k=1$  Wess-Zumino-Witten theory in (1+1) D and critical charge dynamics is in the XY universality class of (2+1) D. We discuss speculations for the high temperature Mott quantum criticality based on this critical field theory.

**8:12AM X22.00002 Quasi-soliton scattering in quantum spin chains**, DAVIDE FIORETTO, Institut für Theoretische Physik, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany, ROGIER VLJIM, Institute for Theoretical Physics, University of Amsterdam, Science Park 904, 1090 GL Amsterdam, The Netherlands, MARTIN GANAHL, Perimeter Institute for Theoretical Physics, 31 Caroline Street North, ON N2L 2Y5, Canada, MICHAEL BROCKMANN, MASUD HAQUE, Max-Planck-Institut für Physik komplexer Systeme, Nthnitzer Strasse 38, 01187 Dresden, Germany, HANS-GERD EVERTZ, Institut für Theoretische Physik, Technische Universität Graz, Petersgasse 16, 8010 Graz, Austria, JEAN-SBASTIEN CAUX, Institute for Theoretical Physics, University of Amsterdam, Science Park 904, 1090 GL Amsterdam, The Netherlands — The quantum scattering of magnon bound states in the anisotropic Heisenberg spin chain is shown to display features similar to the scattering of solitons in classical exactly solvable models. Localized colliding Gaussian wave packets of bound magnons are constructed from string solutions of the Bethe equations and subsequently evolved in time, relying on an algebraic Bethe ansatz based framework for the computation of local expectation values in real space-time. The local magnetization profile shows the trajectories of colliding wave packets of bound magnons, which obtain a spatial displacement upon scattering. Analytic predictions on the displacements for various values of anisotropy and string lengths are derived from scattering theory and Bethe ansatz phase shifts, matching time evolution fits on the displacements. The TEBD algorithm allows for the study of scattering displacements from spin-block states, showing similar displacement scattering features.

**8:24AM X22.00003 Influence of spinons fluctuations near the spin liquid Mott transition**, TSUNG-HAN LEE, Florida State University and National High Magnetic Field Laboratory, SERGE FLORENS, Institut Neel, CNRS and Université Grenoble Alpes, VLADIMIR DOBROSLAVJEVIC, Florida State University and National High Magnetic Field Laboratory — We investigate the metal to Mott-insulator transition (MIT) in the Hubbard-Heisenberg model using the slave-rotor technique, which allows to combine for the first time the dynamical mean field theory (DMFT) with the Resonating Valence Bond (RVB) approach. In the spin-liquid phase at large Coulomb repulsion, the system shows a RVB transition from a trivial paramagnetic Mott insulator towards a low temperature insulating state with long lived spinons, as seen by the emergence of a linear specific heat. This quenching of the entropy in the spin liquid phase provides strong modifications in the shape of the standard DMFT phase diagram for the MIT occurring at intermediate values of the Coulomb repulsion. We find that the RVB transition happens concomitantly with the first order MIT lines at low temperature. This implies that the Mott insulator always accommodates a spinon Fermi surface, even in the coexistence regime of the MIT, and that the metallic state always stays a Fermi-liquid as it rejects the presence of free spinons, due to their strong scattering onto the holons.

**8:36AM X22.00004 Fractionalized Fermi liquids in a quantum dimer model**, JUNHYUN LEE, Harvard University, STEVEN WHITE, University of California, Irvine, SUBIR SACHDEV, Harvard University — We consider a quantum dimer model with bosonic and fermionic dimers, proposed to describe the pseudogap phase of cuprates. <sup>1</sup> By density matrix renormalization group calculations on a finite cylinder, we obtain the ground state density distribution of the fermionic dimers for a number of different total densities. From the Friedel oscillations at open boundaries, we deduce that the Fermi surface consists of small hole pockets near  $(\pi/2, \pi/2)$ , and this feature persists up to 1/8 doping. Our results support the existence of a “fractionalized Fermi liquid” in this model. We also discuss the form factors of the density modulations.

<sup>1</sup>Matthias Punk, Andrea Allais, and Subir Sachdev, Proc. Natl. Acad. Sci. USA **112**, 9552 (2015)

**8:48AM X22.00005 Infinite bandwidth of a Mott-Hubbard insulator**<sup>1</sup>, JAMES FREERICKS, JEFFREY COHN, Georgetown University, PETER VAN DONGEN, University of Mainz, HULIKAL KRISHNAMURTHY, Indian Institute of Science, Bangalore — The conventional viewpoint of the strongly correlated electron metal-insulator transition is that a single band splits into two upper and lower Hubbard bands at the metal-insulator transition. Much work has investigated whether this transition is continuous or discontinuous. Here we focus on another aspect and ask the question of whether there are additional upper and lower Hubbard bands, which stretch all the way out to infinity—leading to an infinite bandwidth for the Mott insulator. While we are not yet able to provide a rigorous proof of this result, we use exact diagonalization studies on small clusters to motivate the existence of these additional bands, and we discuss some different methods that might be utilized to provide a rigorous proof of this result. Even though the extra upper and lower Hubbard bands have very low total spectral weight, those states are expected to have extremely long lifetimes, leading to a nontrivial contribution to the transport density of states for dc transport and modifying the high temperature limit for the electrical resistivity.

<sup>1</sup>JKF supported by the Department of Energy, Office of Basic Energy Sciences, under Grant No. DE-FG02-08ER46542, and by the McDevitt bequest at Georgetown University. HRK supported by the Indian Science Foundation.

**9:00AM X22.00006 Gaps, Pseudogaps, and the Nature of Charge in Holographic Fermion Models**, GARRETT VANACORE, PHILIP PHILLIPS, University of Illinois at Urbana-Champaign — Building on prior holographic constructions of Fermi arcs and Mott physics, we investigate the landscape of gapped and gapless strongly-correlated phases resulting from bulk fermion interactions in gauge/gravity duality. We test a proposed connection between bulk chiral symmetry and gapless boundary states, and discuss implications for discrete symmetry breaking in pseudogapped systems like the cuprate superconductors. Numerical methods are used to treat gravitational backreaction of bulk fermions, allowing more rigorous investigation of the existence of holographic Fermi surfaces and their adherence to Luttinger’s rule. We use these techniques to study deviations from Luttinger’s rule in holography, testing a recent claim that momentum-deconfined charges are at the heart of the Mott state.

**9:12AM X22.00007 Dimensional decoupling at continuous Mott transitions**, LIUJUN ZOU, Department of Physics, Harvard University, T SENTHIL, Department of Physics, Massachusetts Institute of Technology — For continuous Mott metal-insulator transitions in layered two dimensional systems, we demonstrate the phenomenon of dimensional decoupling: the system behaves as a three-dimensional metal in the Fermi liquid side but as a stack of decoupled two-dimensional layers in the Mott insulator. We show that the dimensional decoupling happens at the Mott quantum critical point itself. We derive the temperature dependence of the interlayer electric conductivity in various crossover regimes near such a continuous Mott transition, and discuss experimental implications.

### 9:24AM X22.00008 Doping dependence of ordered phases in the Hubbard-Holstein model

, CHRISTIAN MENDEL, SLAC National Accelerator Laboratory and Stanford University, ELIZABETH NOWADNICK, Cornell University, YVONNE KUNG, BRIAN MORITZ, SLAC National Accelerator Laboratory and Stanford University, STEVEN JOHNSTON, University of Tennessee, THOMAS DEVEREAUX, SLAC National Accelerator Laboratory and Stanford University — Complex phase diagrams of strongly correlated materials are often accessed by the addition or removal of carriers, for example the emergence of high-temperature superconductivity from a charge transfer insulating state in the cuprates, and the metal-insulator transition in the nickelates. In many cases, these doping-dependent transitions are closely linked to the competition between multiple phases of similar energy scales, e.g., charge-stripe and superconducting states in the cuprates. The Hubbard-Holstein model, which includes electron-electron and electron-phonon interactions, provides a framework to study competing phases. In this talk I will present determinant quantum Monte Carlo (DQMC) simulations of the Hubbard-Holstein model and use spin and charge susceptibilities and single-particle spectral functions to elucidate the doping evolution of the competition between spin and charge order.

### 9:36AM X22.00009 An electric field-driven MIT in strongly-correlated thin-film superlattices: an inhomogeneous dynamical mean-field theory study<sup>1</sup>

, PETAR BAKALOV, JEAN-PIERRE LOCQUET, Department of Solid-state physics, KU Leuven — Using an inhomogeneous dynamical mean-field theory (IDMFT) approach to the single-band Hubbard model we investigate the properties of thin-film superlattices made up of alternating strongly ( $U_1$ ) and weakly ( $U_2 < U_1$ ) correlated regions. In particular, we study the influence of temperature, doping, interaction strengths ( $U_1, U_2$ ), superlattice parameters ( $L_1, L_2$ ) and transverse electric field on the correlation driven Mott-Hubbard metal-to-insulator transition. We find that when the periodicity of the superlattice is such that the strongly correlated regions are below a certain thickness, the MIT is suppressed due to proximity effects.

<sup>1</sup>This work was partially funded by the Flemish Fund for Scientific Research (FWO - Vlaanderen) under FWO grant G.0520.10 and by the SITOGA FP7 project. Most of the calculations were performed on KU Leuven's ThinKing HPC cluster.

### 9:48AM X22.00010 Filament Formation and Electric-field-driven Resistive Switching in ordered Mott insulator

, JIAJUN LI, State Univ of NY - Buffalo, CAMILLE ARON, Princeton University, GABRIEL KOTLIAR, Rutgers University, JONG HAN, State Univ of NY - Buffalo — Formation of conductive filaments is widely observed in resistive switching experiments of strongly correlated materials. Although several theoretical scenarios have been suggested, the underlying mechanism is still far from completely understood within microscopic models. In this work, we study the spatial inhomogeneity during electric-field-driven AFI-to-PM transition in a dissipative Hubbard model<sup>1, 2</sup>. We focus on the non-equilibrium steady state, by means of space-dependent Hartree-Fock approximation. It is shown that external field induces a first order insulator-to-metal transition (IMT) even when equilibrium transition is continuous. Disorder turns out to be crucial for formation of filaments. When impurities are placed in lattice, Joule heating assists to create robust conductive paths. Insulator-to-metal transition is then stimulated by conductive paths, with critical field significantly reduced.

[1] J. E. Han and J. Li, Phys. Rev. B **88**, 075113 (2013)

[2] J. Li, C. Aron, G. Kotliar, J. E. Han, Phys. Rev. Lett. **114**, 226403 (2015)

### 10:00AM X22.00011 A Functional Renormalization Group Study of Hubbard Models with Correlated Hopping interactions.

, NAHOM YIRGA, Boston University, ARIANNA MONTORSI, Politecnico di Torino, DAVID CAMPBELL, Boston University — Hubbard Models with correlated hopping interactions have recently been derived from the Floquet Hamiltonian for driven Hubbard models [1]. We consider these models generalized to include an extended Hubbard interaction ( $V$ ) and both with and without particle-hole symmetry. Using the Functional Renormalization Group method, we derive the phase diagram of this class of models in one and two dimensions. In one dimension we reproduce a spin transition to a bond-ordered phase previously seen in DMRG studies [2]. We extend these results to two dimensions. [1] M. Di Liberto, C. E. Creffield, G. I. Japaridze, C. Morais Smith, Phys. Rev. A **89**, 013624 (2014) [2] A.A. Aligia et al., Phys. Rev. Lett. **99**, 206401 (2007)

### 10:12AM X22.00012 Quantum Monte Carlo study of bilayer ionic Hubbard model<sup>1</sup>

, MI JIANG, Institute for Theoretical Physics, ETH Zurich, Switzerland and Swiss National Supercomputing Center, ETH Zurich, 6900 Lugano, Switzerland — The interaction-driven insulator-to-metal transition has been reported in the ionic Hubbard model (IHM) for intermediate interaction  $U$ , which poses fundamental interest in the correlated electronic systems. Here we use determinant quantum Monte Carlo to study the interplay of interlayer hybridization  $V$  and two types of intralayer staggered potentials: one with the same (in-phase) and the other with a  $\pi$ -phase shift (anti-phase) potential in two layers termed as “bilayer ionic Hubbard model”. We demonstrate that the interaction-driven Insulator-Metal transition extends to bilayer IHM with finite  $V$  for both types of staggered potentials. Besides, the system with in-phase potential is prone to metallic phase with turning on interlayer hybridization while that with anti-phase potential tends to insulators with stronger charge density order.

<sup>1</sup>The author thanks CSCS, Lugano, Switzerland for computing facilities.

### 10:24AM X22.00013 Percolative Metal-Insulator transition in the doped Hubbard-Holstein model with the Gutzwiller Approach

, JAMSHID MORADI KURDESTANY, SASHI SATPATHY, Department of Physics and Astronomy, University of Missouri, Columbia, MO 65211-7010, USA. — Motivated by the recent progress in understanding of Mott insulators away from half filling, observed in many perovskite oxides, we study the metal-insulator transition in the Hubbard-Holstein model, which contains both the Coulomb and the electron-lattice (Jahn Teller) interactions by using the Gutzwiller variational method. We find that strong electron-lattice interaction leads to phase separation, which however can be frustrated due to the long-range Coulomb interaction, resulting in a mixed phase consisting of puddles of metallic phases embedded in an insulating matrix. When the dopant concentration exceeds a threshold value  $x_c$ , the metallic part forms a percolating network leading to metallic conduction. Depending on the strength of the electron-lattice interaction,  $x_c$  can be of the order of 0.05 - 0.20 or so, which is the typical value observed in the perovskites.

### 10:36AM X22.00014 Doping evolution of low-energy quasiparticles in the Hubbard model

, BRIAN MORITZ, YAO WANG, CHUNJING JIA, YU HE, SLAC National Accelerator Laboratory and Stanford University, KRZYSZTOF WOHLFELD, University of Warsaw, CHENG-CHIEN CHEN, Argonne National Laboratory, THOMAS P. DEVEREAUX, SLAC National Accelerator Laboratory and Stanford University — We investigate the single-particle spectra of the two-dimensional, single-band Hubbard model using cluster perturbation theory (CPT), paying considerable attention to low doping with a supercluster construction. At half-filling we find two distinct features: a spin polaron band due to strong coupling of a hole to magnons; and a second feature due to strongly renormalized, but effectively free, next-nearest neighbor hopping from additional delocalization pathways. With light hole-doping a third feature forms which disperses across the Fermi level, rapidly stealing spectral weight from the spin polaron. The doping evolution of this third feature is of particular importance as it constitutes the lowest energy degrees of freedom in the model. The three spectral features appear distinct, up to a relatively modest doping (12.5%) where the spectral weight effectively has been exhausted in the spin polaron. We comment on the similarities, differences, and implications for the spectrum in doped cuprates and on competing interpretations of the spectral properties in the Hubbard model.

# Friday, March 18, 2016 8:00AM - 11:00AM –

Session X23 DMP GERA FIAP: Thermoelectrics Theory II 322 - Heiner Linke, Lund University

**8:00AM X23.00001 Thermal and Electronic Transport in Inorganic and Organic Thermoelectric Materials**, ZHITING TIAN, Virginia Tech — In this talk, we will first talk about first-principles calculations of phonon and electron transport in inorganic thermoelectric materials. We will start with rocksalt PbTe and PbSe, and move on to wurtzite ZnO. We will emphasize the strategies to reduce the lattice thermal conductivity. Then we apply first-principles calculations to organic thermoelectric materials. The thermoelectric properties of doped polypyrrole (PPy) will be discussed. In addition, we will cover the chain confinement effects observed in amorphous polymer thin films using molecular dynamics simulations, which highlights the fundamental difference in heat conduction between crystalline polymers and amorphous polymers

**8:36AM X23.00002 Electron-phonon coupling and thermal transport in thermoelectric compound  $\text{Mo}_3\text{Sb}_{7-x}\text{Te}_x$** , DIPANSHU BANSAL, CHEN LI, Oak Ridge National Lab, AYMAN SAID, Argonne National Lab, DOUGLAS ABERNATHY, JIAQIANG YAN, OLIVIER DELAIRE, Oak Ridge National Lab — Complex interactions between solid-state excitations, such as phonon-phonon, phonon-electron, and phonon-magnon couplings are often responsible for unusual material properties. In this presentation, we report on our investigations of phonon propagation and thermal transport in thermoelectric  $\text{Mo}_3\text{Sb}_{7-x}\text{Te}_x$ . We have performed extensive inelastic neutron and x-ray scattering measurements of phonons in  $\text{Mo}_3\text{Sb}_{7-x}\text{Te}_x$ , mapping the phonon dispersions and density of states, as function of temperature and composition. Our first-principles density functional theory simulations, coupled with experimental measurements, reveal the importance of electron-phonon coupling, which dominates the scattering rates over alloy disorder scattering. Doping with Te shifts the Fermi surface near the top of the valence band, suppressing screening and causing phonons to stiffen markedly. Our measurements of acoustic dispersions and linewidths, coupled with DFT simulations and models of phonon scattering enable us to quantify the impact of the electron-phonon coupling on the thermal conductivity.

**8:48AM X23.00003 Vibrational Dynamics of Filled Skutterudites**, SUSMITA BASAK, CHRISTIAN CARBOGNO, MATTHIAS SCHEFFLER, Fritz Haber Institute of the Max Planck Society — Skutterudites are promising candidates for thermoelectric applications, since their cage like structure can be filled with guest atoms to tune the electronic and vibrational properties and so to optimize the thermoelectric transport coefficients. Various conflicting phenomenological models (e.g., incoherent rattling, coherent coupling [1]) have been proposed to explain the interaction between guest and host, but the exact mechanisms are still topic of debate. To clarify this question, we determine the temperature dependence of the geometric, electronic, and vibrational properties for a set of skutterudites ( $\text{CoSb}_3$ ,  $\text{CoAs}_3$ ) and guests (Ga, In, Sn, etc.) using density-functional theory in the quasi-harmonic approximation. We find different coupling mechanisms to be active depending on the guest, which leads to drastically different dynamics ranging from localized to coherent phonon modes. These modes, which are robust against doping and defy the common assumption that the guest's mass primarily determines the coupling, also largely influence the structural and electronic properties. Finally, we discuss the implications of our findings for the control and optimization of the thermoelectric efficiency. [1] M. M. Koza *et al.*, Nat. Mat. 7, 805, (2008).

**9:00AM X23.00004 Low-energy phonon dispersion in  $\text{LaFe}_4\text{Sb}_{12}$** , ANDREAS LEITHE-JASPER, Max Planck Institute for Chemical Physics of Solids, Dresden, Germany, MARTIN BOEHM, HANNU MUTKA, MICHAEL M. KOZA, Institut Laue-Langevin, Grenoble, France — We studied the vibrational dynamics of a single crystal of  $\text{LaFe}_4\text{Sb}_{12}$  by three-axis inelastic neutron spectroscopy. The dispersion of phonons with wave vectors  $q$  along  $[xx0]$  and  $[xxx]$  directions in the energy range of eigenmodes with high amplitudes of lanthanum vibrations, i.e., at  $\hbar\omega < 12\text{ meV}$  is identified. Symmetry-avoided anticrossing dispersion of phonons is established in both monitored directions and distinct eigenstates at high-symmetry points and at the Brillouin-zone center are discriminated. The experimentally derived phonon dispersion and intensities are compared with and backed up by *ab initio* lattice dynamics calculations. results of the computer model match well with the experimental data.

**9:12AM X23.00005 First-principles investigations of phonon anharmonicity and electronic instability in thermoelectric  $\text{SnSe}^1$** , JIAWANG HONG, CHEN W. LI, A. F. MAY, D. BANSAL, S. CHI, T. HONG, G. EHLERS, OLIVIER DELAIRE, Oak Ridge National Laboratory — The promising thermoelectric material SnSe exhibits ultra-low and strongly anisotropic thermal conductivity. By combining first-principles calculations and inelastic neutron scattering measurements, we have investigated the phonon dispersions and phonon scattering mechanisms, and probed the origin of the large anharmonicity in SnSe.<sup>2</sup> We will discuss the connection between the phonon properties and the high-temperature structural phase transition, and how the electronic structure leads to large anharmonic phonon interactions in SnSe. The present results provide a microscopic picture connecting electronic structure and phonon anharmonicity in SnSe, which could help design materials with ultralow thermal conductivity.

<sup>1</sup>Computations were performed using the OLCF at ORNL. Modeling of neutron data was performed in CAMM, measurements were funded by the US DOE, BES, Materials Science and Engineering Division.

<sup>2</sup>C.W. Li\*, J. Hong\*, A.F. May, D. Bansal, S. Chi, T. Hong, G. Ehlers, and O. Delaire, Orbitaly driven giant phonon anharmonicity in SnSe, Nature Physics, (2015)

**9:24AM X23.00006 Phonons Near Lattice Instabilities in Thermoelectric SnSe, SnTe, and PbTe**, OLIVIER DELAIRE, Duke University, Oak Ridge National Laboratory, CHEN LI, JIAWANG HONG, JIE MA, ANDREW MAY, DIPANSHU BANSAL, GEORG EHLERS, SONGXUE CHI, TAO HONG, Oak Ridge National Laboratory — A number of high-performance thermoelectric materials are found in the vicinity of lattice instabilities, including PbTe, SnTe, SnSe, tetrahedrites,  $\text{Cu}_2\text{Se}$ , among others. The large phonon anharmonicity found in such compounds suppresses the lattice thermal conductivity, a key aspect of their thermoelectric efficiency. In this presentation, we will discuss results from our recent investigations of phonons in these materials using inelastic neutron scattering and first-principles simulations, focusing on anharmonic effects near lattice instabilities. Commonalities will be highlighted, including connections between strong anharmonicity and the electronic structure and bonding.

**9:36AM X23.00007 Pressure intrinsically induced thermoelectric enhancement in the SnSe crystal**, YONGSHENG ZHANG, Institute of Solid State Physics, Chinese Academy of Sciences, SHIQIANG HAO, Department of Materials Science and Engineering, Northwestern University, LI-DONG ZHAO, Beihang University, CHRISTOPHER WOLVERTON, Northwestern University, ZHI ZENG, Institute of Solid State Physics, Chinese Academy of Sciences — SnSe is an excellent thermoelectric material due to its high  $ZT$  value ( $\sim 2.6$  along the  $b$  direction) at high temperature  $\sim 923\text{ K}$ . However, in the temperature range of  $300\text{--}773\text{ K}$ , the  $ZT$  values are just  $0.1\text{--}0.9$ . To make this material more efficient, its thermoelectric properties should be large in the entire temperature range. Here, we use DFT calculations to show how pressure intrinsically enhances the thermoelectric properties below  $700\text{ K}$  along the three directions ( $a$ ,  $b$  and  $c$ ) of the crystal (the low- $T$  SnSe- $Pnma$  phase) due to a significant boost in electrical transport. The estimated  $ZT$  values of  $p$ -type along the  $b$  and  $c$  directions can reach as high as  $3.3$  and  $2.1$  at  $6\text{ GPa}$  and  $700\text{ K}$ , respectively. At  $6\text{ GPa}$ , the  $a$  direction shows  $n$ -type properties and its  $ZT$  value is  $1.9$  at  $600\text{ K}$ . It is significant that high-performance both  $n$ -type and  $p$ -type conductors could be available in SnSe just through applying pressure. Our work on SnSe under pressure sheds light on a new mechanism for screening high efficiency thermoelectric materials.

**9:48AM X23.00008 Broadband Phonon Scattering in PbTe-based Materials Driven Near the Peierls Phase Transition by Strain or Alloying<sup>1</sup>**, IVANA SAVIC, RONAN MURPHY, EAMONN MURRAY, STEPHEN FAHY, Tyndall National Institute, Cork, Ireland — Efficient thermoelectric energy conversion is highly desirable as 60% of the consumed energy is wasted as heat. Low lattice thermal conductivity is one of the key factors leading to high thermoelectric efficiency of a material [1]. However, the major obstacle in the design of such materials is the difficulty in efficiently scattering phonons across the frequency spectrum [2]. Using first principles calculations, we predict that driving PbTe materials close to a Peierls-like phase transition could be a powerful strategy to solve this problem. We illustrate this concept by applying tensile [001] strain to PbTe and its alloys with another rock-salt IV-VI material, PbSe; and by alloying PbTe with a IV-VI Peierls-distorted material, GeTe. This induces extremely soft optical modes, which increase acoustic-optical phonon coupling and decrease phonon lifetimes at all frequencies. We show that PbTe, Pb(Se,Te) and (Pb,Ge)Te alloys driven near the phase transition in the described manner could have the lattice thermal conductivity considerably lower than that of PbTe. The proposed concept may open new opportunities for the development of more efficient thermoelectric materials. [1] G. J. Snyder and E. S. Toberer, *Nature Mater.* 7, 105 (2008). [2] K. Biswas et al. *Nature* 489, 414 (2012).

<sup>1</sup>This work was supported by Science Foundation Ireland and the Marie-Curie Action COFUND under Starting Investigator Research Grant 11/SIRG/E2113.

**10:00AM X23.00009 Understanding of phonon anharmonicity in thermoelectric clathrates**, KATSUMI TANIGAKI, JIAZHEN WU, HIDEKAZU SHIMOTANI, KHUONG HUYNH, KAZUTO AKAGI, Tohoku University, AIMR COLLABORATION, DEPARTMENT OF PHYSICS, GRADUATE SCHOOL OF SCIENCE COLLABORATION — Anharmonicity in phonons, apart from the conventional Einstein- or Debye- mode harmonic phonons, is frequently observed for amorphous or glass-like materials. A frontier topic relating to anharmonic phonons revolves around the fact that they are also observed in a single crystal with a void of cage structure. Although the origin of the phonon anharmonicity has been the center of scientific debate for many years, a clear understanding has not yet been achieved. In the present study, we show that the anharmonic oscillations in thermoelectric clathrates can successfully be rationalized in terms of a single unified exponential line for a variety of clathrates by employing a new parameter associated with the freedom of space. The intrinsic nature of phonon anharmonicity is described based on the unified picture with a help of first principles calculations. Although the origin of the anharmonicity appearing in disordered materials is complex to understand due to the missing information on the real structure, the present unified picture gives important information applicable to other systems.

**10:12AM X23.00010 First-principles Study of Guest Impurities of Na and Ba on Lattice Thermal Conductivity of Type-I Si Clathrate**, YI XIA, University of California, Los Angeles, FEI ZHOU, Lawrence Livermore National Laboratory, VIDVUDS OZOLINS, University of California, Los Angeles — The type-I clathrate compounds, known as good thermoelectric materials, exhibit phonon-glass electron-crystal properties with their open cages filled with guest atoms. We present a first-principles study of the intrinsic impact of these rattlers on the lattice thermal conductivity in type-I Si clathrate compounds. We observe both coherent and incoherent coupling between guest and framework acoustic modes which could be ascribed to the difference in atomic radius, confirming the “avoided crossing” behavior. Our calculated lattice thermal conductivities for  $\text{Si}_{46}$  (37.64 W/(m K)),  $\text{Na}_8\text{Si}_{46}$  (2.75 W/(m K)) and  $\text{Ba}_8\text{Si}_{46}$  (1.37 W/(m K)) are in good agreement with experimental measurements and simulations at room temperature. Significant reductions in both phonon lifetime and group velocity due to guest atoms are responsible for the reduction in lattice thermal conductivity. The energy widths of acoustic modes of both empty and filled silicon clathrates are beyond the resolution limit of 0.2 meV of inelastic x-ray scattering and thus cannot be used to exclude the Umklapp scatterings as main cause of reduction in lattice thermal conductivity. In addition, the Umklapp scatterings of acoustic modes are directly mediated by the guest modes.

**10:24AM X23.00011 First-Principles Study of Guest-Host Bonding in the Type-II Clathrate Compounds  $\text{A}_x\text{Si}_{136}$  ( $\text{A} = \text{Na, K, Rb, Cs}$ ;  $0 \leq x \leq 24$ )**, CHARLES MYLES, DONG XUE, Texas Tech University — The Type II clathrate-based materials are interesting due to their potential thermoelectric applications. Recently, a synthesis and characterization of  $\text{Na}_x\text{Si}_{136}$  for various  $x$  has been reported [1]. Powdered X-Ray diffraction (XRD) data and density functional theory (DFT) studies of  $\text{Na}_x\text{Si}_{136}$  have found a lattice contraction as  $x$  increases for  $0 < x < 8$  and an expansion as  $x$  increases for  $x > 8$ . This is explained by XRD data showing that, as  $x$  increases, the 28-atom Si cages are filled first for  $x < 8$  and the 20-atom Si cages are then filled for  $x > 8$ . We report results of first-principles calculations focused on analyzing the underlying mechanisms relevant to guest-host interactions and to understanding the role of the guest atom to host atom size ratio in this material. We have also studied the compounds  $\text{A}_x\text{Si}_{136}$  ( $\text{A} = \text{Na, K, Rb, Cs}$ ;  $0 \leq x \leq 24$ ). Our LDA calculations for  $\text{K}_x\text{Si}_{136}$  ( $0 < x < 16$ ) predict that this material should exhibit a non-monotonic structural response similar to that in  $\text{Na}_x\text{Si}_{136}$ ; the lattice should contract and then expand as  $x$  increases. We find that the heavier guests (Rb, Cs) vibrate nearer to the center of the  $\text{Si}_{28}$  cages than do Na and K. Our results also show that Na and K are both strongly coupled to the Si framework in  $\text{A}_x\text{Si}_{136}$  ( $\text{A} = \text{Na, K}$ ;  $x = 4, 8$ ). [1] S. Stefanoski, C.D. Malliakas, M.G. Kanatzidis, G.S. Nolas, *Inorg. Chem.* 51, 8686 (2012).

**10:36AM X23.00012 Thermoelectric property of a new silicon crystal**, KISUNG CHAE, SEON-MYEONG CHOI, Korea Inst for Advanced Study, DUCK YOUNG KIM, Carnegie Institute of Washington, YOUNG-WOO SON, Korea Inst for Advanced Study — We present ab initio calculations on thermoelectric properties of a recently synthesised allotrope of silicon crystal [1]. A new silicon crystal with 24 Si atoms per unit cell has open channels along the specific crystallographic direction and shows a quasidirect energy gap of 1.3 eV. Using various first-principles calculation techniques for electrical and thermal conductivity as well as Seebeck coefficient, we find large suppression of thermal conductivity and relatively large Seebeck coefficient in the new silicon crystal, thus demonstrating a competitive thermoelectric figure of merit. [1] D. Y. Kim et al, *Nat. Mat.* 14, 169 (2015).

**10:48AM X23.00013 First Principles Study of the Properties of the Type II Clathrate Alloy  $\text{Si}_{136-x}\text{Ge}_x$  ( $x = 8, 32, 96$ )**, DONG XUE, CHARLES MYLES, Texas Tech University — The Type-II clathrate materials based on Si, Ge, and Sn have “open-framework” lattices consisting of large “cages” of atoms covalently bonded together. Due primarily to their potential thermoelectric applications, there has been considerable research on these materials with various guest atoms in the cages and with various substitutional atoms on the lattice framework. Also of interest are the pure Type II clathrates  $\text{M}_{136}$  ( $\text{M} = \text{Si, Ge, Sn}$ ) with neither framework substitution nor guest atoms in the cages. A fundamental understanding of the intrinsic properties of these “guest-free” clathrates is therefore also needed. Mixtures or “alloys” of two different Type II clathrate materials are also potentially interesting. For example, Moriguchi *et al.* [1] have reported the successful synthesis of Type II clathrates with mixtures of Si and Ge on the framework lattice. Motivated by these experiments, we have carried out a computational and theoretical study the properties of the Type II clathrate “alloy”  $\text{Si}_{136-x}\text{Ge}_x$ . We report the results of DFT-based first-principles calculations of the structural, electronic, vibrational, and thermal properties of  $\text{Si}_{136-x}\text{Ge}_x$  for  $x = 8, 32, 96$ . Our calculations have assumed that the ideal lattice symmetry is unaffected by the mixing of Si and Ge. Among other results, we predict that  $\text{Si}_{136-x}\text{Ge}_x$  should have a direct band gap ranging from 1.2 to 2.0 eV. [1]. K. Moriguchi, S. Munetoh, A. Shintani, *Phys. Rev. B* 62, 7138 (2000).

**Friday, March 18, 2016 8:00AM - 10:36AM –**

Session X24 DCOMP GSCCM DMP: Nicholas Metropolis Award: Materials in Extremes 323 -  
Marivi Fernandez-Serra, Stony Brook University

**8:00AM X24.00001 Metropolis Award Talk** , REMI LEHE, LLBL —

**8:36AM X24.00002 First-principles Equations of State and Shock Hugoniot of First- and Second-Row Plasmas**<sup>1</sup> , KEVIN DRIVER, FRANCOIS SOUBIRAN, SHUAI ZHANG, BURKHARD MILITZER, University of California, Berkeley — A first-principles methodology for studying high energy density physics and warm dense matter is important for the stewardship of plasma science and guiding inertial confinement fusion experiments. In order to address this challenge, we have been developing the capability of path integral Monte Carlo (PIMC) for studying dense plasmas comprised of increasingly heavy elements, including nitrogen, oxygen (J. Chem. Phys., 164507 (2015)), and neon (Phys. Rev. B, 91, 045103 (2015)). In recent work, we have extended PIMC methodology beyond the free-particle node approximation by implementing localized nodal surfaces capable of describing bound plasma states in second-row elements, such as silicon (Phys. Rev. Lett. 115, 176403 (2015)). We combine results from PIMC with results from density functional theory molecular dynamics (DFT-MD) calculations to produce a coherent equation of state that bridges the entire WDM regime. Analysis of pair-correlation functions and the electronic density of states reveals an evolving plasma structure and ionization process that is driven by temperature and pressure. We also compute shock Hugoniot curves for a wide range of initial densities, which generally reveal an increase in compression as the second and first shells are ionized.

<sup>1</sup>This work is funded by the NSF/DOE Partnership in Basic Plasma Science and Engineering (DE-SC0010517).

**8:48AM X24.00003 X-Ray Thomson Scattering Without the Chihara Decomposition** , RUDOLPH MAGYAR, ANDREW BACZEWSKI, LUKE SHULENBURGER, STEPHANIE B. HANSEN, MICHAEL P. DESJARLAIS, Sandia National Laboratories, SANDIA NATIONAL LABORATORIES COLLABORATION — X-Ray Thomson Scattering is an important experimental technique used in dynamic compression experiments to measure the properties of warm dense matter. The fundamental property probed in these experiments is the electronic dynamic structure factor that is typically modeled using an empirical three-term decomposition (Chihara, J. Phys. F, 1987). One of the crucial assumptions of this decomposition is that the system's electrons can be either classified as bound to ions or free. This decomposition may not be accurate for materials in the warm dense regime. We present unambiguous first principles calculations of the dynamic structure factor independent of the Chihara decomposition that can be used to benchmark these assumptions. Results are generated using a finite-temperature real-time time-dependent density functional theory applied for the first time in these conditions. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Security Administration under contract DE-AC04-94AL85000.

**9:00AM X24.00004 Comminution of Ceramic Materials Under High-Shear Dynamic Compaction**<sup>1</sup> , MICHAEL HOMEL, Lawrence Livermore Natl Lab, JASON LOISEAU, ANDREW HIGGINS, Dept of Mechanical Engineering, McGill University, ERIC HERBOLD, Lawrence Livermore Natl Lab, JAMIE HOGAN, Dept of Mechanical Engineering, University of Alberta — The post-failure “granular flow” response of high-strength lightweight ceramics has important implications on the materials' effectiveness for ballistic protection. We study the dynamic compaction and shear flow of ceramic fragments and powders using computational and experimental analysis of a collapsing thick-walled cylinder geometry. Using newly developed tools for mesoscale simulation of brittle materials, we study the effect of fracture, comminution, shear-enhanced dilatation, and frictional contact on the continuum compaction response. Simulations are directly validated through particle Doppler velocimetry measurements at the inner surface of the cylindrical powder bed. We characterize the size distribution and morphologies of the initial and compacted material fragments to both validate the computational model and to elucidate the dominant failure processes.

<sup>1</sup>A portion of this work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC. LLNL-ABS-678862.

**9:12AM X24.00005 Real-time dynamics of high-velocity micro-particle impact** , DAVID VEYSSET, Massachusetts Inst of Tech-MIT, ALEX HSIEH, U.S. Army Research Laboratory, STEVE KOOL, ALEX A. MAZNEV, SHENGCHANG TANG, BRADLEY D. OLSEN, KEITH A. NELSON, Massachusetts Inst of Tech-MIT — High-velocity micro-particle impact is important for many areas of science and technology, from space exploration to the development of novel drug delivery platforms. We present real-time observations of supersonic micro-particle impacts using multi-frame imaging. In an all optical laser-induced projectile impact test, a monolayer of micro-particles is placed on a transparent substrate coated with a laser absorbing polymer layer. Ablation of a laser-irradiated polymer region accelerates the micro-particles into free space with speeds up to 1.0 km/s. The particles are monitored during the impact on the target with an ultrahigh-speed multi-frame camera that can record up to 16 images with time resolution as short as 3 ns. In particular, we investigated the high-velocity impact deformation response of poly(urethane urea) (PUU) elastomers to further the fundamental understanding of the molecular influence on dynamical behaviors of PUUs. We show the dynamic-stiffening response of the PUUs and demonstrate the significance of segmental dynamics in the response. We also present movies capturing individual particle impact and penetration in gels, and discuss the observed dynamics. The results will provide an impetus for modeling high-velocity microscale impact responses and high strain rate deformation in polymers, gels, and other materials.

**9:24AM X24.00006 Sensitivity Characterization of Pressed Energetic Materials using Flyer Plate Mesoscale Simulations.** , NIRMAL RAI, H.S. UDAYKUMAR, Univ of Iowa — Heterogeneous energetic materials like pressed explosives have complicated microstructure and contain various forms of heterogeneities such as pores, micro-cracks, energetic crystals etc. It is widely accepted that the presence of these heterogeneities can affect the sensitivity of these materials under shock load. The interaction of shock load with the microstructural heterogeneities may lead to the formation of local heated regions known as “hot spots”. Chemical reaction may trigger at the hot spot regions depending on the hot spot temperature and the duration over which the temperature can be maintained before phenomenon like heat conduction, rarefaction waves withdraws energy from it. There are different mechanisms which can lead to the formation of hot spots including void collapse. The current work is focused towards the sensitivity characterization of two HMX based pressed energetic materials using flyer plate mesoscale simulations. The aim of the current work is to develop mesoscale numerical framework which can perform simulations by replicating the laboratory based flyer plate experiments. The current numerical framework uses an image processing approach to represent the microstructural heterogeneities incorporated in a massively parallel Eulerian code SCIMITAR3D. The chemical decomposition of HMX is modeled using Henson-Smilowitz reaction mechanism. The sensitivity characterization is aimed towards obtaining James initiation threshold curve and comparing it with the experimental results.

**9:36AM X24.00007 Blow Up Exponents and Deviations from Ideal Taylor Cone Shapes in Ultrathin Liquid Metal Films**, THEODORE G. ALBERTSON<sup>1</sup>, SANDRA TROIAN, California Institute of Technology, 1200 E. California Blvd., MC 128-95, Pasadena, CA — We employ a finite element, moving mesh model to investigate the axisymmetric flow of an ultrathin liquid metal film overlay by a thin vacuum layer confined between two circular disks held at a constant potential difference close to field evaporation values. Within nanoseconds, a small Gaussian protrusion centered about the origin evolves into a sharpened cusp elongated by Maxwell stresses and rounded by capillary stresses. Previous analytic studies<sup>2</sup> and numerical simulations based on marker and cell techniques<sup>3,4</sup> have uncovered a self-similar regime in time where the opposing stresses and kinetic energy exhibit blow up behavior with a characteristic exponent of  $-2/3$ , and cusp shapes that deviate from the ideal Taylor cone angle. Our simulations consistently yield exponents in the range  $-3/4$  to  $-4/5$ , with values that depend sensitively on the choice of blowup time. We also find that deviations from the ideal Taylor cone angle become significant all along the film interface as the Gaussian amplitude increases beyond fractions of a micron.

<sup>1</sup>TGA gratefully acknowledges support from a NASA Science and Technology fellowship.

<sup>2</sup>N. M. Zubarev, **JETP Lett.** 73, 613 (2001)

<sup>3</sup>V. G. Suvorov, **Surf. Interface Anal.** 36, 421 (2004)

<sup>4</sup>V. G. Suvorov and N. M. Zubarev, **J. Phys. D: Appl. Phys.** 37, 289 (2004)

**9:48AM X24.00008 A Study of the Multiferroic State Under High Pressure for Co doped MnWO<sub>4</sub>**, MELISSA GOOCH, NARAYAN POUDEL, BERND LORENZ, K. C. LIANG, Texas Center for Superconductivity at the University of Houston, Y. Q. WANG, Y. Y. SUN, Retired, JINCHEN WANG, FENG YE, JAIME FERNANDEZ-BACA, Quantum Condensed Matter Division, Oak Ridge National Laboratory, CHING-WU CHU, Texas Center for Superconductivity at the University of Houston — Multiferroic materials are well understood to be sensitive to small perturbations induced through chemical substitution, magnetic and electric fields, or external pressure. These sensitivities can result in rich and complex phase diagrams to explore; one such system is Co doped MnWO<sub>4</sub>. To gain further insight into this system, high pressure measurements were conducted up to 18 kbars. Results thus far suggest that, in a Co doping range near 13

**10:00AM X24.00009 High Pressure Seebeck Coefficient Measurements Using Paris-Edinburgh Cell**, JASON BAKER, RAVHI KUMAR, HIPSEC and Department of Physics, University of Nevada, Las Vegas, CHANGYONG PARK, CURTIS KENNEY-BENSON, HPCAT, Geophysical Laboratory, Carnegie Institution of Washington, NENAD VELISAVLJEVIC, Shock and Detonation Physics Group, Los Alamos National Laboratory, HIPSEC AND DEPARTMENT OF PHYSICS, UNIVERSITY OF NEVADA, LAS VEGAS COLLABORATION, HPCAT, GEOPHYSICAL LABORATORY, CARNEGIE INSTITUTION OF WASHINGTON COLLABORATION, SHOCK AND DETONATION PHYSICS GROUP, LOS ALAMOS NATIONAL LABORATORY COLLABORATION — We have developed a new type of sample cell assembly for the Paris-Edinburgh (PE) type large volume press for simultaneous x-ray diffraction, electrical resistance, and thermal measurements at high pressures. We demonstrate the feasibility of performing in situ measurements of the Seebeck coefficient over a broad range of pressure-temperature conditions by observing the well-known solid-solid and solid-melt transitions of bismuth (Bi) up to 3GPa and 450 K. We observed a gradual increase in the Seebeck coefficient which becomes positive during transition to the Bi - II phase. Also, we have performed successful Seebeck coefficient measurements on the thermoelectric material PbTe. This new capability enables us to directly correlate pressure-induced structural phase transitions to electrical and thermal properties.

**10:12AM X24.00010 Mechanical Model for Dynamic Behavior of Concrete Under Impact Loading<sup>1</sup>**, YUANXIANG SUN, State Key Laboratory of Explosion Science and Technology, Beijing Institute of Technology, China — Concrete is a geo-material which is used substantively in the civil building and military safeguard. One coupled model of damage and plasticity to describe the complex behavior of concrete subjected to impact loading is proposed in this research work. The concrete is assumed as homogeneous continuum with pre-existing micro-cracks and micro-voids. Damage to concrete is caused due to micro-crack nucleation, growth and coalescence, and defined as the probability of fracture at a given crack density. It induces a decrease of strength and stiffness of concrete. Compaction of concrete is physically a collapse of the material voids. It produces the plastic strain in the concrete and, at the same time, an increase of the bulk modulus. In terms of crack growth model, micro-cracks are activated, and begin to propagate gradually. When crack density reaches a critical value, concrete takes place the smashing destroy. The model parameters for mortar are determined using plate impact experiment with uni-axial strain state. Comparison with the test results shows that the proposed model can give consistent prediction of the impact behavior of concrete. The proposed model may be used to design and analysis of concrete structures under impact and shock loading.

<sup>1</sup>This work is supported by State Key Laboratory of Explosion science and Technology, Beijing Institute of Technology (YBKT14-02)

**10:24AM X24.00011 Jetting mechanisms of particles under shock wave acceleration: the role of force chains**, KUN XUE, Beijing Institute of Technology — The particle jetting phenomenon is widely observed in many problems associated with blast/shock dispersal of granular materials, although its origin is still unidentified. We carried out discrete element simulations of the shock dispersal of two-dimensional particle rings in order to extract the particle-scale evolution of the shocked rings in terms of the velocity profile and the force-chain networks. Initially the force chains distribute uniformly along the circumference, but after several dozens of microseconds, they disseminate into a handful of blobs which mainly consist of long linear or branched chains align with the radial direction. These blobs are separated by zones featuring relatively sparse force chains which take forms of short chains or small compact polygons. The radial-like force chains in blobs serves as the channels transferring the momentum from the inner layers to outer layers, resulting in fast moving blocks without appreciable velocity differences. By contrast, the shock energy in the zones with short force chains is largely dissipated among the particle collision. Thus particles in these zones lag behind those bound by strong force chains. The resultant heterogeneous velocity profile acts as the precursor of the ensuing particle jetting.

**Friday, March 18, 2016 8:00AM - 11:00AM —**

**Session X25 DCMP: Superconductivity: Pseudogap and Related Phenomena** 324 - Lex Kemper, North Carolina State University

**8:00AM X25.00001 ABSTRACT WITHDRAWN —**

**8:12AM X25.00002 Spin order, charge order, and spin liquid in spin-fermion model of cuprates.**, KYUNGMIN LEE, Cornell University, OINAM NGAMBA MEETEL, American Express, STEVEN WHITE, University of California, Irvine, EUN-AH KIM, Cornell University — Recent experimental observations that intra-unit-cell structures play crucial role in the detection of charge order motivates numerical studies that can include strong correlation effects as well as multi-site until cells. However, this costs precious Hilbert space. In this talk I will present our results using a minimal model for cuprates that can access intra-unit-cell information: multi-band spin-fermion model with spins on the copper sites and holes on oxygen sites. For this we used exact diagonalization as well as density matrix renormalization group. In addition to charge and spin order tendencies we test for evidence of the so-called FL\* state.

**8:24AM X25.00003 Interplay of pair density wave and charge density wave order in the cuprate pseudogap phase**, DANIEL AGTERBERG, ADIL AMIN, University of Wisconsin - Milwaukee — Recent x-ray measurements in the cuprate YBCO suggest that the charge density wave (CDW) order seen at high-field has a different c-axis structure than that seen at zero-field and further suggests that CDW order breaks the c-axis mirror plane symmetry of the  $\text{CuO}_2$  layers. We examine pair density wave order that induces CDW order consistent with these observations.

**8:36AM X25.00004 Hybridization of Higgs modes in a bond-density-wave state in cuprates**, ZACHARY RAINES, VALENTIN STANEV, VICTOR GALITSKI, Univ of Maryland-College Park — Recently, several groups have reported observations of collective modes of the charge order present in underdoped cuprates. Motivated by these experiments, we study theoretically the oscillations of the order parameters, both in the case of pure charge order, and for charge order coexisting with superconductivity. We find in the coexistence regime two Higgs modes arising from hybridization of the amplitude oscillations of the different order parameters, one of which has a minimum frequency that is within the single particle energy gap and which is a non-monotonic function of temperature. Additionally, we explore an unusual low-energy damping channel for the collective modes, which relies on the band reconstruction caused by the coexistence of the two orders.

**8:48AM X25.00005 Thermodynamic properties of underdoped  $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$  cuprates for doping values  $x \in (0.5, 0.9)^1$** , P. SALAS, M. A. SOLIS, M. FORTES, Instituto de Física, UNAM, Mexico — We extend the Boson-Fermion superconductivity model to include layered systems, such as underdoped cuprate superconductors  $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$ , with  $x \in (0.5, 0.9)$  ranging from underdoped to optimally doped. We model cuprates as a boson-fermion quantum gas mixture immersed in a layered structure, generated via a Dirac comb potential applied in one direction while the particles move freely in the other two directions. The optimum parameters of the system, which are the impenetrability of the planes and the paired fermion fraction, are obtained by minimizing the Helmholtz free energy and setting the experimental critical temperature  $T_c$ . Using this optimized scheme, we are able to predict the following thermodynamic properties of cuprates as a function of temperature: the entropy; the Helmholtz free energy; the electronic specific heat and the total specific heat for different doping values. Furthermore, we determine the behavior of the jump height in the electronic specific heat, the normal electronic specific heat coefficient  $\gamma(T_c)$ , the quadratic  $\alpha$  and cubic  $\beta$  terms of the specific heat for low temperatures, the ground state energy and the mass anisotropy as a function of doping. Comparison to experimental values reported is analyzed.

<sup>1</sup>We acknowledge the support from grants UNAM-DGAPA-PAPIIT IN-111613 and CONACYT 221030, Mexico.

**9:00AM X25.00006 The roles of antiferromagnetic and nematic fluctuations in cuprate superconductors: a sign-free quantum Monte-Carlo study**, ZIXIANG LI, HONG YAO, Institute for Advanced Study, Tsinghua University, FA WANG, International Center for Quantum Materials, School of Physics, Peking University, DUNG-HAI LEE, Department of Physics, University of California at Berkeley — Superconductivity is an emergent phenomena in the sense that the energy scale at which Cooper pairs form is generically much lower than the bare energy scale, namely the electron kinetic energy bandwidth. Addressing the mechanism of Cooper pairing amounts to finding out the effective interaction (or the renormalized interaction) that operates at the low energies. Finding such interaction from the bare microscopic Hamiltonian has not been possible for strong correlated superconductors such as the copper-oxide high temperature superconductor. In fact even one is given the effective interaction, determining its implied electronic instabilities without making any approximation has been a formidable task. Here, we perform sign-free quantum Monte-Carlo simulations to study the antiferromagnetic, superconducting, and the charge density wave instabilities which are ubiquitous in both electron and hole doped cuprates. Our result suggests only after including both the nematic and antiferromagnetic fluctuation, are the observed properties associated with these instabilities reproduced by the theory.

**9:12AM X25.00007 Strong-coupling approach to nematicity in the cuprates**, PETER PHILIPP ORTH, University of Minnesota, BHILAHARI JEEVANESAN, JOERG SCHMALIAN, Karlsruhe Institute of Technology (KIT), RAFAEL FERNANDES, University of Minnesota — The underdoped cuprate superconductor  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  is known to exhibit an electronic nematic phase in proximity to antiferromagnetism. While nematicity sets in at large temperatures of  $T \approx 150$  K, static spin density wave order only emerges at much lower temperatures. The magnetic response shows a strong in-plane anisotropy, displaying incommensurate Bragg peaks along one of the crystalline directions and a commensurate peak along the other one. Such an anisotropy persists even in the absence of long-range magnetic order at higher temperatures, marking the onset of nematic order. Here we theoretically investigate this situation using a strong-coupling method that takes into account both the localized Cu spins and the holes doped into the oxygen orbitals. We derive an effective spin Hamiltonian and show that charge fluctuations promote an enhancement of the nematic susceptibility near the antiferromagnetic transition temperature.

**9:24AM X25.00008 Interplay between pair density waves and random field disorders in the pseudogap regime of cuprate superconductors**, CHEUNG CHAN, Institute for Advanced Study, Tsinghua University — To capture various experimental results in the pseudogap regime, we propose a four-component pair density wave (PDW) state in which all components compete with each other. Without random field disorders (RFD), globally the PDW components are phase separated and only one of the component survives locally. If the RFD is included, this state becomes a phase separated state with short range PDW stripes, and induces charge density waves (CDW) and loop current order as secondary composite orders. We call this phase-separated pair nematic (PSPN) state. This state could capture a number of important experimental features in the pseudogap, in particular, the predominantly  $d$ -wave CDW with spatial dependent charge smecticity, the unusual ARPES quasiparticle spectrum, and the time reversal symmetry breaking order in polarized neutron diffraction and polar Kerr rotation. We also discuss how the various temperature scales arisen in the pseudogap can be understood in terms of the interplay with the RFD and fluctuating orders.

**9:36AM X25.00009 Breakup of superconducting order parameter into 2 subbands of Cooper pairs increases temperature range of fluctuations in the pseudogap phase**, FU-CHUN ZHANG, Department of Physics, Zhejiang University, Hangzhou 310027, China, YE-HUA LIU, Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland, ROBERT KONIK, Condensed Matter Physics and Material Science Department, Brookhaven National Laboratory, Upton, NY 11973, THOMAS MAURICE RICE, Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland — The opening of the pseudogap in underdoped cuprates breaks up the Fermi surface, into 4 disconnected arcs centered on the nodal directions. In the superconducting phase, the  $d$ -wave order parameter breaks up into 2 subbands of Cooper pairs along  $(1,1)$  and  $(1,-1)$ , with strong intra-subband and weak inter-subband couplings. This multiple-band superconductivity allows a low-energy Leggett mode to emerge due to phase fluctuations between the subbands. We propose that the overdamped Leggett mode is responsible for the highly unusual wide temperature range of superconducting fluctuations observed in the c-axis infrared conductivity in the pseudogap phase.

**9:48AM X25.00010 Giant phonon anomaly associated with strong superconducting fluctuations in the pseudogap phase of underdoped cuprates**, YE-HUA LIU, Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland, ROBERT KONIK, Condensed Matter Physics and Material Science Department, Brookhaven National Laboratory, Upton, NY 11973, THOMAS MAURICE RICE, Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland, FU-CHUN ZHANG, Department of Physics, Zhejiang University, Hangzhou 310027, China — Phonons with wavevectors connecting Fermi-arc ends are strongly damped in the pseudogap phase as  $T \rightarrow T_c$  from above. Below  $T_c$  the anomaly abruptly switches to a dip in the phonon dispersions at the same wavevectors. Based on our proposed 2-subband model of superconductivity, we analyze the coupling between these phonons and the Leggett mode. We consider the phonon self energy arising from a forward scattering of the phonon accompanied by Cooper-pair transfers between the subbands. The intermediate state of this process involves 2 Leggett modes and a forward scattered phonon. Above  $T_c$ , the Leggett mode is overdamped giving rise to the giant phonon damping, while below  $T_c$ , the Leggett mode develops a finite energy turning the phonon anomaly into a dip in the energy dispersion.

**10:00AM X25.00011 Pairing in the presence of a pseudogap<sup>1</sup>**, DOUGLAS SCALAPINO, Univ of California - Santa Barbara, THOMAS MAIER, ORNL, PETER STAAR, IBM Research (Zurich), VIVEK MISHRA, ORNL — After 30 years, the quest to experimentally identify the mechanism responsible for pairing in the high  $T_c$  superconductors continues. Here we discuss an approach in which angle resolved photoemission (ARPES) data for BSCCO 2212 ( $T_c=89K$ ) is used to extract the single particle spectral weight  $A(k,w)$ . This spectral weight is then used to calculate the BCS kernel and estimate the RPA spin-fluctuation d-wave pairing strength. Previously  $A(k,w)$  results at  $T=140K$ , extrapolated to lower temperatures, found that the BSCCO pseudo gap suppressed the logarithmic singularity of the BCS kernel and the spin-fluctuation interaction was too weak to produce superconductivity [V.Mishra et al., Nat. Phys. 10, 357]. Here using results for  $A(k,w)$  at  $T=40K$  for this same system, we find that while the BCS kernel is suppressed, there is a significant increase in the d-wave pairing strength for the spin-fluctuation interaction when the temperature drops from  $T=140K$  and  $40K$ . These results are shown to be consistent with DCA calculations for a 2D Hubbard model of a BSCCO like system which has a pseudo gap. We conclude that in spite of the suppression of the usual BCS logarithmic instability by the pseudo gap, the increase in strength of the spin-fluctuation interaction is sufficient to lead to superconductivity.

<sup>1</sup> Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

**10:12AM X25.00012 Effect of Extended Saddle Point Singularities in Cuprates and Evidences<sup>1</sup>**, GUANG-LIN ZHAO, Physics Department, Southern University and A & M College — First-principles calculations and angle-resolved photoemission spectroscopy measurements showed extended saddle point singularities in the electron structures of some cuprates such as  $YBa_2Cu_3O_7$  (YBCO). The extended saddle point singularities in the electronic structures of the materials can lead to anomalous physical properties. In this work, a new methodology is implemented by integrating first-principles calculations of electronic structures of the materials into the theory of many-body physics for superconductivity. The aim is to seek a unified methodology to calculate the electronic and superconducting properties of the materials. It is demonstrated from first-principles that the extended saddle point singularities in the materials such as YBCO strongly correlate to the anomalous isotope effect in the superconductors.

<sup>1</sup>The work was funded in part by NSF LASIGMA Project (Award EPS-1003897, NSF92010-15-RII-SUBR) and by ARO (Award W911NF-15-1-0483).

**10:24AM X25.00013 Theory of Berry Phases in the Cuprate Pseudogap Phase**, GEREMIA MASSARELLI, TAMAR PEREG-BARNEA, McGill University — The geometric Berry phase is part of the phase accumulated by a quantum system undergoing adiabatic evolution around a closed loop in parameter space <sup>1</sup>. Recently, data from quantum oscillations experiments, in which Berry's phase is accessible via its contribution to the phase offset, were used to determine Berry's phase in certain electron- and hole-doped cuprate superconductors in high-magnetic-field regimes <sup>2</sup>. The data reveal a trivial Berry phase of 0 in the hole-doped materials examined, while a phase of  $\sim 1.4\pi$  was found in the electron-doped material. These findings set new, significant constraints on the possible descriptions of the pseudogap phase of the cuprates. This is used as a test of validity for some proposed models of cuprate superconductors. Berry's phase is computed within the framework of these models in high-field regimes and compared to the experimental findings.

<sup>1</sup>Berry, M. V. Quantal Phase Factors Accompanying Adiabatic Changes. *Proceedings of the Royal Society of London. A. Mathematical and Physical Sciences* **392**, 45-57 (1984).

<sup>2</sup>Doiron-Leyraud, N., et al. Berry Phase in Cuprate Superconductors. *arXiv preprint arXiv:1407.1388* (2014).

**10:36AM X25.00014 Interplay between uni-directional and bi-directional charge orders in underdoped cuprates**, YUXUAN WANG, University of Illinois at Urbana-Champaign, ANDREY CHUBUKOV, University of Minnesota — We analyze the interplay between charge-density-wave (CDW) orders with axial momenta  $(Q, 0)$  and  $(0, Q)$  ( $\Delta_x$  and  $\Delta_y$  respectively), detected in the underdoped cuprates. The CDW order in real space can be uni-directional (either  $\Delta_x$  or  $\Delta_y$  is non-zero) or bi-directional (both  $\Delta_x$  and  $\Delta_y$  are non-zero). To understand which of the two orders develop, we adopt the magnetic scenario, in which the CDW order appears due to spin-fluctuation exchange. We derive the Ginzburg-Landau action to the sixth order in  $\Delta_x$  and  $\Delta_y$  and argue that the CDW order is bi-directional at the onset but changes to uni-directional inside the CDW phase. This implies that, at a given temperature, CDW order is uni-directional at smaller dopings, but becomes bi-directional at larger dopings. These results are consistent with recent x-ray data on YBCO, which detected tendency towards bi-directional order at larger dopings. We also discuss for completeness the effect of yet unobserved intertwined pair-density-wave (PDW) order, which may appear along with CDW.

**10:48AM X25.00015 Dipolon Theory of High Temperature Superconductors— Prediction of the Existence of New Very Low Energy Excitations to be Observed in Photoemission Experiments**, RAM R SHARMA, University of Illinois at Chicago — The dipolon theory [1,2] first discovered [3,4] two high energy kinks in electron energy [5]. It [1-2] has also predicted two superconducting states, symmetric ("s") and anti-symmetric ("as"). Here we report the prediction of very low energy excitations due to transition from "as" state to "s" state ("ass") (or vice versa) which creates (annihilates) the quantum ("asson") of energy  $\hbar\omega_a(\vec{q}_a) = E^s(\vec{k}^i) - E^{as}(\vec{k}^f)$ ; "a" is for "asson" and  $E^s(\vec{k}^i)$  and  $E^{as}(\vec{k}^f)$  are electron energies in "s" and "as" states, respectively ( $E^i(\vec{k}) = \bar{E}_r^i(\vec{k})$  [1-4]). Our theory [1-4] finds in BISCCO at M point on Fermi level at  $T=13$  K asson energy about  $14 \pm 8$  meV. We predict that these assons create a new kink in electron energy at this energy. Also, a single pair transitions are possible which involve two assons. (1) R. R. Sharma, Phys. Rev. B **63**, 054506 (2001). (2) R. R. Sharma, Physica C **439**, 47 (2006). (3) R. R. Sharma, Physica C **468**, 190 (2008). (4) R. R. Sharma, "Dipolon Theory of Kink ...", in "Superconducting ...", Ed. K. N. Courtlandt, P. 81-100, Nova Sc, Pub., Inc., New York, 2009. (5) R. R. Sharma, <http://meetings.aps.org/lnk/BAPS.2015.MAR.D9.15>.

**Friday, March 18, 2016 8:00AM - 11:00AM —**

Session X27 DCMP: New Methods for Strongly Correlated Systems 326 - Gia-Wei Chern, University of Virginia

**8:00AM X27.00001 Non-equilibrium DMFT - Polaritonics** , ANDREAS LUBATSCH, Georg-Simon-Ohm Technical University of Applied Sciences, REGINE FRANK, Serin Physics Laboratory, E273 Department of Physics and Astronomy Rutgers University 136 Frelinghuysen Road Piscataway, NJ 08854-8019, USA — Non-equilibrium physics recently really becomes important with the progress of ultrafast laser sciences. However in our understanding there is still a gap between equilibrium physics and the non-equilibrium, even though numerical methods have been advanced in recent years. We compare in this talk novel results at hand with equilibrium physics. The comparison will show that especially theoretical efforts are needed to explain many - so far - unresolved problems and to predict novel research on the basis of ab initio computing. We specifically discuss several non-equilibrium extensions of DMFT, numerical methods as well as semi-analytical solvers.

**8:12AM X27.00002 Strange metals from quantum geometric fluctuations of interfaces** , JIAN-HUANG SHE, Cornell University, ALAN BISHOP, ALEXANDER BALATSKY, Los Alamos National Lab — The emerging picture of strongly correlated electron systems is that they possess a multiplicity of nearly degenerate ground states. A general theoretical framework for such systems is lacking. Here we explore a new approach based on the observation that different ground states can coexist and fluctuate in real space. Specifying to systems near the Mott metal-insulator transition, we propose a real space picture as itinerant electrons functioning in the fluctuating geometries bounded by interfaces between metallic and insulating regions. The interface fluctuations give rise to non-Fermi liquid behavior for the itinerant electrons, and furthermore mediate Cooper pairing.

**8:24AM X27.00003 A real-time impurity solver for DMFT** , HYUNGWON KIM, Rutgers University, CAMILLE ARON, Laboratoire de Physique Théorique, École Normale Supérieure, CNRS, Paris, France, JONG E. HAN, State University of New York at Buffalo, GABRIEL KOTLIAR, Rutgers University — Dynamical mean-field theory (DMFT) offers a non-perturbative approach to problems with strongly correlated electrons. The method heavily relies on the ability to numerically solve an auxiliary Anderson-type impurity problem. While powerful Matsubara-frequency solvers have been developed over the past two decades to tackle equilibrium situations, the status of real-time impurity solvers that could compete with Matsubara-frequency solvers and be readily generalizable to non-equilibrium situations is still premature. We present a real-time solver which is based on a quantum Master equation description of the dissipative dynamics of the impurity and its exact diagonalization. As a benchmark, we illustrate the strengths of our solver in the context of the equilibrium Mott-insulator transition of the one-band Hubbard model and compare it with iterative perturbation theory (IPT) method. Finally, we discuss its direct application to a nonequilibrium situation.

**8:36AM X27.00004 Constrained Path Monte Carlo with Matrix Product State trial wavefunctions** , CHIA-MIN CHUNG, University California Irvine, MATTHEW FISHMAN, California Institute of Technology, STEVEN WHITE, University California Irvine, SHIWEI ZHANG, College of William and Mary — Constrained path Monte Carlo (CPMC) is a powerful method for simulating strongly correlated systems. By constraining the path with a trial wavefunction, CPMC circumvents the minus sign problem, but at the cost of introducing a bias. The Density Matrix Renormalization Group (DMRG) is an alternative simulation technique, which is immune to the minus sign problem, but which has an analogous "dimensionality problem" for two and three dimensions. Here we present a combination of these techniques, where we use a DMRG matrix product state as a trial wavefunction for CPMC. We demonstrate our method in two-dimensional Hubbard model, and show the comparison to DMRG alone and to CPMC with single-determinant trial functions.

**8:48AM X27.00005 Efficient implementation of the parquet equations - role of the reducible vertex function and its kernel approximation<sup>1</sup>** , GANG LI, NILS WENTZELL, PETRA PUDLEINER, PATRIK THUNSTRÖM, KARSTEN HELD, Vienna University of Technology — We present an efficient implementation of the parquet formalism which respects the asymptotic structure of the vertex functions at both single- and two-particle levels in momentum- and frequency-space. We identify the two-particle reducible vertex as the core function which is essential for the construction of the other vertex functions. This observation stimulates us to consider a two-level parameter-reduction for this function to simplify the solution of the parquet equations. The resulting functions, which depend on fewer arguments, are coined "kernel functions". With the use of the "kernel functions", the open boundary of various vertex functions in the Matsubara-frequency space can be faithfully satisfied. We justify our implementation by accurately reproducing the dynamical mean-field theory results from momentum-independent parquet calculations. The high-frequency asymptotics of the single-particle self-energy and the two-particle vertex are correctly reproduced, which turns out to be essential for the self-consistent determination of the parquet solutions. The current implementation is also feasible for the dynamical vertex approximation.

<sup>1</sup>EU's Seventh Framework Programme (FP/2007-2013)/ERC n. 306447, NSF grant PHY-1066293

**9:00AM X27.00006 Exact Real-time Dynamics with non-equilibrium QMC** , QIAOYUAN DONG, ANDREY ANTIPOV, EMANUEL GULL, University of Michigan — We present an overview of recent methodological progress for non-equilibrium hybridization expansion diagrammatic Monte Carlo impurity solver and we examine the real-time dynamics of a correlated quantum dot in the mixed valence regime. We perform numerically exact calculations of currents and magnetic susceptibilities after a quantum quench from equilibrium by rapidly applying a bias voltage in a wide range of initial temperatures. We observe Kondo signatures both in transient regimes and in the steady state.

**9:12AM X27.00007 Dynamical simulations of strongly correlated electron materials** , JOEL KRESS, KIPTON BARROS, CRISTIAN BATISTA, Los Alamos National Laboratory, GIA-WEI CHERN, University of Virginia, GABRIEL KOTLIAR, Rutgers University — We present a formulation of quantum molecular dynamics that includes electron correlation effects via the Gutzwiller method. Our new scheme enables the study of the dynamical behavior of atoms and molecules with strong electron interactions. The Gutzwiller approach goes beyond the conventional mean-field treatment of the intra-atomic electron repulsion and captures crucial correlation effects such as band narrowing and electron localization. We use Gutzwiller quantum molecular dynamics to investigate the Mott transition in the liquid phase of a single-band metal and uncover intriguing structural and transport properties of the atoms.

**9:24AM X27.00008 Ab Initio Dynamical Correlations from Auxiliary-field quantum Monte Carlo: applications in the Hubbard model<sup>1</sup>** , ETTORE VITALI, HAO SHI, MINGPU QIN, SHIWEI ZHANG, William and Mary College — The possibility of calculating dynamical correlation functions from first principles provides a unique opportunity to explore the manifold of the excited states of a quantum many-body system. Such calculations allow us to predict interesting physical properties like spectral functions, excitation spectra and charge and spin gaps, which are more difficult to access from usual equilibrium calculations. We address the ab-initio calculation of dynamical Green functions and two-body correlation functions in the Auxiliary-field Quantum Monte Carlo method, using the two-dimensional Hubbard model as an example. When the sign problem is not present, an unbiased estimation of imaginary time correlation functions is obtained. We discuss in detail the complexity and the stability of the calculations. Moreover, we propose a new approach which is expected to be very useful when dealing with dilute systems, e.g. for cold gases, allowing calculations with a very favorable complexity in the system size.

<sup>1</sup>Supported by NSF, DOE SciDAC, and Simons Foundation

**9:36AM X27.00009 Bond Order Correlations in the 2D Hubbard Model<sup>1</sup>** , CONRAD MOORE, SAMEER ABU ASAL, SHUXIANG YANG, JUANA MORENO, MARK JARRELL, Louisiana State Univ - Baton Rouge — We use the dynamical cluster approximation to study the bond correlations in the Hubbard model with next nearest neighbor (nnn) hopping to explore the region of the phase diagram where the Fermi liquid phase is separated from the pseudogap phase by the Lifshitz line at zero temperature. We implement the Hirsch-Fye cluster solver that has the advantage of providing direct access to the computation of the bond operators via the decoupling field. In the pseudogap phase, the parallel bond order susceptibility is shown to persist at zero temperature while it vanishes for the Fermi liquid phase which allows the shape of the Lifshitz line to be mapped as a function of filling and nnn hopping. Our cluster solver implements NVIDIA's CUDA language to accelerate the linear algebra of the Quantum Monte Carlo to help alleviate the sign problem by allowing for more Monte Carlo updates to be performed in a reasonable amount of computation time.

<sup>1</sup>Work supported by the NSF EPSCoR Cooperative Agreement No. EPS-1003897 with additional support from the Louisiana Board of Regents.

**9:48AM X27.00010 Entanglement Entropy of U(1) Quantum Spin Liquids** , MICHAEL PRETKO, T SENTHIL, Massachusetts Institute of Technology — We investigate the entanglement structure of the ground state of a (3+1)-dimensional U(1) quantum spin liquid, described by the deconfined phase of a compact U(1) gauge theory. The excitations of the system are a gapless photon and gapped electric/magnetic charges. The elements of the entanglement spectrum can be grouped according to the electric flux between the two regions, leading to an interpretation in terms of particles living on the boundary. The entanglement spectrum is given additional structure due to the presence of the gapless photon. Making use of the Bisognano-Wichmann theorem and a local thermal approximation, these two contributions are recast in terms of boundary and bulk contributions, respectively. Both pieces give rise to universal subleading logarithms in the entanglement entropy, as opposed to the subleading constant in gapped topologically ordered systems. The photon term arises from the low-energy conformal field theory and is essentially local in character. The particle term arises due to the constraint of closed electric loops and is shown to be the natural generalization of topological entanglement entropy to the U(1) spin liquid. This contribution to the entanglement entropy can be isolated by means of a special geometric construction.

**10:00AM X27.00011 Optical Conductivity in Holography with Hyperscaling Violation and Massive Gravity** , BRANDON LANGLEY, PHILIP PHILLIPS, University of Illinois at Urbana-Champaign — One of the long-standing enigmas in the field of strongly-interacting electron systems is the mid-frequency power law form of the optical conductivity in the cuprates,  $|\sigma| \sim \omega^{-\alpha}$ . Many efforts have been put forth to obtain this power law using the AdS/CFT correspondence while maintaining the experimentally observed Drude form of the conductivity at low frequency. Some models have obtained the power law form over a very narrow range but none have matched the robust form lasting over decades as in experimental observations. We expand on previous constructions by introducing the dynamical exponent  $z$  and hyperscaling parameter  $\theta$  in a theory that breaks translational invariance using massive gravity. We seek a form of the optical conductivity that reproduces the functional form of the cuprates over all frequency regimes.

**10:12AM X27.00012 Probing Critical Surfaces in Momentum Space Using Real-Space Entanglement Entropy: Bose versus Fermi<sup>1</sup>** , KUN YANG, Department of Physics and National High Magnetic Field Laboratory, Florida State University, HSIN-HUA LAI, Department of Physics and Astronomy, Rice University — A co-dimension one critical surface in the momentum space can be either a familiar Fermi surface, which separates occupied states from empty ones in the non-interacting fermion case, or a novel Bose surface, where gapless bosonic excitations are anchored. Their presence gives rise to logarithmic violation of entanglement entropy area law. When they are *convex*, we show that the shape of these critical surfaces can be determined by inspecting the leading logarithmic term of real space entanglement entropy. The fundamental difference between a Fermi surface and a Bose surface is revealed by the fact that the logarithmic terms in entanglement entropies differ by a factor of two:  $S_{log}^{Bose} = 2S_{log}^{Fermi}$ , even when they have identical geometry. Our method has remarkable similarity with determining Fermi surface shape using quantum oscillation. We also discuss possible probes of *concave* critical surfaces in momentum space.

<sup>1</sup>HHL and KY acknowledge the National Science Foundation through grants No. DMR-1004545, DMR-1157490, No. DMR-1442366, and State of Florida. HHL is also partially supported by NSF Grant No. DMR -1309531, and the Smalley Postdoctoral Fellowship in Quantum Ma

**10:24AM X27.00013 Entanglement spectrum and entangled modes of highly excited states in random XX spin chains** , MOHAMMAD POURANVARI, KUN YANG, National High Magnetic Field Laboratory and Department of Physics, Florida State University, Tallahassee, Florida 32306, USA — We examine the newly developed real space renormalization group method of finding excited eigenstate (RSRG-X) of the XX spin-1/2 chain, from entanglement perspectives. Eigenmodes of the entanglement Hamiltonian, especially the maximally entangled mode (that contributes the most to the entanglement entropy) and corresponding entanglement energies are studied and compared with predictions of RSRG-X. Our numerical results demonstrate the accuracy of the RSRG-X method in the strong disorder limit, and quantify its error when applied to weak disorder regime. Overall, our results validate the RSRG-X method qualitatively, but as in the case of real space renormalization group method for the ground state (RSRG) there are quantitative errors for weaker randomness, and also such error grows with increasing temperature/excitation energy density.

**10:36AM X27.00014 Two-component Structure in the Entanglement Spectrum of Highly Excited States** , ZHI-CHENG YANG, CLAUDIO CHAMON, Boston University, ALIOSCIA HAMMA, Tsinghua University, EDUARDO MUCCILOLO, University of Central Florida — We study the entanglement spectrum of highly excited eigenstates of two known models which exhibit a many-body localization transition, namely the one-dimensional random-field Heisenberg model and the quantum random energy model. Our results indicate that the entanglement spectrum shows a “two-component” structure: a universal part that is associated to Random Matrix Theory, and a non-universal part that is model dependent. The non-universal part manifests the deviation of the highly excited eigenstate from a true random state even in the thermalized phase where the Eigenstate Thermalization Hypothesis holds. The fraction of the spectrum containing the universal part decreases continuously as one approaches the critical point and vanishes in the localized phase in the thermodynamic limit. We use the universal part fraction to construct a new order parameter for the many-body delocalized-to-localized transition. Two toy models based on Rokhsar-Kivelson type wavefunctions are constructed and their entanglement spectra are shown to exhibit the same structure.

**10:48AM X27.00015 Matrix-product-state method with local basis optimization for nonequilibrium electron-phonon systems<sup>1</sup>** , FABIAN HEIDRICH-MEISNER, LMU Munich, Germany, CHRISTOPH BROCKT, University of Hanover, Germany, FLORIAN DORFNER, LMU Munich, Germany, LEV VIDMAR, Penn State University, USA, ERIC JECKELMANN, University of Hanover, Germany — We present a method for simulating the time evolution of quasi-one-dimensional correlated systems with strongly fluctuating bosonic degrees of freedom (e.g., phonons) using matrix product states [1]. For this purpose we combine the time-evolving block decimation (TEBD) algorithm with a local basis optimization (LBO) approach. We discuss the performance of our approach in comparison to TEBD with a bare boson basis, exact diagonalization, and diagonalization in a limited functional space. TEBD with LBO can reduce the computational cost by orders of magnitude when boson fluctuations are large and thus it allows one to investigate problems that are out of reach of other approaches. First, we test our method on the non-equilibrium dynamics of a Holstein polaron [2] and show that it allows us to study the regime of strong electron-phonon coupling. Second, the method is applied to the scattering of an electronic wave packet off a region with electron-phonon coupling. Our study reveals a rich physics including transient self-trapping and dissipation.

[1] C. Brockt, F. Dorfner, L. Vidmar, F. Heidrich-Meisner, and E. Jeckelmann, arXiv:1508.00694

[2] F. Dorfner, L. Vidmar, C. Brockt, E. Jeckelmann, F. Heidrich-Meisner, Phys. Rev. B 91, 104302 (2015)

<sup>1</sup>Supported by Deutsche Forschungsgemeinschaft (DFG) via FOR 1807

## Friday, March 18, 2016 8:00AM - 10:48AM –

Session X28 DMP DCMP: Topological Semimetals: Theory 327 - Sumanta Tewari, Clemson University.

**8:00AM X28.00001 Weyl Phases in a Three Dimensional Network Model<sup>1</sup>** , HAILONG WANG, YIDONG CHONG, Division of Physics and Applied Physics, Nanyang Technological University, THEORETICAL PHOTONICS TEAM — We study the topological properties of 3D “Floquet” band structures, defined using unitary evolution matrices rather than Hamiltonians. Such band structures can be realized in coherent-wave networks or lattices subjected to time-periodic drives. Previously, 2D Floquet band structures have been shown to exhibit unusual topological behaviors such as topologically-nontrivial zero-Chern-number phases. Here, we analyze the Floquet band structure of a 3D network model, which exhibits an Floquet analogue of a Weyl phase. The surface states exhibit topologically-protected “Fermi” arcs, similar to the recently-discovered Weyl semi-metals; however, the Weyl points in different quasi-energy gaps are related by a particle-hole symmetry which is unique to the Floquet system. By tuning the coupling parameters of the network, we can drive a transition between conventional insulator, weak topological insulator, and Weyl phases. Finally, we discuss the possibility of realizing this model using custom-designed electromagnetic networks.

<sup>1</sup>GRANT: Supported by Singapore National Research Foundation under grant No. NRFF2012-02

**8:12AM X28.00002 Magnetic response in three-dimensional nodal semimetals** , MIKITO KOSHINO, INTAN FATIMAH HIZBULLAH, Tohoku University — We study the magnetic response in various three-dimensional gapless systems, including Dirac and Weyl semimetals and a line-node semimetal. We show that the susceptibility is decomposed into the orbital term, the spin term and also the spin-orbit cross term which is caused by the spin-orbit interaction. We show that the orbital susceptibility logarithmically diverges at the band touching energy in the point-node case, while it exhibits a stronger delta-function singularity in the line node case. The spin-orbit cross term is shown to be paramagnetic in the electron side while diamagnetic in the hole side, in contrast with other two terms which are both even functions in Fermi energy. The spin-orbit cross term in the nodal semimetal is found to be directly related to the chiral surface current induced by the topological surface modes.

**8:24AM X28.00003 Quasi-Topological Electromagnetic Response of Line-node Semimetals<sup>1</sup>** , SRINIDHI RAMAMURTHY, TAYLOR HUGHES, University of Illinois at Urbana-Champaign — Topological semimetals are gapless states of matter which have robust surface states and interesting electromagnetic responses. We consider the electromagnetic response of gapless phases in 3 + 1-dimensions with line nodes. We show through a layering approach that an intrinsic 2-form  $\mathcal{B}_{\mu\nu}$  emerges in the effective response field theory that is determined by the geometry and energy-embedding of the nodal lines. This 2-form is shown to be simply related to the charge polarization and orbital magnetization of the sample. We conclude by discussing the relevance for recently proposed materials and heterostructures with line-node fermi-surfaces.

<sup>1</sup>ONR YIP Award N00014-15-1-2383

**8:36AM X28.00004 Multipolar orders and quantum criticality of a three-dimensional parabolic semimetal** , BITAN ROY, PALLAB GOSWAMI, University of Maryland — Motivated by the observation of multipolar ordering in many heavy fermion compounds and 227 pyrochlore iridates, we investigate the phase diagram of an interacting, three dimensional parabolic semimetal as a paradigmatic toy model for studying the interplay among electronic correlations, topology and quantum critical phenomena. The generic forms of the local order parameters and quartic interactions are constructed according to the irreducible representations of octahedral point group symmetry. Through a renormalization group analysis, we elucidate the competition between time-reversal symmetric quadrupolar and time-reversal symmetry breaking octopolar ordered phases for sufficiently strong interactions. We show that the quadrupolar ordering can give rise to a correlated topological insulator phase, while the octopolar order generically leads to a Weyl semimetal phase. The quantum phase transitions between the semimetal and the broken symmetry phases are controlled by non-Gaussian, itinerant quantum critical points.

**8:48AM X28.00005 Topological ‘Luttinger’ invariants protected by crystal symmetry in semimetals<sup>1</sup>** , S.A. PARAMESWARAN, University of California, Irvine — Luttinger’s theorem is a fundamental result in the theory of interacting Fermi systems: it states that the volume inside the Fermi surface is left invariant by interactions, if the number of particles is held fixed. Although this is traditionally justified using perturbation theory, it can be viewed as arising from a momentum balance argument that examines the response of the ground state to the insertion of a single flux quantum [M. Oshikawa, *Phys. Rev. Lett.* **84**, 3370 (2000)]. This reveals that the Fermi sea volume is a topologically protected quantity. Extending this approach, I show that spinless or spin-rotation-preserving fermionic systems in non-symmorphic crystals possess generalized topological ‘Luttinger invariants’ that can be nonzero even in cases where the Fermi sea volume vanishes. A nonzero Luttinger invariant then forces energy bands to touch, leading to semimetals whose gaplessness is rooted in topology; opening a gap without symmetry breaking automatically triggers fractionalization. The existence of these invariants is linked to the inability of non-symmorphic crystals to host band insulating ground states except at special fillings. I exemplify the use of these new invariants by showing that they distinguish various classes of semimetals.

<sup>1</sup>Supported by the National Science Foundation via Grant No. DMR-1455366.

**9:00AM X28.00006 Ferromagnetic interactions between transition-metal impurities in topological and 3D Dirac semimetals**, TOMASZ DIETL, Inst Phys, Polish Acad of Sci; Inst Theor Phys, Univ Warsaw; WPI-AIMR Tohoku Univ — The magnitude of ferromagnetic coupling driven by inter-band (Bloembergen-Rowland - BR) and intra-band (Ruderman-Kittel-Kasuya-Yoshida - RKKY) spin polarization is evaluated within  $k$ - $p$  theory for topological semimetals  $\text{Hg}_{1-x}\text{Mn}_x\text{Te}$  and  $\text{Hg}_{1-x}\text{Mn}_x\text{Se}$  as well as for 3D Dirac semimetal  $(\text{Cd}_{1-x}\text{Mn}_x)_3\text{As}_2$ . In these systems  $\text{Mn}^{2+}$  ions do not introduce any carriers. Since, however, both conduction and valence bands are built from anion  $p$ -type wave functions, hybridization of Mn  $d$  levels with neighboring anion  $p$  states leads to spin-dependent  $p-d$  coupling of both electrons and holes to localized Mn spins, resulting in sizable inter-band spin polarization and, thus in large BR interactions. We demonstrate that this ferromagnetic coupling, together with antiferromagnetic superexchange, elucidate a specific dependence of spin-glass freezing temperature on  $x$ , determined experimentally for these systems. Furthermore, by employing a multi-orbital tight-binding method, we find that superexchange becomes ferromagnetic when Mn is replaced by Cr or V. Since Cr should act as an isoelectronic impurity in HgTe, this opens a road for realization of ferromagnetic topological insulators based on (Hg,Cr)Te.

**9:12AM X28.00007 Gyrotropic magnetic effect in Weyl semimetals**, SHUDAN ZHONG, JOEL MOORE, Univ of California - Berkeley, IVO SOUZA, Universidad del País Vasco — The transport current  $\mathbf{J}$  induced in a clean metal by a magnetic field  $\mathbf{B}$  is shown to be equivalent to the low-frequency limit of natural optical activity (optical gyrotropy). For a generic multiband Hamiltonian, there is a simple expression for  $\alpha_{ij} = J_i/B_j$  in terms of the intrinsic magnetic moment (orbital plus spin) of the Bloch electrons on the Fermi surface. This “gyrotropic magnetic effect” (GME) is fundamentally different from the chiral magnetic effect (CME) driven by the chiral anomaly, which is only nonzero away from equilibrium and is governed by the Berry curvature. The two effects are compared for a minimal model of a Weyl semimetal. We discuss a simple semiclassical picture of the GME and its possible experimental observation by measuring the rotary power of low-symmetry materials like  $\text{SrSi}_2$ .

**9:24AM X28.00008 Optical conductivity of disordered Weyl semimetals in collisionless regime at zero temperature**, VLADIMIR JURICIC, Nordita, Center for Quantum Materials, KTH Royal Institute of Technology, and Stockholm University, Roslagstullsbacken 23, S-106 91 Stockholm, BITAN ROY, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, MD 20742, USA — Weyl semimetals have recently attracted considerable attention as prime examples of topologically nontrivial gapless states of quantum matter. They have been experimentally found and the chiral anomaly, which represents their hallmark feature, has been measured. In this work, we study transport in the disordered Weyl semimetals using the Kubo formalism. We consider point-like impurity potentials, which are irrelevant in the renormalization-group sense, and compute the corresponding leading correction to the collisionless conductivity at zero temperature. As a result, we find that all eight possible types of the point-like disorder potentials give rise to a correction to the real part of the optical conductivity in the clean limit, which is universal up to a sign. Consequently, the dielectric constant of a Weyl material receives a disorder correction which is linear in frequency. Finally, we discuss some experimental consequences of our findings.

**9:36AM X28.00009 Current at a distance and resonant transparency in Weyl semimetals**, ADY STERN, YUVAL BAUM, EREZ BERG, Weizmann Institute of Science, SIDDHARTH PARAMESWARAN, UC Irvine — Surface Fermi arcs are the most prominent manifestation of the topological nature of Weyl semimetals. In the presence of a static magnetic field oriented perpendicular to the sample surface, their existence leads to unique inter-surface cyclotron orbits. We propose two experiments which directly probe the Fermi arcs: a magnetic field dependent non-local DC voltage and sharp resonances in the transmission of electromagnetic waves at frequencies controlled by the field. We show that these experiments are insensitive to small momentum scattering and do not rely on quantum mechanical phase coherence, which renders them far more robust and experimentally accessible than quantum effects. We also comment on the applicability of these ideas to Dirac semimetals.

**9:48AM X28.00010 Self-consistent theory of electronic states in topological broken-gap quantum wells<sup>1</sup>**, R. WINKLER, Northern Illinois University — Recently broken-gap quantum wells made of  $\text{InAs}/\text{GaSb}/\text{AlSb}$  have raised great interest as they may show a gate-tunable phase transition from a trivial phase to a topologically protected quantum spin Hall phase. We present a quantitative self-consistent theory of electronic states in such systems taking into account the charge transfer between different layers which can substantially modify the level structure including the phase boundary between the inverted and non-inverted regime. We also discuss spin effects and the unusual Landau fans in a quantizing magnetic field.

<sup>1</sup>Work supported by the NSF grant DMR-1310199.

**10:00AM X28.00011 Topological edge states in ultra thin Bi(110) puckered crystal lattice**, BAKKAI WANG, Northeastern University, CHUANGHAN HSU, GUOQING CHANG, HSIN LIN, National University of Singapore, ARUN BANSIL, Northeastern University — We discuss the electronic structure of a 2-ML  $\text{Bi}(110)$  film with a crystal structure similar to that of black phosphorene. In the absence of Spin-Orbit coupling (SOC), the film is found to be a semimetal with two kinds of Dirac cones, which are classified by their locations in the Brillouin zone. All Dirac nodes are protected by crystal symmetry and carry non-zero winding numbers. When considering ribbons, along specific directions, projections of Dirac nodes serve as starting or ending points of edge bands depending on the sign of their carried winding number. After the inclusion of the SOC, all Dirac nodes are gapped out. Correspondingly, the edge states connecting Dirac nodes split and cross each other, and thus form a Dirac node at the boundary of the 1D Brillouin zone, which suggests that the system is a Quantum Spin Hall insulator. The nontrivial Quantum Spin Hall phase is also confirmed by counting the product of parities of the occupied bands at time-reversal invariant points.

**10:12AM X28.00012 Detecting 2D symmetry-protected topological phases with the tensor-network method**, CHING-YU HUANG, TZU-CHIEH WEI, C. N. Yang Institute for Theoretical Physics and Department of Physics and Astronomy, State University of New York at Stony Brook — Symmetry-protected topological (SPT) phases exhibit nontrivial order if symmetry is respected but are adiabatically connected to the trivial product phase if symmetry is not respected. However, unlike the symmetry breaking phase, there is no local order parameter for SPT phases. Here we employ a tensor-network method to compute the topological invariants characterized by the simulated modular  $S$  and  $T$  matrices proposed by Hung and Wen [PRB 89,075121 (2014)] to study a transition in a one-parameter family of wavefunctions which are  $\mathbb{Z}_2$  symmetric. The studied wavefunctions are in some sense the SPT analog of  $\mathbb{Z}_2$  topological states under a string tension. The numerically obtained  $S$  and  $T$  matrices are able to characterize the two different phases and identify the transition point.

**10:24AM X28.00013 Analytical characterization of bulk-boundary separation for non-interacting fermionic Hamiltonians**, EMILIO COBANERA, ABHIJEET ALASE, Dartmouth Coll, GERARDO ORTIZ, Indiana University, LORENZA VIOLA, Dartmouth Coll — In topological quantum matter the notions of bulk and boundary are closely intertwined by the Hamiltonian. For non-interacting systems, the bulk-boundary correspondence relates this phenomenon to topological properties of the single-particle Hamiltonian defined in momentum space, but, so far, no analytic, systematic approach has been put forward to investigate the edge modes themselves. We show how Schrodinger's equation for a confined system of independent fermions may be separated into a bulk and a boundary equation in a manner that depends critically on the nature of the Hamiltonian. The bulk equation may be solved in closed or near closed form, and the Brillouin zone associated to the infinitely extended system emerges naturally embedded in the full complex plane or higher dimensional analogue. The bulk equation determines uniquely all possible zero modes of the system, whereas the boundary equation selects those, if any, compatible with the prescribed boundary.

**10:36AM X28.00014 Prediction of two-dimensional topological insulator by forming surface alloy on Au/Si(111) substrate**, ZHI-QUAN HUANG, FENG-CHUAN CHUANG, CHIA-HSIU HSU, HSIN-LEI CHOU, CHRISTIAN CRISOS-TOMO, SHIH-YU WU, CHIEN-CHENG KUO, Natl. Sun Yat-sen U., WANG-CHI YEH, Natl. Dong Hwa U., HSIN LIN, Natl. U. of Singapore, ARUN BANSIL, Northeastern U. — Two-dimensional (2D) topological insulators (TIs), which can be integrated into the modern silicon industry, are highly desirable for spintronics applications. Here, using first-principles electronic structure calculations, we show that the Au/Si(111)-root3 substrate can provide a new platform for hosting 2D-TIs obtained through the formation of surface alloys with a honeycomb pattern of adsorbed atoms. We systematically examined elements from groups III to VI of the periodic table at 2/3 monolayer coverage on Au/Si(111)-root3, and found that In, Tl, Ge, and Sn adsorbates result in topologically non-trivial phases with band gaps varying from zero to 72 meV. Our scanning tunneling microscopy and low-energy electron diffraction experiments confirm the presence of the honeycomb pattern when Bi atoms are deposited on Au/Si(111)-root3 in accord with our theoretical predictions. Our findings pave the way for using surface alloys as a potential new route for obtaining viable 2D-TI platforms.

**Friday, March 18, 2016 8:00AM - 11:00AM —**

**Session X29 DMP: Topological Insulator - Bi-based Materials** 328 - Rolandes Valdes, Ohio State University

**8:00AM X29.00001 Hidden landscapes in thin film topological insulators: between order and disorder, 2D and 3D, normal and topological phases<sup>1</sup>**, SEONGSHIK OH, Department of Physics and Astronomy, Rutgers, The State University of New Jersey — Topological insulator (TI) is one of the rare systems in the history of condensed matter physics that is initiated by theories and followed by experiments. Although this theory-driven advance helped move the field quite fast despite its short history, apparently there exist significant gaps between theories and experiments. Many of these discrepancies originate from the very fact that the worlds readily accessible to theories are often far from the real worlds that are available in experiments. For example, the very paradigm of topological protection of the surface states on Z2 TIs such as Bi<sub>2</sub>Se<sub>3</sub>, Bi<sub>2</sub>Te<sub>3</sub>, Sb<sub>2</sub>Te<sub>3</sub>, etc, is in fact valid only if the sample size is infinite and the crystal momentum is well-defined in all three dimensions. On the other hand, many widely studied forms of TIs such as thin films and nano-wires have significant confinement in one or more of the dimensions with varying level of disorders. In other words, many of the real world topological systems have some important parameters that are not readily captured by theories, and thus it is often questionable how far the topological theories are valid to real systems. Interestingly, it turns out that this very uncertainty of the theories provides additional control knobs that allow us to explore hidden topological territories. In this talk, I will discuss how these additional knobs in thin film topological insulators reveal surprising, at times beautiful, landscapes at the boundaries between order and disorder, 2D and 3D, normal and topological phases.

<sup>1</sup>This work is supported by Gordon and Betty Moore Foundation's EPiQS Initiative (GBMF4418)

**8:36AM X29.00002 Finite-size driven topological and metal-insulator transition in (Bi<sub>1-x</sub>In<sub>x</sub>)<sub>2</sub>Se<sub>3</sub> thin films**, MARYAM SALEHI, Rutgers University, HASSAN SHAPOURIAN, University of Illinois at Urbana-Champaign, NIKESH KOIRALA, Rutgers University, MATTHEW BRAHLEK, Pennsylvania State University, JISOO MOON, SEONGSHIK OH, Rutgers University — In a topological insulator (TI), if one of its heavy elements is replaced by a light one, the spin-orbit coupling (SOC) strength decreases and eventually the TI transforms into a normal insulator beyond a critical level of substitution. This is the standard description of the topological phase transition (TPT). However, this notion of TPT, driven solely by the SOC (or something equivalent), is not complete for finite size samples considering that the thickness of the topological surface states diverges at the critical point. Here, on specially-engineered (Bi<sub>x</sub>In<sub>1-x</sub>)<sub>2</sub>Se<sub>3</sub> thin films, using systematic transport measurements we show that not only the SOC but also the finite sample size can induce TPT. This study sheds light on the role of spatial confinement as an extra tuning parameter controlling the topological critical point.

**8:48AM X29.00003 Quantum transport of two-species Dirac fermions in dual-gated three-dimensional topological insulators<sup>1</sup>**, YANG XU, IRENEUSZ MIOTKOWSKI, YONG P. CHEN, Department of Physics and Astronomy, Purdue University — Topological insulators (TI) are a novel class of quantum matter with a gapped insulating bulk yet gapless spin helical Dirac fermion conducting surface states. Here, we report local and non-local electrical and magneto transport measurements in dual-gated BiSbTeSe<sub>2</sub> thin film TI devices, with conduction dominated by the spatially separated top and bottom surfaces, each hosting a single species of Dirac fermions with independent gate control over the carrier type and density. We observe many intriguing quantum transport phenomena in such a fully-tunable two-species topological Dirac gas, including a zero-magnetic-field minimum conductivity of  $4e^2/h$  at the double Dirac point, a series of ambipolar two-component "half-integer" Dirac quantum Hall states and an electron-hole total filling factor  $\nu=0$  state (with a zero-Hall plateau), exhibiting dissipationless (chiral) and dissipative (non-chiral) edge conduction respectively. Such a system paves the way to explore rich physics ranging from topological magnetoelectric effects to exciton condensation.

<sup>1</sup>DARPA MESO program

**9:00AM X29.00004 Separation of quantum oscillations from bulk and topological surface states in metallic Bi<sub>2</sub>Se<sub>2.1</sub>Te<sub>0.9</sub><sup>1</sup>**, BERND LORENZ, TCSUH and Dept. of Physics, University of Houston, KESHAV SHRESTHA, TCSUH, University of Houston, DAVID E. GRAF, NHMFL, Florida State University, VERA MARINOVA, Institute of Optical Materials and Technology, Bulgarian Academy of Sciences, PAUL C. W. CHU, TCSUH and Dept. of Physics, University of Houston — Shubnikov-de Haas (SdH) oscillations in metallic Bi<sub>2</sub>Se<sub>2.1</sub>Te<sub>0.9</sub> are studied in magnetic fields up to 35 Tesla. It is demonstrated that two characteristic frequencies determine the quantum oscillations of the conductivity. Angle dependent measurements and calculations of the Berry phase show that the two frequencies  $F_1$  and  $F_2$  describe oscillations from surface and bulk carriers, respectively. At low magnetic fields, only SdH oscillation from topological surface states can be detected whereas at high magnetic field the bulk oscillations dominate. The origin of the separation of bulk and surface SdH oscillations into different magnetic field ranges is revealed in the difference of the cyclotron masses  $m_c$ . The bulk  $m_c$  is nearly three times larger than the surface cyclotron mass resulting in a stronger attenuation of the bulk oscillation amplitude upon decreasing magnetic field. This makes it possible to detect and characterize the surface SdH oscillations in the low-field range.

<sup>1</sup>Supported by the T.L.L. Temple Foundation, the J.J. and R. Moores Endowment, the State of Texas through TCSUH, the US Air Force Office of Scientific Research, the Bulgarian Science Fund, the National Science Foundation, and the State of Florida.

**9:12AM X29.00005 Record surface state mobility and quantum Hall effect in topological insulator thin films via interface engineering**, NIKESH KOIRALA, MATTHEW BRAHLEK, MARYAM SALEHI, Rutgers U., LIANG WU, JHU, JIXIA DAI, Rutgers Univ, JUSTIN WAUGH, THOMAS NUMMY, U. of Colorado, MYUNG-GEUN HAN, BNL, JISOO MOON, Rutgers U., YIMEI ZHU, BNL, DANIEL DESSAU, U. of Colorado, WEIDA WU, Rutgers U., N. PETER ARMITAGE, JHU, SEONGSHIK OH, Rutgers U. — Thin films of topological insulators (TIs) with conduction dominated by high mobility topological surface state (TSS) channel have been difficult to achieve due to increased material defects, thus making it difficult to probe TIs in quantum regime. Here by utilizing a structurally matched buffer layer based on In<sub>2</sub>Se<sub>3</sub>, we have achieved Bi<sub>2</sub>Se<sub>3</sub> films with low defect density resulting in 'order of magnitude' improvement in mobilities and carrier densities. This has led to TSS dominated transport and first observation of quantum Hall effect in Bi<sub>2</sub>Se<sub>3</sub>.

## 9:24AM X29.00006 Differentiation of surface and bulk conductivities in topological insulator via four-probe spectroscopy<sup>1</sup>

AN-PING LI, CORENTIN DURAND, SABAN HUS, XIAOGUANG ZHANG, MICHAEL MCGUIRE, Oak Ridge National Laboratory, YONG CHEN, Purdue University — The direct measurement of the topological surface states (TSS) conductivity is often hard to achieve due to the pronounced contribution from the bulk conduction channel. Here, we show a new method to differentiate conductivities from the surface states and the coexisting bulk states in topological insulators (TI) using a four-probe transport spectroscopy in a multi-probe scanning tunneling microscopy system. In contrast to conventional models that assume two resistors in parallel to count for both the TSS and bulk conductance channels, we derive a scaling relation of measured resistance with respect to varying inter-probe spacing for two interconnected conduction channels, which allows quantitative determination of conductivities from both channels. Using this method, we demonstrate the separation of 2D and 3D conduction in TI by comparing the conductance scaling of Bi<sub>2</sub>Se<sub>3</sub>, Bi<sub>2</sub>Te<sub>2</sub>Se, and Sb-doped Bi<sub>2</sub>Se<sub>3</sub> with that of a pure 2D conductance of graphene on SiC substrate. We also quantitatively show the effect of surface doping carriers on the 2D conductance enhancement in TI. The method offers an approach to understanding not just the topological insulators but also the 2D to 3D crossover of conductance in other complex systems.

<sup>1</sup>This research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

## 9:36AM X29.00007 High magnetic field Shubnikov-de Haas oscillations in BiTeCl<sup>1</sup>

CATALIN MARTIN, Ramapo College of New Jersey, Mahwah, NJ, 07430, L. E. WINTER, R. G. MCDONALD, V. ZAPF, A. V. SUSLOV, National High Magnetic Field Laboratory, Los Alamos, NM, 87545, USA, PHILIPPE BUGNON, ARNAUD MAGREZ, H. BERGER, Crystal Growth Facility, Ecole Polytechnique Federale de Lausanne, Switzerland, D. B. TANNER, University of Florida, Gainesville, Florida, 32611, USA — We report high magnetic field Shubnikov-de Haas oscillations on single crystals of the bulk Rashba compound BiTeCl. Effective mass and scattering rate extracted from temperature and magnetic field dependence of the oscillations amplitude are in good agreement with our previous optical measurements. The present work will focus on the angular dependence study. First, we notice that oscillations were detected for all our measured angles between the magnetic field and the crystallographic z-axis,  $0 \leq \theta \leq 120^\circ$ . This is consistent with a 3D Fermi surface and, in good agreement with optical data, confirms that oscillations originate from bulk carriers. Second, the frequency has unusual angular dependence around  $\theta = 90^\circ$ . We will show that this behavior is consistent with a torus shaped Fermi surface, providing direct evidence for a Rashba spin-split bulk conduction band. Moreover, we extract reliably the bulk Rashba parameters and the anisotropy of BiTeCl.

<sup>1</sup>A portion of this work was supported by the US DOE through contract DE-FG02-02ER45984

## 9:48AM X29.00008 Quantized steps and topological nature of universal conductance fluctuation in Bi<sub>2</sub>Te<sub>2</sub>Se

FENGQI SONG, Nanjing Univ — Here we report the experimental observation of universal conductance fluctuations (UCF) in Bi<sub>2</sub>Te<sub>2</sub>Se. Four aspects were addressed to support the UCF's topological nature of the electronic state. i) The irregular fluctuations are repeatable in different temperature and reversal magnetic fields. ii) All the UCF features coincide after the field is normalized to the perpendicular direction. This points to a two-dimensional electronic state. iii) A parallel field is applied to suppress the bulk coherent paths, while the UCF features stays similar. This excludes a quasi-2D bulk state. iv). The intrinsic UCF magnitude is extracted, which is close to the predicted values of a topological surface state. v). Quantized steps of the UCF magnitudes are observed when the magnetic field is modulated. (*Sci.Rep.* 2012, 2,595; *Appl. Phys. Expre.* 2014,7,065202; arxiv 2015)

## 10:00AM X29.00009 Edge states and integer quantum Hall effect in topological insulator thin films

SONG-BO ZHANG, Department of Physics, The University of Hong Kong, HAI-ZHOU LU, Department of Physics, South University of Science and Technology of China, SHUN-QING SHEN, Department of Physics, The University of Hong Kong — The integer quantum Hall effect is a topological state of quantum matter in two dimensions, and has recently been observed in three-dimensional topological insulator thin films. In this report, I will talk about the Landau levels and edge states of surface Dirac fermions in topological insulators under a strong magnetic field. We examine the formation of the quantum plateaux of the Hall conductance and find two different patterns, in one pattern the filling number covers all integers while only odd integers in the other. We focus on the quantum plateau closest to zero energy and demonstrate the breakdown of the quantum spin Hall effect as a result of the interplay of magnetic field and structure inversion asymmetry. We also reveal that the edge states exist only for the integer Hall conductance while no edge-state solution can be found for the "half-integer" Hall conductance. The addition of top and bottom surface Dirac fermions always form well-defined edge states, and gives an integer quantum Hall effect. This work establishes an intuitive picture of the edge states to understand the integer quantum Hall effect for Dirac electrons in topological insulator thin films.

## 10:12AM X29.00010 Duo gating on a 3D topological insulator - independent tuning of both topological surface states

CHUAN LI, BOB DE RONDE, MARIEKE SNELDER, MARTIN STEHNO, Twente Tech Univ, YINGKAI HUANG, MARK GOLDEN, University of Amsterdam, ALEXANDER BRINKMAN, Twente Tech Univ, ICE TEAM, IOP COLLABORATION — ABSTRACT: Topological insulators are associated with a trove of exciting physics, such as the ability to host robust anyons, Majorana Bound States, which can be used for quantum computation. For future Majorana devices<sup>1</sup> it is desirable to have the Fermi energy tuned as close as possible to the Dirac point of the topological surface state. Based on previous work on gating BSTS<sup>2,3</sup>, we report the experimental progress towards gate-tuning of the top and bottom topological surface states of BiSbTeSe<sub>2</sub> crystal flakes. When the Fermi level is moved across the Dirac point conduction is shown to change from electron dominated transport to hole dominated transport independently for either surface. In the high magnetic field, one can tune the system precisely between the different Landau levels of both surfaces, thus a full gating map of the possible Landau levels combination is established. In addition, we provide a simple capacitance model to explain the general hysteresis behaviors in topological insulator systems.

<sup>1</sup>L. Fu, C.L. Kane, Phys. Rev. Lett **100**, 096407 (2008).

<sup>2</sup>Y. Xu et al. Nat. Phys. **10**, 956-963 (2014).

<sup>3</sup>R. Yoshimi et al., Nat. Comm. **6**, 6627 (2015).

## 10:24AM X29.00011 Weak antilocalization in Bi<sub>2-x</sub>In<sub>x</sub>Te<sub>3</sub> single crystals

HANG CHI, QIANG LI, Brookhaven Natl Lab, CTIRAD UHER, University of Michigan — Bi<sub>2</sub>Te<sub>3</sub> has recently been identified as one of the most promising systems with which to realize a three-dimensional topological insulator. However, the bulk, stoichiometric Bi<sub>2</sub>Te<sub>3</sub> single crystals often exhibit *p*-type metallic electrical conduction due to the Bi<sub>Te</sub>-type antisite defects, which overshadows the contribution of surface states. We have established that, upon group III (indium and/or thallium) doping, the Fermi level of Bi<sub>2</sub>Te<sub>3</sub> can be lifted from the valence band into the band gap, and eventually shifted into the conduction band. Such doping progressively changes the electrical conduction of Bi<sub>2-x</sub>A<sub>x</sub>Te<sub>3</sub> (A = In, Tl, and  $x = 0 - 0.30$ ) single crystals from *p*-type to *n*-type. This is observed via measurements of both the Hall effect and the Seebeck coefficient performed in the (0001) basal plane in the temperature range of 2 - 300 K. At low levels, the temperature dependent in-plane electrical resistivity maintains its metallic character as the density of holes decreases. Heavier doping content,  $x = 0.20$  (0.10) for In (Tl), drives the electrical resistivity into a prominent non-metallic regime displaying the weak anti-localization type of magnetoresistance at the lowest temperatures for Bi<sub>1.80</sub>In<sub>0.20</sub>Te<sub>3</sub>. At the highest concentration, the samples revert back into the metallic state with electron dominated conduction. Thermal conductivity measurements of Bi<sub>2-x</sub>A<sub>x</sub>Te<sub>3</sub> single crystals, as examined by the Debye-Callaway phonon conductivity model, reveal a generally stronger point defect scattering of phonons upon doping.

**10:36AM X29.00012 Induced Superconductivity In Bi<sub>2</sub>Se<sub>3</sub> Nanostructures By Anneal Doping Of Palladium<sup>1</sup>**, JEROME T. MLACK, ATIKUR RAHMAN, NATALIA DRICHKO, NINA MARKOVIC, Johns Hopkins University — Utilizing thermal annealing at temperatures in excess of 100 Celsius we induce superconductivity in Bi<sub>2</sub>Se<sub>3</sub> by palladium doping. Changes in the material structure are analyzed using a combination of AFM, optical microscopy and Raman spectroscopy. The absorption of Pd results in superconductivity in the material with a transition temperature below 1K. The differential conductance as a function of temperature and magnetic field reveals multiple transitions in the material at several applied currents.

<sup>1</sup>This work was supported under the National Science Foundation Grant No.s DGE-1232825 (J.T.M.) and DMR-1106167.

**10:48AM X29.00013 Chromium Doping of the Topological Insulator Bi<sub>1.5</sub>Sb<sub>0.5</sub>Te<sub>1.7</sub>Se<sub>1.3</sub>**, DANIEL DOUGHERTY, ANDREW HEWITT, Department of Physics North Carolina State University, RAJ KUMAR, Department of Materials Science and Engineering North Carolina State University, JONATHAN BOLTERSDORF, PAUL MAGGARD, Department of Chemistry North Carolina State University, FRANK HUNTE, Department of Materials Science and Engineering North Carolina State University — A major materials science challenge is to minimize bulk conductivity in topological insulators so that topological surface state physics can be cleanly accessed. One solution to this problem has been the development of quaternary bismuth chalcogenides Bi<sub>2-x</sub>Sb<sub>x</sub>Te<sub>3-y</sub>Se<sub>y</sub> (BSTS) which can be tuned to place the mid-gap Fermi level near the Dirac point associated with the topological surface state. This is ideal for accessing interesting topological physics including the exotic magnetoelectric effects associated with breaking time reversal symmetry. With this goal in mind, we have grown Cr-doped crystals of Bi<sub>1.5</sub>Sb<sub>0.5</sub>Te<sub>1.7</sub>Se<sub>1.3</sub> to assess the impact of magnetic dopants on the electronic and magnetic properties of this material. For 4 percent Cr doping we find electronic structure modifications measured by angle-resolved ultraviolet photoelectron spectroscopy and observe magnetic ordering below 50 K in bulk magnetometry. Higher doping levels show evidence of phase segregation.

**Friday, March 18, 2016 8:00AM - 10:48AM –**  
**Session X30 DMP: Structural and Functional Imaging of Oxide Interfaces** 329 - Ying-Hao Chu, National Chiao Tung University

**8:00AM X30.00001 A Fresh Twist on The Electron Microscope: Probing Broken Symmetries at a New Level**, JUAN CARLOS IDROBO, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA — The introduction of aberration-correction in scanning transmission electron microscopy (STEM) has allowed the realization of Richard Feynmans long sought dream, atom-by-atom structural and elemental identification of materials by simply looking at the thing. Until now, the goal of aberration-correction in STEM has been to produce the smallest possible electron probes, which essentially corresponds to a near constant phase across the probe. Phases increase the size of electron probes and result in images and spectra with a lower spatial resolution. In this talk, calculations will be presented showing that aberrations in lenses are intrinsic generators of angular momentum, and that phases introduced in atomic-size electron probes can actually be beneficial when studying the symmetry of materials. In particular, examples of mapping magnetic ordering of materials with atomic size electron probes will be shown. Magnetic dichroism is one of the new frontiers where aberration-correction STEM can have a significant impact, and reveal information that is physically out of reach in X-ray and neutron synchrotrons. Current and future limitations in the experiments and requirements to reveal the magnetic moment (orbital and spin), charge ordering, crystal field splitting, spin-orbit-coupling, optical dichroism, and other physical phenomena associated with broken symmetries will be discussed. This research was supported by the Center for Nanophase Materials Sciences (CNMS), which is sponsored at Oak Ridge National Laboratory by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy. Collaborators: J. Rusz, J. Spiegelberg, M.A. McGuire, C.T. Symons, R.R. Vatsavai, C. Cantoni and A.R. Lupini.

**8:36AM X30.00002 Atomic Structure Refinement of *Pbnm*-type Perovskite Oxide Films**, AMBER CHOQUETTE, COLE SMITH, STEVE MAY, Drexel Univ — Complex ABO<sub>3</sub> oxide heterostructures are of interest due to their wide variety of electronic, optical, and magnetic properties. One of the controlling factors to these functionalities is the distortions and rotations of the corner-connected BO<sub>6</sub> octahedral network. This BO<sub>6</sub> octahedra network directly couples to the electronic bandwidth of these materials, but the inability to determine the full atomic structure in thin films has inhibited quantitative understanding of how factors such as epitaxial strain alter the octahedral rotations in this broad class of materials. Earlier work of has demonstrate that half-order diffraction peaks can be used to quantify octahedral rotations in thin strained films. Here, we build on this approach to solve for both the oxygen and A-site positions in films of the commonly occurring *Pbnm* structure type. We present on epitaxial RFeO<sub>3</sub> heterostructures, where *R* is a rare earth element, to demonstrate the feasibility of quantifying oxygen and A-site displacements in films using synchrotron diffraction. This work is supported by the National Science Foundation (DMR-1151649).

**8:48AM X30.00003 Direct measurement of oxygen octahedral rotations in improper ferroelectric superlattices by STEM<sup>1</sup>**, JASON LAPANO, RYAN HAISLMAIER, GREGORY STONE, VENKAT GOPALAN, ROMAN ENGEL-HERBERT, Penn State University — Complex ABO<sub>3</sub> perovskites are an intensely studied class of materials due to their numerous magnetic and electronic functionalities. Using strain and A-site cation, can induce new high temperature functionality known as improper ferroelectricity<sup>1</sup>. Visualizing the interplay between strain, cation ordering and octahedral rotations in improper ferroelectrics is crucial to understand how this property manifests itself in thin films<sup>2</sup>. A series of CaTiO<sub>3</sub><sub>n</sub>/SrTiO<sub>3</sub><sub>n</sub> with periodicities n=2-10 were grown on (La,Sr)(Al,Ta)O<sub>3</sub> by hybrid molecular beam epitaxy. I will discuss how strain and layering affects the cation and oxygen sublattices, and how these distortions propagate through the layers, with direct imaging of the oxygen cations by annular bright field (ABF) STEM. I will then relate these back to understanding how improper ferroelectricity evolves in these films. 1. Rondinelli, J. M. & Fennie, C. J. Octahedral Rotation-Induced Ferroelectricity in Cation Ordered Perovskites. Adv. Mater. 24, 1961–1968 (2012). 2. Biegalski, M. D. et al. Impact of symmetry on the ferroelectric properties of CaTiO<sub>3</sub> thin films. Appl. Phys. Lett. 106, 162904 (2015).

<sup>1</sup>National Science Foundation MRSEC

**9:00AM X30.00004 Effects of local sample bending on atom positions and polarization mapping in HAADF-STEM images**, ZHEN WANG, HANGWEN GUO, LINA CHEN, E.W. PLUMMER, JIANDI ZHANG, Louisiana State Univ - Baton Rouge, JING TAO, LIJUN WU, YIMEI ZHU, Brookhaven National Laboratory — Characterization of the structural distortion/reconstruction in the transition-metal oxide heterostructures play an important role in understanding their novel properties. In recent years, high-angle annular dark field (HAADF) in scanning transmission electron microscopy (STEM) has become a powerful technique to determine local atomic arrangements, particularly near interfaces and boundaries. However, sample bending, especially near the edge of a thin specimen, is often introduced during the TEM sample preparation process. Our recent studies reveal that small sample bending can affect significantly the measurement of atom positions in HAADF-STEM image as a result of channeling effect of the incident electron beam. Here we take SrTiO<sub>3</sub> (STO) as an example to show how to remove sample bending induced artifact from its intrinsic structural distortions. A polar-related artifact in STO at different bending angles were revealed both in our experiments and imaging simulation. This artifact can be removed successfully by quantitative comparing experimental with simulated HAADF-STEM images under the same imaging condition. The bending angle and thickness of the sample can be determined using convergent beam electron diffraction. Our study provide a useful guidance for removing the sample bending-induced artifact in STEM images for the studies of local lattice structures, polarization and distortion of complex materials.

**9:12AM X30.00005 Quantifying the electronic reconstruction in  $\text{LaTiO}_3/\text{LaNiO}_3/(\text{LaAlO}_3)_3$  heterostructures using RIXS<sup>1</sup>**, GILBERTO FABBRIS, Brookhaven Natl Lab, ANKIT S. DISA, SOHAB ISMAIL-BEIGI, FREDERICK J. WALKER, CHARLES H. AHN, Yale University, JONATHAN PELLICIARI, YAobo HUANG, THORSTEN SCHMITT, Swiss Light Source, PSI, LEI XU, LIVIU HOZOI, JEROEN VAN DEN BRINK, IFW Dresden, MARK DEAN, Brookhaven Natl Lab — A novel approach for manipulating the 3d state in transition metal oxide heterostructures has emerged with the growth of trilayer nickelate  $\text{LaTiO}_3/\text{LaNiO}_3/(\text{LaAlO}_3)_3$  (LTNAO) (Disa et al., PRL 114 026801 (2015)). This heterostructure induces a striking reconstruction of the  $\text{LaNiO}_3$  electronic structure, which is due to a combination of charge transfer from Ti's 3d state and octahedral elongation along the *c* axis. We use resonant inelastic x-ray scattering (RIXS) experiments at Ni  $L_{2,3}$  and O K edges to spectroscopically resolve the LTNAO electronic structure. Surprisingly, our results show that the octahedral elongation generates minor changes in crystal fields at Ni's 3d state compared to bulk  $\text{LaNiO}_3$ . Instead, heterostructuring creates an anisotropic reconstruction of the Ni 3d - O 2p hybridization. The  $x^2-y^2$  orbital is significantly more hybridized with O p, leading to a  $3z^2-r^2/x^2-y^2$  hole ratio of  $\sim 0.55$  and large orbital polarization as measured by x-ray absorption spectroscopy. This work establishes RIXS as an ultra-sensitive probe of complex oxide heterostructures.

<sup>1</sup>Work at BNL was supported by the US Department of Energy under Award no DEAC02-98CH10886 and under Early Career Award no 20878.

**9:24AM X30.00006 Electronic Structure near the Interface of Complex Oxide Heterostructure  $\text{SmTiO}_3/\text{SrTiO}_3$** , RYO MORI, University of California, Berkeley and Lawrence Berkeley National Laboratory, BRANDON ISAAC, PATRICK MARSHALL, University of California, Santa Barbara, JONATHAN DENLINGER, Lawrence Berkeley National Laboratory, SUSANNE STEMMER, University of California, Santa Barbara, ALESSANDRA LANZARA, University of California, Berkeley and Lawrence Berkeley National Laboratory — Quantum wells created from oxide heterostructures induce quantum confinement systems at the heterostructure interface, which show unique properties, such as strong electron correlation, two-dimensional superconductivity, high carrier densities and mobility, and/or magnetism. The rare earth titanate,  $\text{SmTiO}_3$ , and the transition metal oxide,  $\text{SrTiO}_3$ , create such confined electron systems at their interface, which has a controllable quantum well length by changing the number of SrO layers in  $\text{SrTiO}_3$ . By Varying the number of SrO layers, we will present the layer-dependent electronic structure of the  $\text{SmTiO}_3/\text{SrTiO}_3$  interface system from angle-resolved photoemission spectroscopy (ARPES) measurements and discuss these results in terms of strong correlations.

**9:36AM X30.00007 Probing Momentum-Resolved Orbital Polarization at the Oxide Interfaces with SW-ARPES**, ARIAN ARAB, Department of Physics, Temple University, SLAVOMIR NEMSAK, Peter-Grunberg-Institut PGI-6, Forschungszentrum Julich, GIUSEPPINA CONTI, Department of Physics, UC Davis; Materials Sciences Division, LBNL, VLADIMIR STROCOV, Swiss Light Source, PSI, MARK HUIJBEN, University of Twente, JAN MINAR, Department Chemie, Universitat Munchen; University of West Bohemia, CHARLES FADLEY, Department of Physics, UC Davis; Materials Sciences Division, LBNL, ALEXANDER GRAY, Department of Physics, Temple University — Interface electronic structure is critical to the functional properties of strongly-correlated multilayer systems such as the  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3/\text{SrTiO}_3$  heterostructure, a promising candidate for a magnetic tunnel junction. Recently it was demonstrated that for periodic superlattice samples controllable depth selectivity in angle-resolved photoemission spectroscopy (ARPES) can be accomplished by setting up an x-ray standing-wave (SW) field in the sample and translating it vertically along the surface normal by varying x-ray incidence angle. Here, by varying polarization of the incident x-rays we add orbital sensitivity to SW-ARPES, thus allowing us to distinguish momentum-resolved electronic dispersions for the electronic states of different symmetries (e.g.  $x^2-y^2$  and  $3z^2-r^2$ ). Distinctly different momentum-resolved orbital polarization maps are obtained for the bulk-like and interface-like Mn 3d electronic states. The results are compared to state-of-the-art first-principles calculations. Future directions and applications are discussed.

**9:48AM X30.00008 Interface properties of  $\text{LaCrO}_3/\text{SrTiO}_3$  superlattices studied by standing-wave excited photoemission spectroscopy**, CHENG-TAI KUO, SHIH CHIEH LIN, Univ of California - Davis, RYAN COMES, Pacific Northwest National Laboratory, JULIEN RAULT, SOLEIL, PETER SUSHKO, Pacific Northwest National Laboratory, AMINA TALEB-IBRAHIMI, SOLEIL, SCOTT CHAMBERS, Pacific Northwest National Laboratory, CHUCK FADLEY, Univ of California - Davis, CHUCK FADLEY TEAM, SCOTT CHAMBERS TEAM, AMINA TALEB-IBRAHIMI TEAM — The interface between  $\text{LaCrO}_3$  (LCO) and  $\text{SrTiO}_3$  (STO) is of interest due to a polar discontinuity, built-in potential [1] and recent evidence of polarization in STO-LCO superlattices (SLs). However, an unambiguous depth profiling of the polarization-induced electronic structure has not been attempted. We here present the quantitative determination of the depth profiles of composition, charge state, potential and momentum-resolved electronic structure for LCO/STO SLs using resonant-excitation x-ray standing wave (SW) photoemission spectroscopy. By varying the incident angle and photon energy around the Bragg condition, the standing wave was moved vertically through the interfaces, giving us the ability to focus on either surface, interface or bulk electronic properties. We are thus able to decompose the valence band spectra into layer-specific contributions for both STO and LCO. We also present momentum-resolved electronic structure using resonant SW angle-resolved photoemission spectroscopy (SW-ARPES) [2] and compare these results to DFT theory for the band dispersions of each layer of the SL. [1] S. Chambers et al. PRL, 107, 206802 (2011) [2] A.X. Gray et al., EPL 104, 17004 (2013)

**10:00AM X30.00009 Built-in electric field and polarization in  $\text{LaCrO}_3\text{-SrTiO}_3$  superlattices**, PETER SUSHKO, RYAN COMES, STEVEN SPURGEON, PHUONG-VU ONG, Pacific Northwest National Laboratory, STEVE HEALD, Argonne National Laboratory, SHIH-CHIEH LIN, CHENG-TAI KUO, CHUCK FADLEY, UC Davis, SCOTT CHAMBERS, Pacific Northwest National Laboratory — Superlattices combining ferroelectric and non-polar materials exhibit an intriguing induced polarization in the non-ferroelectric phase, such as  $\text{SrTiO}_3$  (STO). However, there has been no report of a superlattice where two non-ferroelectric materials combine to produce bulk polarization. We present studies of STO- $\text{LaCrO}_3$  (LCO) superlattices and show that by controlling interfacial termination between layers we can induce a ferroelectric-type polarization in STO. Density functional theory (DFT) predictions show that by alternating terminations between positively charged  $\text{TiO}_2\text{-LaO}$  and negative  $\text{CrO}_2\text{-SrO}$  interfaces a polarization is induced in each material. Using molecular beam epitaxy, we have synthesized superlattices with such interfaces and a built-in electric field is observed using x-ray photoelectron spectroscopy. X-ray absorption spectroscopy and electron microscopy confirmed these results and were used to estimate the polarization within the STO layers. Our results agree well with the DFT predictions for the cation displacements and induced polarization. We also present models of the band dispersion to quantify the electronic structure in each of the STO and LCO layers.

**10:12AM X30.00010 XPS characterization scheme for phase-pure epitaxial  $\text{NbO}_2$** , TOBIAS HADAMEK, AGHAM POSADAS, ALEX DEMKOV, University of Texas at Austin —  $\text{NbO}_2$  shows a semiconductor-to-metal transition with an associated structural transition of Peierls type.  $\text{NbO}_2$  and  $\text{Nb}_2\text{O}_5$  or mixtures thereof have also shown electrically induced insulator-to-metal transitions. To shed light on the nature of the electrically induced insulator-to-metal transition it is important to grow high phase purity  $\text{NbO}_2$  and  $\text{Nb}_2\text{O}_5$  and compare electrical measurements with mixed niobium oxides and with different electrode materials. Processing  $\text{NbO}_2$  and avoiding surface oxidation requires ultra-high vacuum (UHV) conditions. Niobium oxide thin films where grown in UHV by molecular beam epitaxy on 111-oriented STO substrates and analyzed by X-ray photoelectron spectroscopy (XPS). It was shown that the  $\text{NbO}_2$  3d core level spectrum exhibits an asymmetric spin-orbit peak pair with more spectral weight on the high binding energy side. Based on the shape of the Nb 3d core levels, peak positions relative to the oxygen O 1s peak, and the valence band shape and height ratio of the niobium  $4d_{xy}$  split-off band to the oxygen 2p band, an identification scheme for  $\text{NbO}_2$  by XPS was devised. Complementary the  $\text{NbO}_2$  phase was confirmed by reflection high-energy electron and x-ray diffraction analysis.

**10:24AM X30.00011 Thickness-dependent structure variation and novel electronic properties of  $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$  film on  $\text{SrTiO}_3$  (001) substrate<sup>1</sup>**, LINA CHEN, ZHEN WANG, JISUN KIM, GAOMIN WANG, HANGWEN GUO, MOHAMMAD SAGHAYEZHIANE, WARD PLUMMER, JIANDI ZHANG, Louisiana State University, JING TAO, YIMEI ZHU, Brookhaven National Laboratory — In principle,  $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$  (LSMO) is a half metal, which exhibits colossal magnetoresistance. However, it has been observed that the transport properties of LSMO thin films depends on their thickness. By combining *in-situ* scanning tunneling spectroscopy (STS), X-ray photoelectron spectroscopy, and low energy electron diffraction, as well as *ex-situ* scanning transmission electron microscopy, we have studied the structure-property relationship of LSMO on  $\text{SrTiO}_3$ (001) as a function of film thickness and temperature. Studying the electronic properties by STS, we found that LSMO films have the novel zero current bias shifts at low temperature, further enhanced by photons, which can be related to the charging of dielectric layer near the interface and polar surface effect. To figure out it, STS thickness and temperature dependence were systematically studied. Furthermore, film thickness-dependent structure and stoichiometry variation were determined, and their effect to the zero current bias shifts will be discussed.

<sup>1</sup>Supported by U.S. DOE under Grant No. DOE DE-SC0002136

**10:36AM X30.00012 Aberration Corrected Scanning Transmission Electron Microscopy of  $(\text{Ca}, \text{Sr})\text{Fe}_2\text{O}_5$  Brownmillerite superlattices<sup>1</sup>**, DEBANGSHU MUKHERJEE, The Pennsylvania State University, GREG STONE, United States Army Armament Research, Development and Engineering Center, EUN JU MOON, JOSHUA YOUNG, Drexel University, VENKATRAMAN GOPALAN, The Pennsylvania State University, JAMES RONDINELLI, Northwestern University, STEVEN MAY, Drexel University, NASIM ALEM, The Pennsylvania State University — The brownmillerite phase  $\text{A}_2\text{B}_2\text{O}_5$  consists of ordered oxygen vacancies in alternate perovskite layers forming chiral tetrahedral chains. The handedness of these tetrahedral chains control the polarization of the structure. The current study focuses on 1-1 brownmillerite superlattices grown on a  $\text{SrTiO}_3$  substrates using molecular beam epitaxy. The B-site in this structure is iron throughout the superlattice film, while the A-site alternates between calcium and strontium in the superlattice layers. In this study, we use atomic resolution aberration corrected scanning transmission electron microscopy (STEM) to investigate the structure and chemistry of the film-substrate interface as well as the chemical structure of the superlattice. Atom positions are determined to measure displacement vectors of A-site cations in the superlattice structure.

<sup>1</sup>D.M., G.A.S., V.G. and N.A. were supported by the National Science Foundation under grant No. DMR-1420620. E.J.M. and S.J.M. were supported by the National Science Foundation under grant No. DMR-1151649.

**Friday, March 18, 2016 8:00AM - 11:00AM —**

**Session X31 DCP GSOFT: Nanoconfined and Interfacial Water** 331 - Nicolas Giovambattista, CUNY

**8:00AM X31.00001 TBA**, SHEKHAR GARDE, Rensselaer Polytechnic University — No abstract available.

**8:36AM X31.00002 Water in nanoconfined spaces: from superhydrophobicity to Janus interfaces to curved hydrophobes**, ALENKA LUZAR, Department of Chemistry, Virginia Commonwealth University — The talk will review our theoretical and molecular simulation works that predict and elucidate thermodynamic driving forces and kinetic factors pertinent to nanoconfined water. Retrieval of superhydrophobicity on nanostructured surfaces will be one example. We will discuss a new mechanism for water mediated (Laplace) attraction between solutes with contrasting polarities (Janus interfaces) that can play an important role by enabling adhesion between polar and nonpolar particles in both, biophysical systems and heterogeneous nanomaterials. Other examples will show how macroscopic thermodynamics remarkably works down to molecular lengthscales. We will elucidate why water-induced interaction between curved hydrocarbon surfaces can be repulsive.

**9:12AM X31.00003 Behavior of aqueous solutions in hydrophobic confinement studied using molecular simulations**, SUMIT SHARMA, Ohio University — Biological processes, such as formation of cell membranes, vesicles and folding of protein molecules, entail formation of a predominantly hydrophobic interior devoid of water. These processes occur in crowded aqueous environments comprising of amino acids, carbohydrates, ionic species, protein molecules, etc. Kinetics of these processes involve drying of hydrophobic pockets. Previous studies reveal that the kinetics of evaporation of water in hydrophobic confinement significantly slow down as the confinement gap increases. Presumably, the constituents of aqueous environment in biological systems modulate the kinetics of evaporation of confined water. In this work, we employ forward flux sampling in molecular dynamics simulations to study the role of solutes at different concentrations in modulating the kinetics and mechanism of evaporation of water under hydrophobic confinement. The results of these simulations will be useful for understanding optimum conditions for protein folding and other biological self-assembly processes.

**9:24AM X31.00004 Quasi-Elastic Neutron Scattering Study of Characteristic Features of Water Dynamics in Confined Geometries**, SOULEYMANE DIALLO, Oak Ridge National Laboratory Oak Ridge, TN, USA, NARESH OSTI, Oak Ridge National Laboratory, Oak Ridge, TN, USA, ALEXANDRA COTE, University of Miami, FL, USA, EUGENE MAMONTOV, ANIBAL RAMIREZ-CUESTA, DAVID WESOLOWSKI, Oak Ridge National Laboratory, Oak Ridge, TN, USA — Water trapped in restricted environments is ubiquitous in nature and known to influence many biochemical and geophysical processes. Understanding the structural and dynamical properties of nano-confined water (very different than those of the bulk phase) is thus of key fundamental interests. We present a survey of various quasi-elastic neutron (QENS) studies of nano-confined water, which we further analyzed in the context of a proposed universal scaling law. Using this predictive law, we specifically investigate how the diffusive behavior of water changes with changing hydration level, confinement size, or geometry. Finally, we present our recent QENS results of water in nanoporous media evaluated using this scaling law.

**9:36AM X31.00005 Salt Solutions in Carbon Nanotubes: The Role of Cation- $\pi$  Interactions<sup>1</sup>**, TUAN ANH PHAM, Lawrence Livermore Natl Lab, GOLAM MORTUZA, School of Mechanical and Materials Engineering, Washington State University, BRANDON WOOD, EDMOND LAU, TADASHI OGITSU, Lawrence Livermore Natl Lab, STEVEN BUCHSBAUM, ZUZANNA SIWY, Department of Physics and Astronomy, University of California, Irvine, FRANCESCO FORNASIERO, ERIC SCHWEGLER, Lawrence Livermore Natl Lab — Understanding the structure of aqueous electrolytes at interfaces is essential for predicting and optimizing device performances for a wide variety of emerging energy and environmental technologies. In this work, we investigate the structure of two common salt solutions, NaCl and KCl, at a hydrophobic interface within narrow carbon nanotubes (CNTs). Using a combination of first-principles and classical molecular dynamics simulations, we find that the solvation structure of the cations in the CNTs can deviate substantially from the conventional weakly interacting hydrophobic picture. Instead, interactions between solvated ions and the  $\pi$ -orbitals of the CNTs are found to play a critically important role, with the ion solvation structure ultimately determined by a subtle interplay between cation- $\pi$  interactions and the intrinsic flexibility of the solvation shell. In the case of  $\text{K}^+$ , these effects result in an unusually strong propensity to partially desolvate and reside closer to the carbon wall than either  $\text{Na}^+$  and  $\text{Cl}^-$ , in sharp contrast to the known ion ordering at the water-vapor interface.

<sup>1</sup>This work was performed under the auspices of the U.S. Department of Energy by LLNL under Contract DE-AC52-07NA27344.

**9:48AM X31.00006 Confined water between two graphene layers**, FRANCOIS PEETERS, MARIO SOBRINO FERNANDEZ, MEHDI NEEK-AMAL, University of Antwerp, Dept. of Physics, 2020 Antwerp, CONDENSED MATTER THEORY TEAM — Water confined between two layers with a separation of a few Angstrom forms a layered two-dimensional ice structure. Using large scale molecular dynamics simulations with the adoptable ReaxFF interatomic potential we found that monolayer ice with a rhombic-square structure nucleates between graphene layers which is non-polar and non-ferroelectric. We provide different energetic considerations and H-bonding results that explain the inter-layer and intra-layer properties of two-dimensional ice. The controversial AA-stacking found experimentally [G. Algara-Siller et al. Nature 519, 443445 (2015)] is consistent with our minimum energy crystal structure of bilayer ice. Furthermore, we predict that odd-number of layers of ice has the same lattice structure as monolayer ice, while even number of ice layers exhibit the square ice AA-stacking of bilayer ice. We predict that an inplane electric field polarizes the water molecules resulting in distinct-ferroelectricity. Electrical hysteresis in the response of the total dipole moment of monolayer ice is found

**10:00AM X31.00007 Structure, Spectroscopy and Thermodynamics at the Water – Graphene Interface**<sup>1</sup>, TOD PASCAL, The Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA, CRAIG SCHWARTZ, Stanford Synchrotron Radiation Laboratory, Menlo Park, CA 94025, USA, KEITH LAWLER, Department of Chemistry, University of Nevada Las Vegas, Las Vegas, NV 89154, USA, DAVID PRENDERGAST<sup>2</sup>, The Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA — The recent discovery of an ordered two-dimensional phase of water with a square lattice between graphene sheets has led to tremendous interest in the structure of confined water, particularly under pressure.[1] Despite being recently discovered, this finding is fiercely being debated, with other researchers suggesting that the observed structures is due to the presence of NaCl, while various theoretical models predict the formation of water ice between graphene only under enormous external pressures.[1-3] Herein, by examining the EELS data, combined with simulated spectroscopy calculations and molecular dynamic simulations, we examine the thermodynamic properties of nano-encapsulated water, and demonstrate how charge transfer and chemical defects alters the phase diagram. [4]

1. Algara-Siller, G. et al., Nature 519, 443–445 (2015).
2. Mario, S. F., Neek-Amal, M. & Peeters, F. M., arXiv:1509.08242 [cond-mat] (2015)
3. Jiao, S. & Xu, Z., arXiv:1509.07215 [cond-mat] (2015)
4. Schwartz, C. et al., In preparation

<sup>1</sup>This work was performed as a user project at the Molecular Foundry, Lawrence Berkeley National Laboratory supported by the Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231

<sup>2</sup>Lawrence Berkeley Natl Lab

**10:12AM X31.00008 ABSTRACT WITHDRAWN —**

**10:24AM X31.00009 Probing the water on chemically heterogeneous surface: interfacial-structural analysis for surface charge distribution**, SUCHEOL SHIN, ADAM WILLARD, Massachusetts Institute of Technology — We introduce the novel method for predicting the charge distribution of chemically heterogeneous surface, but reconstructed from the perspective of the interfacial water molecules. Our approach is to analyze the response of water to a disordered surface and infer from that response the heterogeneous distribution of surface charge. We accomplish this using a framework that is based on a probabilistic description of waters interfacial molecular structure and maximum likelihood estimation. This framework allows to deduce the apparent charge that is most congruently represented by the set of water configurations over the particular region of a surface. We demonstrate that the estimated charge distribution is consistent to the actual distribution for a static model substrate and hence that our method can be applied to investigate a dynamic fluctuating substrate such as the surface of a hydrated protein. This novel technique provides the useful information that can reflect the influence of fluctuations in the structure of biomolecule.

**10:36AM X31.00010 Enhanced configurational entropy in high-density nanoconfined bilayer ice**, FABIANO CORSETTI, Department of Materials and the Thomas Young Centre for Theory and Simulation of Materials, Imperial College London, London SW7 2AZ, United Kingdom, JON ZUBELTZU, EMILIO ARTACHO, CIC nanoGUNE, 20018 Donostia-San Sebastian, Spain — Understanding the structural tendencies of nanoconfined water is of great interest for nanoscience and biology, where nano/micro-sized objects may be separated by very few layers of water. We present a study of water confined to a 2D geometry by a featureless, chemically neutral potential, in order to characterize its intrinsic behaviour. We use molecular dynamics simulations with the TIP4P/2005 potential, combined with density-functional theory calculations with a non-local van der Waals density functional and an *ab initio* random structure search procedure. We propose a novel kind of crystal order in high-density nanoconfined bilayer ice. A first-order transition is observed between a low-temperature proton-ordered solid and a high-temperature proton-disordered solid. The latter is shown to possess crystalline order for the oxygen positions, arranged on a close-packed triangular lattice with AA stacking. Uniquely amongst the ice phases, the triangular bilayer is characterized by two levels of disorder (for the bonding network and for the protons) which results in a configurational entropy twice that of bulk ice.

**10:48AM X31.00011 Determination of interfacial properties using a PC-SAFT based classical density functional theory for fluid mixtures of industrial interest**, JIAN YANG, DIEGO CRISTANCHO, RAKESH SRIVASTAVA, The Dow Chemical Company — In this paper, a recent development of a PC-SAFT based classical density functional theory (DFT) is applied to the determination of interfacial properties of pure fluids and mixtures of industrial interest. Initially, the DFT formalism is described and the methodology for the property calculations explained. The consistency of this approach allows the determination of interfacial properties for fluids using the PC-SAFT equation of state parameters determined from bulk physical property data, such as vapor-liquid-equilibrium and densities. This methodology is an excellent alternative for the predictions of interfacial property of fluids and extrapolation to high pressure ranges where experimental measurements becomes challenging.

**Friday, March 18, 2016 8:00AM - 10:48AM —**

Session X32 DCP: Plasmonics and Beyond IV: Single particle dynamics 332 - Hrvje Petek, University of Pittsburgh

**8:00AM X32.00001 Plasmonic nano-focused four-wave mixing for femtosecond nano-imaging**, VASILY KRAVTSOV, RONALD ULBRICHT, University of Colorado at Boulder, JOANNA ATKIN, University of North Carolina at Chapel Hill, MARKUS RASCHKE, University of Colorado at Boulder — We experimentally demonstrate efficient and broadband nonlinear optical four-wave mixing (FWM) in a deep sub-wavelength volume using adiabatic nanofocusing of surface plasmon polaritons (SPPs). We couple few-femtosecond laser pulses into SPPs that propagate and experience nanofocusing on a sharp Au tip, and detect blue-shifted intra-pulse FWM response of the nanofocused plasmons. Due to the asymptotic mode volume compression and resulting steep increase in SPP field enhancement when approaching the tip apex, the nonlinear signal is highly localized in a nanoscopic volume at the apex. The simultaneous enhanced generation and further FWM field compression into the tip apex provides for a highly sensitive nano-probe for ultrafast near-field microscopy and spectroscopy. We demonstrate the use of the nano-localized nonlinear frequency conversion to spatially resolve few-femtosecond dynamics in ultrafast coherent spatio-temporal nano-imaging of the localized plasmonic modes of an inhomogeneous Au layer edge. Our results are supported by simulations and provide a perspective for an all-optical implementation of the novel multidimensional nano-spectroscopies.

**8:12AM X32.00002 Femtosecond Snapshots of quantum mechanics at work in plasmonic nano-structures.**<sup>1</sup>, FABRIZIO CARBONE, EPFL — Ultrafast Transmission Electron Microscopy enabled a new technique (Photon-Induced Near Field Electron Microscopy, PINEM), capable of controlling electromagnetic fields confined on the surface of nanostructures and image their properties with nm-resolution in direct space and fs resolution in time. In this presentation, we will show some recent results where the standing wave formed by the plasmonic field confined on the surface of one silver nano-wire was imaged together with its energy exchange with the imaging electrons. In these results, both the interference and the quantization of the plasmonic near field could be imaged simultaneously, revealing both a quantum and a classical aspect of the electromagnetic field in one snapshot. The implications of these results will be discussed, and we will also present new ideas and methodologies to go beyond such an experiment and image the interaction between single electrons and single plasmons. We will also show that shaping the electron density in a thin film via light pulses is possible by taking advantage of the plasmon-plasmon interference and the ability of light polarization to control the excitation of different plasmonic field geometries in ad hoc designed nanostructures. Movies of the propagation of plasmons will also be presented, providing insights into their speed, propagation losses and the effect of confinement.

<sup>1</sup>this work was supported by an ERC grant USED

**8:48AM X32.00003 Ultrafast Nonlinear Plasmonics of Single Nano-Objects**, NATALIA DEL FATTI, Institut Lumiere Matiere, CNRS - Universite Lyon 1 — Investigating, understanding and modeling the physical properties of nano-objects are intense fields of research. Of particular interest are metal-based nano-objects, where their morphology and environment dependent surface plasmon resonances (SPR) have been extensively exploited to design new optical systems. As a SPR is associated to electromagnetic local field enhancement in the nano-object, it also leads to enhancement of its optical nonlinearity, opening many possibilities for investigating fundamental processes at nanoscale [1]. Most of these studies were performed on large ensembles of nano-objects, providing mean information which impedes detailed comparison between experimental data and theoretical models. With the advance of single nanoparticle spectroscopy methods, the linear and nonlinear responses of a single nano-object can now be addressed, which, associated to determination of its morphology by electron microscopy, opens the way to their quantitative modeling [2]. In this context we discuss experimental and theoretical investigations of the ultrafast response of individual model nano-objects, either formed by a single particle (gold nanorod) or by two particles at a nanometric distance (gold-silver nano-dimer). Results obtained in gold nanorods are in excellent quantitative agreement with a model computing the change of the metal dielectric function due to ultrafast electron heating and relaxation. This shows that the nonlinear response of a metal nano-object can be fully described as that of the bulk metal enhanced by plasmonic effects. Extension of these studies to more complex nano-objects, as nano-dimers formed by two different materials, permits analysis of the impact of their interaction. We demonstrate here the existence of Fano effect in the absorption of a single Ag-Au dimer, experimentally proving previous theoretical predictions [3]. Furthermore, we show that ultrafast pump-probe nonlinear spectroscopy permits to selectively address at nanoscale only one of the components of a dimer, paving the way toward quantitative investigations of energy and charge exchanges in multi-material nano-objects. [1] F. Vallée and N. Del Fatti, in "Plasmonics: theory and applications", eds. T.Shahbazyan & M.Stockman, Springer, p. 167 (2013) [2] A. Crut, P. Maioli, N. Del Fatti and F. Vallée, Chem. Soc. Rev. **43**, 3921 (2014) [3] G. Bachelier, I. Russier-Antoine, E. Benichou, C. Jonin, N. Del Fatti, F. Vallée, P.F. Brevet, Phys. Rev. Lett. **101**, 197401 (2008).

**9:24AM X32.00004 Dirac single particle and plasmon excitations in topological insulators**, STEFANO LUPI, Department of Physics, Sapienza University of Rome — Topological Insulators (TIs), like Bi<sub>2</sub>Se<sub>3</sub> and Bi<sub>2</sub>Te<sub>3</sub>, are one of the most intriguing issues at focus in Condensed Matter Physics. TIs exhibit a band gap in the bulk like ordinary insulators, but have intrinsic 2D conducting states on their edge and surface. This means that the topology, associated with the electronic wavefunctions of the system, changes discontinuously when passing from the bulk to the surface. The edge states arise from a strong spin-orbit coupling, and they are backscattering protected, i.e. not sensitive to disorder (except that coming from magnetic impurities). Such as graphene, TIs surface charge transport is carried out by Dirac fermions, with a very high surface carrier density ( $n \geq 10^{13} \text{ cm}^{-2}$ ), compared to typical values on metal surfaces. Apart single particle excitations, Dirac fermions in TIs sustain exotic plasmons (collective) modes whose properties of tunability and temperature dependence can be used for photonics applications at the nanoscale. Moreover, unlike plasmons in metals, Dirac plasmons in TIs are expected to be strongly affected by an external magnetic field B due to fact that the cyclotron frequency is comparable to the plasmon frequency, in particular when plasmons are engineered in the terahertz region of the electromagnetic spectrum. In this talk, after a general review on the properties of Topological Insulators, I will discuss the terahertz linear response of Dirac plasmons in TIs and their behavior under a strong magnetic field up to 30 T. The appearance of strong non-linear optical effects, when the THz electric field reaches values on the order of 1 MV/cm, will be also discussed. In the second part of the talk, I will discuss the sub-ps dynamics of Dirac single-particle and collective excitations as measured by optical-pump THz-probe experiments. Both the steady state and time-resolved experiments provide a unifying picture of single particle and collective electronic excitations in Topological Insulators.

**10:00AM X32.00005 Quantum Plasmonics with Free Electrons**, JAVIER GARCIA DE ABAJO, ICFO - Institut de Ciències Fotoniques, Barcelona, Spain — Fast electrons offer the means to excite and probe plasmons with an unparalleled combination of space and energy resolutions. In particular, electron energy-loss and cathodoluminescence spectral microscopies are widely used to obtain snapshots of these excitations. Additionally, access to ultrafast plasmon dynamics is possible by recording photoelectrons excited with femtosecond light pulses, while recent experiments demonstrate optical pumping followed by electron-beam probing with similar temporal resolution. In this talk, we will review recent highlights of these techniques and present a unified theoretical description. We will further discuss some exciting phenomena enabled by the quantum nature of the electron-plasmon interaction, including quantum nonlinearities, electron-plasmon entanglement, and vacuum fluctuations. Emphasis will be placed on the potential application of these phenomena for improving and extending spectrally resolved electron microscopy, as well as for on-demand creating and probing of plasmons in integrated devices.

**10:36AM X32.00006 ABSTRACT MOVED TO M1.000376 —**

**Friday, March 18, 2016 8:00AM - 11:00AM —**

**Session X33 DPOLY FIAP: Organic Electronics and Photonics - Organic Electronic Devices**

336 - Lei Zhu, Case Western University

**8:00AM X33.00001 Charge Transport Properties in Polymer Brushes.** , MARK MOOG, FRANK TSUI, IAN VONWALD, WEI YOU, University of North Carolina at Chapel Hill — Electrical transport properties in poly(3-methyl)thiophene (P3MT) brushes have been studied. The P3MT brushes correspond to a new type of surface-tethered, vertically oriented conjugated molecular wires, sandwiched between two metallic electrodes to form the electrode-molecule-electrode (EME) devices. P3MT is a highly conjugated polymer, a "workhorse" material for organic electronics and photonics. The P3MT brushes were grown on ITO surfaces with controlled length (between 2 and 100 nm). The top electrodes were transfer-printed Au films with lateral dimensions between 200 nm and 50  $\mu\text{m}$ . I-V and differential conductance measurements were performed using conductive AFM and 4-terminal techniques. Tunneling and field-emission measurements in EME devices with molecular lengths < 5 nm show HOMO mediated direct hole tunneling with energy barriers of 0.3 and 0.5 eV at the respective interfaces with ITO and Au. The transport properties in longer brushes are indicative of the two quasi-Ohmic interfaces with a characteristic offset in the conductance minimum of 0.12 V biased toward the ITO. Temperature dependent parameters have been examined at various molecular lengths. The drift mobility and the interplay between intra- and intermolecular transport have been investigated.

**8:12AM X33.00002 Hall effect and band-like carrier transport in high mobility polymer transistors** , YU YAMASHITA, The University of Tokyo, FELIX HINKEL, TOMASZ MARZALEK, WOJCIECH ZAJACZKOWSKI, WOJCIECH PISULA, MARTIN BAUMGARTEN, Max Planck Institute for Polymer Research, HIROYUKI MATSUI, The University of Tokyo, KLAUS MLLEN, Max Planck Institute for Polymer Research, JUN TAKEYA, The University of Tokyo, PROF. TAKEYA GROUP TEAM, PROF. MLLEN GROUP TEAM — A microscopic understanding of charge carrier transport in polymeric semiconductors is essential to improve the state of the art of flexible or printed electronic devices. In particular, thin-film field-effect transistors based on donor-acceptor polymers are in the focus of current literature reaching high charge-carrier mobility. In this work, we demonstrate the Hall effect and the temperature dependence of the charge carrier mobility based on uniaxially ordered CDT-BTZ donor-acceptor copolymer films. Uniaxially ordered films of CDT-BTZ with hexadecyl (C16) and eicosyl (C20) sidechains showed mobility of 5.6  $\text{cm}^2/\text{Vs}$  and 11.4  $\text{cm}^2/\text{Vs}$  respectively. The activation energy of the mobility decreased with the increasing carrier density, and finally the negative temperature dependence of the mobility was observed. Both polymers showed Hall effect, which also indicates the presence of extended electronic states. The temperature and carrier density dependence will be further discussed in the presentation.

**8:24AM X33.00003 ABSTRACT WITHDRAWN —**

**8:36AM X33.00004 Growth and characterization of organic ferroelectric croconic acid thin films<sup>1</sup>** , XUANYUAN JIANG, HAIDONG LU, YUEWEI YIN, AXEL ENDERS, ALEXEI GRUVERMAN, XIAOSHAN XU, Univ of Nebraska - Lincoln — Using vapor phase evaporation, we have studied the growth of the croconic acid (CCA) thin films, at various conditions such as temperature, thickness, growth speed, and substrates. The morphology of thin film was measured by atomic force microscopy (AFM); the ferroelectric property was confirmed by piezoresponse force microscopy (PFM). A critical thickness of 40 nm and optimal temperature of -30 celsius were found for continuous films, while the substrate and growth speed are found to play a minimal role. According to the reflection high energy electron diffraction (RHEED), the CCA films are polycrystalline. For a 40 nm continuous film, the roughness is about 3 nm, while the coercive voltage for the ferroelectric domain switching is approximately 7V. This is the first molecule ferroelectric thin film. The successful growth of continuous CCA films enhances the applications potential of CCA, which is a molecular crystal of ferroelectricity.

<sup>1</sup>Supported by NSF through UNL MRSEC (DMR-1420645)

**8:48AM X33.00005 Enhance the lifetime and bias stress reliability in organic vertical transistor by UV/Ozone treatment** , HUNG-CHENG LIN, MING-YU CHANG, HSIAO-WEN ZAN, HSIN-FEI MENG, National Chiao Tung University, Taiwan, YU-CHIANG CHAO, Chung-Yuan Christian University, Taiwan — In this paper, we use UV/Ozone treatment to improve the lifetime and bias stress reliability of organic transistor with vertical channel. Even if vertical organic transistor exhibits better bias stress reliability than organic field effect transistor (OFET) due to bulk conduction mechanism, poor lifetime performance is still a challenge. Adding octadecyltrichlorosilane (OTS) to treat the vertical channel can reduce the trapping state and hence improve the bias stress ability. However, off-current is much higher after 6 days and lifetime performance is degraded. On the other hand, after 4000-s on-state bias stress, stable output current and on/off current ratio are demonstrated by using UV/Ozone to treat vertical channels. Threshold voltage shift is only -0.02 V which is much smaller than OFET with the same organic semiconductor material. Furthermore, the output current is also an order enhanced. Nevertheless, unlike device with OTS treatment, no obvious degradation is observed for UV/Ozone treated devices even after 170 days. With UV/Ozone treatment, the output current, bias stress reliability and lifetime were all improved. It makes vertical transistor become a promising device for the further application in display technology and flexible electronics.

**9:00AM X33.00006 Gate-controlled energy barrier at a graphene/molecular semiconductor junction** , S. PARUI, L. PIETROBON, D. CIUDAD, S. VELEZ, X. SUN, P. STOLJAR, CIC nanoGUNE, 20018 Donostia-San Sebastian, Basque Country, Spain, F. CASANOVA, L. E. HUESO, CIC nanoGUNE, 20018 Donostia-San Sebastian, Basque Country, Spain; and IKERBASQUE, Basque Foundation for Science, 48011 Bilbao, Basque Country, Spain — The formation of an energy barrier at a metal/molecular semiconductor junction is both a ubiquitous phenomenon as well as the subject of intense research in order to improve the performance of molecular semiconductor-based electronic and optoelectronic devices. For these devices, a junction with a large energy barrier provides rectification, leading to a diode behavior, whereas a relatively small energy barrier provides nearly-ohmic behavior, resulting in efficient carrier injection (extraction) into the molecular semiconductor. Typically, a specific metal/molecular semiconductor combination leads to a fixed energy barrier; therefore, the possibility of a gate-controlled energy barrier is very appealing for advanced applications. Here [S. Parui *et al*, Adv. Fun. Mat. **25**, 2972 (2015)], we present a graphene/C<sub>60</sub> junction-based vertical field-effect transistor in which we demonstrate control of the interfacial energy-barrier such that the junction switches from a highly rectifying diode at negative gate voltages to a nearly-ohmic behavior at positive gate voltages and at room temperature. We extract an energy-barrier modulation of up to 660 meV, a transconductance of up to five orders of magnitude and a gate-modulated photocurrent.

**9:12AM X33.00007 Influence of Morphological Disorder on In- and Out-of-Plane Charge Transport in Conjugated Polymer Films** , BAN DONG, ANTON LI, PETER GREEN, University of Michigan — We report the unequal impacts of morphological disorder on in- and out-of-plane charge transport in thin films of poly(3-hexylthiophene) (P3HT) fabricated by both conventional spin-casting and the novel technique Matrix-Assisted Pulsed Laser Evaporation (MAPLE). MAPLE produces films with inhomogeneous globular subfeatures with dimensions on the order of 100 nm. Optical absorbance spectroscopy corroborates that MAPLE-deposited films are more energetically disordered, but possesses average conjugation lengths comparable to spin-cast P3HT. Both in- and out-of-plane carrier transport measurements of MAPLE-deposited films show characteristics that reflect a higher degree of energetic disorder and broadened density of states. Whereas in-plane carrier mobilities of MAPLE-deposited thin-film transistors are comparable to spin-cast analogues ( $8.3 \times 10^{-3} \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$  versus  $5.5 \times 10^{-3} \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ ), the out-of-plane mobilities of MAPLE-deposited samples are nearly an order of magnitude lower ( $4.1 \times 10^{-4} \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$  versus  $2.7 \times 10^{-3} \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ ). The unusual ensemble of properties and behaviors arising from the unique morphologies produced by MAPLE provide important perspectives on the extent to which disorder impacts different mechanisms of charge transport in conjugated polymers.

**9:24AM X33.00008 Polarization-induced transport in TIPS-pentacene field-effect transistors<sup>1</sup>**, AMRIT LAUDARI, SUCHI GUHA, University of Missouri, Columbia — The dielectric constant of polymer ferroelectric dielectrics can be tuned by changing the temperature, offering a platform for monitoring the changes in interfacial transport in organic field-effect transistors (FETs), as the polarization strength is tuned. Temperature dependent transport studies of FETs have been carried out from a solution-processed organic semiconductor, 6,13-bis(triisopropylsilyl)ethynylpentacene (TIPS-pentacene), using both ferroelectric and non-ferroelectric gate insulators. Non-polar dielectric based TIPS-pentacene FETs show a clear activated transport in contrast to the ferroelectric dielectric polymer, poly(vinylidene fluoride-trifluoroethylene) (PVDF-TrFE), where a negative temperature coefficient of the mobility is observed in the ferroelectric temperature range. We attribute the weak temperature-dependence of the charge carrier mobility to a polarization fluctuation driven transport resulting from a coupling of the charge carriers to the surface phonons of the polar dielectric. The negative coefficient of mobility ( $\frac{d\mu}{dT} < 0$ ) observed with ferroelectric dielectrics is not a signature of an extended-state conduction but rather denotes polarization fluctuation driven transport.

<sup>1</sup>This work was supported by National Science Foundation under Grant No. ECCS-1305642

**9:36AM X33.00009 Radical Polymer Utilization for Interfacial Improvement of Organic Field-Effect Transistors**, SEUNG HYUN SUNG, NIKHIL BAJAJ, JEFFREY RHOADS, GEORGE CHIU, BRYAN BOUDOURIS, Purdue University — Metal-semiconductor interfacial contact is one of the crucial factors for high-performance organic electronic device applications. In particular, the performance of organic field-effect transistors (OFETs) is critically dependent on the engineering of the interface between the organic semiconductor and the source/drain electrodes. Here, we modulate the performance of pentacene-based OFETs through the inclusion of a specific radical polymer, poly(2,2,6,6-tetramethylpiperidine-1-oxyl methacrylate) (PTMA), at the pentacene-gold electrode interface. Using a simple and fast inkjet printing method, the OFET performance is highly enhanced by the systematic deposition of a thin PTMA layer. The insertion of the radical polymer has an impact on the highly-improved OFET performance due to its redox charge transport ability and the amorphous nature allowing the stable growth of the pentacene. The synergistic effect facilitates the charge injection at the interface of the metal and organic semiconductor, resulting in the highly improved OFET performance. As such, the fundamental insights associated with radical polymers can be widened and their utilization as a highly-improved, low-cost interfacial modifier in myriad organic electronic devices is of great promise.

**9:48AM X33.00010 Small Molecule Doping of Radical Polymers for Enhanced Electronic Performance**, ADITYA BARADWAJ, SI HUI WONG, BRYAN BOUDOURIS, Purdue University — Radical polymers have emerged as a class of conducting polymers that show immense potential for solid state electronic applications. However, very little has been done to explore the small molecule doping of these materials for increased electrical performance. Here, we present the characterization of the charge transport ability of a model radical polymer, poly(2,2,6,6-tetramethylpiperidinyloxy methacrylate) (PTMA), doped with varying levels of the small molecule, 4-Acetamido-2,2,6,6-tetramethyl-1-oxopiperidinium tetrafluoroborate (TEMPO<sup>+</sup>ium). We demonstrate that the addition of the TEMPO<sup>+</sup>ium to PTMA thin films creates a distinct relationship between doping level and electrical conductivity. At optimal doping levels, we find that the electrical conductivity of PTMA thin films increases by over an order of magnitude. Furthermore, we illustrate the competing effects of electrical and ionic conductivity that exists in this system by probing the dependence of current on time in these thin films. Finally, we show that the TEMPO<sup>+</sup>ium doping greatly enhances the film quality of these typically brittle PTMA thin films. We anticipate that these findings will encourage novel methods to enhance the electrical performance of these open shell systems in the solid state.

**10:00AM X33.00011 Understanding the growth of organic semiconductors on semiconducting surfaces**, MINA YOON, CHANGWON PARK, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, BING HUANG, Beijing Computational Science Research Center, SEAN R. WAGNER, PENG PENG ZHANG, Michigan State University — A selective mechanism for tuning the molecule-substrate interaction has been a long sought after goal towards tailored molecular growth. Using first-principles theory and scanning tunneling microscopy, we show that by controlling the strength of orbital hybridization between phthalocyanine molecules and the deactivated Si surface via the selective p-d orbital coupling, we can tune the molecular ordering and molecular orientation at the hetero-interface. This mechanism offers a novel approach to balance the critical interactions, leading to controlled long-ranged ordered molecular growth [1]. [1] S.R. Wagner, B. Huang, C. Park, J. Feng, M. Yoon, and P. Zhang, Phys. Rev. Lett. 115, 096101 (2015). This work was supported by the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy and partly supported by the Materials Sciences and Engineering Divisions, Office of Basic Energy Sciences, U.S. Department of Energy.

**10:12AM X33.00012 Stencil Nano Lithography Based on a Nanoscale Polymer Shadow Mask: Towards Organic Nanoelectronics<sup>1</sup>**, SANG WOOK LEE, HOYEOL YUN, HAKSEONG KIM, KIRSTIE MCALLISTER, DONG HOON SHIN, Konkuk University, JUN SUNG KIM, POSTECH, SEUNGMOON PYO, WI HYOUNG LEE, Konkuk University, ELEANOR CAMPBELL, University of Edinburgh, NENM TEAM — A stencil lithography technique has been developed to fabricate organic-material-based electronic devices with sub-micron resolution. Suspended polymethylmethacrylate (PMMA) membranes were used as shadow masks for defining organic channels and top electrodes. Arrays of pentacene field effect transistors (FETs) with various channel lengths from 50  $\mu\text{m}$  down to 500 nm were successfully produced from the same batch using this technique. Electrical transport measurements showed that the electrical contacts of all devices were stable and the normalized contact resistances were much lower than previously studied organic FETs. Scaling effects, originating from the bulk space charge current, were investigated by analyzing the channel-length-dependent mobility and hysteresis behaviors. This novel lithography method provides a reliable means for studying the fundamental transport properties of organic materials at the nanoscale as well as enabling potential applications requiring the fabrication of integrated organic nanoelectronic devices.

<sup>1</sup>This work was supported by NRF

**10:24AM X33.00013 Ab initio studies of the optoelectronic properties of biphenyl derivatives in OLEDs<sup>1</sup>**, HOSSEIN HASHEMI, AVI BREGMAN, JAEHUN JUNG, MINSANG KWON, JINSANG KIM, JOHN KIEFFER, Univ of Michigan - Ann Arbor, KIEFFER GROUP TEAM, KIM GROUP TEAM — The influence of molecular conformation on electron relaxation and photophysical properties of a series of biphenyl derivatives have been investigated using density functional theory (DFT) and time-dependent DFT (TDDFT). The calculated absorption and emission properties of the series as well as phosphorescence quantum yield are in good agreement with the available experimental data. The spin orbit coupling values and the  $S \rightarrow T$  intersystem-crossing matrix elements and crossing rate constants are also explored as a function of the twist angle between the rings. The  $T \rightarrow S_0$  radiative and non-radiative transition rates are calculated and discussed for each member of the series. In addition, the  $T \rightarrow S_0$  radiative transition rate constant is calculated for twisted biphenyls and compared to those for planar molecules.

<sup>1</sup>Acknowledge support from: National Science Foundation, grant no. DMR-1435965

**10:36AM X33.00014 A Comparison Between Magnetic Field Effects in Excitonic and Exciplex Organic Light-Emitting Diodes**, KEYSER SAHIN TIRAS, YIFEI WANG, NICHOLAS J HARMON, MARKUS WOHLGENANN, MICHAEL E FLATTE, University of Iowa — In flat-panel displays and lighting applications, organic light emitting diodes (OLEDs) have been widely used because of their efficient light emission, low-cost manufacturing and flexibility. The electrons and holes injected from the anode and cathode, respectively, form a tightly bound exciton as they meet at a molecule in organic layer. Excitons occur as spin singlets or triplets and the ratio between singlet and triplet excitons formed is 1:3 based on spin degeneracy. The internal quantum efficiency (IQE) of fluorescent-based OLEDs is limited 25% because only singlet excitons contribute the light emission. To overcome this limitation, thermally activated delayed fluorescent (TADF) materials have been introduced in the field of OLEDs. The exchange splitting between the singlet and triplet states of two-component exciplex systems is comparable to the thermal energy in TADF materials, whereas it is usually much larger in excitons. Reverse intersystem crossing occurs from triplet to singlet exciplex state, and this improves the IQE. An applied small magnetic field can change the spin dynamics of recombination in TADF blends. In this study, magnetic field effects on both excitonic and exciplex OLEDs will be presented and comparison similarities and differences will be made.

**10:48AM X33.00015 Tunable white light emission in Parallel Tandem OLEDs made with silver metal as interlayer**, JORGE OLIVA, Centro de Investigaciones en Optica, ALEXIOS PAPADIMITRATOS, ANVAR ZAKHIDOV, University of Texas at Dallas, UT DALLAS TEAM — Parallel tandem organic light emitting diodes (OLEDs) which consisted in a top and bottom subunits, and joined with a thin layer of silver (interlayer) were fabricated. In this parallel tandem architecture the Ag metal is an active common anode, which permitted to inject holes into top and bottom subunits. Both subunits of the tandem can thus be connected functionally in a new geometry and addressed separately. Those Tandems had a yellow emitter (a mixture of MEH-PPV and TFB polymers) in the bottom subunit and a blue emitting molecule in the top subunit. The simultaneous combination of the emitted yellow and blue light when both subunits are operating produced white light. We could tune the white light from cool (CIE: 0.33, 0.25) to warm (CIE: 0.38, 0.39) by changing the intensity of the yellow light, that in turn depends on the ratio of MEH-PPV/TFB mixture used to make the emitting layer in the bottom subunit. We also compared the performance of the parallel tandem with these in series and we found additional advantages of the parallel architecture over the configuration for the series tandems such as: tunable chromaticity, lower turn on voltage (4V compared to 7V in the in-series tandem) and higher brightness. The best CIE coordinate we obtained for white light was (0.35, 0.35) which is near the ideal coordinate of (0.33,0.33).

**Friday, March 18, 2016 8:00AM - 11:00AM –**

**Session X34 GSOFD DPOLY: Emulsions, Foams, Gels, and Complex Fluids** 337 - Carlos Orellana, Emory University

**8:00AM X34.00001 Experimental measurement of the angle of repose of a pile of soft frictionless grains**, KLEBERT FEITOSA, DANIEL SHORTS, Dept. of Physics and Astronomy, James Madison University — It is well known that dry granular materials can flow like a liquid, but can also behave as a solid and sustain a finite angle of repose, partially as a result of inter-particle friction. Here we investigate the nature of piles formed with soft frictionless grains and measure its angle of repose. The pile is produced by a continuous bubbling of air into a soapy solution in a narrow container of rectangular cross section. We observe a gentle slope at the water-foam interface whose angle depends on the viscosity of the liquid. In contrast with sand piles, the fluidized region along the interface is several layers deep. We also find that, unlike sand piles, upon interruption of the gas flux, the slope relaxes back to zero as a result of bubble rearrangements and liquid drainage.

**8:12AM X34.00002 Rearrangements during slow compression of a jammed 2D emulsion**, XIN DU, CARLOS ORELLANA, XIA HONG, ERIC WEEKS, Department of Physics, Emory University — We experimentally study non-affine motion within an evaporating quasi two-dimensional emulsion system. Our samples are oil-in-water emulsions confined between two close-spaced parallel plates, so that the oil droplets are deformed into pancake shapes. In this system, water slowly evaporates from an open edge of the chamber and, as a consequence, the volume fraction of oil droplets gradually increases. By means of microscopy, we analyzed the motion of droplets and measure the deformation of the droplet's outlines. Based on this information, we calculate the force network and the Voronoi cell when the system approaching jamming state. Using a recently proposed method (J. Rieser et al., arXiv:1509.05496), we calculate the Voronoi cell anisotropy vectors which point from the center of each particle to the corresponding Voronoi cell centroid, and identify void spaces where droplets may be more likely to move toward according to the field of the vectors. These allow us to study the correlations between the force network, the Voronoi vector field, and the non-affine displacements of droplets in our evaporating system.

**8:24AM X34.00003 Self-Assembly of Emulsion Droplets into Polymer Chains**, DYLAN BARGTEIL, ANGUS MCMULLEN, JASNA BRUJIC, New York Univ NYU — We experimentally investigate 'beads-on-a-string' models of polymers using the spontaneous assembly of emulsion droplets into linear chains. Droplets functionalized with surface-mobile DNA allow for programmable 'monomers' through which we can influence the three-dimensional structure of the assembled 'polymer'. Such model polymers can be used to study conformational changes of polypeptides and the principles governing protein folding. In our system, we find that droplets bind via complementary DNA strands that are recruited into adhesion patches. Recruitment is driven by the DNA hybridization energy, and is limited by the energy cost of surface deformation and the entropy loss of the mobile linkers, yielding adhesion patches of a characteristic size with a given number of linkers. By tuning the initial surface coverage of linkers, we control valency between the droplets to create linear or branched polymer chains. We additionally control the flexibility of the model polymers by varying the salt concentration and study their dynamics between extended and collapsed states. This system opens the possibility of programming stable three-dimensional structures, such as those found within folded proteins.

**8:36AM X34.00004 Cellulose Nanocrystals as Water in Water Emulsion Stabilizers**, KARTHIK REDDY PEDDIREDDY, ISABELLE CAPRON, Institut National de la Recherche Agronomique, TACO NICOLAI, LAZHAR BENYAHIA, UMR CNRS Université du Maine — Cellulose is the most abundant polymer on the earth. Thus, it is very much desirable to find as many practical applications as possible for it. Cellulose, in its original form, contains both amorphous and crystalline parts. It is possible to separate both parts by dissolving the amorphous part in concentrated sulfuric acid. The remaining crystalline cellulose part exists in the form of rod-like particles. The dimensions of the particles depend on the source. We produce the particles from the acid hydrolysis of cotton cellulose fibers. It results in cellulose nanocrystals (CNCs) with dimensions of ~150 nm x 6 nm x 6 nm. It is well known that CNCs could very efficiently stabilize oil in water (O/W) emulsions by forming very dense monolayers of CNCs at O-W interfaces. However, it is not yet known whether they could also stabilize water in water (W/W) emulsions. The W/W emulsions can be produced by any two incompatible polymers. It is challenging to find effective stabilizers for W/W emulsions due to ultralow interfacial tension and large interfacial thickness. In this talk, I will show the efficiency and effectiveness of these one-dimensional rods as W/W emulsion stabilizers.

**8:48AM X34.00005 Single droplet-level understanding of flow-induced phase inversion of emulsions**, ANKIT KUMAR, Univ of Pennsylvania, SHIGENG LI, CHIEH-MIN CHENG, Xerox Corp., DAEYEON LEE, Univ of Pennsylvania — Phase inversion emulsification (PIE) is a process of generating emulsions by inverting the continuous and dispersed phases of a pre-existing emulsion. It is particularly useful when it is challenging to generate the target emulsions by conventional emulsification methods. Phase inversion of emulsions by flowing them through precisely engineered conduits is called flow-induced phase inversion emulsification (FIPIE). In this study a fundamental understanding of the underlying mechanism of FIPIE is developed. Phase inversion of monodisperse oil-in-water (O/W) emulsions into water-in-oil (W/O) emulsions is achieved by flowing them through specifically designed microfluidic channels. Based on in situ observation of single droplet-level events which lead to phase inversion, a mechanism of the process has been proposed. The outcome of the process is shown to depend on two dimensionless groups - Capillary number (relative importance of viscous and surface tension effects) and dimensionless droplet deformation ( $D/w$ , ratio of droplet size to channel width). It can be concluded from a state-plot between  $Ca$  and  $D/w$  that lower  $Ca$  and higher ( $D/w$ ) facilitate FIPIE.

**9:00AM X34.00006 Local Rearrangements of Droplets in a Dense Emulsion Under Shear Rearrangements**, VISHWAS VENKATESH, Georgetown University, SUDEEP DUTTA, University of Maryland, EMANUELA DEL GADO, DANIEL BLAIR, Georgetown University — Jammed suspensions can flow when subjected to shear deformation. The flow properties are complex, depend on shear rates and can be inhomogeneous through the material. The microscopic origin of such flow properties is still a subject of intense research. In this work, we present a study of jammed emulsions under shear deformation, using a combination of experiments and molecular dynamics simulations. In the steady state regime, we investigate the local rearrangement of jammed emulsion droplets at a wide range of shear rates and shear strains and characterise the local rearrangement of droplets in terms of mean square displacement (MSD), displacement maps and displacement correlation function. At small shear strains and high shear rates, we find localised flow events and super diffusive motion of droplets. But at low shear rates, we observe emerging shear localisation from plastic events in an elastic background and avalanches. The characterisation of local rearrangements is also done in the stress over-shoot regime as well in the regime approaching the steady state stress. We observe a transient shear banding that progressively disappears as the pressure reaches a steady state value.

**9:12AM X34.00007 Tuneable Rheological Properties of Fluorinated Pickering Emulsions**, LAURA ANDREINA CHACON ORELLANA, CNRS, Univ. Bordeaux, CRPP, UPR 8641, 33600 Pessac, France, BIRTE RIECHERS, Max Plank Institute for Dynamics and Self-organization, Am Fassberg 17, D-37077 Goettingen, Germany, OURIEL CAEN, Univ. Paris Sorbonne Cite, INSERM UMR-S775, 75270 Paris Cedex, France, JEAN-CHRISTOPHE BARET, CNRS, Univ. Bordeaux, CRPP, UPR 8641, 33600 Pessac, France — Pickering emulsions are an appealing approach to stabilize liquid-liquid dispersions without surfactants. Recently, amphiphilic silica nanoparticles have been proposed as an alternative to surfactants for droplet microfluidics applications, where aqueous drops are stabilized in fluorinated oils [1]. This system, proved to be effective in preventing the leakage of resorufin, a model dye that was known to leak in surfactant-stabilized drops [1][2]. The overall capabilities of droplet-based microfluidics technology is highly dependent on the dynamic properties of droplets, interfaces and emulsions [3]. Therefore, fluorinated pickering emulsions dynamic properties need to be characterized, understood and controlled to be used as a substitute of already broadly studied emulsions for droplet microfluidics applications. In this study, fluorinated pickering emulsions have been found to behave as a Herschel Bulkley fluid, representing a challenge for common microfluidic operations as re-injection and sorting of droplets. We found that this behavior is controlled by the interaction between the interfacial properties of the particle-laden interface and the bulk properties of the two phases. [1]M. Pan et al. ACS Appl. Mater 2014 [2]Y. Skhiri et al. Soft Matter 2012 [3]J.C. Baret, Lab Chip 2012

**9:24AM X34.00008 A Computational Study of the Rheology and Structure of Surfactant Covered Droplets**, JOAO MAIA, ARMAN BOROMAND, Case Western Reserve University — Using different types of surface-active agents are ubiquitous in different industrial applications ranging from cosmetic and food industries to polymeric nano-composite and blends. This allows to produce stable multiphase systems like foams and emulsions whose stability and shelf-life are directly determined by the efficiency and the type of the surfactant molecules. Moreover, presence and self-assembly of these species on an interface will display complex dynamics and structural evolution under different processing conditions. Analogous to bulk rheology of complex systems, surfactant covered interfaces will response to an external mechanical forces or deformation differently depends on the molecular configuration and topology of the system constituents. Although the effect of molecular configuration of the surface-active molecules on the planar interfaces has been studied both experimentally and computationally, it remains challenging from both experimental and computational aspects to track efficiency and effectiveness of different surfactant molecules with different molecular geometries on curved interfaces. Using Dissipative Particle Dynamics, we have studied effectiveness and efficiency of different surfactant molecules on a curved interface in equilibrium and far from equilibrium. Interfacial tension is calculated for linear and branched surfactant with different hydrophobic and hydrophilic tail and head groups with different branching densities. Deformation parameter and Taylor plots are obtained for individual surfactant molecules under shear flow.

**9:36AM X34.00009 The origin of power-law rheology in foams**, HYUN JOO HWANG, ROBERT RIGGLEMAN, JOHN CROCKER, University of Pennsylvania — Soft glassy matter (SGM) such as foams, emulsions, and colloids, exhibit interesting rheological properties that have long defied explanation. In particular, the shear modulus of these materials displays weak power law frequency dependence. To understand the origin of this property in more depth, we have built a three-dimensional, modified Bubble Dynamics model. The bubbles interact with a purely repulsive harmonic potential and ripen according to diffusion-based governing equations. Notably, the bubble motion has a Levy flight character, in addition to being spatially correlated in the form of avalanches. Microrheology studies reveal that the power-law shear modulus is the result of constraint release driven by the bubbles' super-diffusive motion combined with simple yield of the resulting stress. The super-diffusive motion of the bubbles, in turn, is the result of the system taking a fractal path in configuration space. We shall discuss the origins of this fractal scaling.

**9:48AM X34.00010 Creep dynamics in soft matter**, RAFFAELA CABRIOLU, Universite' Joseph Fourier — Detecting any precursors of failure in Soft Matter Systems (SMS) is an inter-disciplinary topic with important applications (e.g. prediction of failure in engineering processes). Further, it provides an ideal benchmark to understand how mechanical stress and failure impacts the flow properties of amorphous condensed matter. Furthermore, some SMS are viscoelastic, flowing like viscous liquids or deforming like a solid according to applied forces. Often SMS are fragile and local rearrangements trigger catastrophic macroscopic failure. Despite the importance of the topic little is known on the local creep dynamics [1,2] before the occurrence of such catastrophic events [3,4]. To study creep and failure at an atomic/molecular level and at time scales that are not easily accessible by experiments we chose to carry out microscopic simulations. In this work we present the response of a colloidal system to uniaxial tensile stress applied and we compare our results to experimental works [8]. References: [1] Schurtenberger et al., J. Phys. Chem. 95, 4173 (1991). [2] Bauer et al., Phys. Rev. Lett. 97, 258303 (2006) [3] Chaudhuri P. et al., Phys. Rev. E 88, 040301 (2013). [4] Zausch J. et al., J. Phys. Condens. Matter 20, 404210 (2008).

**10:00AM X34.00011 Modeling Discontinuous Phase Transitions in Gel Membranes: Focus on Hysteresis and Feedback Mechanisms**, OLGA KUKSENOK, Clemson Univ — Feedback mechanisms are vital in a number of processes in biological systems. For example, feedback loops play an essential role during a limb development in mammals and are responsible for the asymmetric cell division to constrain the growth in plants to the specific regions. An integration of well-controlled feedback loops into the fully synthetic materials is an important step in designing a range of biomimetic functionalities. Herein, we focus on hydrogels functionalized with light-sensitive trisodium salt of copper chlorophyllin and study discontinuous phase transitions in these systems. Prior experimental studies had shown that illumination of these functionalized gels results in their heating and in discontinuous, first order phase transition upon the variation in temperature. Herein, we develop the first computational model for these gels; the framework of the model is based on the gel Lattice Spring Model, in this work we account for the gel heating under the illumination. The results of our simulations are in a good agreement with prior experimental studies. We focus on pattern development during the volume phase transitions in membranes of various thicknesses and show that one can effectively utilize light intensity to remotely control feedback loops in these systems.

**10:12AM X34.00012 X-ray speckle measurements of concentrated nanoemulsions under shear**, SAMY ABIDIB, MICHAEL ROGERS, University of Ottawa, ROBERT LEHENY, KUI CHEN, Johns Hopkins University, THOMAS MASON, UCLA, JAMES HARDEN, University of Ottawa — We present in situ X-ray Photon Correlation Spectroscopy (XPCS) measurements of a set of concentrated nanoemulsions subjected to oscillatory shear. The nanoemulsion set contained samples with varying packing fractions of oil droplets ( $r \approx 20\text{nm}$ ) above the jamming transition. In order to study their elasticity, yielding, and flow at various shear amplitudes, we employed stroboscopic coherent X-ray scattering measurements triggered at the maximums of the shear cycle. The degree of correlation between speckle in images taken a full period apart is a direct measurement of particle rearrangements during cycling. A comparison of such XPCS echo measurements with rheological measurements shows an onset of irreversible particle motion at shear strains below the crossover of the storage and loss moduli, which is typically used to indicate the transition to viscoplastic flow. Moreover, the XPCS echo measurements indicate that particle irreversibility increases rapidly with shear amplitude, in contrast to the comparably smooth transition to yielding shown in bulk rheology measurements. However, the macroscopic yield strain observed in rheology and the microscopic yield strain identified from XPCS, which were strong functions of droplet packing fraction, tracked each other closely.

**10:24AM X34.00013 Dynamics of a DNA Gel**, RAMESH ADHIKARI, ANIKET BHATTACHARYA, ARISTIDE DOGARIU, University of Central Florida — We study *in silico* the properties of a gel consisting of DNA strands (modeled as semi-flexible chains) and linkers of varying flexibility, length, and topology. These linkers are envisioned and modeled as active components with additional attributes so as to mimic properties of a synthetic DNA gel containing motor proteins. We use Brownian dynamics to directly obtain frequency dependent complex shear moduli of the gel. We further carry out force spectroscopy on these computer generated gels and study the relaxation properties as a function of the important parameters of the model, e.g., densities and relative ratios of the DNAs and the linkers, the average life time of a link, etc. Our studies are relevant for designing synthetic bio-materials for both materials and medical applications.

**10:36AM X34.00014 Supramolecular Structural Forces in Stratifying Foam Films and Micelle Aggregation Number**, SUBINUER YILIXIATI, YIRAN ZHANG, EWELINA WOJCIK, RABEES RAFIQ, VIVEK SHARMA, Univ of Illinois - Chicago — Understanding and controlling the drainage kinetics of thin films is an important problem that underlies the stability, lifetime and rheology of foams and emulsions. Foam films containing micelles, colloidal particles or polyelectrolyte-surfactant mixtures exhibit step-wise thinning or stratification, due to the influence of non-DLVO forces, including supramolecular oscillatory structural forces. In this study, we use experiments and theory to investigate the drainage and stratification in vertical and horizontal thin foam films ( $<100\text{ nm}$ ) formed by aqueous sodium dodecyl sulfate (SDS) solutions. We determine how the concentration of surfactants and added salt influences the stepwise thinning process for micellar solutions, and how step size can be used for estimating micelle size and interactions. The concentration-dependent aggregation number extracted from our experiments match-up reasonably well with values obtained by other techniques including scattering and fluorescence.

**10:48AM X34.00015 Microrheology using a custom-made AFM<sup>1</sup>**, SEBASTIEN KOSGODAGAN ACHARIGE, UMR CNRS 5672 Laboratoire de Physique de l'Ecole Normale Supérieure de Lyon, 46 Allée d'Italie, 69364 Lyon cedex 07, France, MICHAEL BENZAQUEN<sup>2</sup>, UMR CNRS 7083 Gulliver, ESPCI ParisTech, 10 Rue Vauquelin 75005 Paris, France, AUDREY STEINBERGER, UMR CNRS 5672 Laboratoire de Physique de l'Ecole Normale Supérieure de Lyon, 46 Allée d'Italie, 69364 Lyon cedex 07, France — In the past few years, a new method was developed to measure local properties of liquids (X. Xiong *et al.*, Phys. Rev. E 80, 2009). This method consists of gluing a micron-sized glass fiber at the tip of an AFM cantilever and probing the liquid with it. In ENS Lyon, this method was perfected (C. Devailly *et al.*, EPL, 106 5, 2014) with the help of an interferometer developed in the same laboratory (L. Bellon *et al.*, Opt. Commun. 207 49, 2002 and P. Paolino *et al.*, Rev. Sci. Instrum. 84, 2013), which background noise can reach  $10^{-14}\text{ m}/\sqrt{\text{Hz}}$ . This method allows us to measure a wide range of viscosities ( $1\text{ mPa}\cdot\text{s}$  to  $500\text{ mPa}\cdot\text{s}$ ) of transparent and opaque fluids using a small sample volume ( $\sim 5\text{ mL}$ ). In this presentation, I will briefly describe the interferometer developed in ENS Lyon, then explain precisely the microrheology measurements and then compare the experimental results to a model developed by M. Benzaquen.

<sup>1</sup>This work is supported financially by the ANR project NANOFLUIDYN (grant number ANR-13-BS10-0009).

<sup>2</sup>Currently at Capital Fund Management, 23 Rue de l'Université 75007 Paris, France

## Friday, March 18, 2016 8:00AM - 11:00AM – Session X35 DBIO GSNP: Critical Transitions in Biological Systems 338 - Chen Zeng, GWU

**8:00AM X35.00001 Detecting early-warning signals of critical transitions for complex systems<sup>1</sup>**, LUONAN CHEN, Shanghai Institutes for Life Sciences, Chinese Academy of Sciences — Considerable evidence suggests that during the progression of complex diseases, the deteriorations are not necessarily smooth but are abrupt, and may cause a critical transition from one state to another at a tipping point. Here, we develop a model-free method to detect early-warning signals of such critical transitions, even with only a small number of samples. Specifically, we theoretically derive an index based on a dynamical network biomarker (DNB) for biological systems or dynamical network marker (DNM) for general systems that serves as a general early-warning signal indicating an imminent bifurcation or sudden deterioration before the critical transition occurs. Based on theoretical analyses, we show that predicting a sudden transition from small samples is achievable provided that there are a large number of measurements for each sample, e.g., high-throughput data. We employ microarray data of three diseases to demonstrate the effectiveness of our method for detecting "un-occurred" disease state. The relevance of DNBs with the diseases was also validated by related experimental data and functional analysis.

<sup>1</sup>Detecting early-warning signals of critical transitions for complex systems

**8:36AM X35.00002 The evolution of lossy compression**, SARAH MARZEN, University of California, Berkeley, SIMON DEDEO, Indiana University, Bloomington — In complex environments, there are costs to both ignorance and perception. An organism needs to track fitness-relevant information about its world, but the more information it tracks, the more resources it must devote to memory and processing. As a first step towards an understanding of this tradeoff, we use rate-distortion theory to study large, unstructured environments with fixed, randomly-drawn penalties for stimuli confusion ("distortions"). We find that two different environments will have nearly identical rate-distortion functions (but very different codebooks) when distortions are drawn from the same distribution, suggesting an interesting weak universality. We further identify two distinct regimes for organisms in these structured environments: a high-fidelity regime where perceptual costs grow linearly with environmental complexity, and a low-fidelity regime where perceptual costs are, remarkably, independent of the number of environmental states. This last result suggests that evolution will drive organisms to the threshold between the high- and low-fidelity regimes. In dynamic environments of rapidly-increasing complexity, well-adapted organisms will find themselves able to make, just barely, the most subtle distinctions in their environment.

**8:48AM X35.00003 Dynamics of neuroendocrine stress response: bistability, timing, and control of hypocortisolism** , MARIA D'ORSOGNA, California State University at Northridge, TOM CHOU, LAE KIM , UCLA — The hypothalamic-pituitary-adrenal (HPA) axis is a neuroendocrine system that regulates numerous physiological processes. Disruptions in its activity are correlated with stress-related diseases such as post-traumatic stress disorder (PTSD) and major depressive disorder. We characterize “normal” and “diseased” states of the HPA axis as basins of attraction of a dynamical system describing the inhibition of peptide hormones, corticotropin-releasing hormone (CRH) and adrenocorticotrophic hormone (ACTH), by circulating glucocorticoids such as cortisol (CORT). Our model includes ultradian oscillations, CRH self-upregulation of CRH release, and distinguishes two components of negative feedback by cortisol on circulating CRH levels: a slow direct suppression of CRH synthesis and a fast indirect effect on CRH release. The slow regulation mechanism mediates external stress-driven transitions between the stable states in novel, intensity, duration, and timing-dependent ways. We find that the *timing* of traumatic events may be an important factor in determining if and how the hallmarks of depressive disorders will manifest. Our model also suggests a mechanism whereby exposure therapy of stress disorders may act to normalize downstream dysregulation of the HPA axis.

**9:00AM X35.00004 Dynamics of blood flow in a microfluidic ladder network** , JEEVAN MADDALA, JEVGENIA ZILBERMAN-RUDENKO , OWEN MCCARTY, Oregon Health and Science University — The dynamics of a complex mixture of cells and proteins, such as blood, in perturbed shear flow remains ill-defined. Microfluidics is a promising technology for improving the understanding of blood flow under complex conditions of shear; as found in stent implants and in tortuous blood vessels. We model the fluid dynamics of blood flow in a microfluidic ladder network with dimensions mimicking venules. Interaction of blood cells was modeled using multiagent framework, where cells of different diameters were treated as spheres. This model served as the basis for predicting transition regions, collision pathways, re-circulation zones and residence times of cells dependent on their diameters and device architecture. Based on these insights from the model, we were able to predict the clot formation configurations at various locations in the device. These predictions were supported by the experiments using whole blood. To facilitate platelet aggregation, the devices were coated with fibrillar collagen and tissue factor. Blood was perfused through the microfluidic device for 9 min at a physiologically relevant venous shear rate of  $600 \text{ s}^{-1}$ . Using fluorescent microscopy, we observed flow transitions near the channel intersections and at the areas of blood flow obstruction, which promoted larger thrombus formation. This study of integrating model predictions with experimental design, aids in defining the dynamics of blood flow in microvasculature and in development of novel biomedical devices.

**9:12AM X35.00005 Identifying driving gene clusters in complex diseases through critical transition theory** , NATHANIEL WOLANYK, The Department of Physics University of Alabama at Birmingham, XUJING WANG, NHLBI, NIH, MARTIN HESSNER, Medical College of Wisconsin, SHOUGUO GAO, YE CHEN, NHLBI, NIH, SHUANG JIA, Medical College of Wisconsin — A novel approach of looking at the human body using critical transition theory has yielded positive results: clusters of genes that act in tandem to drive complex disease progression. This cluster of genes can be thought of as the first part of a large genetic force that pushes the body from a curable, but sick, point to an incurable diseased point through a catastrophic bifurcation. The data analyzed is time course microarray blood assay data of 7 high risk individuals for Type 1 Diabetes who progressed into a clinical onset, with an additional larger study requested to be presented at the conference. The normalized data is 25,000 genes strong, which were narrowed down based on statistical metrics, and finally a machine learning algorithm using critical transition metrics found the driving network. This approach was created to be repeatable across multiple complex diseases with only progression time course data needed so that it would be applicable to identifying when an individual is at risk of developing a complex disease. Thusly, preventative measures can be enacted, and in the longer term, offers a possible solution to prevent all Type 1 Diabetes.

**9:24AM X35.00006 Finding the role of time-delays in complex systems<sup>1</sup>** , WEI LIN, School of Mathematical Sciences and Centre Computational Systems Biology, Fudan University — Time delays are omnipresently observed in many nature and artificial systems including physical, biological, and chemical systems. Naturally, two kinds of questions arise: How to identify the time delays when a certain amount of datasets are obtained from the experiments or real world systems whenever the theoretical model is known or unknown? and How to characterize the intrinsic roles of time delays that are played in the critical transition of coupled network systems In this talk, we introduce recent works that address the previous two questions, and show the significance of time delays in dealing with various biological systems.

<sup>1</sup>The work is supported by NNSF of China [Grant No. 11322111 and 61273014] and SCMS.

**9:36AM X35.00007 Detecting critical state before phase transition of complex systems by hidden Markov model** , RUI LIU, PEI CHEN, YONGJUN LI, South China University of Technology, LUONAN CHEN, Shanghai Institutes for Biological Sciences — Identifying the critical state or pre-transition state just before the occurrence of a phase transition is a challenging task, because the state of the system may show little apparent change before this critical transition during the gradual parameter variations. Such dynamics of phase transition is generally composed of three stages, i.e., before-transition state, pre-transition state, and after-transition state, which can be considered as three different Markov processes. Thus, based on this dynamical feature, we present a novel computational method, i.e., hidden Markov model (HMM), to detect the switching point of the two Markov processes from the before-transition state (a stationary Markov process) to the pre-transition state (a time-varying Markov process), thereby identifying the pre-transition state or early-warning signals of the phase transition. To validate the effectiveness, we apply this method to detect the signals of the imminent phase transitions of complex systems based on the simulated datasets, and further identify the pre-transition states as well as their critical modules for three real datasets, i.e., the acute lung injury triggered by phosgene inhalation, MCF-7 human breast cancer caused by heregulin, and HCV-induced dysplasia and hepatocellular carcinoma.

**9:48AM X35.00008 Identification of driving network of cellular differentiation from single sample time course gene expression data.** , YE CHEN, The National Heart, Lung, and Blood Institute (NHLBI), NATHANIEL WOLANYK, University of Alabama at Birmingham, TUNC ILKER, SHOUGUO GAO, XUJING WANG, The National Heart, Lung, and Blood Institute (NHLBI) — Methods developed based on bifurcation theory have demonstrated their potential in driving network identification for complex human diseases, including the work by Chen, et al. Recently bifurcation theory has been successfully applied to model cellular differentiation. However, there one often faces a technical challenge in driving network prediction: time course cellular differentiation study often only contains one sample at each time point, while driving network prediction typically require multiple samples at each time point to infer the variation and interaction structures of candidate genes for the driving network. In this study, we investigate several methods to identify both the critical time point and the driving network through examination of how each time point affects the autocorrelation and phase locking. We apply these methods to a high-throughput sequencing (RNA-Seq) dataset of 42 subsets of thymocytes and mature peripheral T cells at multiple time points during their differentiation (GSE48138 from GEO). We compare the predicted driving genes with known transcription regulators of cellular differentiation. We will discuss the advantages and limitations of our proposed methods, as well as potential further improvements of our methods.

**10:00AM X35.00009 Experimental and theoretical description of higher order periods in cardiac tissue action potential duration** , CONNER HERNDON, FLAVIO FENTON, ILIJA UZELAC, Georgia Tech — Much theoretical, experimental, and clinical research has been devoted to investigating the initiation of cardiac arrhythmias by alternans, the first period doubling bifurcation in the duration of cardiac action potentials. Although period doubling above alternans has been shown to exist in many mammalian hearts, little is understood about their emergence or behavior. There currently exists no physiologically correct theory or model that adequately describes and predicts their emergence in stimulated tissue. In this talk we present experimental data of period 2, 4, and 8 dynamics and a mathematical model that describes these bifurcations. This model extends current cell models through the addition of memory and includes spatiotemporal nonlinearities arising from cellular coupling by tissue heterogeneity.

**10:12AM X35.00010 Theory of advection-driven long range biotic transport** , OLEG KOGAN, KEVIN O'KEEFFE, Cornell University, DAVID SCHNEIDER, United States Department of Agriculture; Cornell University, CHRISTOPHER MYERS, Cornell University — We consider a new reaction-transport framework, and apply it to the problem of advection-driven biotic transport. The are two compartments - the growth layer, coupled to a separate, advective layer. Density fronts propagate in both layers. Crucially, the downwind front speed goes to a finite value as the coupling goes to zero. We next include diffusion in the growth layer, and study the competition between the advective and diffusive transport mechanisms. Advection wins for small diffusion and cannot be ignored, no matter how weak is the coupling. When coupling is not small, both mechanisms work cooperatively, without a clear winner. A further surprise is the existence of a critical diffusion constant at which the front speed is independent of the interlayer coupling.

**10:24AM X35.00011 Geometric phase transition in the cellular network of the pancreatic islets may underlie the onset of type 1 diabetes.** , XUJING WANG, NHLBI, NIH — Living systems are characterized by complexity in structure and emergent dynamic orders. In many aspects the onset of a chronic disease resembles phase transition in a dynamic system: quantitative changes accumulate largely unnoticed until a critical threshold is reached, which causes abrupt qualitative changes of the system. In this study we investigate this idea in a real example, the insulin-producing pancreatic islet  $\beta$ -cells and the onset of type 1 diabetes. Within each islet, the  $\beta$ -cells are electrically coupled to each other, and function as a network with synchronized actions. Using percolation theory we show how normal islet function is intrinsically linked to network connectivity, and the critical point where the islet cellular network loses site percolation, is consistent with laboratory and clinical observations of the threshold  $\beta$ -cell loss that causes islet functional failure. Numerical simulations confirm that the islet cellular network needs to be percolated for  $\beta$ -cells to synchronize. Furthermore, the interplay between site percolation and bond strength predicts the existence of a transient phase of islet functional recovery after disease onset and introduction of treatment, potentially explaining a long time mystery in the clinical study of type 1 diabetes: the honeymoon phenomenon. Based on these results, we hypothesized that the onset of T1D may be the result of a phase transition of the islet  $\beta$ -cell network. We further discuss the potential applications in identifying disease-driving factors, and the critical parameters that are predictive of disease onset.

## Friday, March 18, 2016 8:00AM - 10:24AM —

Session X36 GSOF: Metallic Glasses and Quasicrystals 339 - Fei Wang, Missouri State University

**8:00AM X36.00001 Local growth rules and kinetics for ordered icosahedral quasicrystals** , JOSHUA SOCOLAR, Duke University, CONNOR HANN, Duke University, PAUL STEINHARDT, Princeton University — Icosahedral quasicrystals (IQCs) with extremely high degrees of translational order have been produced in the lab and found in naturally occurring minerals. While the existence of IQCs is well established, questions remain about how IQCs form. We address the question of whether it is possible in principle for nucleation and growth dominated by local growth rules and kinetics to produce a *perfectly* ordered IQC. We find that it is possible to produce an IQC with a vanishing density of defects through a local growth algorithm for sequential, face-to-face addition of tiles of two different shapes to a growing cluster. The choice of how to add a tile at any selected vertex on the surface is based only on short-range information about tiles that share the vertex. The process is analogous to the Onoda growth rule for 2D Penrose tilings [Onoda et al., PRL 60, 2653 (1988)], but new subtleties emerge in three dimensions. The geometric features underlying this algorithm can inform analyses of experimental systems and numerical models that generate highly ordered quasicrystals.

**8:12AM X36.00002 Low participation ratio vibrational modes in a limit-periodic structure<sup>1</sup>** , CATHERINE MARCOUX, JOSHUA E. S. SOCOLAR, Duke University — Motivated by the demonstration that patterned colloidal particles may form a limit-periodic phase<sup>2</sup>, we study the nature of vibrational modes in a toy model based on the Taylor-Socolar tiling. We consider a triangular lattice of identical point masses with nearest neighbors connected by springs of two different strengths, where the pattern of spring constants reflects the limit-periodic structure of the tiling. Using calculations of the phonon spectra for crystalline approximants to the limit-periodic structure, we identify several hierarchies of modes shared by the full limit-periodic system that have arbitrarily low participation ratios. We present a heuristic explanation of the existence of such modes, which are robust in the presence of vacancies and small amounts of disorder in the spring constants.

<sup>1</sup>Supported by the NSF Research Triangle MRSEC (DMR-1121107)

<sup>2</sup>C. Marcoux, T. W. Byington, Z. Qian, P. Charbonneau, and J. E. S. Socolar, *Phys. Rev. E* **90**, 012136 (2014).

**8:24AM X36.00003 Magnetism in the i-R-Cd ( $R = Y, Gd-Tm$ ) binary quasicrystals<sup>1</sup>** , ALAN GOLDMAN, TAI KONG, ANDREAS KREYSSIG, Ames Laboratory, U.S. DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA, TSUNETOMO YAMADA, Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai, Miyagi 980-9870, Japan, HIROYUKI TAKAKURA, Division of Applied Physics, Faculty of Engineering, Hokkaido University, Sapporo, Hokkaido, 060-8628, Japan, SERGEY BUD'KO, PINAKI DAS, WAGEESHA JAYASEKARA, PAUL CANFIELD, Ames Laboratory, U.S. DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA, MARC DE BOISSIEU, SIMAP, Grenoble-INP, UJF, CNRS, Saint Martin d'Heres Cedex, 38402, France — Progress in our understanding of the consequences of aperiodicity for physical phenomena such as the electronic, magnetic, and optical properties has recently seen a surge of activity and new results. A new family of i-R-Cd binary magnetic quasicrystals, exhibiting spin-glass-like behavior, and the closely related  $RCd_6$  crystalline approximants, which manifest long-range magnetic order at low temperature, offer new opportunities for studies of the impact of aperiodicity on magnetic interactions in compounds that have similar local structures. I will discuss their magnetic behavior, as well as recent x-ray diffraction and elastic magnetic neutron scattering investigations that provide some insight into their structural and magnetic properties.

<sup>1</sup>The research was supported by the Office of the Basic Energy Sciences, Materials Sciences Division, US Department of Energy (DOE).

**8:36AM X36.00004 Crystal electric field excitations in quasicrystal approximant TbCd<sub>6</sub> studied by inelastic neutron scattering**<sup>1</sup>, PINAKI DAS, R. FLINT, T. KONG, P.C. CANFIELD, A. KREYSSIG, A.I. GOLDMAN, Ames Laboratory, Iowa State Univ., USA, M. DE BOISSIEU, P.- F. LORY, G. BEUTIER, SIMap, Grenoble-INP, France, T. HIROTO, Tokyo Univ. of Science, Japan — All of the known quasicrystals with local moments exhibit frustration and spin glass-like behavior at low temperature. The onset of the spin freezing temperature is believed to be affected by the crystal electric field (CEF) splitting of the local moments. The quasicrystal approximant TbCd<sub>6</sub> and its related icosahedral quasicrystal phase, i-Tb-Cd, form a set of model systems to explore how magnetism evolves from a conventional lattice (approximant phase) to an aperiodic quasicrystal. Though TbCd<sub>6</sub> shows long-range antiferromagnetic ordering ( $T_N = 24$  K), only spin glass like behavior is observed in i-Tb-Cd with a spin freezing temperature of  $T_F = 6$  K. To investigate further, we have performed inelastic neutron scattering measurements on powder samples of TbCd<sub>6</sub> and observed two distinct CEF excitations at low energies which points to a high degeneracy of the CEF levels related to the Tb surrounding with almost icosahedral symmetry.

<sup>1</sup>Work at Ames Laboratory was supported by the DOE, BES, Division of Materials Sciences & Engineering, under Contract No. DE-AC02-07CH11358. This research used resources at Institut Laue-Langevin, France.

**8:48AM X36.00005 Magnetoresistance in i-R-Cd icosahedral quasicrystals (R=Y, Gd)**<sup>1</sup>, GARIMA SARASWAT, DRAGANA POPOVIĆ, Natl. High Magnetic Field Lab., Florida State Univ., TAI KONG, SERGEY L. BUD'KO, PAUL C. CANFIELD, Ames Laboratory / Iowa State Univ. — We use magnetoresistance (MR) to probe the electronic properties of the recently discovered binary quasicrystals (QCs) i-Gd-Cd and i-Y-Cd, with and without local magnetic moments, respectively. DC magnetization has revealed spin-glass freezing in i-Gd-Cd at a temperature  $T_f = 4.6$  K. MR was measured at  $1.6 \leq T(K) \leq 300$  and in magnetic fields  $H$  up to 12 T. The most interesting behavior is observed in i-Gd-Cd, in which the MR exhibits thermo-magnetic history dependence at low  $T$ . In particular, there is a clear difference between the ZFC and FC values of the low-field positive MR. In contrast, the i-Y-Cd MR does not depend on magnetic history. The onset of the history dependent MR at  $T \sim 20$  K  $> T_f$ , when the QC with local magnetic moments is cooled in a high field of 12 T, may be related to the formation of magnetic clusters above  $T_f$ , as inferred from the magnetization and specific heat studies. Possible mechanisms responsible for the striking coupling between charge transport and local magnetic environment observed in the MR will be discussed.

<sup>1</sup>Work at the NHMFL supported by NSF Grant No. DMR-1307075, the NSF Cooperative Agreement No. DMR-0654118 and the State of Florida. Work at Ames Lab (TK, SLB and PCC) supported by the U.S. D.O.E / B.E.S under Contract No. DE-AC02-07CH11358.

**9:00AM X36.00006 Predicting Novel Bulk Metallic Glasses via High- Throughput Calculations**<sup>1</sup>, E. PERIM, Duke University, D. LEE, Harvard University, Y. LIU, Yale University, C. TOHER, Duke University, P. GONG, Y. LI, Yale University, W. N. SIMMONS, O. LEVY, Duke University, J. VLASSAK, Harvard University, J. SCHROERS, Yale University, S. CURTAROLO, Duke University — Bulk metallic glasses (BMGs) are materials which may combine key properties from crystalline metals, such as high hardness, with others typically presented by plastics, such as easy processability[1]. However, the cost of the known BMGs poses a significant obstacle for the development of applications, which has lead to a long search for novel, economically viable, BMGs[2,3]. The emergence of high-throughput DFT calculations, such as the library provided by the AFLOWLIB consortium[4], has provided new tools for materials discovery. We have used this data to develop a new glass forming descriptor combining structural factors with thermodynamics in order to quickly screen through a large number of alloy systems in the AFLOWLIB database, identifying the most promising systems and the optimal compositions for glass formation. [1] M. F. Ashby, A. L. Greer. Scripta Mater. 54, 321 (2006). [2] A. Inoue Bulk Amorphous Alloys: Preparation and Fundamental Characteristics, Vol. 4. (Trans Tech Publications, Zurich, 1998). [3] T. Egami, Y. Waseda. J. Non-Cryst. Solids 64, 113 (1984). [4] S. Curtarolo et al. Comp. Mater. Sci. 58, 218 (2012).

<sup>1</sup>National Science Foundation (DMR-1436151, DMR-1435820, DMR-1436268)

**9:12AM X36.00007 Stretched Exponential relaxation in pure Se glass.**<sup>1</sup>, S DASH, S RAVINDREN, P BOOLCHAND, University of Cincinnati — A universal feature of glasses is the stretched exponential relaxation,  $f(t) = \exp[-t/\tau]^\beta$ . The model of diffusion of excitations to randomly distributed traps in a glass by Phillips<sup>1</sup> yields the stretched exponent  $\beta = d/[d+2]$  where  $d$ , the effective dimensionality. We have measured the enthalpy of relaxation  $\Delta H_{nr}(t_w)$  at  $T_g$  of Se glass in modulated DSC experiments as glasses age at 300K and find  $\beta = 0.43(2)$  for  $t_w$  in the  $0 < t_w < 8$  months range. The observed  $\beta$  is in harmony with the trap model. The result is consistent with the growth of interchain structural correlations mediated by both long range (van der Waals forces) and short-range (covalent) interactions. A striking consequence of this relaxation is a narrowing of the glass transition width from 7.1C to 1.4C, and the  $\Delta H_{nr}$  term increasing from 0.21 cal/gm to 0.92 cal/gm. In bulk  $Ge_xSe_{100-x}$  glasses as  $x$  increases to 20%, the length of the polymeric  $Se_n$  chains between the Ge-crosslinks decreases to  $n = 2$ . and the striking relaxation effects nearly vanish.

<sup>1</sup>J.C. Phillips, Rep.Prog.Phys. 59, 1133 (1996).  
Supported by NSF grant DMR 08-53957

**9:24AM X36.00008 Low-temperature internal friction in quenched amorphous selenium films**<sup>1</sup>, THOMAS METCALF, XIAO LIU, Naval Research Laboratory, MATTHEW ABERNATHY, NRC Postdoc, RICHARD STEPHENS, University of Pennsylvania — Using ultra-high-quality-factor silicon mechanical resonators, we have measured the internal friction and shear modulus of amorphous selenium (a-Se) films at liquid helium temperatures. The glass transition temperature of selenium lies at a conveniently accessible  $40 - 50^\circ\text{C}$ , facilitating a series of in- and ex-situ annealing and quench cycles. The a-Se films exhibit the low-temperature internal friction plateau ( $10^{-4} \leq Q^{-1} \leq 10^{-3}$ ) found in almost all amorphous solids, which is a result of (and direct measure of) a broad distribution of two-level tunneling systems (TLS), whose origin is still unknown. We find a clear correlation between the post-anneal quench rate and the value of this plateau. The implications of these observations for understanding the microscopic origin of TLS will be discussed. Principally, the observed changes in the internal friction plateau could show the way in which the density of TLS could be manipulated or suppressed in other amorphous systems.

<sup>1</sup>Work supported by the Office of Naval Research and the University of Pennsylvania Materials Research Science and Engineering Center

### 9:36AM X36.00009 Non-Gaussian resistance noise in misfit layer compounds: Bi-Se-Cr , LINTAO

PENG, Electrical Engineering and Computer Science & Applied Physics, Northwestern University, Evanston, IL 60208, USA, ALEX FREEDMAN, Electrical Engineering and Computer Science, Northwestern University, Evanston, IL 60208, USA, SAMANTHA CLARKE, DANNA FREEDMAN, Department of Chemistry, Northwestern University, Evanston, IL 60208, USA, M GRAYSON, Electrical Engineering and Computer Science & Applied Physics, Northwestern University, Evanston, IL 60208, USA — Misfit layer ternary compounds Bi-Se-Cr have been synthesized and structurally and magnetically characterized [1]. However, the nature of the magnetic ordering below the transition temperature remains debatable between ferromagnetic and spin-glass. These misfit layer compounds consist of two alternating chalcogenide layers of CrSe<sub>2</sub> and BiSe along the c-axis. Whereas the a-axis is lattice matched, the lattice mismatch along the b-axis introduces non-periodic modulation of atomic position leading to quasi-crystalline order along the b-axis alone. We explore unconventional electrical transport properties in the noise spectrum of these compounds. After thinning down the compounds to nanoscale, Van der Pauw devices are fabricated with standard electron beam lithography process. Large resistance noise was observed at temperature below the Curie temperature. The magnitude of resistance noise is much greater than trivial intrinsic noises like thermal Johnson noise and increases as temperature decreases. The probability density function of the relative noise shows 2-4 peaks among different observations which indicate strong non-Gaussian statistic property suggesting glassy behaviors in this material. [1] S. M. Clarke and D. E. Freedman, Inorg. Chem. 54, 2765-2771 (2015)

### 9:48AM X36.00010 Synthesis, optical and thermal characterization of NaPO<sub>3</sub> glass.<sup>1</sup> , C MOHANTY,

R CHBEIR, A WELTON, P BOOLCHAND, Univ of Cincinnati — We have synthesized the stoichiometric bulk glass by reacting equimolar amounts of Na<sub>2</sub>CO<sub>3</sub> and P<sub>2</sub>O<sub>5</sub>, and handling the anhydrous starting materials and reacted product in a dry ambient environment. The bulk glass displays a T<sub>g</sub> of 306(2)C and an enthalpy of relaxation of 0.26 cal/gm using MDSC. In a previous report a T<sub>g</sub> = 287C was obtained<sup>1</sup> using DSC. The glass was crystallized and characterized by XRD and revealed a powder pattern that is in excellent agreement with the known structure (CSD 174021). Raman scattering of the glass revealed prominent modes of symmetric vibration of the PO<sub>4</sub> tetrahedra bearing P-O<sub>br</sub> and P-O<sub>ter</sub> bonds near 684 cm<sup>-1</sup> and 1162 cm<sup>-1</sup> respectively. The integrated intensity ratio R of the 1162 cm<sup>-1</sup>/684 cm<sup>-1</sup> modes is close to 1.0(1) in the crystal but increases to 1.4(1) in the glass reflecting the finite length of the P-O-P chains in the latter. The highest frequency mode is a weak feature near 1268 cm<sup>-1</sup>, which coincides with the TO response in IR reflectivity of the glass, suggesting that it represents the TO mode of the NaPO<sub>3</sub> glass.

<sup>1</sup>J.J. Hudgens et al. JNCS 223, 21 (1998).

Supported by NSF grant DMR 08-53957

### 10:00AM X36.00011 Raman scattering and Medium Range Structure of (BaO)<sub>x</sub>(B<sub>2</sub>O<sub>3</sub>)<sub>100-x</sub>-

glasses.<sup>1</sup> , CHAD HOLBROOK, Air Force Research Labs, RALPH CHBEIR, ANDREW CZAJA, PUNIT BOOLCHAND, University of Cincinnati — In Raman scattering of titled glasses we observe a triad of modes (770 cm<sup>-1</sup>, 750 cm<sup>-1</sup>, 705 cm<sup>-1</sup>) on the low frequency side of the famous Boroxyl-Ring (BR) mode (808 cm<sup>-1</sup>) as the BaO content x increases in the 0 < x < 40% range. Raman polarization experiments reveal that the triad of modes show a rather low depolarization ratio ( $\rho < 0.25$ ) suggesting that each mode results from a symmetric stretch of O atoms in mixed-3-member-rings, analogous to the BR-mode. In the 0 < x < 15% range, the conspicuous absence of these mixed-ring modes is consistent with the composition range representing the immiscibility range. At x > 15%, the 770 cm<sup>-1</sup> mode scattering strength grows precipitously to show a maximum near x<sub>c</sub> = 20%, consistent with presence of Ba-tetraborate structural grouping (SG). At x > 15%, we also observe scattering strength of the 750 cm<sup>-1</sup> mode to increase with x and show a maximum near x<sub>c</sub> = 33%, consistent with formation of Ba-diborate SG. Finally, a mode near 705 cm<sup>-1</sup>, whose scattering strength increases linearly with x in the 15% < x < 40% range, we identify with Ba-metaborate SG. FTIR measurements permit a measurement of the B<sub>4</sub>/B<sub>3</sub> fraction and also the LO-TO splittings.

<sup>1</sup>NSF grant DMR-08-53957

### 10:12AM X36.00012 The effect of spherical inclusions in metallic glass nanowires under tensile test and its relation to atomic structure<sup>1</sup> , MATIAS SEPULVEDA, GONZALO GUTIERREZ, NICOLAS AMIGO, Departamento de

Física, Facultad de Ciencias, Universidad de Chile — The plastic behavior of crystalline metals is well understood. It is known that this regime is mainly mediated by nucleation and propagation of dislocations as well as by grain boundary sliding. In metallic glasses (MGs) the plastic behavior is quite different from their crystalline counterparts and a relationship between atomic-micro structure and properties remains one of the barriers that has hampered the progress to wide applications of MGs. In particular it would be desirable to have studies which directly relate the evolution of the shear bands (SBs) and glass matrix structure to each step of the applied strain, which would allow us to easily connect the evolution of the atomic structure to the stress-strain curve. Here we present a computational tensile test which shows the evolution of the atomic structure according to the strain is applied for a Cu<sub>50</sub>Zr<sub>50</sub> metallic glass nanowire at 300 K with a Cu-Zr b2 inclusion in the center of the system with three different radius from 20 to 60 Å. The system consists of a million atoms and the local structure is analyzed by means of the Voronoi polyhedral technique and the nucleation and propagation of SBs by monitoring the local atomic shear strain.

<sup>1</sup>CONICYT PhD Fellowship No. 21140904

## Friday, March 18, 2016 8:00AM - 10:48AM –

Session X37 GSOF: Liquid Crystals: Defects, Theory and Simulations 340 - Chenhui Zhu, Lawrence Berkeley Laboratory

### 8:00AM X37.00001 Topological defects in liquid crystals as templates for molecular self-assembly. , XIAO GUANG WANG, DANIEL MILLER, EMRE BUKUSOGLU, University of Wisconsin-Madison, JUAN DE PABLO, University of Chicago,

NICHOLAS ABBOTT, University of Wisconsin-Madison — Topological defects in liquid crystals (LCs) have been widely used to organize colloidal dispersions and template polymerizations, leading to a range of elastomers and gels with complex mechanical and optical properties. However, little is understood about molecular-level assembly processes within defects. This presentation will describe an experimental study that reveals that nanoscopic environments defined by LC defects can selectively trigger processes of molecular self-assembly. By using fluorescence microscopy, cryogenic transmission electron microscopy and super-resolution optical microscopy, key signatures of molecular self-assembly of amphiphilic molecules in topological defects are observed - including cooperativity, reversibility, and controlled growth of the molecular assemblies. By using polymerizable amphiphiles, we also demonstrate preservation of molecular assemblies templated by defects, including nanoscopic o-rings synthesized from Saturn-ring disclinations. Our results reveal that topological defects in LCs are a versatile class of three-dimensional, dynamic and reconfigurable templates can direct processes of molecular self-assembly in a manner that is strongly analogous to other classes of macromolecular templates.

**8:12AM X37.00002 Molecular nature of liquid crystal defects**, MOHAMMAD RAHIMI, Institute for Molecular Engineering, University of Chicago, NICHOLAS L. ABBOTT, Department of Chemical Engineering, University of Wisconsin - Madison, JUAN J DE PABLO, Institute for Molecular Engineering, University of Chicago, RUI ZHANG, University of Chicago — Distortion of liquid crystal (LC) director creates defects which can be easily observed and controlled experimentally. Liquid crystal defects, which are a consequence of symmetry breaking, have significant influence on the macroscopic properties of liquid crystals, and many of the features that make LCs particularly exciting for new applications can be traced back to the existence of liquid crystal defects. However, the molecular nature of liquid crystal defects remains largely unknown. In this work, we perform large-scale atomistic simulations of 5CB/8CB mixture with a cylinder with strong homeotropic anchoring. The presence of the cylinder distorts the nematic field around the cylinder surface and creates two line defects. The local order parameter and biaxiality are calculated to characterize these defects. The results of this study indicate that, the density and the order parameter are correlated, and at the defect both parameters are low.

**8:24AM X37.00003 Topological defects and self-assembly of cuboidal colloidal particles with sharp edges in a nematic liquid crystal.**, JUAN J. DE PABLO, MONIRO SADAT, JULIO C. ARMAS-PEREZ, The University of Chicago, Institute for Molecular Engineering, VISHAL SONI, WILLIAM T. M. IRVINE, The University of Chicago, James Franck Institute — The geometry of colloidal particles defines the topology and self-assembly of colloidal superstructures in nematic liquid crystals. Past research has largely focused on the defects that arise around spherical colloids, and the defect-induced aggregation between them. In this work, we examine experimentally and theoretically, the effect of edge curvature of colloidal particles on their defect configurations and self-assembly in a nematic liquid crystal (5CB). The polarized images of the particles with homeotropic surface anchoring in 5CB show that the presence of sharp edges can reshape completely the defect ring. The defect makes sharp turns and follows the edge of the cube particles, which significantly affects the interaction between particles and their eventual self-assembly. In agreement with our experimental results, our computational studies indicate that the gradual increase of the edges sharpness that occurs as we transition from spheres to cubes, changes the defect structure from a Saturn ring to a twisted ring, which is pinned to the edges of the cube particle. The wide variety of topological defects achievable by changing the curvature could provide new tools to tune colloidal self-assembly.

**8:36AM X37.00004 Nematic liquid crystal bridges**, SUSANNAH DOSS, PERRY ELLIS, Georgia Institute of Technology, JAYALAKSHMI VALLAMKONDU, National Institute of Technology, Warangal (India), EDWARD DANEMILLER, MARK VERNON, ALBERTO FERNANDEZ-NIEVES, Georgia Institute of Technology — We study the effects of confining a nematic liquid crystal between two parallel glass plates with homeotropic boundary conditions for the director at all bounding surfaces. We find that the free surface of the nematic bridge is a surface of constant mean curvature. In addition, by changing the distance between the plates and the contact angle with the glass plates, we transition between loops and hedgehogs that can be either radial or hyperbolic.

**8:48AM X37.00005 Fine structure of the topological defect core: Disclination in lyotropic chromonic liquid crystal<sup>1</sup>**, SHUANG ZHOU, SERGIY SHYANOVSKI, HEUNG-SHIK PARK, YOUNG-KI KIM<sup>2</sup>, Liquid crystal institute, Kent State University, Kent, Ohio 44242, USA, TRISTAN HEARN, LOTHAR REICHEL, Department of Mathematical Science, Kent State University, Kent, Ohio 44242, USA, OLEG LAVRENTOVICH, Liquid crystal institute, Kent State University, Kent, Ohio 44242, USA — Topological defects represent an important concept in many branches of modern physics ranging from cosmology and optics to hard and soft matter. One of the most difficult problems is the fine structure of the so-called core region of defects, where the deformations of the order parameter are so strong that the phenomenological description valid in the far field becomes invalid. Experimental exploration of the fine core structure is usually hindered by the small size (atomic/molecular level) of the core, where optical or even electron microscopy techniques are invalid. In this work, we take advantage of the peculiar nature of the so-called lyotropic chromonic liquid crystals (LCLC) of a nematic type that carry disclinations with a core extending over macroscopic distances (tens of micrometers), large enough to explore their spatial variation by optical and electron microscopy. We demonstrate that the director and the scalar order parameter (associated with the degree of orientational order) show a profound change in the core region. In particular, as one approaches the center of the defect, the azimuthal dependency of the director field changes dramatically and the scalar order parameter shows a strong dependence on the strength of splay and bend deformations.

<sup>1</sup>This work is supported by NSF grant DMS-1434185.

<sup>2</sup>Now at Department of Chemical & Biological Engineering, University of Wisconsin-Madison, Madison, WI 53706, USA

**9:00AM X37.00006 Lassoing the Saddle-Splay: Harnessing  $K_{24}$  Distortions to Line Up Disclinations**, LISA TRAN, MAXIM LAVRENTOVICH, Department of Physics, University of Pennsylvania, DANIEL BELLER, School of Engineering and Applied Sciences, Harvard University, NINGWEI LI, KATHLEEN STEBE, Department of Chemical and Biomolecular Engineering, University of Pennsylvania, RANDALL KAMIEN, Department of Physics, University of Pennsylvania — Systems with holes, such as colloidal handlebodies and toroidal droplets, have been studied in the nematic liquid crystal (NLC) 4-cyano-4-pentylbiphenyl (5CB). It was found that point or ring topological defects occur within each hole and around the system, such that the overall topological charge of the system is conserved. However, what has not been fully appreciated is the ability of the hole geometry with homeotropic (perpendicular) anchoring conditions to induce a saddle-like deformation in the NLC bulk. We exploit this by creating an array of many holes suspended in an NLC cell with oriented planar (parallel) anchoring at the cell boundaries. Through simulations and experiments, we study how the bulk saddle deformations of each hole interact to create novel defect structures, including an array of  $\frac{1}{2}$  disclination lines, reminiscent of those that occur in LC blue phases. The locations of these disclination lines are tunable via the geometry of the cell and hole array, which has potential for controlled, three-dimensional self-assembly in NLCs.

**9:12AM X37.00007 The weirdest martensite: Smectic liquid crystal microstructure and Weyl-Poincaré invariance**, DANILO LIARTE, MATTHEW BIERBAUM, Cornell University, RICARDO MOSNA, Universidade Estadual de Campinas, RANDALL KAMIEN, University of Pennsylvania, JAMES SETHNA, Cornell University — We propose a generalization of the mathematical theory of martensites to describe the complex assembly of focal conics in smectic liquid crystals. Smectics are remarkable, beautiful examples of materials microstructure, with ordered patterns of geometrically perfect ellipses and hyperbolas. The solution of the complex problem of filling three-dimensional space with domains of focal conics under constraining boundary conditions yields a set of strict rules, which are similar to the compatibility conditions in a martensitic crystal. Here we present the rules giving compatible conditions for the concentric circle domains found at two-dimensional smectic interfaces with planar boundary conditions. Using configurations generated by numerical simulations, we develop a clustering algorithm to decompose the planar boundaries into domains. The interfaces between different domains agree well with the smectic compatibility conditions. We also discuss generalizations of our approach to describe the full three-dimensional smectic domains, where the variant symmetry group is the restricted Weyl-Poincaré group of Lorentz boosts, translations, rotations, and dilatations.

**9:24AM X37.00008 4 x 4 Matrix Method Simulations of Swinging Nematic Liquid Crystals**, IGHODALO IDEHENRE, Univ of Dayton, DEAN EVANS, Air Force Research Laboratory, PARTHA BANERJEE, Univ of Dayton, TIMOTHY BUNNING, Air Force Research Laboratory — We present the results of numerical simulations of swinging nematic liquid crystal (SNLC) systems using the 4 x 4 Berreman matrix method. SNLCs are a special class of cholesteric liquid crystals that periodically change handedness when propagating along the helical axis. Unlike standard cholesterics which can only reflect one circular polarization state allowing the other to pass, SNLCs are able to reflect both simultaneously. Our simulations explore the advantages and disadvantages of various periodic functions (sinusoidal, square wave, triangular, etc...), the influence of pitch and optical birefringence on the reflection central wavelength and bandwidth, as well as the overall impact incidence angle has on the reflection spectra.

**9:36AM X37.00009 Phase transitions and order parameters of complex liquid crystalline ordered systems** , KE LIU, JAAKKO NISSINEN, ROBERT-JAN SLAGER, Instituut-Lorentz for Theoretical Physics, Universiteit Leiden, KAI WU, Stanford Institute for Materials and Energy Sciences, Stanford University, JAN ZAAENEN, Instituut-Lorentz for Theoretical Physics, Universiteit Leiden — Liquid crystalline states of matter possess rich phase diagrams, exotic topological defects and unique responses to external fields. Traditionally the focus has been on liquid crystal phases with uniaxial  $D_{\infty h}$  symmetry and biaxial  $D_{2h}$  symmetry. However, in full generality liquid crystalline orders are associated with breaking the  $O(3)$  rotational symmetry to any point group symmetry  $G \subset O(3)$ . We present a general theory for arbitrary three dimensional point group symmetries that allows to derive order parameters and investigate phase transitions of liquid crystalline states. The theory is constructed on symmetry grounds, and adapts to the description of both thermal and quantum liquid crystal systems. The realization of the model in experimental systems are also discussed.

**9:48AM X37.00010 Coarsening Dynamics of Inclusions and Thermocapillary Phenomena in Smectic Liquid Crystal Bubbles** , CHEOL PARK, JOSEPH MACLENNAN, MATTHEW GLASER, NOEL CLARK, University of Colorado, TORSTEN TRITTEL, ALEXEY EREMIN, RALF STANNARIUS, University of Magdeburg, PADETHA TIN, NANCY HALL, NASA Glenn Research Center — The Observation and Analysis of Smectic Islands in Space (OASIS) project comprises a series of experiments that probe interfacial and hydrodynamic behavior of thin spherical-bubbles of smectic liquid crystal in microgravity. Smectic films are the thinnest known stable condensed phase structures, making them ideal for studies of two-dimensional (2D) coarsening dynamics and thermocapillary phenomena in microgravity. The OASIS flight hardware was launched on SpaceX-6 in April 2015 and experiments were carried out on the International Space Station using four different smectic A and C liquid crystal materials in separate sample chambers. We will describe the behavior of collective island dynamics on the bubbles, including temperature gradient-induced thermomigration, and the diffusion and coalescence-driven coarsening dynamics of island emulsions in microgravity. This work was supported by NASA Grant No. NNX-13AQ81G, and NSF MRSEC Grants No. DMR-0820579 and DMR-1420736.

**10:00AM X37.00011 Competition of lattice and basis for alignment of nematic liquid crystals** , ANDREW DEBENEDICTIS, Department of Physics and Astronomy, Tufts University, CANDY ANQUETIL-DECK, DOUGLAS J. CLEAVER, Materials and Engineering Research Institute, Sheffield Hallam University, DAVID B. EMERSON, MATHEW WOLAK, JAMES H. ADLER, Department of Mathematics, Tufts University, TIMOTHY J. ATHERTON, Department of Physics and Astronomy, Tufts University — Due to elastic anisotropy, two-dimensional patterning of substrates can promote weak azimuthal alignment of adjacent nematic liquid crystals. We consider a periodic square lattice of elliptical motifs to examine ways in which the lattice and motif can combine to favor differing orientations. Using semi-analytic elastic continuum theory and Monte Carlo simulations, we find, for circular motifs, that the coverage fraction controls both the polar anchoring angle and a transition in the azimuthal orientation. If the circles are generalized to ellipses, arbitrary control of the effective easy axis and effective anchoring potential becomes achievable by appropriate tuning of the orientation of the ellipse motif relative to the lattice vectors. To determine the behavior of liquid crystals near the domain boundaries, we additionally formulate and solve the full 3D Euler-Lagrange equations directly. We additionally comment on the role of weak anchoring and saddle-splay elasticity.

**10:12AM X37.00012 ABSTRACT MOVED TO P36.013 —**

**10:24AM X37.00013 Particles and curvatures in nematic liquid crystals.** , FRANCESCA SERRA, YIMIN LUO, SHU YANG, RANDALL D. KAMIEN, KATHLEEN J. STEBE, University of Pennsylvania — Elastic interactions in anisotropic fluids can be harnessed to direct particle interactions. A strategy to smoothly manipulate the director field in nematic liquid crystals is to vary the topography of the bounding surfaces. A rugged landscape with peaks and valleys create local deformations of the director field which can interact with particles in solution. We study this complex interaction in two different settings. The first consists of an array of shallow pores in a poly-dimethyl-siloxane (PDMS) membrane, whose curvature can be tuned either by swelling the PDMS membrane or by mechanical stretching. The second is a set of grooves with wavy walls, fabricated by photolithography, with various parameters of curvature and shapes. In this contexts we study how the motion of colloidal particles in nematic liquid crystals can be influenced by their interaction with the peaks and valleys of the bottom substrate or of the side walls. Particles with different associated topological defects (hedgehogs or Saturn rings) behave differently as they interact with the topographical features, favoring the docking on peaks or valleys. These experimental systems are also ideal to study the “lock and key” mechanism of particles in holes and to investigate a possible route for particle sorting.

**10:36AM X37.00014 Effect of an applied electric field on a weakly anchored non-planar Nematic Liquid Crystal (NLC) layer<sup>1</sup>** , ENSELA MEMA, LINDA J. CUMMINGS, LOU KONDIC, New Jersey Institute of Technology — We consider a mathematical model that consists of a NLC layer sandwiched between two parallel bounding plates, across which an external field is applied. We investigate its effect on the director orientation by considering the dielectric and flexoelectric contributions and varying parameters that represent the anchoring conditions and the electric field strength. In particular, we investigate possible director configurations that occur in weakly anchored and non-planar systems. We observe that non-planar anchoring angles destroy any hysteresis seen in a planar system by eliminating the fully vertical director configuration and the “saturation threshold” seen in weakly anchored planar Freedericksz cells.

<sup>1</sup>Supported by NSF Grant No. DMS-1211713

**Friday, March 18, 2016 8:00AM - 10:48AM —**

**Session X38 DPOLY: Block Copolymer Thin Films: Directed Assembly** 341 - Ryan Hayward, U Mass Amherst

**8:00AM X38.00001 Out-of-plane Block Copolymer Microdomains in High Aspect-Ratio Templates** , KARIM GADELRAH, WUBIN BAI, ALFREDO ALEXANDER-KATZ, CAROLINE ROSS, Massachusetts Inst of Tech-MIT — The use of directed self-assembly DSA of block copolymers BCP proved to be a power approach for nanoscale fabrication. It combines the ability of BCPs to self-assemble into nanoscale features with the use of lithographic tools to create controlled long range order. In addition, BCP with highly incompatible blocks (high Flory-Huggins interaction parameter ( $\chi$ )) offer improvement in resolution, and line edge fluctuations of the self-assembled patterns. Unfortunately, high- $\chi$  BCPs usually exhibit large differences in surface affinity between the two blocks, leading to the formation of a surface layer of the lower surface energy block and favoring in-plane orientation of lamellae or cylindrical microdomains. Here, we explore the conditions under which a high  $\chi$  BCP creates an out-of-plane lamellar structure using functionalized high aspect ratio trenches with preferential walls. We employ the free energy analysis of self-consistent field theory SCFT to identify whether an in-plane or out-of-plane structure is stable for a particular trench width. In addition, we employ the single mode expansion of Ginzburg-Landau free energy expression in the weak segregation limit to analytically construct a phase diagram of the in-plane and out-of-plane lamellae as a function of aspect ratio and surface attraction strength. It is found that achieving an out of plane lamellar structure necessitates a coupling between aspect ratio and surface functionality. In particular, strong side wall attraction results in out-of-plane lamellae when the trench aspect ratio is greater than unity. The results are validated for a lamellar forming polystyrene-block-polydimethylsiloxane (PS-b-PDMS) within trenches made using interference lithography.

**8:12AM X38.00002 Characterizing the interfaces of block copolymers with high  $\chi$** , DANIEL SUNDAY, NIST - Natl Inst of Stds & Tech, MICHAEL MAHER, Department of Chemistry, University of Texas, GREGORY BLACHUT, YUSUKE ASANO, SUMMER TEIN, Department of Chemical Engineering, University of Texas, C. GRANT WILLSON, Department of Chemistry/Chemical Engineering, University of Texas, CHRISTOPHER ELLISON, Department of Chemical Engineering, University of Texas, R. JOSEPH KLINE, NIST - Natl Inst of Stds & Tech — In order for block copolymer (BCP) directed self-assembly (DSA) to be able to pattern features below 10 nm there must be materials which can spontaneously assemble at the required length scales. For the smallest features this will require phase separation where the total chain lengths are under 50 monomer units, demanding very large interaction parameters ( $\chi$ ) to have an order-disorder transition. One of the key parameters for DSA will be the interfacial width between the blocks, which is expected to be correlated to the interaction parameter and will help determine the line edge roughness (LER). We have used resonant soft X-ray reflectivity to investigate a series of high  $\chi$  BCPs with different compositions and molecular weights to determine the interfacial width and degree of phase separation. We use these results to estimate the value of  $\chi$  and determine relationships between  $\chi$  and the interfacial mixing.

**8:24AM X38.00003 Reducing Line Edge Roughness of PS-*b*-PMMA pattern by inducing hydrogen bonding at the interface of the block copolymer microdomains**, KYU SEONG LEE, SUNG HYUN HAN, SANGSHIN JANG, JICHEOL PARK, JONGHEON KWAK, JIN KON KIM, POSTECH — Sharp interface between two blocks in block copolymer nano pattern is one of the important issues in industrial applications to nano-patterning. We utilized hydrogen bonding between N-(4-aminomethyl-benzyl)-4-hydroxymethyl-bezamide (BA) and urea (U) at the interface of polystyrene-*block*-poly(methyl methacrylate) copolymer (PS-PMMA). For this purpose, we first synthesized PS by ATRP, then the end group was converted to amino group. Next, it was reacted with BA, followed by reaction with 4-pentynoic acid, resulting in alkyne-terminated group (PS-U-BA-alkyne). Also, azide-terminated PMMA was prepared by anionic polymerization followed by end functionalization. Finally, by the azide-alkyne click reaction between PS-U-BA-alkyne and PMMA-azide, PS-U-BA-PMMA was synthesized. We prepared vertical oriented lamellar nanopatterns on pre-patterned wafers and investigated line edge roughness (LER) after removing PMMA block by dry etching process. We found that LER was reduced compared with PS-PMMA without hydrogen bonding.

**8:36AM X38.00004 Photothermal assembly of block copolymers**, KEVIN YAGER, Center for Functional Nanomaterials, Brookhaven National Laboratory — This talk will discuss recent work on the use of photothermal methods to control the ordering of block copolymer thin films. Photothermal methods can be used to generate temperature gradients and shear fields, which have a strong influence on block copolymer assembly. For example, assembly can be accelerated, and morphology can be aligned. These methods also highlight the non-equilibrium, pathway-dependence of self-assembly. We present examples of exploiting these effects to control alignment, and to iteratively construct arbitrary lattice symmetries.

**9:12AM X38.00005 Numerical Simulations of Directed Self-Assembly in Diblock Copolymer Films using Zone Annealing and Templating Techniques**, JOSEPH HILL, PAUL MILLETT, Univ of Arkansas-Fayetteville — Bulk fabrication of surface patterns with sub-20 nm feature sizes is tremendously desirable for many existing and emerging technologies. Directed self-assembly (DSA) of block copolymers (BCPs) has been a recently demonstrated approach to achieve such feature resolution over large-scale areas with minimal defect populations. Much work however remains to understand and optimize DSA methods in order to move this field forward. This talk will present results from large-scale numerical simulations of zone annealing and topological template processing of BCP films to achieve long-range orientational order. The simulations utilize a Time-Dependent Ginzburg-Landau model and parallel processing to elucidate relationships between thermal gradient velocities and domain orientations as well as defect densities. Additional simulations have been conducted to study to what degree orientational order can be further enhanced with both zone annealing and topological templating techniques. It is found that these two DSA methods do synergistically enhance long-range order with a particular relationship between thermal gradient velocity and topological template spacing.

**9:24AM X38.00006 Rapid microwave annealing for perpendicular oriented cylinders in PS-*b*-PMMA thin films**, ZHE QIANG, KEVIN CAVICCHI, BRYAN VOGT, University of Akron, UNIVERSITY OF AKRON TEAM — Self-assembly of block copolymer (BCP) has been extensively studied for decades due to their wide range of potential applications such as lithography. Direct microwave annealing provides rapid ordering kinetics. However, the knowledge regarding the structural and orientation evolution of morphology during microwave annealing without solvents remains sparse. Herein, we report on how microwave-annealing conditions impact the morphology developed in cylinder forming PS-*b*-PMMA films on unmodified silicon wafers. The fraction of perpendicular cylinders developed during microwave annealing is primarily determined by temperature ramp from microwave heating itself. The heating of the substrate during microwave annealing is varied from 0.5 C/s to 2.8 C/s by two factors: (1) the microwave output energy and (2) the local heating position of BCP film in the microwave reaction vessel. A maximum in the fraction of perpendicular cylinders (97 %) occurs at 1.83 C/s and appears independent of the microwave power used. This work demonstrates the importance of controlling conditions of microwave annealing in the morphology developed.

**9:36AM X38.00007 Directed Self-assembly of Block Copolymer with Sub-15 nm Domain Spacing Using Nanoimprinted Photoresist Templates**, ZHIWEI SUN, Univ of Mass - Amherst, ZHENBIN CHEN, Lanzhou University of Technology, WENXU ZHANG, E. BRYAN COUGHLIN, Univ of Mass - Amherst, SHUAIGANG XIAO, Seagate Technology, THOMAS RUSSELL, Univ of Mass - Amherst — There has been increasing interest in preparing block copolymer thin films with ultra-small domain spacings for use as etching masks for ultra-high resolution nanolithography. One method to prepare block copolymer materials with small feature sizes is salt doping, increasing the Flory-Huggins interaction and allowing microphase separation to be maintained at lower molecular weights. Lamellae-forming P2VP-*b*-PS-*b*-P2VP block copolymer with various molecular weight was synthesized using RAFT polymerization with a dual functional chain transfer agent. Copper (II) Chloride or Gold (III) chloride was found to be selectively associated with P2VP block and increase the unfavorable interactions between PS and P2VP blocks, driving the disordered block copolymer into the ordered state. A 14 nm lamellar spacing of P2VP-*b*-PS-*b*-P2VP thin film was prepared using copper (II) Chloride doping after acetone vapor annealing on neutral brushes. Metallic nano-wire arrays were prepared after selective infiltration of platinum salt into the P2VP domain and oxygen plasma treatment. The directed self-assembly of salt doped P2VP-*b*-PS-*b*-P2VP triblock copolymer having long-range lateral order on nanoimprinted photoresist templates with shallow trenches was also studied.

**9:48AM X38.00008 Exploring the Use of Additives to Optimize the Directed Self-Assembly of Block Copolymers via Self-Consistent Field Theory Simulations**, ADAM HANNON, DANIEL SUNDAY, R. JOSEPH KLINE, National Institute of Standards and Technology — The directed self-assembly (DSA) of block copolymers (BCPs) is being investigated for the fabrication of next generation memory and integrated circuit technologies. Much progress has been made showing how these materials can be processed to produce a variety of transferable patterned morphologies that meet the requirements for fabricating integrated circuit geometries. One lingering issue in using these materials to produce sub-10 nm structures is finding new BCPs with a high enough  $\chi$  Flory-Huggins interaction parameter to create small resolution features with low interfacial widths that are also easily processable. An alternative approach to synthesizing new materials is to instead blend the BCP with additives that strongly interact with one of the blocks. Here we present findings on how the addition of a hydrogen bonding homopolymer affects the overall effective  $\chi$ , the periodicity, and the morphology of the BCP. Self-consistent field theory simulations are used to explore how the relative  $\chi$  values and degrees of polymerization between the BCP and homopolymer affect these parameters and suggest optimal blending conditions. Results are compared with experimental X-ray and neutron scattering studies of a polystyrene-*b*-poly(methyl methacrylate)/poly(vinyl phenol) blend.

**10:00AM X38.00009 Controlled Ordering of Long-range Perpendicular Lamellae by Block Copolymer Self-assembly**, DU YEOL RYU, KYUNGINN KIM, SUNGMIN PARK, YEONGSIK KIM, Yonsei Univ, YONSEI UNIV TEAM — We introduce a simple approach to fabricating highly stable, perpendicularly oriented lamellae through the self-assembly of high-molecular-weight polystyrene-*b*-poly(methyl methacrylate) (PS-*b*-PMMA). The desired morphology was achieved over a narrow annealing period (5–10 min) under solvent vapor, since the SVA process need to terminate immediately before the saturated BCP films begin to dewet the substrate. This narrow processing period impeded practical applications to continuous industrial processes. A controlled SVA process at a selected temperature gap was found to show the excellent long-term stability, at which highly ordered line-arrays of perpendicularly oriented lamellae were confined to topographic line patterns.

**10:12AM X38.00010 Using chemically patterned substrates to suppress thermal placement errors in the directed self-assembly of block copolymer multi-cylinder linear arrays**, CORINNE CARPENTER, KRIS DELANEY, GLENN FREDRICKSON, Univ of California - Santa Barbara — Directed self assembly (DSA) of block copolymers is a promising alternative approach for ~10nm microelectronics patterning, both for feature-size reduction and rectification. One prototypical application of DSA is the use of vertical interconnect access (VIA) cylinders for fabricating conducting channels between circuit layers. Typically a compromise exists between the fidelity and low defect density obtained by using a small number of cylinders per pre-pattern guide and the objective to further increase feature density. In particular for 1D linear arrays of multiple VIAs in a single prepattern, prior experimental and theoretical work has demonstrated that thermal fluctuations in larger arrays cause cylinder placement to vary widely around the equilibrium positions in a manner analogous to the collective excitations in a simple 1D coupled oscillator model (Landau-Peierls instability). In the present work, we assess the efficacy of using chemically patterned substrates to suppress the thermal placement errors using both a phenomenological oscillator model and full field theoretic simulations.

**10:24AM X38.00011 Minimal Topographic Patterns for Guiding Hexagonal Arrays of Cylindrical Microdomains in Block Copolymer Thin Films**, JAEWON CHOI, YINYONG LI, University of Massachusetts Amherst, ILJA GUNKEL, Lawrence Berkeley National Laboratory, ZHIWEI SUN, University of Massachusetts Amherst, FENG LIU, Lawrence Berkeley National Laboratory, KENNETH CARTER, THOMAS RUSSELL, University of Massachusetts Amherst — Topographically patterned substrates have been widely studied to control the lateral order of block copolymer (BCP) microdomains in thin films. However, most studies have been focused on deep topographic patterns, where a confinement depth is comparable to or larger than domain spacing of BCP, limiting the grain size of BCP due to the confinement width. Also, the investigation of BCP microdomains using grazing incidence small angle X-ray scattering (GISAXS) is limited because the scattering peaks from BCP are generally hidden by the strong scattering peaks from the deep topographic pattern. Here, we present the use of minimal topographic patterns for guiding hexagonal arrays of cylindrical microdomains of poly(styrene-*b*-ethylene oxide) (PS-*b*-PEO) thin films. Since the confinement depth of the minimal pattern is much smaller than domain spacing of BCP, this enables cylindrical microdomains to overcome the confined width, generating macroscopic ordered hexagonal arrays. In the GISAXS experiment, we confirmed that the (10) plane of hexagonal arrays was parallel to the direction of the trench by rotating the sample stage and changing the incident angle of X-ray.

**10:36AM X38.00012 Polarized Resonant Critical Dimension Small Angle X-Ray Scattering for the Characterization of Polymer Patterns**, CHRISTOPHER LIMAN, DANIEL SUNDAY, HYUN WOOK RO, LEE RICHTER, ADAM HANNON, R. JOSEPH KLINE, National Institute of Standards and Technology — Critical dimension small angle X-ray scattering (CDSAXS) is a recently developed technique that enables the characterization of the three-dimensional shape of periodic patterns, such as directed self-assembled (DSA) block copolymer (BCP) lamellae thin films. Information about the polymer patterns is extracted by fitting simulated scattering patterns to the experimental ones using an inverse iterative algorithm. Conducting CDSAXS at resonant energies near the carbon or nitrogen edge can enhance the strength of the scattering, but also causes the scattering to be influenced by any anisotropic orientation of the polymer chains. In this work, to assess the degree to which the scattering may be influenced by orientation, we simulate polarized resonant CDSAXS patterns for BCP lamellae with varying degrees of orientation, as well as orientation as a function of location within the lamellae, for different polarizations of the incident X-rays. Also, to assess the influence of a higher degree of orientation, we use capillary force lithography to pattern nanogratings of two semiconducting homopolymers which are known to orient strongly. We characterize these nanogratings, which have similar length scales to DSA BCP lamellae, with polarized resonant CDSAXS and spectroscopic ellipsometry. Finally, we fit simulated CDSAXS and ellipsometric data to the experimental data to obtain information about the shape and the orientation of the nanogratings.

## **Friday, March 18, 2016 8:00AM - 11:00AM –**

**Session X39 DBIO: Method in Molecular Biophysics: DBIO Doctoral Thesis Award** 342 - Henrik Flyvbjerg, Danish Technical University

**8:00AM X39.00001 How to determine local stretching and tension in a flow-stretched DNA molecule**, JONAS N. PEDERSEN, RODOLPHE MARIE, ANDERS KRISTENSEN, HENRIK FLYVBJERG, Tech Univ of Denmark — We determine the nonuniform stretching of and tension in a Mbp-long fragment of DNA that is flow-stretched in a nanofluidic chip. We use no markers, do not know the contour length of the DNA, and do not have the full DNA molecule inside our field-of-view. Instead we analyze the transverse thermal motion of the DNA. Tension at the center of the DNA adds up to 16 pN, giving almost fully stretched DNA. Fitted parameters agree well with simplified expressions, where the DNA is modeled as a cylinder in a parallel flow.

**8:12AM X39.00002 Magnetic Actuation of Self-Assembled DNA Hinges**, S. LAUBACK, K. MATTIOLI, M. ARMSTRONG, C. MILLER, C. PEASE, C. CASTRO, R. SOORYAKUMAR, The Ohio State University — DNA nanotechnology offers a broad range of applications spanning from the creation of nanoscale devices, motors and nanoparticle templates to the development of precise drug delivery systems. Central to advancing this technology is the ability to actuate or reconfigure structures in real time, which is currently achieved primarily by DNA strand displacement yielding slow actuation times (about 1-10min). Here we exploit superparamagnetic beads to magnetically actuate DNA structures which also provides a system to measure forces associated with molecular interactions. DNA nanodevices are folded using DNA origami, whereby a long single-stranded DNA is folded into a precise compact geometry using hundreds of short oligonucleotides. Our DNA nanodevice is a nanohinge from which rod shaped DNA nanostructures are polymerized into micron-scale filaments forming handles for actuation. By functionalizing one arm of the hinge and the filament ends, the hinge can be attached to a surface while still allowing an arm to rotate and the filaments can be labeled with magnetic beads enabling the hinge to be actuated almost instantaneously by external magnetic fields. These results lay the groundwork to establish real-time manipulation and direct force application of DNA constructs.

**8:24AM X39.00003 Nanopore DNA sequencing using kinetic proofreading<sup>1</sup>**, XINSHENG LING, Southeast University (Nanjing China) and Brown University — We propose a method of DNA sequencing by combining the physical method of nanopore electrical measurements and Southern's sequencing-by-hybridization. The new key ingredient, essential to both lowering the costs and increasing the precision, is an asymmetric nanopore sandwich device capable of measuring the DNA hybridization probe twice separated by a designed waiting time. Those incorrect probes appearing only once in nanopore ionic current traces are discriminated from the correct ones that appear twice. This method of discrimination is similar to the principle of kinetic proofreading proposed by Hopfield and Ninio in gene transcription and translation processes. An error analysis of this nanopore kinetic proofreading (nKP) technique for DNA sequencing is carried out in comparison with the most precise 3' dideoxy termination method developed by Sanger.

<sup>1</sup>Nanopore DNA sequencing using kinetic proofreading

**8:36AM X39.00004 Genetic Assessment of the Space Environment using MEMS Technologies**<sup>f1</sup>, DILIP JANA, DILEON SAINT JEAN, SIYOVUSH ABDURAKHIMOV, VARUN KOPPARTHY, GERGAN NESTOROVA, NABAMITA PAL, NAM NGUYEN, PEDRO DEROSA, LEE SAWYER, NIEL CREWS, MARK DECOSTER, Louisiana Tech University, LOUISIANA TECH UNIVERSITY TEAM — *h-abstract-* For decades, researchers have studied the damage to DNA by high-energy radiation. Radiation induced damage include DNA strand breaks, base damage and base substitution. Currently, though, scientists are discovering that it is, in fact, the non-irradiated cells adjacent to the irradiated cells are the primary source of carcinogenesis. To address these "bystander effects", we developed a radiation detector using multi-clad scintillating fibers and silicon pixel arrays to study the effect of radiation on gene expression changes using Microelectromechanical systems (MEMS) technology. The efficiency of proton energy deposition on each of the different layers of the radiation tracking detector has been simulated using GEANT4 toolkit and tested experimentally using the detector. The position of the proton beam was determined from the intensity of the output signal from orthogonal planes of the tracking detector. We have developed and tested an instrument that automates the extraction and quantification of RNA from living cells that automates the collection, purification, and reverse transcription (RT) of RNA from a precisely-defined area of the biological sample. *-pard-/abstract-*

<sup>1</sup>NASA EPSCOR GRANT 13-EPSCoR-0027

**8:48AM X39.00005 Fabrication and characterization of nanopore sandwich devices for DNA kinetic proofreading studies**, ZHISHAN YUAN, JIAJIA YE, HONGWEN WU, XIAO XIE, Southeast University (Nanjing China), QIANJIN WANG, Nanjing University (Nanjing China), JINGJIE SHA, YUNFEI CHEN, ZHONGHUA NI, Southeast University (Nanjing China), XINSHENG LING, Southeast University and Brown University — It has been proposed [1] that solid-state nanopores can be used as a kinetic proofreading mechanism for oligonucleotide hybridization on ssDNA molecules. We describe the first generation of nanopore sandwich structures consisted of two nanopores of different thicknesses of Si<sub>3</sub>N<sub>4</sub> separated by a SiO<sub>2</sub> cavity. We will discuss the results of helium ion-beam and Ga FIB drilling and TEM characterization of the nanopore sandwiches devices. This work was supported by the National 1000-People Plan of China and Jiangsu-985 Fund, and NSFC grant no.51302037. [1] X.S. Ling, "Methods of sequencing nucleic acids using nanopores and active kinetic proofreading", WO/2013/119784, International Application No.: PCT/US2013/025106.

**9:00AM X39.00006 Confinement-induced Molecular Templating and Controlled Ligation**, DANIEL BERARD, MARJAN SHAYEGAN, FRANCOIS MICHAUD, GIL HENKIN, SHANE SCOTT, JASON LEITH, SABRINA LESLIE, McGill University, LESLIE LAB TEAM — Loading and manipulating long DNA molecules within sub-50 nm cross-section nanostructures for genomic and biochemical analyses, while retaining their structural integrity, present key technological challenges to the biotechnology sector, such as device clogging and molecular breakage. We overcome these challenges by using Convex Lens-induced Confinement (CLiC) technology to gently load DNA into nanogrooves from above. Here, we demonstrate single-fluorophore visualization of custom DNA barcodes as well as efficient top-loading of DNA into sub-50 nm nanogrooves of variable topographies. We study confinement-enhanced self-ligation of polymers loaded in circular nanogrooves. Further, we use concentric, circular nanogrooves to eliminate confinement gradient-induced drift of stretched DNA.

**9:12AM X39.00007 Computational and Experimental Characterization of Ribosomal DNA and RNA G-Quadruplexes**, SAMUEL CHO, Wake Forest University — DNA G-quadruplexes in human telomeres and gene promoters are being extensively studied for their role in controlling the growth of cancer cells. Recent studies strongly suggest that guanine (G)-rich genes encoding pre-ribosomal RNA (pre-rRNA) are a potential anticancer target through the inhibition of RNA polymerase I (Pol I) in ribosome biogenesis. However, the structures of ribosomal G-quadruplexes at atomic resolution are unknown, and very little biophysical characterization has been performed on them to date. Here, we have modeled two putative rDNA G-quadruplex structures, NUC 19P and NUC 23P, which we observe via circular dichroism (CD) spectroscopy to adopt a predominantly parallel topology, and their counterpart rRNA. To validate and refine the putative ribosomal G-quadruplex structures, we performed all-atom molecular dynamics (MD) simulations using the CHARMM36 force field in the presence and absence of stabilizing K<sup>+</sup> or Na<sup>+</sup> ions. We optimized the CHARMM36 force field K<sup>+</sup> parameters to be more consistent with quantum mechanical calculations (and the polarizable Drude model force field) so that the K<sup>+</sup> ion is predominantly in the G-quadruplex channel. Our MD simulations show that the rDNA G-quadruplex have more well-defined, predominantly parallel-topology structures than rRNA and NUC 19P is more structured than NUC 23P, which features extended loops. Our study demonstrates that they are both potential targets for the design of novel chemotherapeutics.

**9:24AM X39.00008 Observation of an angular change in the structure of an RNA complex using Fluorescence Resonance Energy Transfer<sup>1</sup>**, SHEEMA RAHMANSERESHT, PEKER MILAS, LOUIS PARROT, LORI S. GOLDNER, University of Massachusetts, Amherst, Physics Department — Single-molecular-pair FRET is often used to study distance fluctuations of single molecules. It is harder to capture angular changes using FRET, because rotational motion of the dyes tends to wash out the angular sensitivity. Using a dye labeling scheme that minimizes the rotational motion of the dyes with respect to the RNA, we use spFRET to measure an angular change in structure of an RNA kissing complex upon protein binding. The model system studied here, R1inv-R2inv, is derived from the RNAI-RNAII complex in *E.coli*. RNA II is a primer for replication of the ColE1 plasmid; its function is modulated by interaction with RNA I, Rop protein is known to stabilize the bent R1inv-R2inv kissing complex against dissociation. The effect, if any, of Rop protein on the conformation of the kissing complex is not known. The eight minimized-energy NMR structures reported for R1inv-R2inv show a small difference in end-to-end distances and much larger differences in twist and bend angles. We compare a first-principles model with spFRET data to determine if the observed change in FRET is consistent with an angular change in structure, as suggested by the model.

<sup>1</sup>Grant number: NSF DBI-1152386

**9:36AM X39.00009 Two-color spectroscopy of UV excited ssDNA complex with a single-wall nanotube (SWNT) probe: Fast nucleobase autoionization mechanism<sup>1</sup>**, SLAVA V ROTKIN, Lehigh University, TETYANA IGNATOVA, UC Irvine, ALEXANDER BALAEFF, University of Central Florida, MING ZHENG, National Institute of Standards and Technology, MICHAEL BLADES, Lehigh University, PETER STOECKL, University of Rochester — DNA autoionization is a fundamental process wherein UV-photoexcited nucleobases dissipate energy to the environment without undergoing chemical damage. SWNT is shown to serve as a photoluminescent reporter for studying the mechanism and rates of DNA autoionization. Two-color photoluminescence (PL) spectroscopy revealed a strong SWNT PL quenching when the UV pump is resonant with the DNA absorption [Nano Research, 2015]. Semiempirical calculations of the DNA-SWNT electronic structure, combined with a Green's function theory for charge transfer, show a 20 fs autoionization rate, dominated by the hole transfer. Rate-equation analysis of the spectroscopy data confirms that the quenching rate is limited by the thermalization of the free charge carriers transferred to the nanotube reservoir. The developed approach has a great potential for monitoring DNA excitation, autoionization, and chemical damage both *in vivo* and *in vitro*.

<sup>1</sup>NSF ECCS-1509786 (S.V.R.,T.I.) and PHY-1359195 (P.S.), NIST and UCF facilities

**9:48AM X39.00010 Mapping DNA methylation by transverse current sequencing: Reduction of noise from neighboring nucleotides**, JOSE ALVAREZ, Department of Physics, University of Puerto Rico, San Juan, PR 00931-3344, USA, STEVEN MASSEY, Department of Biology, University of Puerto Rico, San Juan, PR 00631-3360, USA, ALAN KALITSOV, JULIAN VELEV, Department of Physics, University of Puerto Rico, San Juan, PR 00931-3344, USA — Nanopore sequencing via transverse current has emerged as a competitive candidate for mapping DNA methylation without needed bisulfite-treatment, fluorescent tag, or PCR amplification. By eliminating the error producing amplification step, long read lengths become feasible, which greatly simplifies the assembly process and reduces the time and the cost inherent in current technologies. However, due to the large error rates of nanopore sequencing, single base resolution has not been reached. A very important source of noise is the intrinsic structural noise in the electric signature of the nucleotide arising from the influence of neighboring nucleotides. In this work we perform calculations of the tunneling current through DNA molecules in nanopores using the non-equilibrium electron transport method within an effective multi-orbital tight-binding model derived from first-principles calculations. We develop a base-calling algorithm accounting for the correlations of the current through neighboring bases, which in principle can reduce the error rate below any desired precision. Using this method we show that we can clearly distinguish DNA methylation and other base modifications based on the reading of the tunneling current.

**10:00AM X39.00011 Amylin Detection with a Miniature Optical-Fiber Based Sensor**, ZHAOWEN LIU, MATSKO ANN, ADAM HUGHES, MARK REEVES, George Washington University — We present results of a biosensor based on shifts in the localized surface plasmon resonance of gold nanoparticles self-assembled on the end of an optical fiber. This system allows for detection of protein expression in low sensing volumes and for scanning in cell cultures and tissue samples. Positive and negative controls were done using biotin/avidin and the BSA/Anti-BSA system. These demonstrate that detection is specific and sensitive to nanomolar levels. Sensing of amylin, an important protein for pancreatic function, was performed with polyclonal and monoclonal antibodies. The measured data demonstrates the difference in sensitivity to the two types of antibodies, and titration experiments establish the sensitivity of the sensor. Further experiments demonstrate that the sensor can be regenerated and then reused.

**10:12AM X39.00012 A Nanocoaxial-Based Electrochemical Sensor for the Detection of Cholera Toxin<sup>1</sup>**, MICHELLE ARCHIBALD, BINOD RIZAL, TIMOTHY CONNOLLY, MICHAEL J. BURNS, MICHAEL J. NAUGHTON, THOMAS C. CHILES, Boston College, BIOLOGY AND PHYSICS COLLABORATION — We report a nanocoax-based electrochemical sensor for the detection of bacterial toxins using an electrochemical enzyme-linked immunosorbent assay (ELISA) and differential pulse voltammetry (DPV). The device architecture is composed of vertically-oriented, nanoscale coaxial electrodes, with coax cores and shields serving as integrated working and counter electrodes, respectively. Proof-of-concept was demonstrated for the detection of cholera toxin (CT), with a linear dynamic range of detection was 10 ng/ml - 1 g/ml, and a limit of detection (LOD) of 2 ng/ml. This level of sensitivity is comparable to the standard optical ELISA used widely in clinical applications. The nanocoax array thus matches the detection profile of the standard ELISA while providing a simple electrochemical readout and a miniaturized platform with multiplexing capabilities, toward point-of-care (POC) implementation. In addition, next generation nanocoax devices with extended cores are currently under development, which would provide a POC platform amenable for biofunctionalization of ELISA receptor proteins directly onto the device.

<sup>1</sup>This work was supported by the National Institutes of Health (National Cancer Institute award No. CA137681 and National Institute of Allergy and Infectious Diseases award No. AI100216).

**10:24AM X39.00013 DBIO Doctoral Thesis Award: Enabling multivariate investigation of single-molecule dynamics in solution by counteracting Brownian motion**, QUAN WANG, Stanford University

**Friday, March 18, 2016 8:00AM - 11:00AM –**

**Session X40 GSNP: General Statistical and Nonlinear Physics 343 - Flavio Fenton**

**8:00AM X40.00001 Chaotic dynamics of a candle oscillator**, MARY ELIZABETH LEE, Georgia Inst of Tech, GREG BYRNE, FDA, FLAVIO FENTON, Georgia Inst of Tech — The candle oscillator is a simple, fun experiment dating to the late nineteenth century. It consists of a candle with a rod that is transverse to its long axis, around which it is allowed to pivot. When both ends of the candle are lit, an oscillatory motion will initiate due to different mass loss as a function of the flame angle. Stable oscillations can develop due to damping when the system has friction between the rod and the base where the rod rests. However, when friction is minimized, it is possible for chaos to develop. In this talk we will show periodic orbits found in the system as well as calculated, maximal Lyapunov exponents. We show that the system can be described by three ordinary differential equations (one each for angle, angular velocity and mass loss) that can reproduce the experimental data and the transition from stable oscillations to chaotic dynamics as a function of damping.

**8:12AM X40.00002 Spike Bursts from an Excitable Optical System<sup>1</sup>**, JOSE R RIOS LEITE, EDISON J ROSERO, WENDSON A S BARBOSA, Depto. Física- Univ. Fed. de Pernambuco-Recife, JORGE R TREDICCE, INLN-Univ de Nice-Sophie Antipolis -France — Diode Lasers with double optical feedback are shown to present power drop spikes with statistical distribution controllable by the ratio of the two feedback times. The average time between spikes and the variance within long time series are studied. The system is shown to be excitable and present bursting of spikes created with specific feedback time ratios and strength. A rate equation model, extending the Lang-Kobayashi single feedback for semiconductor lasers proves to match the experimental observations. Potential applications to construct network to mimic neural systems having controlled bursting properties in each unit will be discussed.

<sup>1</sup>Brazilian Agency CNPQ

**8:24AM X40.00003 Singular probability distribution of a parametric oscillator driven by Poisson noise** , PAVEL M. POLUNIN, Michigan State University, PANPAN ZHOU, Hong Kong University of Science and Technology, STEVEN W. SHAW, Michigan State University, HO BUN CHAN, Hong Kong University of Science and Technology, MARK I. DYKMAN, Michigan State University — We provide the results of the theoretical and experimental studies of the probability distribution of a parametric oscillator, which is additionally driven by a Poisson-like noise. The noise consists of pulses at the vibration frequency with duration small compared to the oscillator relaxation time but long compared to the vibration period. We find that the stationary probability distribution of an oscillator quadrature can display a self-similar structure of sharp peaks, almost symmetrical with respect to the maximum, or can have a strongly asymmetric two-peak structure. The form of the distribution depends on the oscillator dynamics in the rotating frame and the rate of the noise pulses. In particular, the self-similar multi-peak structure emerges if the oscillator dynamics in the rotating frame is underdamped. The peaks have a singular power-law shape. We show that the singularity is smeared by thermal noise, which makes the peaks Gaussian near the maxima. We also discuss the frequently encountered situation where the Poisson noise describes fluctuations of the oscillator eigenfrequency. The theoretical and experimental results are in excellent agreement.

**8:36AM X40.00004 Quantum Boltzmann Machine** , BOHDAN KULCHYTSKYI, Univ of Waterloo, EVGENY ANDRIYASH, MOHAMMED AMIN, D-Wave Systems Inc, ROGER MELKO, Univ of Waterloo, Perimeter Institute — The field of machine learning has been revolutionized by the recent improvements in the training of deep networks. Their architecture is based on a set of stacked layers of simpler modules. One of the most successful building blocks, known as a restricted Boltzmann machine, is an energetic model based on the classical Ising Hamiltonian. In our work, we investigate the benefits of quantum effects on the learning capacity of Boltzmann machines by extending its underlying Hamiltonian with a transverse field. For this purpose, we employ exact and stochastic training procedures on data sets with physical origins.

**8:48AM X40.00005 Quantum Feynman Ratchet** , KETAN GOYAL, RYOICHI KAWAI, Univ of Alabama - Birmingham — As nanotechnology advances, understanding of the thermodynamic properties of small systems becomes increasingly important. Such systems are found throughout physics, biology, and chemistry manifesting striking properties that are a direct result of their small dimensions where fluctuations become predominant. The standard theory of thermodynamics for macroscopic systems is powerless for such ever fluctuating systems. Furthermore, as small systems are inherently quantum mechanical, influence of quantum effects such as discreteness and quantum entanglement on their thermodynamic properties is of great interest. In particular, the quantum fluctuations due to quantum uncertainty principles may play a significant role. In this talk, we investigate thermodynamic properties of an autonomous quantum heat engine, resembling a quantum version of the Feynman Ratchet, in non-equilibrium condition based on the theory of open quantum systems. The heat engine consists of multiple subsystems individually contacted to different thermal environments.

**9:00AM X40.00006 Reversibility in Quantum Models of Stochastic Processes** , DAVID GIER, University of Kansas, JAMES CRUTCHFIELD, JOHN MAHONEY, RYAN JAMES, University of California at Davis — Natural phenomena such as time series of neural firing, orientation of layers in crystal stacking and successive measurements in spin-systems are inherently probabilistic. The provably minimal classical models of such stochastic processes are  $\varepsilon$ -machines, which consist of internal states, transition probabilities between states and output values. The topological properties of the  $\varepsilon$ -machine for a given process characterize the structure, memory and patterns of that process. However  $\varepsilon$ -machines are often not ideal because their statistical complexity ( $C_\mu$ ) is demonstrably greater than the excess entropy ( $E$ ) of the processes they represent. Quantum models (q-machines) of the same processes can do better in that their statistical complexity ( $C_q$ ) obeys the relation  $C_\mu \geq C_q \geq E$ . q-machines can be constructed to consider longer lengths of strings, resulting in greater compression. With code-words of sufficiently long length, the statistical complexity becomes time-symmetric — a feature apparently novel to this quantum representation. This result has ramifications for compression of classical information in quantum computing and quantum communication technology.

**9:12AM X40.00007 Finding stability domains and escape rates in kicked Hamiltonians** , ARCHISHMAN RAJU, SAYAN CHOUDHURY, DAVID RUBIN, JAMES SETHNA, Cornell University — We use an effective Hamiltonian to characterize particle dynamics and find escape rates in a one dimensional system with a periodically kicked Hamiltonian. We study a model of particles in storage rings which is given by a symplectic map where the chaos is described by the KAM theorem. Ignoring the resonances, the dynamics typically has a finite region in phase space where it is stable. Photon noise in the system leads to particle loss from this stable region. Determining this 'aperture' and finding escape rates is therefore an important physical problem. We characterize the stable region in phase space using a perturbation theory developed in the context of quantum mechanics. We then derive analytical expressions for the escape rate in the small damping regime and compare them with numerical simulations. We discuss the possibility of extending the procedure to include higher dimensions and more complicated noise terms.

**9:24AM X40.00008 The canonical ensemble revisited: a projection operator approach** , WIM MAGNUS, Universiteit Antwerpen / Imec, FONS BROSENS, Universiteit Antwerpen, CONDENSED MATTER THEORY TEAM, THEORY OF QUANTUM SYSTEMS AND COMPLEX SYSTEMS TEAM — Constraining the particle number  $N$  in the canonical ensemble hampers the systematic calculation of the partition function  $Z_N$  for non-interacting fermions and bosons, unlike in the case of the grand-canonical ensemble. Recently, we have shown that this task can be accomplished by invoking a projection operator that automatically imposes the particle number constraint in the many-particle Hilbert space. As a result, an integral representation is obtained for  $Z_N$ , as well as for the two-point and four-point correlation functions. As an illustration, the Helmholtz free energy and the chemical potential are calculated for a two-dimensional electron gas typically residing in the inversion layer of a field-effect transistor.

**9:36AM X40.00009 Novel dynamics and thermodynamics of a new Hamiltonian mean field model<sup>1</sup>** , SERGIO CURILEF, BORIS ATENAS, Universidad Catlica del Norte — Statistical systems are idealized by the hypothesis that the particles do not interact among them, or the range of interactions is short enough, reaching very fast the statistical state that we know as equilibrium. However, systems with long-range interactions are common in nature because of they are observed from the atomic scale to the astronomical scale, exhibiting some anomalies as inequivalence of ensembles, negative heat capacity, ergodicity breaking, non equilibrium phase transitions, quasi-stationarity, anomalous diffusion, etc. We present in this contribution a new Hamiltonian mean field model whose potential is inspired in the dipole-dipole interactions. The equilibrium is analytically studied in the canonical ensemble and coincides with the one obtained from molecular dynamics simulations (microcanonical ensemble). We notice, this model presents a kind of inequivalence of ensembles in long-standing states before arriving at equilibrium. However, the novelty, compared to other models presented in recent literature, is that two quasi-stationary states appear in the behavior of this system. The first quasi-stationary state decays to a second one, which is different to the first, before going to the equilibrium. We characterize them by its dynamics and thermodynamics.

<sup>1</sup>We acknowledge partial financial support by Anillo ACT-1204, VRIDT-UCN105/2015. We appreciate the computational assistance of A. Pluchino.

**9:48AM X40.00010 Optimization of finite-size errors in finite-temperature calculations of unordered phases** , DEEPAK IYER, Bucknell University, MARK SREDNICKI, University of California Santa Barbara, MARCOS RIGOL, Pennsylvania State University — It is common knowledge that the microcanonical, canonical, and grand canonical ensembles are equivalent in thermodynamically large systems. Here, we study finite-size effects in the latter two ensembles. We show that contrary to naive expectations, finite-size errors are exponentially small in grand canonical ensemble calculations of translationally invariant systems in unordered phases at finite temperature. Open boundary conditions and canonical ensemble calculations suffer from finite-size errors that are only polynomially small in the system size. We further show that finite-size effects are generally smallest in numerical linked cluster expansions. Our conclusions are supported by analytical and numerical analyses of classical and quantum systems.

**10:00AM X40.00011 Complex Pole Approach in Thermodynamic Description of Fluid Mixtures with Small Number of Molecules**, TIMUR ASLYAMOV, OLEG DINARIEV, Schlumberger Moscow Research — Physically consistent description of equilibrium small molecular systems requires the extension of thermodynamics. The reason is the absence of thermodynamic limit, which is mandatory for the applicability of classical thermodynamics. New theoretical method of complex pole decomposition for the statistical description of small multicomponent molecular systems is implemented. Similar approach has been previously developed and applied in nuclear physics for finite systems of nucleons. We have significantly transformed and extended the original formulation to make it work for multicomponent molecular mixtures in small systems. The aim of this research is to provide new comprehensive description of small equilibrium molecular systems with numerous scientific and industrial applications for artificial and natural materials with nanopores. Several cases for molecular systems in small cavities are studied. In particular size-dependent additional pressure for small systems is evaluated analytically and numerically. The obtained results are in correspondence to published experimental data and molecular dynamics simulations.

**10:12AM X40.00012 Exact  $\Phi^4$  Critical Exponents via the Limit of Finite Periodic Systems**, ANTHONY HEGG, PHILIP PHILLIPS, University of Illinois at Urbana-Champaign — We formulate an RG procedure to nonperturbatively calculate the critical exponents of  $\Phi^4$  theory in arbitrary dimension. Our method first calculates the exact RG equations for a finite but arbitrarily large system with periodic boundary. We then take the limit as that boundary diverges to simplify the equations and recover a true critical point of the system. In particular this provides the 3d critical Ising exponents to high precision. This method is not specific to  $\Phi^4$  theory and thus should apply to many other systems.

**10:24AM X40.00013 The three-dimensional  $O(n \rightarrow \infty)$   $\phi^4$  model on a strip with free boundary conditions: exact results for a nontrivial dimensional crossover**, HANS WERNER DIEHL, SERGEI RUTKEVICH, Univ Duisburg-Essen — The  $O(2)$   $\phi^4$  model on a 3D film of thickness  $L$  with free boundaries is relevant for the explanation of the thinning of wetting layers of  $^4\text{He}$  caused by critical Casimir forces near and below the  $\lambda$ -transition. Just as its  $O(n)$  analog, the model has long-range order below the bulk critical temperature  $T_c$  if  $L = \infty$ , but remains disordered for all  $T > 0$  when  $L < \infty$ . A proper analysis of its scaling behavior near  $T_c$  is challenging: it involves a nontrivial dimensional crossover in addition to bulk, boundary, and finite-size critical behaviors. The  $n \rightarrow \infty$  limit of the model can be solved exactly in terms of the eigenvalues and eigenfunctions of a self-consistent Schrödinger equation whose potential  $v(z)$  becomes singular at the boundary planes. Complementing recent numerically exact results, we derive various exact analytical results for series expansion coefficients of  $v(z)$ , its  $L = \infty$  scattering data for all values  $m_0$  of the temperature scaling field, and the low-temperature asymptotic behavior of the residual free energy and the Casimir force using a combination of boundary-operator and short-distance expansions, proper extensions of inverse scattering theory, new trace formulae, and semi-classical expansions.

**10:36AM X40.00014 A Molecular Model for Chiral Symmetry Breaking**, FOLARIN LATINWO, FRANK STILLINGER, PABLO DEBENEDETTI, Princeton University — In this work, we present a new class of molecular models for chiral phenomena in condensed matter systems. A key feature of these models is the ability of the four-site (tetramer) “molecules” to inter-convert between two distinct chiral forms (enantiomers). Given this feature, we use analytical theory and computer simulations to investigate the emergent chiral properties (including symmetry breaking) over a range of conditions. In particular, we consider the single-molecule level and condensed-phase behavior of our model system. Interestingly, we find that our liquid-phase predictions are in excellent agreement with recent experimental reports on chiral self-sorting in isotropic liquids. From this perspective, our model demonstrates accurate predictive capabilities, as well as a platform for understanding the microscopic origins of a variety of chiral phenomena. In a broader context, we anticipate that this class of models will be relevant to chirality-dominated areas such as the pharmaceutical industry and pre-biotic geochemistry.

**10:48AM X40.00015 Thermal diffusion and colored energy dissipation in hydrogen bonded liquids.**, RICCARDO DETTORI, Department of Physics - University of Cagliari (I), CLAUDIO MELIS, Department of Physics - University of Cagliari, MICHELE CEROTTI, Ecole Polytechnique Federale de Lausanne (CH), DAVIDE DONADIO, Department of Chemistry - UC Davis (USA), LUCIANO COLOMBO, Department of Physics - University of Cagliari (I) — H-bonded liquids show a manifold energy dissipation dynamics due to: strong directionality of H-bonds and complexity of their network. This affects both thermal diffusion and energy dissipation mechanisms in pump-probe spectroscopy experiments. By nonequilibrium molecular dynamics (MD) simulations we investigate such phenomena in liquid methanol. While heat transport is studied by approach-to-equilibrium MD, energy dissipation is investigated by making use of a novel Generalized Langevin Equation (GLE) colored noise thermostat, which can generate a non-equilibrium frequency-resolved dynamics by using a correlated noise. The colored thermostat can thermally excite a narrow range of vibrational modes, typically the stretching mode of the OH involved in H-bonding, leaving the other degrees of freedom at the equilibrium temperature. The energy dissipation is then observed as a function of time, by probing the excitation decay and the energy transfer to other modes. In particular, by monitoring in time the different contributions to the potential energy of the system, we evaluate how energy is transferred from the excited mode to other modes of the nearby molecules and provide understanding on the dynamics of H-bonded liquids, as resulting from current experimental investigations

**Friday, March 18, 2016 8:00AM - 11:00AM –**

**Session X41 DBIO DPOLY DCOMP: Physics of Proteins: Structure and Dynamics II** 344 - Yi Cao, Nanjing University

**8:00AM X41.00001 Dual-resolution modeling demonstrates greater conformational heterogeneity of CENP-A/H4 dimer than that of H3/H4**, HAIQING ZHAO, University of Maryland — Centromere protein A (CENP-A) is a centromere-specific H3 histone variant and shares only about 50% amino acid sequence identity with the canonical H3 protein. CENP-A is required for packaging the centromere and for the proper separation of chromosomes during mitosis. Despite their discrete functions, previously reported crystal structures of the CENP-A/H4 and H3/H4 dimers reveal surprising similarity. In this work, we characterize the structure and dynamics of CENP-A/H4 and H3/H4 dimers with a dual-resolution approach, using both all-atom and coarse-grained (CG) molecular dynamics (MD) simulations. Interestingly, the histone dimer containing CENP-A is more structurally variable than the canonical H3 dimer. Furthermore, our calculations revealed significant conformational distinctions between the interface profiles of CENP-A/H4 and H3/H4. In addition, the presence of the CENP-A-specific chaperone HJURP dramatically reduced the conformational heterogeneity of CENP-A/H4. Overall, these results are in general agreement with the available experimental data and provide new dynamic insights into the mechanisms underpinning the chaperone-mediated assembly of CENP-A nucleosomes *in vivo*.

**8:12AM X41.00002 Aggregation of alpha-synuclein by a coarse-grained Monte Carlo simulation**, BARRY FARMER, Air Force Research Laboratory, RAS PANDEY, University of Southern Mississippi — Alpha-synuclein, an intrinsic protein abundant in neurons, is believed to be a major cause of neurodegenerative diseases (e.g. Alzheimer, Parkinson's disease). Abnormal aggregation of ASN leads to Lewy bodies with specific morphologies. We investigate the self-organizing structures in a crowded environment of ASN proteins by a coarse-grained Monte Carlo simulation. ASN is a chain of 140 residues. Structure detail of residues is neglected but its specificity is captured via unique knowledge-based residue-residue interactions. Large-scale simulations are performed to analyze a number local and global physical quantities (e.g. mobility profile, contact map, radius of gyration, structure factor) as a function of temperature and protein concentration. Trend in multi-scale structural variations of the protein in a crowded environment is compared with that of a free protein chain.

**8:24AM X41.00003 Network Analysis Reveals the Recognition Mechanism for Mannose-binding Lectins**, YUNJIE ZHAO, YIREN JIAN, CHEN ZENG, Department of Physics, The George Washington University, COMPUTATIONAL BIOPHYSICS LAB TEAM — The specific carbohydrate binding of mannose-binding lectin (MBL) protein in plants makes it a very useful molecular tool for cancer cell detection and other applications. The biological states of most MBL proteins are dimeric. Using dynamics network analysis on molecular dynamics (MD) simulations on the model protein of MBL, we elucidate the short- and long-range driving forces behind the dimer formation. The results are further supported by sequence coevolution analysis. We propose a general framework for deciphering the recognition mechanism underlying protein-protein interactions that may have potential applications in signaling pathways.

**8:36AM X41.00004 Unliganded EphA3 dimerization promoted by the SAM domain**, KALINA HRISTOVA, DEO SINGH, CHRISTOPHER KING, FOZIA AHMED, Johns Hopkins University, ELENA PASQUALE, Sanford-Burnham Medical Research Institute — The EphA3 receptor tyrosine kinase regulates morphogenesis during development, and is overexpressed and mutated in a variety of cancers. EphA3 activation is believed to follow a “seeding mechanism” model, in which ligand binding to the monomeric receptor acts as a trigger for signal-productive receptor clustering. We use a novel approach to study EphA3 lateral interactions on the surface of live cells, and we demonstrate that EphA3 forms dimers in the absence of ligand binding. We further show that these dimers are stabilized by interactions involving the EphA3 SAM domain. The discovery of unliganded EphA3 dimers challenges the current understanding of the chain of EphA3 activation events, and suggests that EphA3 may follow the “pre-formed dimer” model of activation known to be relevant for other receptor tyrosine kinases. This work also establishes a new role for the SAM domain in promoting Eph receptor lateral interactions and signaling on the cell surface.

**8:48AM X41.00005 Dissecting the active site of a photoreceptor protein**, WOUTER HOFF, MIWA HARA, JIE REN, FARZANEH MOGHADAM, AIHUA XIE, MASATO KUMAUCHI, Oklahoma State University — While enzymes are quite large molecules, functionally important chemical events are often limited to a small region of the protein: the active site. The physical and chemical properties of residues at such active sites are often strongly altered compared to the same groups dissolved in water. Understanding such effects is important for unraveling the mechanisms underlying protein function and for protein engineering, but has proven challenging. Here we report on our ongoing efforts on using photoactive yellow protein (PYP), a bacterial photoreceptor, as a model system for such effects. We will report on the following questions: How many residues affect active site properties? Are these residues in direct physical contact with the active site? Can functionally important residues be recognized in the crystal structure of a protein? What structural resolution is needed to understand active sites? What spectroscopic techniques are most informative? Which weak interactions dominate active site properties?

**9:00AM X41.00006 Statistical mechanics of hydrophobic amino acids in aqueous solution: A joint experimental scattering and computational study**, LINGSHUANG SONG, Case Western Reserve University, LIN YANG, Brookhaven National Laboratory, WEI HUANG, Case Western Reserve University, JIE MENG, Peking University, SICHUN YANG, Case Western Reserve University — How hydrophobic amino acids interact with each other is still a fundamental question in understanding protein dynamics and folding. Here, we describe an integrative experimental-computational approach of combining x-ray solution scattering and atomistic molecular simulations to determine the molecular properties of a hydrophobic leucine amino acid in an aqueous solution. First, scattering data were acquired at a series of amino acid and salt concentrations and these scattering profiles were further used to calibrate atomistic molecular simulations via a single parameter for solute-solvent interaction. Second, these accurate data of atomistic leucine simulations were used to quantify the effective interacting potentials via a structural simplification of one-bead-per-residue and two-bead-per-residue representations. Third, comparative energetic analyses between the one-bead and two-bead representations were performed to reach a simple picture of residue-residue interactions with an accurate energy function. Taken together, this joint experimental-computational study provides critical insights into microscopic interactions of hydrophobic amino acids in solution with a profound application for studying molecular dynamics of, e.g., intrinsically disordered proteins and their folding.

**9:12AM X41.00007 Mapping the temperature-dependent conformational landscapes of the dynamic enzymes cyclophilin A and urease<sup>1</sup>**, ROBERT THORNE, Cornell University, DANIEL KEEDY, University of California, San Francisco, MATTHEW WARKENTIN, Cornell University, JAMES FRASER, University of California, San Francisco, DAVID MOREAU, HAKAN ATAKISI, PETER RAU, Cornell University — Proteins populate complex, temperature-dependent ensembles of conformations that enable their function. Yet in X-ray crystallographic studies, roughly 98% of structures have been determined at 100 K, and most refined to only a single conformation. A combination of experimental methods enabled by studies of ice formation and computational methods for mining low-density features in electron density maps have been applied to determine the evolution of the conformational landscapes of the enzymes cyclophilin A and urease between 300 K and 100 K. Minority conformations of most side chains depopulate on cooling from 300 to ~200 K, below which subsequent conformational evolution is quenched. The characteristic temperatures for this depopulation are highly heterogeneous throughout each enzyme. The temperature-dependent ensemble of the active site flap in urease has also been mapped. These all-atom, site-resolved measurements and analyses rule out one interpretation of the protein-solvent glass transition, and give an alternative interpretation of a dynamical transition identified in site-averaged experiments. They demonstrate a powerful approach to structural characterization of the dynamic underpinnings of protein function.

<sup>1</sup>Supported by NSF MCB-1330685

**9:24AM X41.00008 Computational modeling of the side chain dihedral angle distributions of methionine using hard-sphere repulsive and short-range attractive interactions<sup>1</sup>**, ALEJANDRO VIRRUETA, COREY O'HERN, LYNNE REGAN, Yale University — Methionine (Met) is a versatile amino acid found frequently both in protein cores and at protein-protein interfaces. Thus, a complete description of the structure of Met is tantamount to a fundamental understanding of protein structure and design. In previous work, we showed that our hard-sphere dipeptide model is able to recapitulate the side chain dihedral angle distributions observed in high-resolution protein crystal structures for the 8 amino acids we have studied to date: Val, Thr, Ser, Leu, Ile, Cys, Tyr, and Phe. Using the same approach, we can predict the observed Met side chain dihedral angle distributions  $P(\chi_1)$  and  $P(\chi_2)$ , but not  $P(\chi_3)$ . In this manuscript, we investigate the possible origins of the discrepancy and identify the minimal additions to the hard-sphere dipeptide model necessary to quantitatively predict  $P(\chi_3)$  of Met. We find that applying a Lennard-Jones potential with weak attraction between hydrogen atoms is sufficient to achieve predictions that match the observed  $\chi_3$  side chain dihedral angle probability distributions for Met, Nle, and Mse without negatively affecting our results for the 8 previously studied amino acids.

<sup>1</sup>A. V. is supported by an NSF Graduate Research Fellowship and a Ford Foundation Fellowship.

**9:36AM X41.00009 Model comparison in X-ray crystallography**, DAVID SIVAK, NATHAN BABCOCK, Dept. of Physics, Simon Fraser University, DANIEL KEEDY, JAMES FRASER, Dept. of Bioengineering and Therapeutic Sciences, University of California, San Francisco — X-ray crystallographers conventionally infer a single best-fit structure from experimental data. Recently, attention has turned to inference of multiple structures and more generally to more complex model types that improve quality of fit—yet potentially increase overfitting to experimental noise. Significant research effort has been focused on inferring the best-fit parameters within a given model type, yet comparatively little attention has been given to selection between model types. Using metrics from the statistics community, we develop a model comparison framework for statistically-rigorous inference of protein conformational heterogeneity. We compare these information criteria to conventional model comparison criteria, and we assess their utility for judging different model types on their balance between quality of fit and model parsimony.

## 9:48AM X41.00010 Small-Angle Neutron Scattering study of the NIST mAb reference material

, MARIA MONICA CASTELLANOS, NIST Center for Neutron Research, IBBR, YUN LIU, NIST Center for Neutron Research, Univ. Delaware, SUSAN KRUEGER, JOSEPH CURTIS, NIST Center for Neutron Research — Monoclonal antibodies (mAbs) are of great interest to the biopharmaceutical industry because they can be engineered to target specific antigens. Due to their importance, the biomanufacturing initiative at NIST is developing an IgG1 mAb reference material 'NIST mAb', which can be used by industry, academia, and regulatory authorities. As part of this collaborative effort, we aim at characterizing the reference material using neutron scattering techniques. We have studied the small-angle scattering profile of the NIST mAb in a histidine buffer at 0 and 150 mM NaCl. Using Monte Carlo simulations, we generate an ensemble of structures and calculate their theoretical scattering profile, which can be directly compared with experimental data. Moreover, we analyze the structure factor to understand the effect of solution conditions on the protein-protein interactions. Finally, we have measured the solution scattering of the NIST mAb, while simultaneously performing freeze/thaw cycles, in order to investigate if the solution structure was affected upon freezing. The results from neutron scattering not only support the development of the reference material, but also provide insights on its stability and guide efforts for its development under different formulations.

**10:00AM X41.00011 Replica-exchange Wang-Landau simulations of the HOP lattice protein model<sup>1</sup>**, GUANGJIE SHI, Center for Simulation Physics, The University of Georgia, THOMAS WÜST, ID Scientific IT Services, ETH Zürich, Switzerland, YING WAI LI, National Center for Computational Sciences, Oak Ridge National Laboratory, DAVID P. LANDAU, Center for Simulation Physics, The University of Georgia — The hydrophobic-polar (HP) lattice protein model has been the subject of intensive investigation in an effort to aid our understanding of protein folding. However, the high ground state degeneracies caused by its simplification stands in contrast to the generally unique native states of natural proteins. Here we proposed a simple modification, by introducing a new type of "neutral" monomer, 0, i.e. neither hydrophobic nor polar, thus rendering the model more realistic without increasing the difficulties of sampling significantly<sup>2</sup>. With the replica exchange Wang-Landau (REWL) scheme<sup>3</sup> we investigated several widely studied HP proteins and their HOP counterparts. Dramatic differences in both ground state and thermodynamic properties have been found. For example, the HOP version of Crambin shows more clear two-step folding and 3 order of magnitudes less ground state degeneracy than its HP counterpart.

<sup>1</sup>Supported by NSF

<sup>2</sup>G. Shi, T. Wüst, Y. W. Li and D. P. Landau J. Phys.: Conf. Ser. 640, 012017 (2015)

<sup>3</sup>T. Vogel, Y. W. Li, T. Wüst, and D. P. Landau, Phys. Rev. Lett., 110, 210603 (2013)

## 10:12AM X41.00012 Experimental and Computational Study of Beta-Galactosidase Inhibition

, ANTHONY COOPER, LUCA LARINI, Rutgers University-Camden — In this study, we combine experiments and simulations to design novel inhibitors of enzymes. We aim to characterize the inhibition mechanism which we show to be dependent on the aggregation of inhibitor peptides. As a model system we chose to use  $\beta$ -galactosidase. We selected four peptides out of 10,000 initially screened using microarrays and that show the greatest Michaelis-Menten constant and highest solubility. Molecular dynamics simulations were performed to identify the exact mechanism of action of these peptides. We show that the positive residues, like arginine and lysine, are crucial for inhibiting enzyme activity. According to simulations, these residues are also responsible for the conformations adopted by the peptide in solution. Dynamic light scattering study revealed that the aggregation of peptides with the enzyme takes place and is responsible for inhibiting enzyme activity.

## 10:24AM X41.00013 ABSTRACT MOVED TO M1.392 —

## 10:36AM X41.00014 Dynamic switching mechanisms of a CC chemokine, CCL5 (RANTES).

**A simulation study.**, EMANUEL PETER, IGOR PIVKIN, University of Lugano — CCL5 (RANTES) belongs to the class of pro-inflammatory chemokines which are part of the human immune-response. It is known to activate leukocytes through its associated chemokine receptor 5 (CCR5) and plays a key role in several malignancies, including HIV-1 infections and cancer. In this talk, we present our results from enhanced sampling simulations of the CCL5 (RANTES) monomer. We find that this protein can adopt 2 different conformations: a globular form, with an orthogonal alignment of the N-terminal part, and a 'cis' form, in which the N-terminus is aligned parallel to the  $\beta$ -strand interface. A detailed analysis of the structure reveals that each of these states is stabilized by salt-bridges along the sequence, and corresponds to a defined dihedral-geometry of the 2 disulfide bridges Cys10-34 and Cys11-50. We derive a uniform distribution of transitions from the globular form of CCL5 (RANTES), and find that each of the main conformers adopts different electrostatic patterns.

## 10:48AM X41.00015 Using Excel To Study The Relation Between Protein Dihedral Angle Omega And Backbone Length<sup>1</sup>

, CHRISTOPHER SHEW, SAMARI EVANS, XIUPING TAO, Winston-Salem State University — How to involve the uninitiated undergraduate students in computational biophysics research? We made use of Microsoft Excel to carry out calculations of bond lengths, bond angles and dihedral angles of proteins. Specifically, we studied protein backbone dihedral angle omega by examining how its distribution varies with the length of the backbone length. It turns out Excel is a respectable tool for this task. An ordinary current-day desktop or laptop can handle the calculations for midsized proteins in just seconds. Care has to be taken to enter the formulas for the spreadsheet column after column to minimize the computing load.

<sup>1</sup>Supported in part by NSF grant 1238795

## Friday, March 18, 2016 8:00AM - 11:00AM —

Session X42 DPOLY: Semicrystalline Polymers 345 - Ahmed Ismail, University of West Virginia

## 8:00AM X42.00001 Crystallization of atactic polystyrene.

, YU CHAI, JAMES FORREST, Univ of Waterloo — Atactic polystyrene is often used as an archetypical example of a material that has no crystalline ground state due to the lack of order in the arrangement of phenyl groups along the backbone. However, even in polymers with perfect Bernoullian (random) statistics, there is a probability that a given molecule will have larger blocks of a given stereoregularity. These blocks, in turn, could allow the formation of nanocrystalline domains. As a model system to investigate whether such blocks could lead to nanoscale crystallinity, we consider PS with Mw less than 1000 where there is a reasonable probability of a molecule having all meso or racemo diads. For the case of Mw 600, there are clear indications of crystal growth with two characteristic temperatures below which two different crystal species can nucleate and grow. Similar crystal growth and melting behavior is observed for Mw 1000.

## 8:12AM X42.00002 Bisoxalamide Clarifiers to Improve Optical Performance of Polyethylene

**Resins<sup>1</sup>**, LIN WANG, MARTIN HILL, NESTOR SANTOS JR, ANDREW BANKS, JESSICA HUANG, ELLEN KEENE, RICH KEATON, Dow chemical — The use of special nucleating agents, often referred to as clarifying agents, to improve optical performance of polyethylene is not widely used in the industry. A series of bisoxalamide compounds were synthesized and mixed with linear low density polyethylene (LLDPE) to test clarification effects. In this talk, we will discuss structure/property relationship of these molecules on optical and thermal properties of LLDPE.

<sup>1</sup>Bisoxalamide clarifiers to improve optical performance of polyethylene resins

**8:24AM X42.00003 Coincident Crystallization of PEO-*b*-PCL Copolymers with Similar Block Molecular Weights**, RYAN VAN HORN, NATASHA BRIGHAM, CHRISTOPHER NARDI, Allegheny College — Poly(ethylene oxide)-*block*-poly(epsilon-caprolactone) (PEO-*b*-PCL) copolymers have garnered much attention for their use in the biomedical field due to their biocompatibility and the degradation of PCL. The applications of this polymer are heavily dependent on the polymer's physical properties, including crystalline content. One complicating factor is the relatively similar transition temperatures for PEO and PCL. We have studied the coincident crystallization behavior of 5k-5k and 10k-10k g/mol samples using FTIR. Both samples were isothermally crystallized at varying temperatures to track the development of crystallinity over time. Experiments showed that the crystallization of both blocks occurred nearly simultaneously over all temperatures. Each block's crystallization behavior was affected by the other block's crystallization.

**8:36AM X42.00004 Self Nucleation and Crystallization of Poly(vinyl alcohol)<sup>1</sup>**, DAVID THOMAS, PEGGY CEBE, Tufts Univ — Polyvinyl alcohol (PVA) is a hydrophilic, biodegradable, semi-crystalline polymer with uses ranging from textiles to medicine. Film samples of PVA were investigated to assess crystallization and melting behavior during self-nucleation experiments, and thermal degradation, using differential scanning calorimetry (DSC) and thermogravimetric (TG) analysis, respectively. TG results show that degradation occurred at temperatures close to the observed peak melting temperature of 223 C. Using conventional DSC, PVA was heated at a rate of 10 C/min to various self-nucleation temperatures,  $T_s$ , within its melting range, briefly annealed, cooled and reheated. Three distinct crystallization regimes were observed upon cooling, depending upon self nucleation temperature. At low values of  $T_s$ , below 227 C, PVA only partially melts; residual crystal anneals while new, less perfect crystals form during cooling. Between 228 C and 234 C, PVA was found to crystallize exclusively by self-nucleation. For  $T_s$  above 235 C the PVA melts completely. Fast scanning chip-based calorimetry was used to heat and cool at 2000 K/s, to prevent degradation. Results of self nucleation experiments using fast scanning and conventional DSC will be compared.

<sup>1</sup>NSF DMR-1206010

**8:48AM X42.00005 Folding of Polymer Chains in Early Stage of Crystallization<sup>1</sup>**, SHICHEN YUAN, TOSHIKAZU MIYOSHI, Univ of Akron — Understanding the structural formation of long polymer chains in the early stage of crystallization is one of the long-standing problems in polymer science. Using solid state NMR, we investigated chain trajectory of *isotactic* polypropylene in the mesomorphic nano-domains formed via rapid and deep quenching. Comparison of experimental and simulated <sup>13</sup>C-<sup>13</sup>C Double Quantum (DQ) buildup curves demonstrated that instead of random re-entry models and solidification models, individual chains in the mesomorphic form *i*PP adopt adjacent reentry sequences with an average folding number of  $\langle n \rangle = 3-4$  (assuming an adjacent re-entry fraction of  $\langle F \rangle$  of 100%) during mesomorphic formation process via nucleation and growth in the early stage.

<sup>1</sup>This work was financially supported by the National Science Foundation (Grant DMR-1105829 and 1408855) and startup funds from the UA.

**9:00AM X42.00006 Flow-Induced Crystallization of Poly(ether ether ketone).**, BEHZAD NAZARI, ALICYN RHOADES, RALPH COLBY, Pennsylvania State University — The effects of an interval of shear above the melting temperature  $T_m$  on subsequent isothermal crystallization below  $T_m$  is reported for the premier engineering thermoplastic, poly(ether ether ketone) (PEEK). The effect of shear on the crystallization rate of PEEK is investigated by means of rheological techniques and differential scanning calorimetry (DSC) under a protocol of imposing shear in a rotational cone and plate rheometer and monitoring crystallization after quenching. The rate of crystallization at 320 C was not affected by shear for shear rates  $< 7 \text{ s}^{-1}$  at 350 C, whereas intervals of adequate shear at higher shear rates prior to the quench to 320 C accelerated crystallization significantly. As the duration of the interval of shear above  $7 \text{ s}^{-1}$  is increased, the crystallization time decreases but at each shear rate eventually saturates once the applied specific work exceeds  $\sim 120 \text{ MPa}$ . The annealing of the flow-induced precursors was also investigated. The nuclei were fairly persistent at temperatures close to 350 C, however very unstable at temperatures above 375 C. This suggests that the nanostructures formed under shear might be akin to crystalline lamellae of greater thickness, compared to quiescently crystallized lamellae.

**9:12AM X42.00007 Fluoropolymer Microstructure and Dynamics: Influence of Molecular Orientation Induced by Uniaxial Drawing<sup>1</sup>**, DANIEL MIRANDA, CHAOQING YIN, JAMES RUNT, Pennsylvania State Univ — Fluorinated semi-crystalline polymer films are attractive for dielectric film applications due to their chemical inertness, heat resistance, and high thermal stability. In the present investigation we explore the influence of orientation induced by uniaxial drawing on the crystalline microstructure and relaxation processes of poly(ethylene-tetrafluoroethylene) (ETFE), in order to ascertain how morphological control can benefit polymer dielectric design. When drawn below or near the  $T_g$ , the crystallinity of the drawn films is unchanged, and oriented amorphous structures and crystalline microfibrils form at high draw ratios. This orientation slows segmental relaxation, reflected by an increase in the dynamic  $T_g$ , and also delays the transition to the high temperature crystalline form of ETFE. When drawing above the  $T_g$ , the films undergo strain-induced crystallization at high draw ratios. For these films an increase in the dynamic  $T_g$  is also observed, in addition to a second segmental relaxation process, appearing as a shoulder on the primary process. We propose that this represents a contribution from a rigid amorphous fraction, having slowed chain dynamics.

<sup>1</sup>Supported by Office of Naval Research

**9:24AM X42.00008 Structure of Poly(3-(2'-ethyl)hexylthiophene) (P3EHT) Containing Diblock Copolymers Controlled via Thermal Processing**, EMILY DAVIDSON, UC Berkeley, RACHEL SEGALMAN, UC Santa Barbara — Poly(3-alkylthiophene)s with modified alkyl side chains crystallize confined within block copolymer microphases, serving as a good model system for the confined crystallization of semiflexible polymers. We hypothesize that the diblock structure may impose an equilibrium degree of crystalline conjugated chain folding which here is only accessible for small degrees of undercooling. Crystallization of these P3ATs in soft confinement drives microdomain expansion; here, we show that this expansion is minimized for crystallization at small degrees of undercooling. Upon heating, domains return to their melt structure over three distinct regimes. These regimes directly correspond to thermal features we assign to the relaxation of a rigid-amorphous fraction at the diblock interface, melt-recrystallization which reorganizes the degree of chain folding, and a final complete melting transition.

**9:36AM X42.00009 Annealing effects on the crystalline structures of syndiotactic polystyrene after the crystalline  $\beta$  to  $\alpha$  form structural transition induced by mechanical strain.**, FUYUAKI ENDO, ATSUSHI HOTTA, Department of Mechanical Engineering, Keio University — The thermal effects on the polymorphic behavior of syndiotactic polystyrene (sPS) after the crystalline structural transition from  $\beta$  to  $\alpha$  were investigated. Our group has previously reported that  $\beta$  form crystals of sPS could transform into  $\alpha$  form crystals by mechanical strain at about 200C. In this study, we investigated possible crystalline structural transitions of pre-stretched sPS by thermal treatments. More specifically, the samples containing  $\beta$  form crystals were stretched at temperatures above the glass transition temperature ( $T_g$ ) before annealing. The crystalline structures in the sPS samples were characterized by Fourier-transform infrared spectroscopy and X-ray diffraction analyses. Before the annealing treatment, the samples stretched at near  $T_g$  possessed mesomorphic  $\alpha$  form crystals, whereas the samples stretched at higher temperatures had more perfect  $\alpha$  form crystals. It was also found that the mesomorphic  $\alpha$  form crystals, produced by the mechanical strain at lower temperatures, could transform into perfect  $\alpha$  form crystals by annealing, and that the amount of  $\alpha$  form crystals slightly increased with the increase in the annealing temperature.

**9:48AM X42.00010 Investigating the Equilibrium Melting Temperature of Polyethylene Using the Non-Linear Hoffman-Weeks Analysis: Effect of Molecular Weight**, HADI MOHAMMADI, HERVE MARAND, Virginia Tech, Department of Chemistry — The limiting equilibrium melting temperature for infinite molar mass linear polyethylene,  $T_m^o$ , has been a point of controversy for about five decades. On one hand, Broadhurst and Flory-Vrij extrapolated melting data for short alkanes to a value of ca. 145°C. On the other hand, Wunderlich proposed a value of 141°C from melting studies of extended-chain PE crystals formed under high pressure. While a difference in  $T_m^o$  by 4°C might seem superfluous, it has significant implication for the analysis of the temperature and chain length dependences of crystal growth kinetic data. In this work we estimate the equilibrium melting temperatures,  $T_m$  for three linear narrow molecular weight distribution polyethylenes using the non-linear Hoffman-Weeks treatment. The resulting  $T_m$  values thus obtained are significantly lower than these predicted by the Flory-Vrij treatment and are within experimental uncertainty indistinguishable from those reported by Wunderlich and Hikosaka et al. Our results also suggest that the constant  $C_2$  in the expression for the undercooling dependence of the initial lamellar thickness ( $l_g^* = C_1/\Delta T + C_2$ ) increases linearly with chain length.

**10:00AM X42.00011 Free surfaces overcome superheating in simulated melting of isotactic polypropylene<sup>1</sup>**, QIN CHEN, Department of Chemical Engineering, The Pennsylvania State University, ERIC B. SIROTA, ExxonMobil Research and Engineering, MIN ZHANG, T.C. MIKE CHUNG, Department of Materials Science and Engineering, The Pennsylvania State University, SCOTT T. MILNER, Department of Chemical Engineering, The Pennsylvania State University — The equilibrium melting point ( $T_m$ ) is a challenging experimental benchmark for molecular dynamics simulation of polymer melting and crystallization.  $T_m$  obtained from melting simulation of  $\alpha$  phase isotactic polypropylene (iPP) can exhibit superheating of over 100°C. Superheating has been attributed to the use of periodic boundary conditions and ultrafast simulated heating rates, both of which inhibit melting. We have developed a simple method to overcome superheating; we replace the periodic crystal structure with a periodic array of finite thickness slabs, separated by vacuum gaps. Thermal disorder at the slab surface promotes nucleation of the melt phase. Above  $T_m$ , we observe that the melting front advances into the crystal with a velocity proportional to  $T - T_m$ . This correspond to a quadratic rise in the system energy versus temperature, at constant heating rate. We obtain  $T_m$  as the onset of this quadratic rise in energy, which give values consistent with experimental melting points for iPP oligomers. The same simulations allow reasonable estimates of the crystal-vacuum interfacial free energy, from the energy difference between crystalline slabs and periodic crystals.

<sup>1</sup>The authors acknowledge support from National Science Foundation DMR-1507980.

**10:12AM X42.00012 Yield Stress Enhancement in Glassy-Polyethylene Block Copolymers.**, WILLIAM MULHEARN, RICHARD REGISTER, Princeton University — Polyethylene (PE) has the highest annual production volume of all synthetic polymers worldwide, and is valuable across many applications due to its low cost, toughness, processability, and chemical resistance. However, PE is not well suited to certain applications due to its modest yield stress and Young's modulus (approximately 30 MPa and 1 GPa, respectively for linear, high-density PE). Irreversible deformation of PE results from dislocation of crystal stems and eventual crystal fragmentation under applied stress. The liquid-like amorphous fraction provides no useful mechanical support to the crystal fold surface in a PE homopolymer, so the only method to enhance the force required for crystal slip, and hence the yield stress, is crystal thickening via thermal treatment. An alternative route towards modifying the mechanical properties of PE involves copolymerization of a minority high-glass transition temperature block into a majority-PE block copolymer. In this work, we investigate a system of glassy/linear-PE block copolymers prepared via ring-opening metathesis polymerization of cyclopentene and substituted norbornene monomers followed by hydrogenation. We demonstrate that a large change in mechanical properties can be achieved with the addition of a short glassy block (e.g. a doubling of the yield stress and Young's modulus versus PE homopolymer with the addition of 25 percent glassy block). Furthermore, owing to the low interaction energy between PE and the substituted polynorbornene blocks employed, these high-yield PE block copolymers can exhibit single-phase melts for ease of processability.

**10:24AM X42.00013 On the structure and morphology of poly (vinylidene fluoride) nanoscrolls**, GABRIEL BURKS, SARAH GLEESON, SHAN MEI, HAO QI, CHRISTOPHER LI, Drexel University — Beyond its widely popular piezoelectric effect and  $\beta$ -phase molecular conformation, poly (vinylidene fluoride) PVDF also offers great intrigue as it relates to understanding its intrinsic crystallization behavior and morphological preference. It has been suggested that the  $\gamma$ -phase of PVDF adopts a highly regular scrolling lamellar habit which can be attributed to small differences in the folding volume of atomic level hydrogen and fluorine atoms resulting in the evolution of highly curved polymer lamellae. To date this scrolled morphology of  $\gamma$ -phase PVDF has been witnessed via high temperature melt crystallization of crystalline thin films and via severe chemical etching of PVDF bulk films. Here we show the first growth of free-standing  $\gamma$ -phase PVDF scrolls via the solution crystallization technique. Differential scanning calorimetry (DSC), X-Ray Diffraction (XRD), Fourier Transformed-Infrared Spectroscopy (FT-IR), and Atomic Force Microscopy (AFM) have been used to both characterize and to further understand the fundamental preferred crystalline habit of the  $\gamma$ -phase of poly (vinylidene fluoride).

**10:36AM X42.00014 Structure and Properties of Tactic Hydrogenated Polynorbornenes**, ADAM B. BURNS, RICHARD A. REGISTER, Princeton University — Tacticity is one of the most important structural parameters for determining the physical properties of a polymer. A high degree of stereoregularity typically promotes crystallization, with different tacticities giving rise to differences in crystal structure, melting point, and degree of crystallinity. In polynorbornene (PN) made by ring-opening metathesis polymerization (ROMP), tacticity is determined by the relative configuration of the nonplanar cyclopentylene rings enchain in the backbone. Traditional ROMP initiators yield *atactic* polymers (*aPN*); however, recent advances in catalyst design have produced both *isotactic* and *syndiotactic* PN. Newly reported *cis, isotactic*- and *cis, syndiotactic*-PNs were catalytically hydrogenated (abbreviated *ihPN* and *shPN*, respectively) without altering the tacticity. The thermal and structural characteristics of *ihPN* and *shPN* were studied by differential scanning calorimetry (DSC) and wide-angle x-ray scattering (WAXS) and compared to that of *ahPN*. Remarkably, all three polymers are semicrystalline, each with a distinct crystal structure. *ihPN* has a nominal melting point of 165 C, more than 20 C above that of *ahPN*. WAXS patterns of melt-drawn fibers of *ihPN* show few strong reflections indicative of either a highly symmetric unit cell or poor long-range order. *ihPN* fibers also exhibit a crystal-crystal transition near 130 C, which is not fully reversible on subsequent cooling. On the other hand, *shPN* has a nominal melting point some 15 C below that of *ahPN*, and *shPN* fibers show no evidence of polymorphism.

**10:48AM X42.00015 Crystallization and recrystallization behavior study on biopolymer composites with polymer grafted halloysite nanotubes<sup>1</sup>**, YA-TING HSIEH, KEN KOJIO, ATSUSHI TAKAHARA, Institute for Materials Chemistry and Engineering, Kyushu University — We study the crystallization and recrystallization behavior of poly(lactic acid) (PLA) in PLA/halloysite composites. Specifically, we are interested in finding the additional effect of interface properties variation in composites except for enhancing filler dispersion. Halloysite nanotubes are grafted with polymer to create different surface properties at their surface. These polymer grafted halloysite nanotubes are then spread into PLA via solvent mixing. Using differential scanning calorimeter, we track and analyze the influence of halloysite surface properties on the crystallization and recrystallization behavior of PLA composites under several conditions. We also present investigations of polarizing optical microscopy, in-situ Fourier transform infrared spectroscopy, and in-situ synchrotron X-ray diffraction measurements. The investigations provide insight into interface effect on PLA composites.

<sup>1</sup>The synchrotron WAXD measurements were performed on BL02B2 beamline at Spring-8 with the approval of the Japan Synchrotron Radiation Institute (JASRI) (Proposal No. 2015B1541)

# Friday, March 18, 2016 8:00AM - 11:00AM –

Session X43 GSNP: Statistical Mechanics of Social Systems 346 - Eli Ben Naim, Los Alamos National Laboratory

**8:00AM X43.00001 Microscopic to Macroscopic Dynamical Models of Sociality<sup>1</sup>**, CITLALI SOLIS SALAS, THOMAS WOOLLEY, Mathematical Institute, University of Oxford, EILUNED PEARCE, ROBIN DUNBAR, Department of Experimental Psychology, University of Oxford, PHILIP MAINI, Mathematical Institute, University of Oxford, SOCIAL AND EVOLUTIONARY NEUROSCIENCE RESEARCH GROUP (SENRG) COLLABORATION — To help them survive, social animals, such as humans, need to share knowledge and responsibilities with other members of the species. The larger their social network, the bigger the pool of knowledge available to them. Since time is a limited resource, a way of optimising its use is meeting amongst individuals whilst fulfilling other necessities. In this sense it is useful to know how many, and how often, early humans could meet during a given period of time whilst performing other necessary tasks, such as food gathering. Using a simplified model of these dynamics, which comprehend encounter and memory, we aim at producing a lower-bound to the number of meetings hunter-gatherers could have during a year. We compare the stochastic agent-based model to its mean-field approximation and explore some of the features necessary for the difference between low population dynamics and its continuum limit. We observe an emergent property that could have an inference in the layered structure seen in each person's social organisation. This could give some insight into hunter-gatherer's lives and the development of the social layered structure we have today.

<sup>1</sup>With support from the Mexican Council for Science and Technology (CONACyT), the Public Education Secretariat (SEP), and the Mexican National Autonomous University's Foundation (Fundacion UNAM).

**8:12AM X43.00002 Impact of Bursty Communication Patterns on Naming Game Competitions.<sup>1</sup>**, CASEY DOYLE, GYORGY KORNISS, BOLESŁAW SZYMANSKI, Rensselaer Polytech Inst — The currently dominant model of opinion spread dynamics chooses speakers randomly, giving rise to an exponentially distributed wait time between speaking events. Many studies, however, suggest that a more appropriate distribution would be a power law since it captures the bursty nature of communication<sup>2,3,4,5,6</sup>. Here we study how adjusting the wait times for agents to speak to fit various distributions affects the dynamics of the naming game. Specifically, we show that by creating a system with competition between two groups (each with a different wait time distribution but the same mean), the symmetry of the system is broken and in the infinite system the 'burstier' community always wins. In contrast, when this burstiness is studied in the voter model, the symmetry breaking does not occur. Lastly, we show that burstiness in the naming game with committed agents shifts downwards the critical population required for consensus.

<sup>1</sup>Supported in part by ARO, ARL NS-CTA, and ONR.

<sup>2</sup>J. Candia, M. Gonzalez, P. Wang et al., J. Phys. A, 41 22 (2008).

<sup>3</sup>J. Iribarren, E. Moro, PRL. 103, 038702 (2009).

<sup>4</sup>P. Van Mieghem, R. van de Bovenkamp, PRL 110, 108701 (2013).

<sup>5</sup>A. Vazquez, B. Racz, A. Lukacs et al., PRL 98, 158702 (2007).

<sup>6</sup>M. Karsai et al. PRE 83, 025102(R) (2011).

**8:24AM X43.00003 Comparison of human mobility patterns in different settings<sup>1</sup>**, XIANGWEN WANG, MICHEL PLEIMLING, Virginia Tech — The development of location tracking technologies and big-data analysis capacities makes it possible to understand human mobility patterns at the global level through the analysis of huge datasets made available by open-data communities. Working with millions of empirical world-wide GPS trajectories, we examine users' mobility patterns in urban, rural and intermediate scenarios. Similar scaling properties are found in the analysis of several quantities, including end-to-end distance, radius of gyration, mean-squared displacement, and fixed-interval step-length. The impact of cities is elucidated by comparing mobility patterns in major cities worldwide.

<sup>1</sup>This work is in part supported by the US National Science Foundation through grant DMR-1205309.

**8:36AM X43.00004 Effects of long-range interactions in the one-dimensional Sznajd model**, JOSEPH GARCIA, University of Maine, THOMAS STONE, Husson University, SUSAN MCKAY, University of Maine — The Sznajd model is a one-dimensional, binary, voter-like model used to study consensus in systems where information flows outward from like-minded agent pairs. Here, we introduce long-range interactions to the Sznajd model, quantified by the parameter  $p$  in analogy with the dynamic and static small-world rewiring parameter ( $p \rightarrow 1$  is the mean-field limit,  $p \rightarrow 0$  is the 1-D limit). We use Monte Carlo simulations and finite-size scaling analyses to characterize the exit probability for  $p \neq 0$ , finding a step function that depends on two  $p$ -dependent exponents. By examining the  $p \rightarrow 0$  limit of these exponents, we comment on the functional form of the exit probability in one dimension, which has been an open question. We complement this limiting approach (letting  $p \rightarrow 0$ , which offers considerable computational speedup over the pure  $p=0$  case) by also simulating the  $p=0$  case via a parallel algorithm. This investigation also probes the dependence of consensus time and system magnetization on  $p$ .

**8:48AM X43.00005 Selection Strategies for Social Influence in the Threshold Model<sup>1</sup>**, PANAGIOTIS KARAMPOURNIOTIS, BOLESŁAW SZYMANSKI, GYORGY KORNISS, Rensselaer Polytech Inst — The ubiquity of online social networks makes the study of social influence extremely significant for its applications to marketing, politics and security. Maximizing the spread of influence by strategically selecting nodes as initiators of a new opinion or trend is a challenging problem. We study the performance of various strategies for selection of large fractions of initiators on a classical social influence model, the Threshold model (TM). Under the TM, a node adopts a new opinion only when the fraction of its first neighbors possessing that opinion exceeds a pre-assigned threshold. The strategies we study are of two kinds: strategies based solely on the initial network structure (Degree-rank, Dominating Sets, PageRank etc.) and strategies that take into account the change of the states of the nodes during the evolution of the cascade, e.g. the greedy algorithm. We find that the performance of these strategies depends largely on both the network structure properties, e.g. the assortativity, and the distribution of the thresholds assigned to the nodes<sup>2</sup>. We conclude that the optimal strategy needs to combine the network specifics and the model specific parameters to identify the most influential spreaders.

<sup>1</sup>Supported in part by ARL NS-CTA, ARO, and ONR.

<sup>2</sup>Karampourniotis et al., PLOS ONE (in press); arXiv:1506.00986

**9:00AM X43.00006 Pattern Selection and Super-Patterns in Opinion Dynamics** , ELI BEN-NAIM, Los Alamos National Laboratory, ARND SCHEEL, University of Minnesota — We study pattern formation in the bounded confidence model of opinion dynamics. In this random process, opinion is quantified by a single variable. Two agents may interact and reach a fair compromise, but only if their difference of opinion falls below a fixed threshold. Starting from a uniform distribution of opinions with compact support, a traveling wave forms and it propagates from the domain boundary into the unstable uniform state. Consequently, the system reaches a steady state with isolated clusters that are separated by distance larger than the interaction range. These clusters form a quasi-periodic pattern where the sizes of the clusters and the separations between them are nearly constant. We obtain analytically the average separation between clusters  $L$ . Interestingly, there are also very small quasi-periodic modulations in the size of the clusters. The spatial periods of these modulations are a series of integers that follow from the continued-fraction representation of the irrational average separation  $L$ .

**9:12AM X43.00007 Spatially clustered zealots in a two-dimensional voter model** , THOMAS STONE, Husson University, MATTHEW LUDDEN, SUSAN MCKAY, University of Maine — The voter model, solvable in all dimensions in its standard form, has been extensively used to study behavior dynamics by using the tools of statistical mechanics. Recently, much work has been focused on determining the effects of zealots in the voter model, where a zealot is an agent that maintains its opinion (akin to an Ising spin variable) no matter the local environment. Here we investigate the effects of spatially clustered zealots in the standard voter model on a two-dimensional square lattice. The clustering of zealots is quantified by the conditional probability that a zealot of the  $+1$  state appears on an adjacent site to a randomly chosen zealot. (All zealots are of the  $+1$  state.) We determine the functional forms of the system consensus time with respect to system size, clustering, and zealot density, and compare these findings to previous results that do not include clustering. We also discuss an interesting random walk problem that arises when one attempts to calculate how clustering affects the consensus time for fixed zealot density and system size.

**9:24AM X43.00008 Highlighting impact: Do editors' selections identify influential papers?** , MANOLIS ANTONOYIANNAKIS, (1) Columbia University (2) American Physical Society — A recent trend in scientific publishing is that journal editors highlight each week a select set among the papers published (usually) in their respective journals. The highlighted papers are deemed of higher quality, importance, or interest than the 'average' paper and feature prominently in the publishers' websites. We perform a citation analysis of the highlighted papers for a number of journals from various publishers in physics. By comparing the performance of highlighted papers relative to (a) typical papers and (b) highly cited papers in their source journals and in other journals in the field, we explore whether, and to what extent, the selection process at the time of publication identifies papers that will turn out to be influential. We discuss the broader implications for research assessment.

**9:36AM X43.00009 Measuring diversity and coherence using hierarchical APS-PACS classification of sub fields of physics and their impact on citations.** , SHIVAKUMAR JOLAD, MURALI KRISHNA ENDURI, I. VINOD REDDY, IIT Gandhinagar — American Physical Society introduced Physics and Astronomy Classification Scheme (PACS) in 1975 to classify different subfields of physics in a hierarchical tree structure. Since 1985, almost all the physical review articles include the PACS code to refer different subfields it belongs to. In this work, we define the notion of diversity of articles and authors based on the PACS codes they are associated with, using Weitzmann diversity index, from 1985-2012. We find that the fraction of authors with high diversity is increasing with time, whereas the fraction of least diversity are decreasing, and moderate diversity authors have higher tendency to switch over to other diversity groups. By measuring the interconnectedness among the PACS codes, we define measures of coherence of papers and authors. The diversity and coherence captures the dimensions of Interdisciplinarity. Based on which we study the correlation between Interdisciplinarity (within sub fields of physics) and citations. We find that the diversity index of articles is correlated with the citations they received in a given time period from their publication year. Articles with lower and higher end of diversity index receive lesser citations than the moderate diversity papers.

**9:48AM X43.00010 Untangling Performance from Success<sup>1</sup>** , BURCU YUCESoy, ALBERT-LASZLO BARABASI, Northeastern University — Fame, popularity and celebrity status, frequently used tokens of success, are often loosely related to, or even divorced from professional performance. This dichotomy is partly rooted in the difficulty to distinguish performance, an individual measure that captures the actions of a performer, from success, a collective measure that captures a community's reactions to these actions. Yet, finding the relationship between the two measures is essential for all areas that aim to objectively reward excellence, from science to business. Here we quantify the relationship between performance and success by focusing on tennis, an individual sport where the two quantities can be independently measured. We show that a predictive model, relying only on a tennis player's performance in tournaments, can accurately predict an athlete's popularity, both during a player's active years and after retirement. Hence the model establishes a direct link between performance and momentary popularity. The agreement between the performance-driven and observed popularity suggests that in most areas of human achievement exceptional visibility may be rooted in detectable performance measures.

<sup>1</sup>This research was supported by Air Force Office of Scientific Research (AFOSR) under agreement FA9550-15-1-0077.

**10:00AM X43.00011 A simple model for research interest evolution patterns** , TAO JIA, Southwest University, China, DASHUN WANG, Pennsylvania State University, BOLESŁAW SZYMANSKI, Rensselaer Polytechnic Institute — Sir Isaac Newton supposedly remarked that in his scientific career he was like "... a boy playing on the sea-shore ... finding a smoother pebble or a prettier shell than ordinary". His remarkable modesty and famous understatement motivate us to seek regularities in how scientists shift their research focus as the career develops. Indeed, despite intensive investigations on how microscopic factors, such as incentives and risks, would influence a scientist's choice of research agenda, little is known on the macroscopic patterns in the research interest change undertaken by individual scientists throughout their careers. Here we make use of over 14,000 authors' publication records in physics. By quantifying statistical characteristics in the interest evolution, we model scientific research as a random walk, which reproduces patterns in individuals careers observed empirically. Despite myriad of factors that shape and influence individual choices of research subjects, we identified regularities in this dynamical process that are well captured by a simple statistical model. The results advance our understanding of scientists' behaviors during their careers and open up avenues for future studies in the science of science.

**10:12AM X43.00012 Development of kink jams in traffic flow** , DOUGLAS KURTZE, Saint Joseph's Univ — Near the threshold of absolute stability of uniform, steady traffic flow, car-following models can often be reduced to a modified Korteweg-deVries (mKdV) equation plus small corrections. The mKdV equation has a continuous family of hyperbolic-kink solutions describing boundaries between regions of different traffic densities, i.e. the edges of traffic jams. A solvability calculation picks out the one member of this family which is consistent with the correction terms; this is usually labelled the "selected" kink. This identification is problematic, however, since it must be the downstream boundary condition that determines which kink solution is realized. We display a two-parameter family of mKdV solutions which has the kink solutions as one limit and uniform flow as another, and show how the correction terms can lead to kinks developing from initially near-uniform traffic. We then clarify the meaning of the usual solvability calculation and of the "selected" kink.

**10:24AM X43.00013 A Langevin model for low density pedestrian dynamics**, ALESSANDRO CORBETTA, Eindhoven University of Technology, CHUNG-MIN LEE, California State University Long Beach, ROBERTO BENZI, University of Rome Tor Vergata, ADRIAN MUNTEAN, Karlstad University, Sweden, FEDERICO TOSCHI, Eindhoven University of Technology — The dynamics of pedestrian crowds shares deep connections with statistical physics and fluid dynamics. Reaching a quantitative understanding, not only of the average behaviours but also of the statistics of (rare) fluctuations would have major impact, for instance, on the design and safety of civil infrastructures. A key feature of pedestrian dynamics is its strong intrinsic variability, that we can already observe at the single individual level. In this work we aim at a quantitative characterisation of this statistical variability by studying individual fluctuations. We consider experimental observations of low-density pedestrian flows in a corridor within a building at Eindhoven University of Technology. Few hundreds of thousands of pedestrian trajectories with high space and time resolutions have been collected via a Microsoft Kinect 3D-range sensor and automatic head tracking techniques. From these observations we model pedestrians as active Brownian particles by means of a generalised Langevin equation. With this model we can quantitatively reproduce the observed dynamics including the statistics of ordinary pedestrian fluctuations and of rarer U-turn events. Low density, pair-wise interactions between pedestrians are also discussed.

**10:36AM X43.00014 A Hierarchy of Multi-Lane Driven Diffusive Systems with Unfair Resource Availability**<sup>1</sup>, AYSE YESIL, CEMAL YALABIK, Bilkent University — We present a model system for objects which have the ability to move along columns with the availability of a low entropy resource which is provided abundantly to a first column. The unused part of this resource is available to objects in neighbouring consecutive columns. This forms a hierarchy of multi-lane driven diffusive systems, which displays interesting dynamics. We present results from Monte Carlo simulations of the system.

<sup>1</sup>Turkish Academy of Sciences (TUBA)

**10:48AM X43.00015 Kinetic model for dilute traffic flow**, ASHKAN BALOUCHI, DANA A. BROWNE, Louisiana State University, Department of Physics and Astronomy — The flow of traffic represents a many-particle non-equilibrium problem with important practical consequences. Traffic behavior has been studied using a variety of approaches, including fluid dynamics models, Boltzmann equation, and recently cellular automata (CA). The CA model for traffic flow that Nagel and Schreckenberg (NS) introduced can successfully mimic many of the known features of the traffic flow. We show that in the dilute limit of the NS model, where vehicles exhibit free flow, cars show significant nearest neighbor correlation primarily via a short-range repulsion. introduce an approximate analytic model to describe this dilute limit. We show that the distribution of the distance between consecutive vehicles obeys a drift-diffusion equation. We compared this model with direct simulations. The steady state solution and relaxation of this model agrees well with direct simulations. We explore how this model breaks down as the transition to jams occurs.

**Friday, March 18, 2016 8:00AM - 10:12AM –**  
**Session X44 GQI: Measurement, Characterization, and Emulation** 347 - Ken Brown, Georgia Institute of Technology

**8:00AM X44.00001 Consecutive Measurements in Quantum Mechanics**<sup>1</sup>, JENNIFER R. GLICK, CHRISTOPH ADAMI, Michigan State University — The physics of quantum measurement still continues to puzzle with no resolution in sight between competing interpretations, in particular because no interpretation has so far produced predictions that would be falsifiable via experiment. Here we present an analysis of consecutive projective measurements performed on a quantum state using quantum information theory, where the entanglement between the quantum system and a measuring device is explicitly taken into account, and where the consecutive measurements increase the joint Hilbert space while the wavefunction of the joint system never collapses. Using this relative-state formalism we rederive well-known results for the pairwise correlation between any two measurement devices, but show that considering the joint as well as conditional entropy of three devices reveals a difference between the collapse and no-collapse pictures of quantum measurement that is experimentally testable.

<sup>1</sup>This research was funded by a Michigan State University Enrichment Fellowship.

**8:12AM X44.00002 Hidden Variables Theorems with Fewer Measurements**, JAY LAWRENCE, Dartmouth College and University of Chicago — A Greenberger-Horne-Zeilinger (GHZ) contradiction may be thought of as a sequence of measurements on a system of  $N$  particles, for which each may be duplicated by local hidden variables up to, but not including the last of an irreducible set. Each measurement consists of  $N$  spatially separated local measurements on individual particles. Existing contradictions require more such measurements than there are particles, the minimum number being  $N + 1$ . By allowing successive measurements to impose incremental local constraints on the hidden variables (as opposed to global constraints associated with products of hidden variables), we derive contradictions that require fewer measurements. We have found protocols for which the number of measurements,  $N_m$ , grows more slowly than linearly with the number of particles: Asymptotically,  $N_m \sim \sqrt{2N}$  for large  $N$  if the particles are qubits, and a similar relation holds for particles of higher spins.

**8:24AM X44.00003 Statistical and optimal behaviours of weak continuous quantum measurement using stochastic path integral formalism**, AREEYA CHANTASRI, University of Rochester, ANDREW JORDAN, University of Rochester, Chapman University — We study stochastic behaviour and optimal dynamics of quantum systems under weak continuous measurement. Using the stochastic path integral formalism and action principle introduced in [Phys. Rev. A 88, 042110 (2013) and Phys. Rev. A 92, 032125 (2015)], the optimal evolution, such as the most likely paths, can be obtained by extremizing the action of the stochastic path integral. We also show that any statistical information, such as multi-time correlation functions for quantum state variables, can be derived by applying functional methods and a perturbative approach to the stochastic path integral. Examples are given in one-qubit and two-qubit case. Moreover, we consider an example of qubit measurement with feedback control, using the action principle to investigate the global dynamics of its most likely paths, and finding that qubit state stabilization at any desired pure state is possible with linear feedback.

**8:36AM X44.00004 Localizing and observing Kochen-Specker quantum contextuality using weak measurements.**<sup>1</sup>, MORDECAI WAEGELL, JEFF TOLLAKSEN, Institute for Quantum Studies, Chapman University, YUJI HASEGAWA, STEPHAN SPONAR, TOBIAS DENKMAYR, HERMANN GEPPERT, Atominstitut, TU-Wien, INSTITUTE FOR QUANTUM STUDIES COLLABORATION, RESEARCH GROUP OF DR. YUJI HASEGAWA COLLABORATION — Experimental tests of the Kochen-Specker (KS) theorem conventionally require a set of different measurement settings, and the test can furthermore be applied to an arbitrary prepared state. These experiments show that nature is contextual, but they do not indicate which specific observables must behave nonclassically. We show that, using pre- and post-selected states from within a set of projectors that prove the KS theorem, it is possible to identify another specific projector in the set that behaves nonclassically, in this case because it has an anomalous weak value. We explore specific KS sets that gives rise to the Quantum Pigeonhole Effect (QPE), and use weak measurements on a large ensemble of identically pre- and post-selected neutrons to verify the QPE, and also to measure the anomalous weak value of the nonclassical projector. We construct a new contextuality inequality based on the recent result of Pusey showing that any projector with a negative weak value is a proof of contextuality, and show that our measured weak value is many standard deviations below zero.

<sup>1</sup>Fetzer-Franklin Fund

**8:48AM X44.00005 Direct Characterization of Quantum Dynamics with Noisy Ancilla**<sup>1</sup>, EUGENE DUMITRESCU, TRAVIS HUMBLE, Oak Ridge National Laboratory, University of Tennessee — We present methods for the direct characterization of quantum dynamics (DCQD) in which both the principal and ancilla systems undergo noisy processes. Using a concatenated error detection code, we discriminate between located and unlocated errors on the principal system in what amounts to filtering of ancilla noise. The example of composite noise involving amplitude damping and depolarizing channels is used to demonstrate the method, while we find the rate of noise filtering is more generally dependent on code distance. Our results indicate the accuracy of quantum process characterization can be greatly improved while remaining within reach of current experimental capabilities.

<sup>1</sup>We acknowledge support from the IC postdoctoral research program.

**9:00AM X44.00006 Realizing quantum advantage without entanglement in single-photon states**, ALEJANDRA MALDONADO-TRAPP, PABLO SOLANO, Joint Quantum Institute, ANZI HU, American University, CHARLES W. CLARK, Joint Quantum Institute — Correlations allow us to measure, and quantitatively study, the properties of physical systems, their evolution and their interactions. Quantum discord expresses quantum correlations beyond those associated with entanglement.<sup>1</sup> However, discord has not yet been adopted as a standard subject of study by the experimental community. Here we propose a feasible optical setup to generate symmetric two-qubit  $X$ -states with controllable coherences, where the two qubits correspond to the spin and path of a photon. With these states we show how a classical random variable  $K$  can be encoded by Alice and decoded by Bob. Using our previous results<sup>2</sup> we study the correlations between the spin and path qubits and its relation with the information about  $K$  that can be decoded by Bob using local measurements with or without two-qubit gate operations.<sup>3</sup> Discord is the mutual information contained in the coherences of the system, and it is possible to exploit it for quantum advantage even in the absence of entanglement.

<sup>1</sup>K Modi, *et al.*, *Rev. Mod. Phys.* **84**, 1655 (2012)

<sup>2</sup>A. Maldonado-Trapp, *et al.*, *Quantum Inf. Process* **14** 1947 (2015)

<sup>3</sup>M. Gu, *et al.*, *Nature Phys.* **8**, 671 (2012)

**9:12AM X44.00007 A novel computational approach towards the certification of large-scale boson sampling**<sup>1</sup>, JOONSUK HUH, Pohang University of Science and Technology — Recent proposals of boson sampling and the corresponding experiments exhibit the possible disproof of extended Church-Turning Thesis. Furthermore, the application of boson sampling to molecular computation has been suggested theoretically [1]. Till now, however, only small-scale experiments with a few photons have been successfully performed. The boson sampling experiments of 20-30 photons are expected to reveal the computational superiority of the quantum device. A novel theoretical proposal for the large-scale boson sampling using microwave photons is highly promising due to the deterministic photon sources and the scalability [2]. Therefore, the certification protocol of large-scale boson sampling experiments should be presented to complete the exciting story. We propose, in this presentation, a computational protocol towards the certification of large-scale boson sampling. The correlations of paired photon modes and the time-dependent characteristic functional with its Fourier component can show the fingerprint of large-scale boson sampling. [1] J. Huh, G. G. Guerreschi, B. Peropadre, J. R. McClean, and A. Aspuru-Guzik. *Nature Photon.* 9 (2015): pp 615-620. [2] B. Peropadre, G. G. Guerreschi, J. Huh, and A. Aspuru-Guzik. Preprint: arXiv:1510.08064.

This work was supported by Basic Science Research Program through the National Research Foundation of Korea(NRF) funded by the Ministry of Education, Science and Technology(NRF-2015R1A6A3A04059773), the ICT RD program of MSIP/IITP [2015-019, Fundamental Research Toward Secure Quantum Communication] and Mueunjae Institute for Chemistry (MIC) postdoctoral fellowship.

1

**9:24AM X44.00008 Occupation number entanglement in mesoscopic conductors**, DAVID DASENBROOK, University of Geneva, Switzerland, CHRISTIAN FLINDT, Aalto University, Finland — The controlled entanglement of electrons in mesoscopic conductors has been theoretically investigated before using the spin- and orbital degrees of freedom. By contrast, entanglement of two spatially separated electronic channels using the fermionic occupation number has mostly been considered inaccessible due to the charge superselection rule. However, using non-local measurements or combining several copies of occupation number entangled states, the superselection rules can be lifted and the entanglement can be detected using current and noise measurements. We present the theory for an interferometric setup to detect entanglement in the electron-hole degree of freedom of electronic excitations [1] as well as a mesoscopic setup that demonstrates entanglement and non-locality of a single electron. [1] D. Dasenbrook and C. Flindt, *Phys. Rev. B* **92**, 161412(R) (2015)

### 9:36AM X44.00009 Neutron interferometry for precise characterization of quantum systems<sup>1</sup>

, DUSAN SARENAC, Institute for Quantum Computing, CHANDRA SHAHI, Tulane University, TAI SIYA MINEEVA, CHRISTOPHER J. WOOD, Institute for Quantum Computing, MICHAEL G. HUBER, MUHAMMAD ARIF, National Institute of Standards and Technology, CHARLES W. CLARK, Joint Quantum Institute, DAVID G. CORY, DMITRY A. PUSHIN, Institute for Quantum Computing — Neutron interferometry (NI) is among the most precise techniques used to test the postulates of quantum mechanics. It has demonstrated coherent spinor rotation and superposition, gravitationally induced quantum interference, the Aharonov-Casher effect, violation of a Bell-like inequality, and generation of a single-neutron entangled state. As massive, penetrating and neutral particles neutrons now provide unique capabilities in classical imaging applications that we seek to extend to the quantum domain. We present recent results on NI measurements of quantum discord in a bipartite quantum system<sup>2</sup> and neutron orbital angular momentum multiplexing,<sup>3</sup> and review progress on our commissioning of a decoherence-free-subspace NI user facility at the NIST Center for Neutron Research.<sup>4</sup>

<sup>1</sup>Supported in part by CERC, CIFAR, NSERC and CREATE.

<sup>2</sup>“Quantum correlations in a noisy neutron interferometer,” C. J. Wood *et al.*, *Phys. Rev. A* **90**, 032315 (2014)

<sup>3</sup>“Controlling neutron orbital angular momentum,” C. W. Clark *et al.*, *Nature* **525**, 504 (2015)

<sup>4</sup>“Experimental realization of decoherence-free subspace in neutron interferometry,” D. A. Pushin *et al.*, *Phys. Rev. Lett.* **107**, 150401 (2011)

### 9:48AM X44.00010 Recovering the ideal results of a perturbed quantum emulator , MICHAEL

MARTHALER, Karlsruhe Institute of Technology, LIN TIAN, University of California, Merced, IRIS SCHWENK, Karlsruhe Institute of Technology — We consider a quantum emulator which is a model of an ideal Hamiltonian of interest  $H_S$ . However, inevitably the system is perturbed by coupling to additional degrees of freedom. We study the case where we are interested in extracted a correlator from the emulated system in equilibrium. We show that it is possible to extract the ideal correlator from a perturbed system under certain conditions. The ideal correlator can be reconstructed if any n-time correlator of the ideal system can be written as a product of two-time correlators.

### 10:00AM X44.00011 Experimental observation of melting of the effective Minkowski

spacetime<sup>1</sup> , IGOR SMOLYANINOV, University of Maryland, VERA SMOLYANINOVA, Towson University — Cobalt nanoparticle-based ferrofluid in the presence of an external magnetic field forms a self-assembled hyperbolic metamaterial, which may be described as an effective 3D Minkowski spacetime for extraordinary photons. Moreover, such extraordinary photons perceive thermal gradients in the ferrofluid as an effective gravitational field, which obeys the Newton law. If the magnetic field is not strong enough, the effective Minkowski spacetime gradually melts under the influence of thermal fluctuations. On the other hand, it may restore itself if the magnetic field is increased back to its original value. Here we present direct microscopic visualization of such a Minkowski spacetime melting/crystallization, which is somewhat similar to hypothesized formation of the Minkowski spacetime in loop quantum cosmology [1]. [1] M. Bojowald, J. Mielczarek, “Some implications of signature-change in cosmological models of loop quantum gravity”, arXiv:1503.09154 [gr-qc]

<sup>1</sup>This work was supported in part by NSF grant DMR-1104676

## Friday, March 18, 2016 8:00AM - 11:12AM –

### Session X47 DCMP: Thin Insulating Adlayers and Films 312 -

### 8:00AM X47.00001 Oxidic copper on the Au(111) surface:A theoretical surface science ap-

proach , TAEHUN LEE, Yonsei University, YONGHYUK LEE, KISUNG KANG, ALOYSIUS SOON, Department of Materials Science and Engineering, Yonsei University — Recently, via reactive Cu deposition in an oxygen ambience, high quality gold-supported cuprous oxide ( $\text{Cu}_2\text{O}$ ) ultrathin nanofilms [1] have been prepared as a model system to further such catalytic studies. Nonetheless, an accurate atomic picture of these ultrathin  $\text{Cu}_2\text{O}$  nanofilms, which largely depends on its immediate oxygen environment, is currently lacking. In this work, we perform density-functional theory (DFT) calculations using the Vienna ab initio Simulation Package in combination with *ab initio* atomistic thermodynamics [2] to investigate stability of  $\text{Cu}_2\text{O}$  thin films on Au(111) as a function of oxygen chemical potential. Our results indeed show that some of the surface structures suggested in Ref. [1] are energetically more stable than the traditional copper oxide thin film structures on copper substrate, and elucidated the electronic structure of these ultrathin copper oxide films on gold, in comparison with available experimental data. [1] H. Str  er et al., J. Phys. Chem. C **119**, 5975 (2015); [2] A. Soon et al., Phys. Rev. B **73**, 165424 (2006)

### 8:12AM X47.00002 Interaction of Molecular Oxygen with Au (001) Surface<sup>1</sup> , MICHAEL PIERCE,

ANDREW LOHEAC<sup>2</sup>, Rochester Institute of Technology, ANDI BARBOUR, Brookhaven National Laboratory, VLADIMIR KOMANICKY, Safarik University, ANTHONY RUFFINO, Rochester Institute of Technology, HOYDOO YOU, Argonne National Laboratory — Kinetics of dioxygen - Au (001) surface interaction has been studied at high temperature and near atmospheric pressures with in situ x-ray scattering measurements. We find that the hexagonal reconstruction (hex) of Au (001) surface lifts to (11) in the presence of dioxygen. The measured lifting rate constant vs. temperature shows a ‘volcano’-type behavior indicating that oxygen adsorption limits at high temperature while activation barrier of the lifting limits at low temperature. The pressure–temperature (PT) phase diagram obtained in our study shows three regions: hex at low P and T, (11) at high P and T, and coexistence of the hex and the (11) at the intermediate P and T.

<sup>1</sup>Funding provided by Research Corporation for Science Advancement. Work done at the Advanced Photon Source supported by the U.S. Department of Energy.

<sup>2</sup>\* Now at University of North Carolina - Chapel Hill

### 8:24AM X47.00003 Stabilization of the O p2x2 phase on Cu(001) sheltered by wrinkled BN

over-layer<sup>1</sup> , YONG-SUNG KIM, Korea Research Institute of Standards and Science, Yuseong, Daejeon 305-340, Korea, CHUANXU MA, AN-PING LI, MINA YOON, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA — The  $2\sqrt{3}\times\sqrt{3}R45^\circ$  phase of oxygen (O) on the Cu(001) surface has been observed in scanning tunneling microscopy (STM) measurements. Although the p2x2 phase of O on the Cu(001) surface has been proposed theoretically to be the most stable in O-lean conditions, it has not been observed in experiments for a long time. Recently, the O p2x2 phase has been found in STM on the Cu(001) surface with an overlying BN monolayer. In this theoretical study, we investigate what the role of BN over-layer is to stabilize the O p2x2 phase on the Cu(001) surface. The BN over-layer is lattice-matched with the Cu(001) surface and the BN mono-layer sheet is periodically wrinkled along the BN arm-chair direction and along the [100] or [010] direction on the Cu(001) surface. The interlayer space between the Cu(001) surface and the bulge of the wrinkled BN sheet is found to play as a preferential shelter for O to be adsorbed, and the boundary of the BN inner wall along the [010] or [100] direction makes the p2x2 phase more favorable against the  $45^\circ$ -tilted  $2\sqrt{3}\times\sqrt{3}R45^\circ$  phase of O on the Cu(001) surface.

<sup>1</sup>This was supported by Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility, and the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U. S. DOE.

**8:36AM X47.00004 Multiscale Investigations of the Early Stage Oxidation on Cu Surfaces**, QING ZHU, University of Pittsburgh, PENGHAO XIAO, XIN LIAN, SHEN-CHE YANG, GRAME HENKELMAN, University of Texas at Austin, WISSAM SAIDI, JUDITH YANG, University of Pittsburgh, UNIVERSITY OF PITTSBURGH TEAM, UNIVERSITY OF TEXAS AT AUSTIN TEAM — Previous *in situ* TEM experiments have shown that the oxidation of the three low index Cu surfaces (100), (110) and (111) exhibit different oxide nucleation rates, and the resulting oxides have 3-dimensional (3D) island shapes or 2D rafts under different conditions. In order to better understand these results, we have investigated the early stages of Cu oxidation using a multiscale computational approach that employs density functional theory (DFT), reactive force field (ReaxFF), and kinetic Monte Carlo (KMC). With DFT calculation, we have compared O<sub>2</sub> dissociation barriers on Cu (100), (110) and (111) surfaces at high oxygen coverage to evaluate the kinetic barrier of sublayer oxidation. We found that O<sub>2</sub> dissociation barriers on Cu(111) surface are all lower than those on (110) and (100) surfaces. This trend agrees with experimental observations that (111) surface is easier to oxidize. These DFT calculated energy barriers are then incorporated into KMC simulations. The large scale ReaxFF molecular dynamics and KMC simulations detail the oxidation dynamics of the different Cu surfaces, and show the formation of various oxide morphologies that are consistent with experimental observations.

**8:48AM X47.00005 Inducing electric polarization in ultrathin insulating layers**, JOSE MARTINEZ-CASTRO, London Center for Nanotechnology, London, MARTEN PIANTEK, Instituto de Nanociencia de Aragn and Laboratorio de Microscopias Avanzadas, Universidad de Zaragoza, MATS PERSSON, SSRC, University of Liverpool, Liverpool, DAVID SERRATE, Instituto de Nanociencia de Aragn and Laboratorio de Microscopias Avanzadas, Universidad de Zaragoza, CYRUS F. HIRJIBEHDIN, London Center for Nanotechnology, London — Studies of ultrathin polar oxide films have attracted the interest of researchers for a long time due to their different properties compared to bulk materials. However they present several challenges such as the difficulty in the stabilization of the polar surfaces and the limited success in tailoring their properties. Moreover, recently developed Van der Waals materials have shown that the stacking of 2D-layers trigger new collective states thanks to the interaction between layers. Similarly, interface phenomena emerge in polar oxides, like induced ferroelectricity. This represents a promising way for the creation of new materials with customized properties that differ from those of the isolated layers. Here we present a new approach for the fabrication and study of atomically thin insulating films. We show that the properties of insulating polar layers of sodium chloride (NaCl) can be engineered when they are placed on top of a charge modulated template of copper nitride (Cu<sub>2</sub>N). STM studies carried out in ultra-high vacuum and at low temperatures over NaCl/Cu<sub>2</sub>N/Cu(001) show that we are able to build up and stabilize interfaces of polar surface at the limit of one atomic layer showing new properties not present before at the atomic scale.

**9:00AM X47.00006 Role of oxygen diffusion at Ni/Cr<sub>2</sub>O<sub>3</sub> interface in intergranular oxidation of Ni-Cr alloy<sup>1</sup>**, BHARAT MEDASANI, MARIA SUSHKO, DANIEL SCHREIBER, KEVIN ROSSO, STEPHEN BRUEMMER, PACIFIC NORTHWEST NATIONAL LAB — Certain Ni-Cr alloys used in nuclear systems experience intergranular oxidation and stress corrosion cracking when exposed to high-temperature water leading to their degradation and unexpected failure. To develop a mechanistic understanding of grain boundary oxidation processes, we proposed a mesoscale metal alloy oxidation model that combines quantum Density Functional Theory (DFT) with mesoscopic Poisson-Nernst-Planck/classical DFT. This framework encompasses the chemical specificity of elementary diffusion processes and mesoscale reactive dynamics, and allows modeling oxidation processes on experimentally relevant length scales from first principles. As a proof of concept, a preliminary model was previously employed that limited oxygen diffusion pathways to those through the oxide phase and did not allow oxygen diffusion in the alloy or across oxide/alloy interfaces. In this work, we expand the model to include oxygen diffusion pathways along Ni/Cr<sub>2</sub>O<sub>3</sub> interfaces and demonstrate the increasing importance of such pathways for intergranular oxidation of Ni-Cr alloys with high Cr content.

<sup>1</sup>This work is supported by the U.S. Dept. of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division. Simulations are performed using PNNL Institutional Computing facility.

**9:12AM X47.00007 Theoretical Investigation of Supported Ultra-Thin Cobalt/Nickel/Iron/Manganese Oxides**, MICHAL BAJDICH, MAX GARCA MELCHOR, ALEXANDRA VOJVODIC, SLAC National Accelerator Laboratory — In the last decade, a number of experiments have shown that ultra-thin layers of transition metal oxides (TMOs) can be stabilized when interfaced with precious metal supports such as Au(111) and Pt(111) or Ir(100). Moreover, gold supported Co/Ni/Mn-based catalysts have been experimentally proven to exhibit higher oxygen evolution reaction (OER) activities than other metal supported oxide catalysts. However, the synergistic effect of contact with gold support is yet to be fully understood. In this talk, I will report on our recent investigation of thermodynamic stability and and high water reactivity of ultra-thin cobalt oxide nanoislands supported on Au(111). Furthermore, the stability trends, scaling of the metal-support interaction and charge transfer of several Mn/Fe/Co/Ni supported oxides on all FCC(111) metals will be analyzed. The type and role of different edge sites for the OER activity of these nanoislands will be discussed.

**9:24AM X47.00008 A DFT study of metastable *h*-WO<sub>3</sub> surfaces**, YONGHYUK LEE, TAEHUN LEE, WOOSUN JANG, ALOYSIUS SOON, Department of Materials Science and Engineering, Yonsei University — Polycrystalline WO<sub>3</sub> has gained considerable interest as an efficient oxide material for photoreactions [1], and its surface-dependent catalytic properties have been exploited by shape-control crystal engineering of this oxide for photochemistry reactions e.g. water-splitting. Recently, hexagonal single crystal WO<sub>3</sub> nanorods with dominant (0001) and (11 $\bar{2}$ 0) facets were synthesized and these nanorods are found to be highly effective photoanode [2] However, the precise local atomic structures and surface orientations of this metastable *h*-WO<sub>3</sub>, which are important for understanding surface-dependent photoreactions, are not well studied. In this work, using first-principles density-functional theory (DFT), we consider the various orientations and terminations of *h*-WO<sub>3</sub> surfaces and address the predicted nanomorphologies under corresponding experimental conditions based on the DFT-derived Gibbs-Wulff polyhedrons. We provide a microscopic perspective for its potential applications in photoreactions by studying the surface energetics and electronic structure. [1] Y. Ping and G. Galli, *J. Phys. Chem. C* **118**, 6019 (2014); [2] P. M. Rao *et al.*, *Nano Lett.* **14**, 1099 (2014)

**9:36AM X47.00009 Structural and electrical characterization of NbO<sub>2</sub> vertical devices grown on TiN coated SiO<sub>2</sub>/Si substrate<sup>1</sup>**, TOYANATH JOSHI, PAVEL BORISOV, West Virginia University, Morgantown, WV, DAVID LEDERMAN, West Virginia University, Morgantown, WV, University of California, Santa Cruz, CA — Due to its relatively high MIT temperature (1081 K) and current-controlled negative differential resistance, NbO<sub>2</sub> is a robust candidate for memory devices and electrical switching applications. In this work, we present in-depth analysis of NbO<sub>2</sub> thin film vertical devices grown on TiN coated SiO<sub>2</sub>/Si substrates using pulsed laser deposition (PLD). Two of the films grown in 1 mTorr and 10 mTorr O<sub>2</sub>/Ar (~7% O<sub>2</sub>) mixed growth pressures were studied. The formation of NbO<sub>2</sub> phase was confirmed by Grazing Incidence X-ray Diffractometry (GIXRD), X-ray Photoelectron Spectroscopy (XPS) and current vs. voltage measurements. A probe station tip (tip size ~2  $\mu$ m) or conductive AFM tip was used as a top and TiN bottom layer was used as a bottom contact. Device conductivity showed film thickness and contact size dependence. Current pulse measurements, performed in response to applied triangular voltage pulses, showed a non-linear threshold switching behavior for voltage pulse durations of ~100 ns and above. Self-sustained current oscillations were analyzed in terms of defect density presented in the film.

<sup>1</sup>Supported by FAME (sponsored by MARCO and DARPA, Contract 2013-MA-2382), WV Higher Education Policy Commission grant (HEPC.dsr.12.29), and WVU SRF. We also thank S. Kramer from Micron for providing the TiN-coated Si substrates.

**9:48AM X47.00010 Multiferroic fluoride BaCoF<sub>4</sub> Thin Films Grown Via Molecular Beam Epitaxy<sup>1</sup>**, PAVEL BORISOV, TRENT JOHNSON, West Virginia University, CAMILO GARCA-CASTRO, Universite de Liege, Belgium, AMIT KC, DUSTIN SCHRECONGOST, CHENG CEN, ALDO ROMERO, West Virginia University, DAVID LEDERMAN, West Virginia University; University of California, Santa Cruz — Multiferroic materials exhibit exciting physics related to the simultaneous presence of multiple long-range orders, in many cases consisting of antiferromagnetic (AF) and ferroelectric (FE) orderings. In order to provide a new, promising route for fluoride-based multiferroic material engineering, we grew multiferroic fluoride BaCoF<sub>4</sub> in thin film form on Al<sub>2</sub>O<sub>3</sub> (0001) substrates by molecular beam epitaxy. The films grow with the orthorhombic b-axis out-of-plane and with three in-plane structural twin domains along the polar c-axis directions. The FE ordering in thin films was verified by FE remanent hysteresis loops measurements at T = 14 K and by room temperature piezoresponse force microscopy (PFM). An AF behavior was found below Neel temperature T<sub>N</sub> ~ 80 K, which is in agreement with the bulk properties. At lower temperatures two additional magnetic phase transitions at 19 K and 41 K were found. First-principles calculations demonstrated that the growth strain applied to the bulk BaCoF<sub>4</sub> indeed favors two canted spin orders, along the b- and a-axes, respectively, in addition to the main AF spin order along the c-axis.

<sup>1</sup>supported by FAME (Contract 2013-MA-2382), WV Research Challenge Grant (HEPC.dsr.12.29), and DMREF-NSF 1434897

**10:00AM X47.00011 Transport Physics in Thin-Film Oxides: From Capacitors to Memristors<sup>1</sup>**, BRIAN TIERNEY, HAROLD HJALMARSON, MICHAEL MCLAIN, DAVID HUGHART, MATTHEW MARINELLA, DENIS MAMALUY, XUJIAO GAO, Sandia Natl Labs — A physics-based model of transport mechanisms in metal-insulator-metal (M-I-M) systems is developed to explain transport through the metal-oxide interfaces and in the bulk of the insulating oxide. Interface tunneling, such as that between the metal to the conduction band or bound defect states, is accounted for by a WKB model. Our model also incorporates the evolution of the associated oxide defect chemistry. Continuum calculations are performed for both Ta<sub>2</sub>O<sub>5</sub> M-I-M capacitors and TaO<sub>x</sub>-Based M-I-M memristors, as both devices are structurally similar and can be characterized by a common set of transport mechanisms. However, due to the electroforming process for which memristors are subjected, different transport mechanisms dominate for each type of device. Also, the effects of pulsed ionizing radiation from an external source are included in the model. It is shown that such radiation can be used to probe whether the M-I-M system is in a capacitive or memristive state. <sup>1</sup>Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

**10:12AM X47.00012 The effect of Si impurities on the effective work function at TiN/tetragonal-HfO<sub>2</sub> interface.**, GEUN-MYEONG KIM, YOUNG JUN OH, KEE JOO CHANG, Department of Physics, KAIST — The TiN/monoclinic-HfO<sub>2</sub> (TiN/m-HfO<sub>2</sub>) interface structure is widely used in high-k/metal gate stacks of metal-oxide-semiconductor field-effect transistors. As the device size is continuously reduced, high-k dielectric materials are required to reduce the gate leakage current. The tetragonal HfO<sub>2</sub> (t-HfO<sub>2</sub>) is beneficial in high-k/metal gate stacks because its dielectric constant is much higher than that of m-HfO<sub>2</sub>. It is known that Si doping can reduce the crystalline temperature of t-HfO<sub>2</sub>. However, there is a lack of studies for the effect of Si impurities at TiN/t-HfO<sub>2</sub> interface. Here we perform first-principles density functional calculations to investigate the effect of Si impurities on the work function at TiN/t-HfO<sub>2</sub> interface. It is energetically favorable for Si atoms to substitute for interface N atoms. The change of interface bonds by the Si atoms enhances the effective work function(EWF). On the other hand, when the Si atoms replace the N atoms in bulk region, the EWF is almost unchanged. Our results indicate that the Si impurities incorporated in the interface region mostly affect the work function at TiN/t-HfO<sub>2</sub> interface.

**10:24AM X47.00013 Absolute surface energy calculations of Wurtzite (0001)/(000-1): a study of ZnO and GaN<sup>1</sup>**, JINGZHAO ZHANG, YIOU ZHANG, KINFAT TSE, BEI DENG, Chinese Univ of Hong Kong, HU XU, South University of Science and Technology of China, JUNYI ZHU, Chinese Univ of Hong Kong — The accurate absolute surface energies of (0001)/(000-1) surfaces of wurtzite structures are crucial in determining the thin film growth mode of important energy materials. However, the surface energies still remain to be solved due to the intrinsic difficulty of calculating dangling bond energy of asymmetrically bonded surface atoms. We used a pseudo-hydrogen passivation method to estimate the dangling bond energy and calculate the polar surfaces of ZnO and GaN. The calculations were based on the pseudo chemical potentials obtained from a set of tetrahedral clusters or simple pseudo-molecules, using density functional theory approaches, for both GGA and HSE. And the surface energies of (0001)/(000-1) surfaces of wurtzite ZnO and GaN we obtained showed relatively high self-consistencies. A wedge structure calculation with a new bottom surface passivation scheme of group I and group VII elements was also proposed and performed to show converged absolute surface energy of wurtzite ZnO polar surfaces.

<sup>1</sup>Part of the computing resources was provided by the High Performance Cluster Computing Centre, Hong Kong Baptist University. This work was supported by the start-up funding and direct grant with the Project code of 4053134 at CUHK

**10:36AM X47.00014 The Effect of Gate -Bias Stress and Light illumination on the performance of ZnO Thin-Film Field Effect Transistors<sup>1</sup>**, PRAKASH GAJUREL, Department of Physics and Astronomy, West Virginia University, MICHAEL ALDRIDGE, Department of Biology, West Virginia University, YURI GLINKA, PAVEL BORISOV, Department of Physics and Astronomy, West Virginia University, KEVIN DALY, Department of Biology, West Virginia University, DAVID LEDERMAN, Department of Physics and Astronomy, West Virginia University, Department of Physics, University of California, Santa Cruz, 95064 — We have investigated the stability of ZnO thin film field effect transistors (TFETs) grown on Si/SiO<sub>2</sub> under the application of positive gate bias stress and light illumination at room temperature. A gate voltage applied over a few seconds in ZnO TFET devices is known to induce a positive shift in the threshold voltage as a consequence of charge trapping at or near the conducting channel / insulator interface. This bias stress remains unchanged even if a negative gate voltage stress is applied. A negative shift of the transfer curve for stressed devices was achieved while exposing the transistor to light in the presence of a small source voltage. The negative shift in threshold voltage depended on the photon energy and exposure time. Our experimental results indicate that the traps responsible for the stress are approximately 2.1 eV below the bottom of the ZnO conduction band with an energy distribution width of 3.40 eV. Stressed devices recovered their original characteristics with the photon energy of UV light (365 nm, 3.6 mW/cm<sup>2</sup>) at room temperature within 1818s. This approach could be used to reset stressed TFETs using light sources.

<sup>1</sup>This work was supported by the National Science Foundation (grant 1003907), NanoSAFE, and the West Virginia University Shared Research Facilities.

**10:48AM X47.00015 Tuning electrical transport in rare-earth delta-doped SrTiO<sub>3</sub> epitaxially grown on Si (001)**, KAMYAR AHMADI MAJLAN, MOHAMMADREZA JAHANGIR MOGHADAM, University of Texas at Arlington, XUAN SHEN, Brookhaven National Laboratory, RICKY HENSLEY, PATRICK CONLIN, ZHENG HUI LIM, University of Texas at Arlington, DONG SU, Brookhaven National Laboratory, JOSEPH H. NGAI, University of Texas at Arlington — The monolithic integration of crystalline oxides on semiconductors provides a pathway to integrate new functionalities into semiconductor devices. In particular, strongly correlated oxides that exhibit metal-insulator transitions are technologically important due to their potential use in a variety of applications. Here we present transport characteristics of strongly correlated, ultra-thin layers of Re<sub>x</sub>Sr<sub>1-x</sub>TiO<sub>3</sub> (Re = rare earth) that have been epitaxially imbedded, or “delta-doped”, into SrTiO<sub>3</sub> grown on Si(100). We will discuss how the interplay of dimensionality, rare-earth composition, and strain affects the transport characteristics and metal-insulator behavior of such correlated oxides.

**11:00AM X47.00016 Sand effects on thermal barrier coatings for gas turbine engines.**<sup>1</sup>, MICHAEL WALOCK, BLAKE BARNETT, ANINDYA GHOSHAL, MUTHUVEL MURUGAN, JEFFREY SWAB, MARC PEPI, DAVID HOPKINS, GEORGE GAZONAS, US Army Rsch Lab - Aberdeen, KEVIN KERNER, US Army Aviation and Missile Research Development and Engineering Center — Accumulation and infiltration of molten/ semi-molten sand and subsequent formation of calcia-magnesia-alumina-silicate (CMAS) deposits in gas turbine engines continues to be a significant problem for aviation assets. This complex problem is compounded by the large variations in the composition, size, and topology of natural sands, gas generator turbine temperatures, thermal barrier coating properties, and the incoming particulate's momentum. In order to simplify the materials testing process, significant time and resources have been spent in the development of synthetic sand mixtures. However, there is debate whether these mixtures accurately mimic the damage observed in field-returned engines. With this study, we provide a direct comparison of CMAS deposits from both natural and synthetic sands. Using spray deposition techniques, 7% yttria-stabilized zirconia coatings are deposited onto bond-coated, Ni-superalloy discs. Each sample is coated with a sand slurry, either natural or synthetic, and exposed to a high temperature flame for 1 hour. Test samples are characterized before and after flame exposure. In addition, the test samples will be compared to field-returned equipment.

<sup>1</sup>This research was sponsored by the US Army Research Laboratory, and was accomplished under Cooperative Agreement W911NF-12-2-0019.

**Friday, March 18, 2016 8:00AM - 11:00AM –**  
**Session X48 GQI: Scalable Hardware for Superconducting Qubits** 349 - William Oliver, Massachusetts Institute of Technology, Lincoln Laboratory

**8:00AM X48.00001 High-Q 3D coaxial resonators for cavity QED**, TAEKWAN YOON, JOHN C OWENS, RAVI NAIK, AMAN LACHAPPELLE, RUICHAO MA, JONATHAN SIMON, DAVID I SCHUSTER, Univ of Chicago — Three-dimensional microwave resonators provide an alternative approach to transmission-line resonators used in most current circuit QED experiments [1]. Their large mode volume greatly reduces the surface dielectric losses that limits the coherence of superconducting circuits, and the well-isolated and controlled cavity modes further suppress coupling to the environment. In this work, we focus on unibody 3D coaxial cavities which are only evanescently coupled and free from losses due to metal-metal interfaces, allowing us to reach extremely high quality-factors. We achieve quality-factor of up to 170 million using 4N6 Aluminum at superconducting temperatures, corresponding to an energy ringdown time of ~4ms. We extend our methods to other materials including Niobium, NbTi, and copper coated with Tin-Lead solder. These cavities can be further explored to study their properties under magnetic field or upon coupling to superconducting Josephson junction qubits, e.g. 3D transmon qubits. Such 3D cavity QED system can be used for quantum information applications, or quantum simulation in coupled cavity arrays. References: [1] Matthew Reagor et al., A quantum memory with near-millisecond coherence in circuit QED. arXiv: 1508.05882 (2015)

**8:12AM X48.00002 Three-Dimensional Architecture at Chip Level for Large-Scale-Integration of Superconducting Quantum Electronic Devices**, MARTIN GÖPPL, Sensirion AG, PHILIPP KURPIERS, ANDREAS WALL-RAFF, ETH Zurich — We propose a novel way to realize three-dimensional circuit QED systems at chip level. System components such as qubits, transmission lines, capacitors, inductors or cross-overs can be implemented as suspended, electromagnetically shielded and optionally, as hermetically sealed structures. Compared to known state-of-the-art devices, volumes of dielectrics penetrated by electromagnetic fields can be drastically reduced. Our intention is to harness process technologies for very-large-scale-integration, reliably applied and improved over decades in micro-sensor- and semiconductor industry, for the realization of highly integrated circuit QED systems. Process capabilities are demonstrated by fabricating first exploratory devices using the back-end-of-line part of a commercial 180 nm CMOS foundry process in conjunction with HF vapor phase release etching.

**8:24AM X48.00003 3D Integration for Superconducting Qubits**, DANNA ROSENBERG, DONNA-RUTH YOST, RABINDRA DAS, DAVID HOVER, LIVIA RACZ, STEVEN WEBER, JONILYN YODER, ANDREW KERMAN, MIT Lincoln Laboratory, WILLIAM OLIVER, MIT Lincoln Laboratory; Research Laboratory of Electronics, MIT — As the field of superconducting quantum computing advances from the few-qubit stage to large-scale fault-tolerant devices, scalability requirements will necessitate the use of standard 3D packaging and integration processes. While the field of 3D integration is well-developed, relatively little work has been performed to determine the compatibility of the associated processes with superconducting qubits. Qubit coherence time could potentially be affected by required process steps or by the proximity of an interposer that could introduce extra sources of charge or flux noise. As a first step towards a large-scale quantum information processor, we have used a flip-chip process to bond a chip with flux qubits to an interposer containing structures for qubit readout and control. We will present data on the effect of the presence of the interposer on qubit coherence time for various qubit-chip-interposer spacings and discuss the implications for integrated multi-qubit devices. This research was funded by the ODNI and IARPA under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as representing the official policies or endorsements, either expressed or implied, of ODNI, IARPA, or the US Government.

**8:36AM X48.00004 Extensible circuit QED processor architecture with vertical I/O**<sup>1</sup>, ALESSANDRO BRUNO, STEFANO POLETTTO, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, Delft, The Netherlands, NADIA HAIDER, QuTech, Delft University of Technology, and Netherlands Organisation for Applied Scientific Research (TNO), Delft, The Netherlands, LEONARDO DICARLO, QuTech and Kavli Institute of Nanoscience, Delft University of Technology, Delft, The Netherlands — Achieving quantum fault tolerance in an extensible architecture is an outstanding challenge across experimental quantum computing platforms today. Traditionally, circuit QED processors have millimeter dimensions and lateral coupling for all input/output (I/O) signals, precluding the increase in qubit numbers beyond ~10. We present a scalable footprint for circuit QED processors with vertically coupled I/O. Our demonstration using centimeter scale chips can accommodate the ~50 qubits needed in next-generation processors targeting the experimental demonstration of quantum fault tolerance.

<sup>1</sup>We acknowledge funding from FOM, NWO and the EU FP7 Project SCALEQIT

**8:48AM X48.00005 The Quantum Socket: Wiring for Superconducting Qubits - Part 1**, T.G. MCCONKEY, J.H. BEJANIN, J.R. RINEHART, J.D. BATEMAN, C.T. EARNEST, C.H. MCRAE, Y. ROHANIZADEGAN, D. SHIRI, M. MARIANTONI, University of Waterloo, B. PENAVA, P. BREUL, S. ROYAK, M. ZAPATKA, Ingun, A.G. FOWLER, Google Inc. — Quantum systems with ten superconducting quantum bits (qubits) have been realized, making it possible to show basic quantum error correction (QEC) algorithms. However, a truly scalable architecture has not been developed yet. QEC requires a two-dimensional array of qubits, restricting any interconnection to external classical systems to the third axis. In this talk, we introduce an interconnect solution for solid-state qubits: The quantum socket. The quantum socket employs three-dimensional wires and makes it possible to connect classical electronics with quantum circuits more densely and accurately than methods based on wire bonding. The three-dimensional wires are based on spring-loaded pins engineered to insure compatibility with quantum computing applications. Extensive design work and machining was required, with focus on material quality to prevent magnetic impurities. Microwave simulations were undertaken to optimize the design, focusing on the interface between the micro-connector and an on-chip coplanar waveguide pad. Simulations revealed good performance from DC to 10 GHz and were later confirmed against experimental measurements.

**9:00AM X48.00006 The Quantum Socket: Wiring for Superconducting Qubits - Part 2** , J.H. BEJANIN, T.G. MCCONKEY, J.R. RINEHART, J.D. BATEMAN, C.T. EARNEST, C.H. MCRAE, Y. ROHANIZADEGAN, D. SHIRI, M. MARIANTONI, University of Waterloo, B. PENAVA, P. BREUL, S. ROYAK, M. ZAPATKA, Ingun, A.G. FOWLER, Google Inc. — Quantum computing research has reached a level of maturity where quantum error correction (QEC) codes can be executed on linear arrays of superconducting quantum bits (qubits). A truly scalable quantum computing architecture, however, based on practical QEC algorithms, requires nearest neighbor interaction between qubits on a two-dimensional array. Such an arrangement is not possible with techniques that rely on wire bonding. To address this issue, we have developed the quantum socket, a device based on three-dimensional wires that enables the control of superconducting qubits on a two-dimensional grid. In this talk, we present experimental results characterizing this type of wiring. We will show that the quantum socket performs exceptionally well for the transmission and reflection of microwave signals up to 10 GHz, while minimizing crosstalk between adjacent wires. Under realistic conditions, we measured an  $S_{21}$  of -5 dB at 6 GHz and an average crosstalk of -60 dB. We also describe time domain reflectometry results and arbitrary pulse transmission tests, showing that the quantum socket can be used to control superconducting qubits.

**9:12AM X48.00007 The Quantum Socket: Wiring for Superconducting Qubits - Part 3** , M. MARIANTONI, J.H. BEJANIN, T.G. MCCONKEY, J.R. RINEHART, J.D. BATEMAN, C.T. EARNEST, C.H. MCRAE, Y. ROHANIZADEGAN, D. SHIRI, University of Waterloo, B. PENAVA, P. BREUL, S. ROYAK, M. ZAPATKA, Ingun, A.G. FOWLER, Google Inc. — The implementation of a quantum computer requires quantum error correction codes, which allow to correct errors occurring on physical quantum bits (qubits). Ensemble of physical qubits will be grouped to form a logical qubit with a lower error rate. Reaching low error rates will necessitate a large number of physical qubits. Thus, a scalable qubit architecture must be developed. Superconducting qubits have been used to realize error correction. However, a truly scalable qubit architecture has yet to be demonstrated. A critical step towards scalability is the realization of a wiring method that allows to address qubits densely and accurately. A quantum socket that serves this purpose has been designed and tested at microwave frequencies. In this talk, we show results where the socket is used at millikelvin temperatures to measure an on-chip superconducting resonator. The control electronics is another fundamental element for scalability. We will present a proposal based on the quantum socket to interconnect a classical control hardware to a superconducting qubit hardware, where both are operated at millikelvin temperatures.

**9:24AM X48.00008 Development of superconducting bonding for multilayer microwave integrated quantum circuits** , TERESA BRECHT, CHRISTOPHER AXLINE, YIWEN CHU, WOLFGANG PFAFF, LUIGI FRUNZIO, MICHEL DEVORET, ROBERT SCHOELKOPF, Yale University — Future quantum computers are likely to take the shape of multilayer microwave integrated quantum circuits.[1] The proposed physical architecture retains the superb coherence of 3D structures while achieving superior scalability and compatibility with planar circuitry and integrated readout electronics. This hardware platform utilizes known techniques of bulk etching in silicon wafers and requires metallic bonding of superconducting materials. Superconducting wafer bonding is a crucial tool in need of development. Whether micromachined in wafers or traditionally machined in bulk metal, 3D cavities typically possess a seam where two parts meet. Ideally, this seam consists of a perfect superconducting bond. Pursuing this goal, we have developed a new understanding of seams as a loss mechanism that is applicable to 3D cavities in general.[2] We present quality factor measurements of both 3D cavities and 2D stripline resonators to study the losses of superconducting bonds. [1]Brecht, T. *et al.*, arXiv:1509.01127 (2015) [2]Brecht, T. *et al.*, arXiv:1509.01119 (2015)

**9:36AM X48.00009 High speed on-chip current measurement using a low-Q tunable LC resonator** , BROOKS CAMPBELL, Z. CHEN, B. CHIARO, A. DUNSWORTH, C. NEILL, P.J.J. O'MALLEY, C. QUINTANA, A. VAINSENER, J. WENNER, UC Santa Barbara, R. BARENDTS, Y. CHEN, A. FOWLER, E. JEFFREY, J. KELLY, E. LUCERO, A. MEGRANT, J. MUTUS, M. NEELEY, P. ROUSHAN, D. SANK, Google, Santa Barbara, T.C. WHITE, JOHN M. MARTINIS, UC Santa Barbara and Google, Santa Barbara — Superconducting quantum computing technology requires precise high frequency analog waveforms to perform single and multi-qubit gates. Due to signal path irregularities, gates are tuned-up by perturbing the drive signal until qubit state populations indicate the desired gate function. A more direct approach is to measure the effect of circuit imperfections by sampling control waveforms directly, as seen by the qubits. We proceed by measuring the resonant frequency shift of a capacitively shunted SQUID and converting the control waveform to DC flux applied to the SQUID. By measuring the reflected phase of a CW tone applied to this resonant circuit while applying the resonance-shifting flux pulse, we are able to reconstruct the current waveform of the input pulse at the SQUID loop. This device's geometry is the same as the z-control lines used in qubit experiments to control the qubit frequency. I will present this method of on-chip waveform sampling for superconducting circuits in addition to proof of concept data. This technique opens the door for improved gate bring up and a deeper understanding of qubit control as well as the circuit parasitics that deform these waveforms.

**9:48AM X48.00010 Maintaining Qubit Coherence in the face of Increased Superconducting Circuit Complexity** , DAVID HOVER, STEVE WEBER, DANNA ROSENBERG, GABRIEL SAMACH, ADAM SEARS, JEFFREY BIRENBAUM, WAYNE WOODS, JONILYN YODER, LIVIA RACZ, JAMIE KERMAN, MIT Lincoln Laboratory, WILLIAM D. OLIVER, MIT Lincoln Laboratory; Research Laboratory of Electronics, Massachusetts Institute of Technology — Maintaining qubit coherence in the face of increased superconducting circuit complexity is a challenge when designing an extensible quantum computing architecture. We consider this challenge in the context of inductively coupled, long-lived, capacitively-shunted flux qubits. Specifically, we discuss our efforts to mitigate the effects of radiation loss, parasitic chip-modes, cross-coupling, and Purcell decay. Our approach employs numerical modeling of the ideal Hamiltonian and electromagnetic analysis of the circuit, both of which are independently shown to be consistent with experimental results. This research was funded by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA) and by the Assistant Secretary of Defense for Research & Engineering under Air Force Contract No. FA8721-05-C-0002. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of ODNI, IARPA, or the US Government.

**10:00AM X48.00011 Time Reversal Symmetry Breaking Microwave Resonators** , JOHN C OWENS, AMAN LACHAPPELLE, TAEKWAN YOON, RUICHAO MA, DAVID SCHUSTER, JONATHAN SIMON, University of Chicago — In this talk we present our work towards realizing high Q, superconducting circulators to be employed in topological circuit QED lattices. These circulators generate gauge fields that produce protected edge states. We couple magnon excitations in spheres of the ferrite Yttrium Iron Garnet (YIG) to microwave cavity fields in order to break the degeneracy between modes that precess with different handedness. The YIG sphere only couples strongly (1 GHz) to cavity modes that precess with the same handedness. We tune the YIG sphere into resonance with degenerate cavity modes to shift only the frequency of the modes with the same handedness, leaving the uncoupled mode at its original frequency. Since this mode is dark to the YIG excitation, its quality factor is dependent only on the characteristics of the cavity. We make the cavities out of the Type II superconductor Niobium Titanium so that we achieve high quality factors while also tolerating the large magnetic fields acting on the YIG spheres within the cavities. These cavities can be evanescently coupled to create topologically nontrivial lattices. Photon-photon interactions can then be added via couplings to qubits to create fractional quantum hall states for microwave photons.

**10:12AM X48.00012 On Chip Josephson Junction Microwave Switch** , OFER NAAMAN, MOHAMED ABU-TALEB, CHRIS KIRBY, MICHAEL RENNIE, Northrop Grumman Systems Corp. — We report on the design and measurement of a reflective single-pole single-throw microwave switch based on a superconducting circuit containing a single Josephson junction. The device has no internal power dissipation, minimal insertion loss, and is controlled by  $\Phi_0$ -level base-band signals. The data demonstrates the device operation with 2 GHz instantaneous bandwidth centered at 10 GHz and better than 20 dB on/off ratio for input powers up to -100 dBm.

**10:24AM X48.00013 Realization of an on-chip superconducting microwave switch**, MAREK PECHAL, SIMONE GASPARINETTI, MINTU MONDAL, MARKUS OPPLIGER, ANDREAS WALLRAFF, ETH Zurich — As state-of-the-art superconducting quantum devices get increasingly complex, they require a growing number of control and detection channels. On-chip routing and multiplexing of signals presents a way to realize these without requiring an unrealistically large number of microwave lines. The ability to route signals on a chip will also be a useful tool for fast in-situ characterization of superconducting devices. Here, we describe and experimentally demonstrate a superconducting on-chip microwave switch which can be integrated with current superconducting quantum circuits. The device is based on interference effects and is in principle lossless, making it well-suited for operation in dilution cryostats and for routing of signals at the single quantum level with near-unity efficiency. The first proof-of-principle device has a bandwidth of 150 MHz, a 1 dB compression point of  $-80$  dBm and turn-on/off times on the order of 5 ns. On/off power ratios reach values of approximately 30 dB. We expect that our device will find use in (de)multiplexing of control and readout in superconducting circuits and routing of microwave fields in quantum optical experiments and quantum communication applications.

**10:36AM X48.00014 Coherent control of a linear microwave cavity via single flux quantum pulses**, SHAOJIANG ZHU, GUILHEM RIBEILL, TED THORBECK, EDWARD LEONARD, MAXIM VAVILOV, Department of Physics, University of Wisconsin Madison, BRITTON PLOURDE, Department of Physics, Syracuse University, ROBERT MCDERMOTT, Department of Physics, University of Wisconsin Madison — Classical Josephson digital logic based on single flux quantum (SFQ) pulses offers a path to robust, low-latency control of a large-scale quantum processor. Here we describe the coherent control of a linear superconducting cavity by direct excitation via SFQ pulses. Resonant trains of SFQ pulses are capacitively coupled to a thin-film coplanar waveguide cavity. We examine the resulting cavity states as a function of subharmonic drive and temperature. In addition, we describe first steps toward the coherent control of a superconducting qubit with SFQ pulses.

**10:48AM X48.00015 Development of Integrated Single Flux Quantum - Superconducting Qubit Circuits**, EDWARD LEONARD JR., TED THORBECK, SHAOJIANG ZHU, Univ of Wisconsin, Madison, CALEB HOWINGTON, MATTHEW HUTCHINGS, JJ NELSON, BRITTON PLOURDE, Syracuse University, ROBERT MCDERMOTT, Univ of Wisconsin, Madison — Significant theoretical and experimental progress has been made in recent years towards a scalable superconducting quantum circuit architecture. Here we present a first attempt to integrate classical control elements from the single flux quantum (SFQ) digital logic family with a superconducting transmon qubit on a single chip. The SFQ driving circuit is fabricated in a six-layer high- $J_c$  Nb/Al-AIOx/Nb junction process while the transmon qubit is subsequently formed using submicron Al-AIOx-Al junctions grown by double-angle evaporation. We investigate sources of decoherence associated with the more complex fabrication process and describe first attempts to perform coherent qubit manipulations using resonant trains of SFQ pulses.

## Friday, March 18, 2016 8:00AM - 11:00AM –

**Session X50 DAMOP GQI: Quantum Information with Cold Atoms and Ions** Hilton Baltimore Holiday Ballroom 1 - Zhexuan Gong, Joint Quantum Institute, University of Maryland

**8:00AM X50.00001 Entanglement area law for long-range interacting systems**, ZHEXUAN GONG, MICHAEL FOSS-FEIG, Joint Quantum Institute, FERNANDO G.S.L. BRANDAO, Microsoft Research, ALEXEY V. GORSHKOV, Joint Quantum Institute — Area laws for entanglement provide crucial insight into the low-energy behavior of many-body systems and are intimately connected to the efficiency of classical computational methods. For 1D systems, an area law was rigorously proven for ground states of gapped Hamiltonians with local interactions and for states with exponentially decaying correlations. In the presence of long-range interactions, the proof of an area law for gapped ground states becomes much more challenging because long-range interactions can change the effective dimensionality of the system and introduce correlations decaying slower than an exponential. Based on recent theoretical advances that reveal strong remnants of locality in quenched systems with power-law decaying interactions, we prove an area law for a large class of gapped Hamiltonians with long-range interactions. As an intermediate step, we prove tight bounds on the decay of ground-state correlations.

**8:12AM X50.00002 A System For High Flexibility Entangling Gates With Trapped Ions**, ALISTAIR MILNE, CLAIRE EDMUNDS, SANDEEP MAVADIA, TODD GREEN, MICHAEL BIERCUK, Univ of Sydney — Trapped ion qubits may be entangled via coupling to shared modes of motion using spin-dependent forces generated by optical fields. Residual qubit-motional coupling at the conclusion of the entangling operation is the dominant source of infidelity in this type of gate. For synchronously entangling increasing numbers of ions, longer gate times are required to minimise this residual coupling. We present a scheme that enables the state of each qubit to be simultaneously decoupled from all motional modes in an arbitrarily chosen gate time, increasing the gate fidelity and scalability. This is achieved by implementing discrete phase shifts in the optical field moderating the entangling operation. We describe an experimental system based on trapped ytterbium ions and demonstrate this scheme for two-qubit entangling gates on ytterbium ion pairs.

**8:24AM X50.00003 Phase-modulated spin-motional decoupling with trapped ions**, CLAIRE EDMUNDS, ALISTAIR MILNE, SANDEEP MAVADIA, TODD GREEN, MICHAEL BIERCUK, Univ of Sydney — We present a technique to minimize residual spin-motional entanglement after a phonon-mediated entangling gate in trapped  $^{171}\text{Yb}^+$  ion qubits. Phonon-mediated gates, such as the Mølmer-Sørensen gate, engineer spin-spin entanglement by coupling the qubits to their collective modes of motion. Consequently, a major experimental limitation is residual motional entanglement at the conclusion of the gate, resulting in a degradation of the final spin state purity. Our work utilizes phase-modulated pulse sequences to decouple the qubits from multiple motional modes simultaneously at a variable gate time. In addition, we extend this technique to the suppression of time-dependent noise using concatenated gate sequences, which allows for the recovery of a higher purity spin state. Using a single, experimentally controllable modulation parameter we are able to achieve more optimal quantum control in these gate sequences.

**8:36AM X50.00004 The effect of electrode surface roughness on the motional heating rate of electromagnetic trapped ions**, KUANG-YU LIN, GUANG HAO LOW, ISAAC CHUANG, Massachusetts Inst of Tech-MIT — Electric field noise is a major source of motional heating in trapped ion quantum computation. While it is well known that this noise is influenced by trap electrode geometry in patch potential and surface adsorbate models, this has only been analyzed for smooth surfaces. We investigate the dependence of electric field noise on the roughness of surface electrodes by deriving a Greens function describing this roughness, and evaluating its effects on adsorbate-surface binding energies. At cryogenic temperature, surface roughness is found to exponentially enhance or suppress heating rate, depending on the density distribution of surface adsorbates. Our result suggests that heating rates can be tuned over orders of magnitude by careful engineering of electrode surface profiles.

Reference  
[1] Q. Turchette, B. King, D. Leibfried, D. Meekhof, C. Myatt, M. Rowe, C. Sackett, C. Wood, W. Itano, C. Monroe, et al., Physical Review A 61, 063418 (2000).

**8:48AM X50.00005 Universal critical phenomena of the cloud  $\rightarrow$  crystal phase transition in the Paul trap: Powerlaws**, DANIEL WEISS, YUNSEONG NAM, REINHOLD BLMEL, Wesleyan University —  $N$  charged particles, simultaneously stored in a radio-frequency (rf) Paul trap, exhibit deterministic heating. Depending on the damping ( $\gamma$ ) imparted to the system, these particles can exist in multiple phases, the most commonly found being the cloud and crystal phases. With a small  $\gamma$ , the particles exhibit gas-like behavior, where the heating and cooling equilibrate and a stable cloud results. For larger  $\gamma$ , the damping overcomes the heating and the particles are forced into the crystalline state. We explore the cloud  $\rightarrow$  crystal transition as a critical phenomenon. We find that the transition occurs at a critical value  $\gamma_c$  of the damping constant  $\gamma$ . We find that as a function of  $N$ ,  $\gamma_c$  scales approximately like an iterated log law. We also present a universal power law,  $\bar{\tau}_m \sim (\gamma - \gamma_c)^{-\beta}$ ,  $\gamma > \gamma_c$ ,  $\beta > 0$ , independent of both  $N$  and the Paul trap parameter  $a$ , depending only on the Paul trap parameter  $q$ , that describes the number of cycles necessary for the system to crystallize as a function of  $\gamma - \gamma_c$ .

**9:00AM X50.00006 Ion-crystal metamorphoses in the Paul trap**, VARUN URSEKAR, YUN SEONG NAM, REINHOLD BLMEL, Wesleyan Univ — We construct a generalized time-independent pseudo potential to describe the crystal morphologies and transitions between them for a three-ion Coulomb-interacting system in a Paul trap. The derivation of this pseudo potential extends a similar method that was already successfully constructed for the two-ion case to the case of three ions. Our method is based on keeping second-order micro-motion terms in the derivation of the pseudo potential. The resulting improved pseudo potential predicts ion-crystal morphologies that are corroborated by numerical simulations but are not captured by the standard pseudo potential. We provide a general method for extending this improved pseudo potential to a system of  $N$  Coulomb-interacting ions in a Paul trap.

**9:12AM X50.00007 Storage of multiple single-photon pulses emitted from a quantum dot in a solid-state quantum memory.**, JIAN-SHUN TANG, ZONG-QUAN ZHOU, YI-TAO WANG, CHUAN-FENG LI, GUANG-CAN GUO, University of Science and Technology of China — Quantum repeaters are critical components for distributing entanglement over long distances in presence of unavoidable optical losses during transmission. Stimulated by Duan-Lukin-Cirac-Zoller protocol, many improved quantum-repeater protocols based on quantum memories have been proposed, which commonly focus on the entanglement-distribution rate. Among these protocols, the elimination of multi-photons (multi-photon-pairs) and the use of multimode quantum memory are demonstrated to have the ability to greatly improve the entanglement-distribution rate. Here, we demonstrate the storage of deterministic single photons emitted from a quantum dot in a polarization-maintaining solid-state quantum memory; in addition, multi-temporal-mode memory with 1, 20 and 100 narrow single-photon pulses is also demonstrated. Multi-photons are eliminated, and only one photon at most is contained in each pulse. Moreover, the solid-state properties of both sub-systems make this configuration more stable and easier to be scalable. Our work will be helpful in the construction of efficient quantum repeaters based on all-solid-state devices.

**9:24AM X50.00008 Towards the coupling of single photons from dye molecules to a photonic waveguide.**, CLAUDIO POLISSENI, KIANG WEI KHO, KYLE MAJOR, SAMUELE GRANDI, SEBASTIEN BOISSER, JAESUK HWANG, ALEX CLARK, EDWARD HINDS, Imperial College London — Single photons are very attractive for quantum information processing given their long coherence time and their ability to carry information in many degrees of freedom. A current challenge is the efficient generation of single photons in a photonic chip in order to scale up the complexity of quantum operations. We have proposed that a dibenzoterrylene (DBT) molecule inside an anthracene (AC) crystal could couple lifetime-limited indistinguishable single photons into a photonic waveguide if deposited in its vicinity. In this talk I describe the recent progress towards the realization of this proposal. A new method has been developed for evaporating AC and DBT to produce crystals that are wide and thin. The crystals are typically several microns across and have remarkably uniform thickness, which we control between 20 and 150 nm. The crystal growth is carried out in a glove bag in order to exclude oxygen, which improves the photostability of the DBT molecules by orders of magnitude. We image the fluorescence of single DBT molecules using confocal microscopy and analyse the polarization of this light to determine the alignment of the molecules. I will report on our efforts to control the alignment of the molecules by aligning the host matrix with the substrate.

**9:36AM X50.00009 Ultra-Low Power Cross-Phase Shifts using Metastable Xenon in a High-Finesse Cavity**<sup>1</sup>, GARRETT HICKMAN, TODD PITTMAN, JAMES FRANSON, University of Maryland, Baltimore County — Many important applications in quantum information and quantum communications make use of weak single-photon nonlinearities. These nonlinearities have been produced using a number of methods, but they generally require a complicated experimental setup. We demonstrate a relatively simple system for producing ultra-low power cross-phase modulation, by using metastable xenon as the nonlinear medium within an optical cavity. Using metastable xenon prevents the degradation of optical surfaces which typically occurs with the use of alkali vapors such as rubidium. We produce phase shifts of up to 10 mrad using 4.5-fJ control pulses. We discuss the performance of this system and outline the planned improvements that will allow the cavity to produce single-photon phase shifts on the order of 1 mrad.

<sup>1</sup>This work was supported in part by DARPA DSO Grant No. W31P4Q-12-1-0015 and by NSF Grant No. PHY-1402708.

**9:48AM X50.00010 Electric-Field Noise above a Thin Dielectric Layer on Metal Electrodes**, MUIR KUMPH, IBM, CARSTEN HENKEL, Universitaet Potsdam, PETER RABL, TU Wien, MICHAEL BROWNNUTT, The University of Hong Kong, RAINER BLATT, University of Innsbruck — The electric-field noise above a layered structure composed of a planar metal electrode covered by a thin dielectric is evaluated and it is found that the dielectric film considerably increases the noise level, in proportion to its thickness. Importantly, even a thin (mono) layer of a low-loss dielectric can enhance the noise level by several orders of magnitude compared to the noise above a bare metal. Close to this layered surface, the power spectral density of the electric field varies with the inverse fourth power of the distance to the surface, rather than with the inverse square, as it would above a bare metal surface. Furthermore, compared to a clean metal, where the noise spectrum does not vary with frequency (in the radio-wave and microwave bands), the dielectric layer can generate electric-field noise which scales in inverse proportion to the frequency. For various realistic scenarios, the noise levels predicted from this model are comparable to those observed in trapped-ion experiments. Thus, these findings are of particular importance for the understanding and mitigation of unwanted heating and decoherence in miniaturized ion traps.

**10:00AM X50.00011 Carving complex many-atom entangled states by single-photon detection**, JIAZHONG HU, WENLAN CHEN, YIHENG DUAN, BORIS BRAVERMAN, HAO ZHANG, VLADAN VULETIC, Massachusetts Inst of Tech-MIT — We propose a versatile and efficient method to generate a broad class of complex entangled states of many atoms via the detection of a single photon. For an atomic ensemble contained in a strongly coupled optical cavity illuminated by weak single- or multi-frequency light, the atom-light interaction entangles the frequency spectrum of a transmitted photon with the collective spin of the atomic ensemble. Simple time-resolved detection of the transmitted photon then projects the atomic ensemble into a desired pure entangled state. This method can be implemented with existing technology, yields high success probability per trials, and can generate complex entangled states such as multicomponent Schrödinger cat states with high fidelity.

### 10:12AM X50.00012 Exponentially small dependence of the Q-function on quantum coherence<sup>1</sup>

, R. A. BREWSTER, J. D. FRANSON, University of Maryland Baltimore County — We show that the Huisimi Q-function has an exponentially small dependence on the relative phase of a Schrodinger cat state, as might be expected from its definition. This raises the question as to whether or not the Q-function provides a complete description of the coherence of quantum states. We calculate the Q-function for a cat state and then invert it by first calculating the Glauber-Sudarshan P-function using a Fourier transform, which can then be used to calculate the state itself. This process is shown to multiply the small phase-dependent terms in the Q-function by an exponentially large factor as needed in order to obtain the original state once again. This exponential factor is strongly degraded by decoherence, such as by amplification of the original state.

<sup>1</sup>Funded by the Office of Naval Research.

### 10:24AM X50.00013 Generation and multi-pass propagation of a squeezed vacuum field in hot Rb vapor<sup>1</sup>

, MI ZHANG, College of William and Mary, R. NICHOLAS LANNING, ZHIHAO XIAO, JONATHAN P. DOWLING, Louisiana State University, IRINA NOVIKOVA, EUGENIY E. MIKHAILOV, College of William and Mary — We study a squeezed vacuum field (with reduced quantum noise level) generated in hot Rb vapor via the polarization self-rotation effect. By propagating the strong laser beam through a vapor cell once, we were able to achieve a noise suppression of 1.5-2 dB below shot noise. Our previous experiments showed that the amount of observed squeezing may be limited by the contamination of the squeezed vacuum output with higher-order spatial modes, also generated inside the cell. Here, we investigate whether or not the squeezing can be improved by making the light interact several times with a less dense atomic ensemble. We carry out a comparison of various conditions, e.g. injection power, atomic density, passing numbers etc., and studied their effect on squeezing level and the spatial structure of the output squeezed vacuum field. We believe(or show) optimization of the conditions can lead to higher achievable squeezing which would be very useful for precision metrology and quantum memory applications.

<sup>1</sup>This project is supported by AFOSR grant FA9550-13-1-0098.

### 10:36AM X50.00014 Bright Single Photon Emitter in Silicon Carbide

, BENJAMIN LIENHARD, TIM SCHROEDER, SARA MOURADIAN, FLORIAN DOLDE, Massachusetts Inst of Tech-MIT, TOAN TRONG TRAN, IGOR AHARONOVICH, University of Technology Sydney, Australia, DIRK ENGLUND, Massachusetts Inst of Tech-MIT — Efficient, on-demand, and robust single photon emitters are of central importance to many areas of quantum information processing. Over the past 10 years, color centers in solids have emerged as excellent single photon emitters. Color centers in diamond are among the most intensively studied single photon emitters, but recently silicon carbide (SiC) has also been demonstrated to be an excellent host material. In contrast to diamond, SiC is a technologically important material that is widely used in optoelectronics, high power electronics, and microelectromechanical systems. It is commercially available in sizes up to 6 inches and processes for device engineering are well developed. We report on a visible-spectrum single photon emitter in 4H-SiC. The emitter is photostable at both room and low temperatures, and it enables 2 million photons/second from unpatterned bulk SiC. We observe two classes of orthogonally polarized emitters, each of which has parallel absorption and emission dipole orientations. Low temperature measurements reveal a narrow zero phonon line with linewidth  $< 0.1$  nm that accounts for more than 30% of the total photoluminescence spectrum. To our knowledge, this SiC color emitter is the brightest stable room-temperature single photon emitter ever observed.

### 10:48AM X50.00015 Ring-shaped Wigner crystals of trapped ions at the microscale

, HAOKUN LI, ERIK URBAN, CRYSTAL NOEL, ALEXANDER CHUANG, YANG XIA, BORGE HEMMERLING, YUAN WANG, XIANG ZHANG, HARTMUT HAEFFNER, University of California, Berkeley — Trapped ion crystals are ideal platforms to study many-body physics and quantum information processing, with both the internal electronic states and external motional degree-of-freedom controllable at the single quantum level. In contrast to conventional, finite, linear chains of ions, a ring topology exhibiting periodic boundary conditions and rotational symmetry opens up a new directions to diverse topics. However, previous implementations of ion rings result in small aspect ratios ( $< 0.07$ ) of ion-electrode distance to ring diameter, making the rotational symmetry of the ion crystals prone to stray electric fields from imperfections of the trap electrodes, particularly evident at low temperatures. Here, using a new trap design with a 60-fold improvement of this aspect ratio, we demonstrate crystallization of  $^{40}\text{Ca}^+$  ions in a ring with rotational energy barriers comparable to the thermal energy of Doppler laser cooled ion crystals. When further reducing the rotational energy barriers, we observe delocalization of the ion rings. With this result, we enter a regime where quantum topological effects can be studied and novel quantum computation and simulation experiments can be implemented.

## Friday, March 18, 2016 8:00AM - 11:00AM –

Session X51 FIAP: Fractional QHE: Measurement Methodologies Hilton Baltimore Holiday Ballroom 2 - John Cumings, University of Maryland

### 8:00AM X51.00001 Surface Acoustic Wave Study of Exciton Condensation in Bilayer Quantum Hall Systems<sup>1</sup>

, J. POLLANEN, J.P. EISENSTEIN, Institute for Quantum Information and Matter and Department of Physics, California Institute of Technology, Pasadena, California 91125, USA, L.N. PFEIFFER, K.W. WEST, Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544, USA — In bilayer two-dimensional electron systems (2DES) in GaAs a strongly correlated many-electron state forms at low temperature and high magnetic field when the total electron density  $n_T$  becomes equal to the degeneracy of a single spin split Landau level. This state corresponds to a total filling factor  $\nu_T = 1$  and can be described in terms of pseudospin ferromagnetism, or equivalently, Bose condensation of bilayer excitons. We have simultaneously measured magneto-transport and the propagation of pulsed surface acoustic waves (SAWs) at a frequency of 747 MHz to explore the phase transition between two independent layers at  $\nu_T = 1/2 + 1/2$  and the correlated state at  $\nu_T = 1$  in a high quality double quantum well device. We tune through this transition by varying the total electron density in our device with front and backside electrostatic gates.

<sup>1</sup>We acknowledge funding provided by the Institute for Quantum Information and Matter, an NSF Physics Frontiers Center (NFS Grant PHY-1125565) with support of the Gordon and Betty Moore Foundation (GBMF-12500028).

### 8:12AM X51.00002 Vibrational modes in the quantum Hall system<sup>1</sup>

, RACHEL WOOTEN, BIN YAN, Purdue University, KEVIN DAILY, Wolfram Research, CHRIS H. GREENE, Purdue University — The hyperspherical adiabatic technique is more familiar to atomic and nuclear few-body systems, but can also be applied with high accuracy to the many-body quantum Hall problem<sup>2</sup>. This technique reformulates the Schrödinger equation for  $N$  electrons into hyperspherical coordinates, which, after extracting the trivial center of mass, describes the system in terms of a single global size coordinate known as the hyperradius  $R$ , and  $2N - 3$  remaining internal angular coordinates. The solutions are approximately separable in the hyperradial coordinate, and solutions in the system are found by treating the hyperradius as an adiabatic coordinate. The approximate separability of the wave functions in this coordinate suggests the presence of hyperradial vibrational modes which are not described in conventional theories. The vibrationally excited states share the internal geometry of their quantum Hall ground states, and their excitation frequencies may vary with the number of participating particles or the strength of the confinement. We plan to discuss the features of these vibrational modes and their possible detection in quantum Hall systems.

<sup>1</sup>NSF

<sup>2</sup>K. M. Daily, R. E. Wooten, and C. H. Greene, Phys. Rev. B, **92** 125427 (2015).

**8:24AM X51.00003 Surface acoustic waves as a probe of the Wigner crystal in n-GaAs/AlGaAs in vicinity of  $\nu = 1/5, 1$ , and  $2^1$** , A.V. SUSLOV, NHMFL, Tallahassee, FL 32310, USA, I.L. DRICHKO, I.YU. SMIRNOV, A. F. Ioffe PTI of RAS, 194021 St.-Petersburg, Russia, L.N. PFEIFFER, K.W. WEST, Princeton University, Princeton, NJ 08544, USA, Y.M. GALPERIN, University of Oslo, 0316 Oslo, Norway — Both attenuation of a surface acoustic wave (SAW) and variation of its speed due to interaction with 2D electrons in n-GaAs/GaAlAs structures are measured versus perpendicular magnetic field of up to 18 T in the frequency range of (28.5 – 306) MHz and at temperatures (40 – 380) mK. The study is performed on  $\delta$ -doped from both sides 65 nm wide GaAs quantum well with the carrier density of  $n = 5 \cdot 10^{10} \text{ cm}^{-2}$  and their mobility of  $\mu = 8 \cdot 10^6 \text{ cm}^2/\text{Vs}$ . The complex AC conductance,  $\sigma$  is calculated. Analysis of  $\sigma$  shows that at low temperatures and at the filling factor of 2, 1, and 1/5 the electron system resides in the integer and fractional quantum Hall states, respectively. However, in vicinities to these values, namely at  $\nu = 1.9$ , (1.1 and 0.9), (0.21 and 0.19), the electron states can be interpreted as so-called pinning modes of Wigner crystal (WC). Temperature dependences of  $\sigma$  indicates a crossover between the localized modes (at  $\nu = 1$  and 2) and a pinned WC. When the temperature (or the SAW intensity) increases the behavior of the complex conductance can be understood as manifestation of WC melting.

<sup>1</sup>Acknowledgements to E. Palm, T. Murphy, J.-H. Park, and G. Jones; RFBR grant 14-02-00232 for ILD; NSF DMR-1157490 and the State of Florida for NHMFL; Gordon and Betty Moore Foundation grant GBMF2719 and NSF MRSEC-DMR-0819860 for Princeton University.

**8:36AM X51.00004 Examining the Influence of Alloy Disorder on the  $\nu = 7/3$  Fractional Quantum Hall State**, ETHAN KLEINBAUM, NIANPEI DENG, GEOFFREY GARDNER, MICHAEL MANFRA, GABOR CSATHY, Purdue University — The fractional quantum Hall states of the second Landau level elicit interest from their potential to realize novel many-body ground states. In addition to the notable even denominator FQHS, the odd denominator states in this region are worthy of considerable attention. Specifically, the nature of the most prominent odd denominator state,  $\nu = 7/3$ , remains unknown – admitting both the conventional Laughlin-Jain state and more exotic candidate states. We examine the  $\nu = 7/3$  state in a series of samples with alloy disorder intentionally added during MBE growth. In these samples, we measure the energy gap at  $\nu = 7/3$  to explore the influence of disorder on the  $\nu = 7/3$  FQHS. A comparison of these data to the energy gap measurements of the even denominator  $\nu = 5/2$ . This work was supported by DOE DE-SC000671.

**8:48AM X51.00005 Diagnosis of phase transitions in disordered fractional quantum Hall liquids using quantum entanglement<sup>1</sup>**, ZHAO LIU, Dahlem Center for Complex Quantum Systems and Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany, R. N. BHATT, Department of Electrical Engineering, Princeton University, Princeton, NJ 08540 — The conventional method to study phase transitions from fractional quantum Hall (FQH) liquids to a localized phase induced by disorder has relied on the collapse of the mobility gap and Hall conductance [1,2]. Here, we scrutinize this issue from the perspective of quantum entanglement. We consider electrons in the disordered lowest Landau level at Laughlin filling fractions  $\nu = 1/m$  with either Haldane's pseudopotentials or Coulomb interaction. We find that the derivative of the orbital-cut von-Neumann entropy with respect to the disorder strength has a sharp peak, which diverges with system size, providing a clear fingerprint of the transition from FQH liquids to a localized phase. Further, the fluctuation of the entropy with different cut boundaries is utilized to examine whether the ground states are localized in some region. We also investigate the level statistics of the entanglement spectrum, as well as the low-lying spectrum of the Hamiltonian to extract more information about the phase transition. Our method can be applied to study many-body localization in other topological systems. [1] D. N. Sheng *et al.*, Physical Review Letters **90**, 256802 (2003). [2] Xin Wan *et al.*, Physical Review B **72**, 075325 (2005).

<sup>1</sup>This work was supported by US Department of Energy, Office of Basic Energy Sciences, through Grant No. DE-SC0002140.

**9:00AM X51.00006 Excitation spectra of unconventional FQHE states in the SLL from Light Scattering Experiments<sup>1</sup>**, URSULA WURSTBAUER, Walter Schottky Institut TU München, ANTONIO LEVY, ARON PINCZUK, Columbia University, JOHN WATSON, GEOFF GARDNER, MICHAEL MANFRA, Purdue University, KEN WEST, LOREN PFEIFFER, Princeton University — The fascinating interaction physics in the second Landau level (SLL) supports the emergence of exotic quantum phases and unconventional possibly FQHE states such as e.g. at  $\nu = 5/2$  and  $2+1/3$  and the weaker state at  $\nu = 2+3/8$  and  $2+2/5$ . We observe clear signatures for gapped collective excitations in inelastic light scattering experiments just for these 'magic' filling factors and only for low temperatures substantiating access to the physics of the incompressible quantum fluids [1]. The lowest excitation feature in the spectrum at  $2+1/3$  occurs at around 70  $\mu\text{eV}$ . The analysis of spectral lineshapes suggests magnetoroton features that are characteristic of 2D neutral excitations in a perpendicular magnetic field. The striking polarization dependence observable in light scattering experiments in the SLL are consistent with nematic FQHE states. [1] U. Wurstbauer *et al.*, arXiv:1507.04939v2 (2015).

<sup>1</sup>Supported by award NSF-DMR-1306976

**9:12AM X51.00007 High Pressure Studies of the Second Landau Level Region of a Two-Dimensional Electron System<sup>1</sup>**, KATHERINE SCHREIBER, Purdue University Dept. of Physics, NODAR SAMKHARADZE, Delft University of Technology, GEOFFREY GARDNER, Purdue University Birck Nanotechnology Center, EDUARDO FRADKIN, University of Illinois Urbana-Champaign Dept. of Physics, MICHAEL MANFRA, GABOR CSATHY, Purdue University Dept. of Physics — Hydrostatic pressure has become a prevalent tool in condensed matter systems because the application of pressure to crystalline structures results in the shrinking of the lattice constant. This allows one to tune the Bloch wavefunction of the electrons and therefore all band parameters such as effective carrier mass, carrier density, and effective g-factor. In this manner, pressure acts as a probe into various strongly interacting electronic states. Motivated in particular by the capability to discern the spin polarization of quantum Hall states, we apply hydrostatic pressure up to 10 kbar to a two dimensional electron system (2DES) in a high-mobility GaAs/AlGaAs quantum well. This 2DES is subjected to milliKelvin temperatures and strong magnetic fields to observe the effect of pressure on fractional quantum Hall states, especially those in higher Landau levels, a regime not previously studied under pressure. We report our findings, focusing on the observation of a pressure-driven transition from a fractional quantum Hall state to the quantum Hall nematic phase in the second Landau level.

<sup>1</sup>Grants: Researchers at Purdue and N. Samkharadze: US DOE, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, DE-SC0006671. E. Fradkin: US NSF, DMR 1408713

**9:24AM X51.00008 Spatially resolved breakdown in reentrant quantum Hall states**, OLEKSANDR ROSSOKHATY, JOSHUA FOLK, University of British Columbia, YUVAL BAUM, ADY STERN, Weizmann Institute of Science, JOHN WATSON, GEOFFREY GARDNER, MICHAEL MANFRA, Purdue University — Electrons in a two dimensional electron gas in the fractional quantum Hall regime may rearrange into a quasi-crystalline structure that gives rise to a reentrant Integer Quantum Hall (RIQH) effect in transport. As bias current increases, longitudinal and Hall resistivities measured for these states show multiple sharp breakdown transitions, a signature that is unique to RIQH states and has previously been ascribed to pinning-depinning transitions or to the development of bias-induced anisotropy. We present an alternate interpretation of the characteristic features of RIQH breakdown at high bias, based on spatially-resolved measurements that indicate a phase boundary between broken-down and unbroken regions propagating chirally from source and drain contacts as a function of bias current. As the phase boundary passes various contacts, its spreading generates multi-stage breakdown signatures like those reported elsewhere. Confirming numerical simulations, the chiral sense of the spreading is set not by the chirality of the edge state itself, but instead depends on electron- or hole-like character of the RIQH state.

### 9:36AM X51.00009 Observation of an Even-odd Anisotropic Transport in High Landau Levels<sup>1</sup>

, GUANGTONG LIU, CHANGLI YANG, QIN WANG, YUYING ZHU, YUAN PANG, JIE FAN, XIUNIAN JING, ZHONGQING JI, LI LU, Institute of Physics, Chinese Academy of Sciences, RUI-RUI DU, International Center for Quantum Materials, Peking University, Beijing 100871, China, LOREN PFEIFFER, KEN WEST, Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544, USA, INSITITUTE OF PHYSICS, CHINESE ACADEMY OF SCIENCES TEAM, INTERNATIONAL CENTER FOR QUANTUM MATERIALS, PEKING UNIVERSITY, BEIJING 100871, CHINA COLLABORATION — Magnetotransport experiments (including tilt fields) were performed on ultrahigh mobility L-shaped Hall-bar samples of GaAs/AlGaAs quantum wells. The low-temperature longitudinal resistance  $R_{xx}$  data demonstrate that a striking even-odd anisotropic transport exists only along the [110] direction at half filling in  $N \geq 2$  high Landau levels. Although the origin for the peculiar even-odd anisotropy remains unclear, we propose that the coupling strength between electrons within the same Landau level and between the neighboring two Landau levels should be considered in future studies. The tilt field data show that the in-plane field can suppress the formation of both bubble and stripe phases.

<sup>1</sup>The work at IOP was supported by the National Basic Research Program of China under the grant No.2014CB920904 and 2011CB921702. The work at Princeton University was funded by the Gordon and Betty Moore Foundation through the EPIQS initiative Grant GBMF4420

### 9:48AM X51.00010 ABSTRACT MOVED TO L51.012 —

### 10:00AM X51.00011 New Method for Studying Localization effects in Quantum Hall Systems

, R. N. BHATT, SCOTT GERAEDTS, Department of Electrical Engineering, Princeton University, Princeton, NJ 08544 — Disorder is central to the study of the fractional quantum Hall effect. It is responsible for the finite width of the quantum Hall plateaus, and it is of course present in experiment. Numerical studies of the disordered fractional quantum Hall effect are nonetheless very difficult, because the lack of symmetry present in clean systems limits the size of systems that can be studied [1,2]. We introduce a new method for studying the integer and fractional quantum Hall effect in the presence of disorder that allows larger system sizes to be studied. The method relies on truncating the single particle Hilbert space, which leads to an exponential reduction in the Hilbert space of the many-particle system while preserving the essential topological nature of the state. We apply the model to the study of disorder transitions in the quantum Hall effect, both for the ground state and excited states. This work was supported by the US Department of Energy, Office of Basic Energy Sciences, through Grant DE-SC0002140. [1] D. N. Sheng, Xin Wan, E. H. Rezayi, Kun Yang, R. N. Bhatt and F. D. M. Haldane, Physical Review Letters 90, 256802 (2003) [2] Xin Wan, D. N. Sheng, E. H. Rezayi, Kun Yang, R. N. Bhatt and F. D. M. Haldane, Physical Review B 72, 075325 (2005).

### 10:12AM X51.00012 Reorientation of the anisotropic phase of a 2D electron system using a very small density modulation

, MD SHAFAYAT HOSSAIN, M A MUEED, HAO DENG, MANSOUR SHAYEGAN, LOREN PFEIFFER, K.W. WEST, KIRK BALDWIN, Princeton University — A high-quality two-dimensional electron system (2DES) confined to a GaAs quantum well typically exhibits isotropic transport coefficients when the Fermi level resides in the first excited ( $N = 1$ ) Landau level. Adding an in-plane magnetic field ( $B_{||}$ ) leads to an anisotropic (stripe) phase with the stripes oriented perpendicular to the  $B_{||}$  direction. We study how a periodic density modulation of the 2DES, induced by a surface strain grating from lines of negative electron-beam resist, affects the orientation of the  $\nu = 7/2$  stripe phase. Our results reveal that the external potential modulation competes against the  $B_{||}$ -induced orientational order of the stripe phase. Even a minute ( $\sim 0.5\%$ ) density modulation is sufficient to reorient the stripes at  $\nu = 7/2$  along the direction of the surface grating.

### 10:24AM X51.00013 Edge mode velocities in the quantum Hall effect from a dc measurement<sup>1</sup>

, PHILIP ZUCKER, D. E. FELDMAN, Brown University — Because of the bulk gap, low energy physics in the quantum Hall effect is confined to the edges of the 2D electron liquid. The velocities of edge modes are key parameters of edge physics. They were determined in several quantum Hall systems from time-resolved measurements and high-frequency ac transport. We propose a way to extract edge velocities from dc transport in a point contact geometry defined by narrow gates. The width of the gates assumes two different sizes at small and large distances from the point contact. The Coulomb interaction across the gates depends on the gate width and affects the conductance of the contact. The conductance exhibits two different temperature dependencies at high and low temperatures. The transition between the two regimes is determined by the edge velocity. An interesting feature of the low-temperature  $I - V$  curve is current oscillations as a function of the voltage. The oscillations emerge due to charge reflection from the interface of the regions defined by the narrow and wide sections of the gates. This work is available at arXiv:1510.01725

<sup>1</sup>This work was supported by the NSF under Grant No. DMR-1205715.

### 10:36AM X51.00014 Composite Fermion States near 3/2 Hosted by a High-Mobility 2D Hole System<sup>1</sup>

, PO ZHANG, Peking Univ, RUIYUAN LIU, Rice University, JIANLI WANG, CHI ZHANG, Peking Univ, CHANGLI YANG, LI LU, IOP, Chinese Academy of Sciences, LOREN PFEIFFER, KEN WEST, Princeton University, RUI-RUI DU, Rice University — Magnetotransport experiments of Carbon-doped GaAs/AlGaAs 2D hole gas (2DHG) have revealed a variety of interesting phenomena previous not seen in the 2DEG counterpart. For example, it was found that the effective  $g$ -factor of 2DHG is large enough to cause Landau level crossing even at  $\sim 1$  T, and the product of  $gm^*$  (where  $m^*$  is the hole effective mass) increases with total magnetic field (Yuan et al, Appl. Phys. Lett. 94, 052103 (2009)). Such level crossings could have profound influences on the fractional quantum Hall states in the relevant magnetic fields. We systematically investigate the composite fermion states near 3/2 in C-doped high-mobility 2DHG by tilted-magnetic field experiments, and map out the Landau levels and composite fermion spectra as a function of hole density and tilt angles. Preliminary results and brief discussions will be presented.

<sup>1</sup>The work at Peking University were supported by National Basic Research Program of China grants 2012CB921301 and 2014CB920901, and by Collaborative Innovation Center of Quantum Matter.

### 10:48AM X51.00015 Quantum Hall plateau-plateau transition probed by magnon quantum Hall insulator

, BAOLONG XU, School of Physics, Peking University, TOMI OHTSUKI, Department of Physics, Sophia University, RUIYCHI SHINDOU, School of Physics, Peking University — Based on a generalization of quantum Hall physics to quasi-particle boson system, we introduce a magnetic superlattice structure in the dipolar regime whose lowest gapped magnon bands mimic magnon quantum Hall insulator in strong out-of-plane magnetic fields. By calculating two-terminal conductance and localization length, we characterize the critical nature of the localization-delocalization transition in the magnon quantum Hall insulator. Especially, we show that the calculated conductance distribution at the 'plateau-plateau' transition in our system exhibits essentially the same distribution as that in the critical point of the Chalker-Corrington network model, demonstrating the 'universality' of the conductance distribution at the quantum Hall critical point beyond Fermion system.

**Friday, March 18, 2016 8:00AM - 11:00AM —**

**Session X52 DAMOP: Atomic Physics: New Frontiers | Hilton Baltimore Holiday Ballroom 3 -**

**8:00AM X52.00001 Comparison between two models of time-dependent absorption of matter waves<sup>1</sup>**, MAXIMILIEN BARBIER, Northumbria University, UK, MATHIEU BEAU, University of Massachusetts Boston, USA, and Dublin Institute for Advanced Studies, Ireland, ARSENI GOUSSEV, Northumbria University, UK — The interaction between an atom and a laser might give rise to transitions between two, or more, internal states of the atom. Such processes can be efficiently described within the framework of matter wave absorption, in which the laser beam is mimicked by an absorbing barrier. In this talk we present a quantitative comparison between two models describing the interaction between a non-relativistic quantum particle and a thin time-dependent absorbing barrier. The first model represents the barrier by time-dependent discontinuous matching conditions imposed on both the wave function of the particle and its spatial derivative. The second model treats the particle as a spinor submitted to a time-dependent off-diagonal  $\delta$ -potential. We show the two models to be in excellent agreement in a semiclassical regime. Reference: M. Barbier, M. Beau, A. Goussev, arXiv:1510.06996, *Phys. Rev. A* (in press).

<sup>1</sup>EPSRC Grant No. EP/K024116/1

**8:12AM X52.00002 Bell Experiment with Classical Optical Fields<sup>1</sup>**, BETHANY LITTLE, XIAO-FENG QIAN, JOHN HOWELL, J. H. EBERLY, University of Rochester — We theoretically and experimentally explore the implications of entanglement in statistically classical optical fields<sup>2</sup>. The description of these fields in terms of polarization and amplitude degrees of freedom can take a non-separable form which employs a mathematical description of entanglement often associated with quantum phenomena. By subjecting these optical fields to a Bell analysis, we examine the role of entanglement in marking the quantum-classical boundary. We report a value of the Bell parameter greater than  $B = 2.54$ , many standard deviations outside the limit  $B = 2$  established by the Clauser-Horne-Shimony-Holt Bell inequality<sup>3</sup>. This suggests that Bell violation has less to do with quantum theory than previously thought, but everything to do with entanglement.

<sup>1</sup>University of Rochester Research Award, NSF PHY-1203931, NSF PHY-1505189, and NSF/INSPIRE PHY-1539859

<sup>2</sup>X.-F. Qian, Bethany Little, John Howell, and J. H. Eberly, *Optica* **2**, 611-615 (2015).

<sup>3</sup>John F. Clauser, Michael A. Horne, Abner Shimony, and Richard Holt. *Phys. Rev. Lett.* **23**, 880-884 (1969)

**8:24AM X52.00003 Non-equilibrium Transport of Light**, CHIAO-HSUAN WANG, JQI/UMD/QuICS, JACOB TAYLOR, JQI/NIST/QuICS — Non-equilibrium Transport of Light The thermalization of light under conditions of parametric coupling to a bath provides a robust chemical potential for light [1]. We study non-equilibrium transport of light using non-equilibrium Green's function approach under the parametric coupling scheme, and explore a potential photonic analogue to the Landauer transport equation. Our results provide understandings of many-body states of photonic matter with chemical potential imbalances. The transport theory of light paves the way for quantum simulation and even practical applications of diode-like circuits using quantum photonic sources in the microwave and optical domain.

[1] M. Hafezi, P. Adhikari, J. M. Taylor, arXiv:1405.5821v2 (2014)

**8:36AM X52.00004 Determination of Zak phase by reflection phase in 1D photonic crystals**, WENSHENG GAO, HKUST, MENG XIAO COLLABORATION, CHETING CHAN COLLABORATION, WINGYIM TAM TEAM — For a one-dimensional (1D) periodic system with inherent mirror symmetry, the value of the geometric “Zak” phase in a bulk band is related to the sign of reflection phase for wavelengths inside the bandgaps sandwiching the bulk band. We designed an interference setup which allows us to measure the reflection phase of 1D photonic crystal fabricated for the optical range, and this in turn enabled us to determine the Zak phases of the bands. We then found interface states whose existence can be traced to the topological properties of the bandgaps and the geometric phases of the bulk bands. (accepted by optics letters)

**8:48AM X52.00005 Experimental Apparatus for the Observation of the Topological Change Associated with Dynamical Monodromy**, DANIEL SALMON, M. PERRY NEREM, SETH AUBIN, JOHN DELOS, William & Mary Coll — Monodromy means once around a path, therefore systems that have non-trivial monodromy are systems such that, when taken around a closed circuit in some space, the system has changed state in some way. Classical systems that exhibit non-trivial Hamiltonian monodromy have action and angle variables that are multivalued functions. A family, or loop, of trajectories of this system has a topological change upon traversing a monodromy circuit. We present an experimental apparatus for observing this topological change. A family of particles moving in a cylindrically symmetric champagne-bottle potential exhibits non-trivial Hamiltonian monodromy. At the center of this system is a classically forbidden region. By following a monodromy circuit, a loop of initial conditions on one side of the forbidden region can be made to evolve continuously into a loop that surrounds the forbidden region. We realize this system using a spherical pendulum, having at its end a permanent magnet. Magnetic fields generated by coils can then be used to create the champagne-bottle potential, as well as drive the pendulum through the monodromy circuit.

**9:00AM X52.00006 Topological Charge Screening in Disordered Aharonov-Bohm Wavefunctions**, ALEXANDER HOUSTON, JOHN HANNAY, ALEXANDER TAYLOR, MARK DENNIS, University of Bristol — Free electrical charges are typically subject to screening relations. For example, in ionic fluids and Coulomb gases there is screening (both global and local) of the electrical charges, described by the first and second Stillinger-Lovett sum rules [1]. A topological analogy governs the statistical behaviour of the nodal points in Gaussian random superpositions of plane waves. These nodal points are integer topological charges, i.e. vortices and antivortices of the complex wavefunction, whose sign is that of the phase circulation. Such superpositions are known to model high energy eigenfunctions in the presence of wave chaos [2], and display topological charge screening in the bulk [3]. We investigate how these screening relations are affected by the introduction of a magnetic flux line [4], which may be fractional in strength. We find that the global screening relation is broken, with the average total topological charge of the vortices given by the flux strength, and that the local screening of the flux itself shows unexpected features. [1] F. H. Stillinger and R. Lovett, *J. Chem. Phys.* **49**, 1991-94 (1968) [2] M. V. Berry, *J. Phys. A* **10**, 2083-91 (1977) [3] M. V. Berry and M. R. Dennis, *Proc. R. Soc. A* **456**, 2059-79 (2000) [4] Y. Aharonov and D. Bohm, *Phys. Rev.* **115**, 485-91 (1959)

**9:12AM X52.00007 Synthetic gauge flux and Weyl points in acoustic systems.<sup>1</sup>**, MENG XIAO, stanford university, WEN-JIE CHEN, WEN-YU HE, C. T. CHAN, the Hong Kong University of Science and Technology — We consider acoustic systems comprising a honeycomb lattice in the xy plane and periodic along the z direction. As  $k_z$  is a good quantum number here, for each fixed  $k_z$ , this system can be treated as a reduced two-dimensional system. By engineering the interlayer coupling in the z-direction, we show that we can realize effective inversion symmetry breaking and synthetic staggered gauge flux in the reduced two-dimensional system. The realizations of chiral edge states for fixed values of  $k_z$  are direct consequences of the staggered gauge flux. And we then show that the synthetic gauge flux is closely related to the Weyl points in the three-dimensional band structure.

<sup>1</sup>This work was supported by the Hong Kong Research Grants Council (grant no. AoE/P-02/12)

**9:24AM X52.00008 Atomic collisions, inelastic indeed.** , HERVE BERCEGOL, GWENAEL FERRANDO, ROLAND LEHOUCQ, CEA — At the turn of the twentieth century, a hot controversy raged about the ability of Boltzmann's framework to take care of irreversibility. The so-called Loschmidt's paradox progressively faded with time during the last hundred years, due to the predictive efficiency of statistical mechanics. However, one detail at the origin of the controversy – the elasticity of atomic collisions – was not completely challenged. A semi-classical treatment of two atoms interacting with the vacuum zero-point field permits to predict a friction force acting against the rotation of the pair of atoms [Bercegol H. & Lehoucq R., *Phys. Rev. Lett.* **115**, 090402 (2015)]. By its form and its level, the calculated torque is a candidate as a physical cause for diffusion of energy and angular momentum, and consequently for entropy growth. It opens the way to a revision of the standard vision of irreversibility. This presentation will focus on two points. First we will discuss the recent result in a broader context of electromagnetic interactions during microscopic collisions. The predicted friction phenomenon can be compared to and distinguished from Collision-Induced Emission and other types of inelastic collisions. Second we will investigate the consequences of the friction torque on calculated trajectories of colliding atoms, quantifying the generation of dimers linked by dispersion forces.

**9:36AM X52.00009 Hydrogen Dissociation in Generalized Hartree-Fock Theory: Breaking the diatomic bond<sup>1</sup>** , JONATHAN JERKE, Texas Southern University, SAMINA MASOOD, University of Houston Clear Lake, CJ TYMCZAK, Texas Southern University — Generalized Hartree Fock theory predicts molecular Hydrogen dissociation without correlation. A variational Gaussian-Sinc linear superposition is the basis of 50 calculations with 3-4 significant digits of quality. The spin singlet covalent bond spontaneously breaks into a pair of uncorrelated doublets at atomic separation of 1.22 Angstroms. Quantum spin numbers and energetic comparison with Configuration Interaction theory—correlation—point to a first order phase transition in the molecular Hydrogen bond without correlation.

<sup>1</sup>Welch Foundation (Grant J-1675), the ARO (Grant W911Nf-13-1-0162), the Texas Southern University High Performance Computing Center (<http://hpcc.tsu.edu/>; Grant PHY-1126251) and NSF-CREST CRCN project (Grant HRD-1137732)

**9:48AM X52.00010 Stretching of Picosecond Laser Pulses with Uniform Reflecting Volume Bragg Gratings.** , SERGIY MOKHOV, CREOL - the College of Optics and Photonics, Univ. of Central Florida — It is shown that a uniform reflecting volume Bragg grating (VBG) can be used as a compact monolithic stretcher of high-power picosecond laser pulses in cases when chirped Bragg gratings with an appropriate chirp rate are difficult to fabricate. A chirp-free reflected stretched pulse is generated of almost rectangular shape when incident short pulse propagates along a grating and experiences local Bragg diffraction. The increase in duration of the reflected pulse is approximately equal to twice the propagation times along the grating. We derived the analytic expression for diffraction efficiency, which incorporates incident pulse duration, grating thickness, and amplitude of refractive index modulation, enabling an optimum selection of the grating for pulse stretching. The typical expected theoretical value of diffraction efficiency is about 10% after taking into account the spectral narrowing of the reflected emission. We believe that the relatively low energy efficiency of the proposed method is more than offset by a number of advantages, which are chirp-free spectrum of a stretched pulse, compactness, robustness, preservation of setup alignment and beam quality, and tolerance to high power. Obtained pulses of several tens of picoseconds can be amplified by standard methods which are not requiring special measures to avoid undesirable non-linear effects. We propose a simple and reliable method to control the temporal parameters of the high-power picosecond pulses using the same laser source and the VBG of variable thickness that can significantly simplify the experiments requiring different pulse durations.

**10:00AM X52.00011 Ablation-cooled material removal with ultrafast bursts of pulses** , F. MER ILDAY, Department of Electrical and Electronics Engineering, Bilkent University, Ankara, Turkey, C. KERSE, H. KALAYCIOGLU, P. ELAHI, Department of Physics, Bilkent University, Turkey, S. YAVAS, FiberLAST, Inc., Ankara, Turkey, D. KESIM, . AKAALAN, Department of EEE, Bilkent University, Turkey, B. ETIN, Department of Mechanical Engineering, Bilkent University, Turkey, B. KTEM, Department of Physics, Bilkent University, Turkey, M. ASIK, Nanotechnology and Nanomedicine Department, Hacettepe University, Turkey, H. HOOGLAND, R. HOLZWARTH, Department of Physics, University of Erlangen-Nuremberg, Germany — Use of femtosecond pulses allows precise and thermal-damage-free material removal with broad applications. However, its potential is limited by low material removal speeds and complexity of the required lasers. The laser complexity arises from the high pulse energy threshold for ablation. Physics of the laser-material interaction precludes a straightforward scaling up of the removal rate by using more powerful lasers due to shielding and collateral damage from heat accumulation. Here, we exploit ablation cooling, a technique used in aerospace engineering since 1950s, to circumvent this limitation. We apply rapid successions of pulses from specially developed lasers to ablate the target material before the residual heat deposited by previous pulses diffuse away from the interaction region. This constitutes a new physical regime of laser-material interactions, where heat removal due to ablation is comparable to conduction. Proof-of-principle experiments demonstrate reduction of required pulse energies by 1000x, while simultaneously increasing efficiency and speed by 10x.

**10:12AM X52.00012 Formation of ultrashort pulses from monochromatic XUV radiation via interaction with a medium of IR-dressed He atoms.** , TIMUR AKHMEDZHANOV, Texas A&M University and Institute for Quantum Studies and Engineering, College Station, TX, VLADIMIR ANTONOV, Institute of Applied Physics of the Russian Academy of Sciences, Nizhny Novgorod, Russia, OLGA KOCHAROVSKAYA, Texas A&M University and Institute for Quantum Studies and Engineering, College Station, TX — Trains of high intensity ultrashort XUV pulses could find a lot of applications. Recently, a mechanism of high efficiency formation of a train of XUV pulses from quasi-monochromatic XUV field was suggested [Opt. Lett. **36**, 2296 (2011)]. XUV field propagates through the medium of atoms, which are space-time modulated by IR field. The field scattered by modulated atoms contains sidebands of incident XUV field frequency and, for properly chosen parameters, train of ultrashort pulses is formed at the output of the medium. In this contribution, we study formation of ultrashort pulses in the medium of He atoms. Contrary to our recent work [Phys. Rev. A **91**, 023830 (2015)], IR field is chosen to be weak enough, so that pulses are formed due to modulation of excited atomic levels, rather than tunnel ionization. The suggested method allows to form train of pulses with high efficiency and can be scaled to He-like ions in order to get even shorter pulses.

**10:24AM X52.00013 Chiral Molecular Optical Response to Nano-Shaped Light<sup>1</sup>** , PRASOON SAURABH, Univ of California - Irvine, VLADIMIR CHERNYAK, Wayne State University, JEREMY ROUXEL, SHAUL MUKAMEL, Univ of California - Irvine — Chiral linear optical signals are an important spectroscopic tool for biomolecules and chemical sensing applications. Exact expressions are derived which express these signals as a convolution of a non-local linear susceptibility of matter with a non-local intrinsic property of the electric field. The chiral response can be enhanced and optimized using nano-optical fields with strong spatial variation. The approach is based on a gauge invariant calculation using the minimal coupling Hamiltonian. The multipolar expansion is avoided and all multipoles are naturally incorporated. We apply these expression to achiral (planar) and chiral (dihedral angle of 45°) bi-phenyl as a physically intuitive illustration.

<sup>1</sup>The support of National Science Foundation (Grant No. CHE-1361516) and the Chemical Sciences, Geosciences and Biosciences Division, Office of Basic Energy Sciences, Office of Science, U.S. Dept. of Energy (award DE-FG02-4ER15571)

**10:36AM X52.00014 Study of Rydberg blockade mediated optical non-linearity in thermal vapor<sup>1</sup>** , ARUP BHOWMICK, Senior Research Fellow, ASHOK MOHAPATRA, Reader-F — We demonstrate Rydberg blockade by coupling to Rydberg state via two-photon excitation in rubidium thermal vapor. The probe beam coupling to the  $D2$  transition was blue detuned by 1.3 GHz and a coupling beam was scanned to excite the atoms to Rydberg state via two-photon transition ( $5s_{1/2} \rightarrow ns_{1/2}$ ). The dispersion of the probe beam is modified due to the 2-photon excitation and is measured using an optical heterodyne detection technique in the experiment. We have observed that the dispersion of the probe beam depends linearly on atomic vapor density while coupling to a Rydberg state with principal quantum number,  $n = 30$ . However, density dependent suppression of the dispersion is observed while coupling to the Rydberg state with  $n = 60$ . Since the dispersion of the probe beam due to 2-photon excitation depends on the Rydberg population, the density dependent suppression is explained by introducing the concept of blockade. The blockade radius is measured to be about  $2.2 \mu\text{m}$  which is consistent with the scaling due to Doppler width of the 2-photon resonance in thermal vapor. Our result promises the realization of single photon source and strong single photon non-linearity based on Rydberg blockade in thermal vapor.

<sup>1</sup>National Institute of Science Education and Research

**10:48AM X52.00015 'Relativistic' corrections to the mass of a plucked guitar string** , MICHAEL KOLODRUBETZ, Univ of California - Berkeley, ANATOLI POLKOVNIKOV, Boston University — Quantum systems respond non-adiabatically when parameters controlling them are ramped at a finite rate. If the parameters themselves are dynamical for instance the position of a box that defines the boundary of a quantum field the feedback of these excitations gives rise to effective Newtonian equations of motion for the parameter. For the age old problem of photons in a box, this correction gives rise to a mass proportional to the energy of the photons. We show that a similar correction arises for a classical guitar string plucked with energy  $E$ ; moving clamps at the ends of the string requires inertial mass  $m = 2E/c_s^2$ , where  $c_s$  is the speed of sound. This quasi-relativistic effect should be observable in freshman physics level experiments. We then comment on how these simple methods have been readily extended to treat problems such as ramps and quenches of strongly-interacting superconductors and dynamical trapping near a quantum critical point.

**Friday, March 18, 2016 8:00AM - 11:00AM –**

**Session X53 FIAP: Electricity and Hydrogen Production, Storage and Delivery** Hilton Baltimore Holiday Ballroom 4 - Ernesto Marinero, Purdue University

**8:00AM X53.00001 Generation of Electric Energy and Desalinating Water from Solar Energy and the Oceans Hydropower** , NIAZI ELFIKKY<sup>1</sup>, Saudi Electricity Company — Brief. All warnings and fears about the environment in our Earth planet due to the serious effects of the industrial revolution were certainly predicted early. But the eager contest and the powerful desire for more profits beside the human interest for welfare and development closed all minds about the expected severe destructive impacts on our earth planet. Also, we have to remember that the majority of the African, Asian and Latin American countries are still in the first stage of their development and if they will be left to generate all their demand of energy by the conventional machine e.g (Fossil Fuel, Biofuel and Nuclear Fuel), then our Earth planet will confront an endless and ceaseless severe destructive impacts due to the encroachment of the released hot Carbon Dioxide and hot vapours of Acids which will never forgive any fruitful aspect in our Earth Planet from destruction. 1. Importance of the New Project. Building the Extra cheap, clean Power plants with safe and smooth Operation in addition to the long life time in service for generating enough and plentiful electric energy the sustainable renewable resources will invigorate the foresaking of all Nuclear, Fossil and Biofuel power plants to avoid the nuclear hazards and stop releasing the hot carbon dioxide, hot acids for the recovery of our ill environment. Also, the main sustainable, renewable, and cheap resources for generating the bulky capacity of the electric energy in our project are the Sun and the Oceans in addition to all Seas Surrounding all Continents in our Earth planet. Therefore, our recourses are so much enormous plentiful, clean, and renewable. 2. Generation of Electricity from Solar Energy by Photovoltaic Cells (PVCs) or Concentrated Solar Power (CSP). Characteristics of Photovoltaic Cells (PVCs). It is working only by Sun's Light (Light photons) and its efficiency will decrease as the Solar Thermal Radiation will increase, i.e. as the temperature of the Solar Voltiac will increase, its output will decrease or when the Solar thermal radiation of the Sun will increase, the efficiency of the Solar Voltiac Cells will nearly fully degrade at the ambient temperature  $55^\circ\text{C}$  ( $131^\circ\text{Fahrenheit}$ ). As known, in the African countries near the Atlantic Ocean like Mauritania, Senegal, South Africa and Guinea .etc, also the middle east countries like Morocco, Tuniz, Lybia, Algeria, Egypt, Sudan, Saudi Arabia, Kuwait, United Arab Emirates and Iraqetc. the range of the ambient temperature in the Summer seasons especially in the Desert near the Atlantic Ocean, the Mediterranean Sea, Red Sea and the Persian Gulf is around  $(60-70)^\circ\text{C}$  or  $(140^\circ\text{F}-158^\circ\text{F})$ . Similarly the majority of the Latin American countries with India and China. So, all the environments of the antecedent countries are not the suitable environment for generating electric energy from the Solar Voltiac cells in all seasons along the year. Characteristics of the Concentrated Solar Power (CSP). It uses half cylindrical mirrors to reflect with concentration the Solar thermal Radiation around a pipe to heat a special liquid. When the liquid will be heated it will pass through a water tank to exchange its heat in water tank to evaporate the water and create a steam to drive the Power Turbine for generating electricity. Also the capacity of the electric power generated by such technique is so much limited with respect to the wide area (3000 acres, about five miles end to end) occupied by the Concentrated Solar Power Plant. 3. The New Project Profile. Employing the water from the Oceans, Mediterranean Sea, Red Sea and Chinese sea to generate the bulky Hydraulic power capacity which will be delivered directly to the electric power Grid without any inverters. The Salt water will be drawn for desalination after driving A Steam Power Turbine for generating additional electric power.

<sup>1</sup>P. P. 5, P. O. Box 57 Riyadh 11411

**8:36AM X53.00002 Suppressing diborane production during the hydrogen release in metal borohydrides: The example of doped  $\text{Al}(\text{BH}_4)_3$ <sup>1</sup>** , DAVID HARRISON, TIMO THONHAUSER, Wake Forest University — Aluminum borohydride ( $\text{Al}(\text{BH}_4)_3$ ) is an example of a promising hydrogen storage material with exceptional hydrogen densities by weight and volume and a low hydrogen desorption temperature. But, unfortunately its production of diborane ( $\text{B}_2\text{H}_6$ ) gases upon heating restricts its practical use. To elucidate this issue, we investigate the properties of a number of metal borohydrides with the same problem and find that the electronegativity of the metal cation is not the best descriptor of diborane production. We show that, instead, the closely related formation enthalpy is a much better descriptor and we find that diborane production is an exponential function thereof. We conclude that diborane production is sufficiently suppressed for formation enthalpies of  $-80 \text{ kJ/mol BH}_4$  or lower, providing specific design guidelines to tune existing metal borohydrides or synthesize new ones. We then use first-principles methods to study the stabilizing effects of Sc alloying in  $\text{Al}(\text{BH}_4)_3$ , predicting that with sufficient alloying diborane can be fully suppressed. We conclude that stabilizing  $\text{Al}(\text{BH}_4)_3$  and similar borohydrides via alloying or other means is a promising route to suppress diborane production and thus develop viable hydrogen storage materials.

<sup>1</sup>Supported by NSF DMR-1145968

**8:48AM X53.00003 Improving ammonia borane as a hydrogen storage material with B-group substitutions<sup>1</sup>**, E. WELCHMAN, T. THONHAUSER, Wake Forest Univ — We present *ab initio* results for substitutions intended to lower the hydrogen desorption temperature of  $\text{NH}_3\text{BH}_3$  (ammonia borane or AB), already a promising hydrogen storage material. Substitutions in the  $\text{NH}_3$  group have previously been investigated with success; we propose a different route, instead performing substitutions in the  $\text{BH}_3$  group. To keep gravimetric density high, we focus on the second period elements C, N, O, and F, all with higher electronegativities than H. We also investigate Cu and S as possible substituents. Results include hydrogen binding energies and kinetic barriers for the hydrogen release in the gas phase as well as the solid. Of the substituents studied, we identify Cu as the most promising substituent, which lowers the reaction barrier for the hydrogen release by 38% compared to pure AB and we estimate a new hydrogen desorption temperature between  $-10^\circ\text{C}$  and  $40^\circ\text{C}$ .

<sup>1</sup>This work was supported in full by NSF Grant No. DMR-1145968

**9:00AM X53.00004 Stability of alkali-metal hydrides: effects of n-type doping<sup>1</sup>**, MONICA ARACELI OLEA AMEZCUA, OMAR DE LA PEÑA SEAMAN, JUAN FRANCISCO RIVAS SILVA, Institute of Physics, Benemérita Universidad Autónoma de Puebla (IFUAP-BUAP), ROLF HEID, KLAUS-PETER BOHNEN, Institute of Solid State Physics, Karlsruhe Institute of Technology (IFP-KIT) — Metal hydrides could be considered ideal solid-state hydrogen storage systems, they have light weight and high hydrogen volumetric densities, but the hydrogen desorption process requires excessively high temperatures due to their high stability. Efforts have been performed to improve their dehydrogenation properties, based on the introduction of defects, impurities and doping. We present a systematic study of the n-type (electronic) doping effects on the stability of two alkali-metal hydrides:  $\text{Na}_{1-x}\text{Mg}_x\text{H}$  and  $\text{Li}_{1-x}\text{Be}_x\text{H}$ . These systems have been studied within the framework of density functional perturbation theory, using a mixed-basis pseudopotential method and the self-consistent version of the virtual crystal approximation to model the doping. The full-phonon dispersions are analyzed for several doping content, paying special attention to the crystal stability. It is found a doping content threshold for each system, where they are close to dynamical instabilities, which are related to charge redistribution in interstitial zones. Applying the quasiharmonic approximation, the vibrational free energy, the linear thermal expansion and heat capacities are obtained for both hydrides systems and are analyzed as a function of the doping content.

<sup>1</sup>This work is partially supported by the VIEP-BUAP 2016 and CONACYT-México (No.221807) projects

**9:12AM X53.00005 Transition metal dichalcogenides as a catalyst for hydrogen-evolution reaction**, JUN-HO LEE, YOUNG-WOO SON, Korea Inst for Advanced Study, JINBONG SEOK, HEEJUN YANG, Department of Energy Science and IBS Center for Integrated Nanostructure Physics, Institute for Basic Science, Sungkyunkwan University — Hydrogen evolution using electrochemical reaction of water with specific catalysts has been considered as next-generation energy resources. The best-known and most productive electrochemical catalyst is platinum. However, there has been a continuous struggle to replace the precious Pt-based catalysts by inexpensive and earth-abundant materials such as transition metal dichalcogenides (TMDs). We investigated catalytic performances of various TMDs for hydrogen-evolution reaction (HER) by using first-principles density functional theory calculation. We calculate Gibbs free energy, most widely used descriptor of catalytic activity, of hydrogen atom on TMDs and analyze an origin of significant performance of HER.

**9:24AM X53.00006 Computational study on the hydrogen storage in 2-dimensional potential well using K-intercalated graphite oxide**, JAEHYUN BAE, JISOON IHM, Seoul National University, SEOUL NATIONAL UNIVERSITY TEAM — Here, we present a new hydrogen storage strategy based on a diffusive equilibrium of gas molecules under the external potential we show that density of a gas inside the potential well increases exponentially relative to the ambient gas by the corresponding Boltzmann factor. In this mechanism, hydrogen molecules reside in the delocalized gas form in the potential well, in contrast to the conventional storage localized to specific binding sites. As a realization of the potential well, we choose K-intercalated graphite oxide (KGO) as a scaffold material and show that a relatively uniform potential well arises in between KGO layers. The average potential well depth is much enhanced due to the induced dipole interaction by the electric field generated by K ions and functional groups. The grand canonical Monte-Carlo calculation is employed to obtain the equilibrium hydrogen molecule density in the room temperature and the simulation results are explained by the density enhancement due to the attractive potential inside the KGO layers.

**9:36AM X53.00007 ABSTRACT WITHDRAWN —**

**9:48AM X53.00008 Hydrogen production by thermal water splitting using ferroelectric  $\text{PbTiO}_3$** , ARVIN KAKEKHANI, SOHRAB ISMAIL-BEIGI, Yale University — The increasing demand for renewable energy sources is a prominent challenge facing humanity in 21st century. In this regard, hydrogen production by splitting water has received great attention. Here, we theoretically propose a catalytic cycle that by leveraging the pyroelectric properties of ferroelectric  $\text{PbTiO}_3$ , and using a controlled temperature modulation around Curie temperature as a switch for surface chemical properties, can thermally split  $\text{H}_2\text{O}$  into  $\text{O}_2$  and  $\text{H}_2$ . Since the Curie temperature of  $\text{PbZr}_{1-x}\text{Ti}_x\text{O}_3$  class of materials is tunable and usually in the range of 250-450 degree Celsius; the energy needed to drive this catalytic cycle can be provided by low/intermediate grade heat, for instance: geothermal, industrial waste heat or concentrated solar power. Since no precious metal is needed in this scheme, and all the elements are earth abundant, this can potentially become an economically viable method for hydrogen production.

**10:00AM X53.00009 Engineering and characterization of high surface area graphitic carbon nitrides for hydrogen sorption**, DAVID STALLA, FLORIAN SEYDEL, ANDREW GILLESPIE, THOMAS LAM, MARK SWEANY, MARK LEE, PETER PFEIFER, University of Missouri, Columbia — Theoretical calculations predict graphitic carbon nitride to produce a binding energy to hydrogen ( $6.4\text{ kJ/mol}$ ) which is greater than that of pure graphene, making it attractive as a storage medium. However, the prohibitively small surface areas characteristic of g-CN materials dramatically limit  $\text{H}_2$  uptake. We discuss efforts to increase surface areas through physical/chemical exfoliation and templating.  $\text{N}_2$  sorption directly determines improvements to surface area, EF/TEM maps the thickness of aggregated planes, powder XRD indicates a novel, 2-phase structure, and XPS quantifies in-plane chemistry largely independent of the literature, which fails in a consensus regarding binding energy assignments.

**10:12AM X53.00010 Hydrogen Storage Studies of Palladium-Cobalt alloy nanoparticles dispersed Nitrogen Doped Graphene**, ASHOK PULLAMSETTY, Research scholar, RAMAPRABHU SUNDARA, Professor — Solid state hydrogen storage has significant importance in the present scenario of depleting conventional energy sources. Recent studies reveal that nanomaterials can play a significant role in the performance enhancement of energy conversion and storage device. Carbon based nanomaterials are considered as suitable candidates for hydrogen storage due to their high porosity, large surface area and high chemical stability. The two dimensional graphene, which has been discovered recently, consists of a single layer of atoms arranged in a honeycomb lattice, exhibits surface area. In the present work, we have been studied the hydrogen storage properties of Palladium-Cobalt alloy nanoparticles dispersed nitrogen doped graphene ( $\text{Pd}_3\text{Co}/\text{NG}$ ). Graphitic oxide was prepared by Hummers method and mixed with Palladium Cobalt and melamine precursors. The compound was reduced in hydrogen atmosphere at  $500^\circ\text{C}$  for 5 h. Structural and micro-structural characterization of these samples has been carried out by X-ray diffraction pattern (XRD), Raman spectroscopy, scanning electron microscope (SEM), transmission electron microscopy (TEM) and X-ray photo electro spectroscopy (XPS). The hydrogen adsorption measurements were carried out for NG as well as  $\text{Pd}_3\text{Co}/\text{NG}$  at different temperatures ( $25\text{--}100^\circ\text{C}$ ) and pressures ( $5\text{--}40\text{ bar}$ ) using a high pressure Sieverts apparatus. The material  $\text{Pd}_3\text{Co}/\text{NG}$  exhibits high storage capacity compared to NG due to spillover mechanism and the results have been discussed.

**10:24AM X53.00011 Direct Measurement of the Adsorbed Film Volume for Estimating Heats of Adsorption**, ANDREW GILLESPIE, ELMAR DOHNKE, TYLER RASH, DAVID STALLA, ERNEST KNIGHT, FLORIAN SEYDEL, MARK SWEANY, PETER PFEIFER, Univ of Missouri - Columbia — Compressed hydrogen and methane require extremely high pressures or low temperatures in order to compete with the energy density of conventional fossil fuels. Adsorbent materials provide a means to increase the energy density of these gasses up to 6 times that of compressed gas at the same temperature and pressure. One major concern in engineering adsorbed gas systems is thermal management during charging and discharging. Adsorption is an exothermic process, releasing heat during charging and absorbing heat during discharging. To estimate the heat of adsorption, it is common to analyze excess adsorption isotherms by converting to absolute adsorption and employ the Clausius Clapeyron relation. However, this method requires an assumed volume of the adsorbed state. It is common for researchers to assume that the adsorbed film occupies the entire pore volume of the adsorbent material. However, the adsorbed film only occupies a fraction of the total pore volume. This yields heats of adsorption that are underestimated by as much as 10kJ/mol at high coverage. In this talk, we present a method to directly measure the adsorbed film volume as a function of temperature and present the resulting heats of adsorption for both methane and hydrogen.

**10:36AM X53.00012 Anticipated detection of favorable periods for wind energy production by means of information theory**, EUGENIO VOGEL, GONZALO SARAVIA, Universidad de La Frontera, Temuco, Chile, SIGISMUND KOBE, ROLF SCHUMANN, Technische Universität Dresden, Dresden, Germany, ROLF SCHUSTER, Driedorf, Germany — Managing the electric power produced by different sources requires mixing the different response times they present. Thus, for instance, coal burning presents large time lags until operational conditions are reached while hydroelectric generation can react in a matter of some seconds or few minutes to reach the desired productivity. Wind energy production (WEP) can be instantaneously fed to the network to save fuels with low thermal inertia (gas burning for instance), but this source presents sudden variations within few hours. We report here for the first time a method based on information theory to handle WEP. This method has been successful in detecting dynamical changes in magnetic transitions [J. Mag. Mag. Mater. 372 (2014) 173] and variations of stock markets [Eur. Phys. J. B 87 (2014) 177]. An algorithm called wzip based on information recognition is used to recognize the information content of a time series. We make use of publically available energy data in Germany to simulate real applications. After a calibration process the system can recognize directly on the WEP data the onset of favorable periods of a desired strength. Optimization can lead to a few hours of anticipation which is enough to control the mixture of WEP with other energy sources, thus saving fuels.

**10:48AM X53.00013 Quasi-Elastic Neutron Scattering (QENS) Studies of Hydrogen Dynamics for Nano-Confined NaAlH<sub>4</sub>**<sup>1</sup>, TABBETHA DOBBINS, Rowan University, Dept. of Physics, SHATHABISH NARASEGOWDA<sup>2</sup>, Louisiana Tech University, CRAIG BROWN, MADHUSUDAN TYAGI, TIMOTHY JENKINS<sup>3</sup>, National Institute for Standards and Technology, Center for Neutron Research — The hydrogen dynamics of nano-confined sodium alanate (NaAlH<sub>4</sub>) has been studied using quasi-elastic neutron scattering (QENS). Results indicate thermodynamic destabilization is responsible for reduced desorption temperatures of NaAlH<sub>4</sub> upon confinement within the nanopores of a metal organic framework (MOF). Both the bulk (microscale) NaAlH<sub>4</sub> and the nanoconfined NaAlH<sub>4</sub> data were fitted to re-orientation models which yielded corresponding percent mobile hydrogen and jump lengths. The jump lengths calculated from the nano-NaAlH<sub>4</sub> were  $\approx 2.5$  Å, and in conformity with those jump lengths determined for bulk NaAlH<sub>4</sub> of  $\approx 2.3$  Å. As much as 18 % of the hydrogen atoms were estimated to be mobile in the nano-NaAlH<sub>4</sub> sample even at relatively low temperatures of 350 K. In contrast, bulk NaAlH<sub>4</sub> shows less than 7 % mobile H-atoms even at higher temperatures of  $\approx 450$  K. The activation energy for the long range is 3.1meV.

<sup>1</sup>Quasi-Elastic Neutron Scattering (QENS) Studies of Hydrogen Dynamics for Nano-Confined NaAlH<sub>4</sub>

<sup>2</sup>currently at Intel Corporation

<sup>3</sup>currently at: Army Research Laboratory

## Friday, March 18, 2016 8:00AM - 11:00AM –

Session X55 DBIO GSNP: Principles of Cell to Cell Communication Hilton Baltimore Holiday Ballroom

6 - Ned S. Wingreen, Princeton University

**8:00AM X55.00001 Optimal census by quorum sensing**, THIBAUD TAILLEFUMIER, Princeton University — Bacteria regulate their gene expression in response to changes in local cell density in a process called quorum sensing. To synchronize their gene-expression programs, these bacteria need to glean as much information as possible about local density. Our study is the first to physically model the flow of information in a quorum-sensing microbial community, wherein the internal regulator of the individuals response tracks the external cell density via an endogenously generated shared signal. Combining information theory and Lagrangian optimization, we find that quorum-sensing systems can improve their information capabilities by tuning circuit feedbacks. At the population level, external feedback adjusts the dynamic range of the shared input to individuals detection channels. At the individual level, internal feedback adjusts the regulators response time to dynamically balance output noise reduction and signal tracking ability. Our analysis suggests that achieving information benefit via feedback requires dedicated systems to control gene expression noise, such as sRNA-based regulation.

**8:36AM X55.00002 Using memory to enforce stereotyped behavior in a bacterial community**, RICHARD LOSICK, Harvard University — Bacteria communicate with each other by the exchange of chemical cues. I will describe a simple system in which bacteria form a one-dimensional community in which behavior in the community is enforced by trans-generational memory inherited from a founder cell rather than by intercellular signaling. The bacterium *B. subtilis* held under constant conditions of exponential phase growth switches between a unicellular, motile state and a sessile state in which individual cells are held together in a chain. I will show that cells enter the chaining state spontaneously by a stochastic competition mechanism involving tight binding between two proteins and remain in that state for a stereotyped number of generations due to the action of a third protein that is responsible for memory. The motile state, in contrast, is memoryless. Reconstruction of the principal features of the two states in an unrelated bacterium, *E. coli*, provides evidence that the three proteins are necessary and sufficient to account for the alternative behaviors. Thus, *B. subtilis* is capable of cell-cell communication by an epigenetic information is transmitted to progeny cells for a characteristic number of cell divisions.

**9:12AM X55.00003 Design principles of paradoxical signaling in the immune system**, YUVAL HART, Physics department, School of Engineering and Applied Sciences, Harvard University — A widespread feature of cell-cell signaling systems is paradoxical pleiotropy: the same secreted signaling molecule can induce opposite effects in the responding cells. For example, the cytokine IL-2 can promote proliferation and death of T-cells. The role of such paradoxical signaling remains unclear. We suggest that this mechanism provides homeostatic concentration of cells, independent of initial conditions. The crux of the paradoxical mechanism is the combination of a positive and a negative feedback loops creating two stable states - an OFF state and an ON state. Experimentally, we found that CD4+ cells grown in culture with a 30-fold difference in initial concentrations reached a homeostatic concentration nearly independent of initial cell levels (ON-state). Below an initial threshold, cell density decayed to extinction (OFF-state). Mathematical modeling explained the observed cell and cytokine dynamics and predicted conditions that shifted cell fate from homeostasis to the OFF-state. We suggest that paradoxical signaling provides cell circuits with specific dynamical features that are robust to environmental perturbations.

**9:48AM X55.00004 The BMP Pathway is a Programmable Multi-Ligand Signal Processing System**, YARON ANTEBI, Caltech — The BMP signaling pathway comprises multiple ligands and receptors that interact promiscuously and appear in combinations. This feature is often understood in the context of redundancy and tissue specificity, but it has remained unclear whether it enables specific signal processing capabilities. Here, we show that the BMP pathway performs a specific set of computations, including sums, ratios, and balance and imbalance detection, across the multi-dimensional space of ligand concentrations. These computations can arise directly from receptor-ligand interactions without requiring transcriptional regulation. Furthermore, cells can re-program the type of computation performed on specific ligands through changes in receptor expression, allowing different cell types to perceive distinct signals in the same ligand environment. Together, these results may help explain the prevalence of promiscuous ligand-receptor architectures across pathways and enable predictive understanding and control of BMP signaling.

**10:24AM X55.00005 A positional code and anisotropic forces control tissue remodeling in Drosophila**, JENNIFER ZALLEN, Sloan Kettering Institute — A major challenge in developmental biology is to understand how tissue-scale changes in organism structure arise from events that occur on a cellular and molecular level. We are using cell biological, biophysical, and quantitative live-embryo imaging approaches to understand how genes encode the forces that shape tissues, and to identify the mechanisms that modulate cell behavior in response to local forces. In many animals, the elongated head-to-tail body axis is achieved by rapid and coordinated movements of hundreds of cells. We found that in the fruit fly, these cell movements are regulated by subcellular asymmetries in the localization of proteins that generate contractile and adhesive forces between cells. Asymmetries in the force-generating machinery are in turn controlled by a positional code of spatial information provided by an ancient family of Toll-related receptors that are widely used for pathogen recognition by the innate immune system. I will describe how this spatial system systematically orients local cell movements and collective rosette-like clusters in the Drosophila embryo. Rosettes have now also been shown to shape the body axis in chicks, frogs, and mice, demonstrating that rosette behaviors are a general mechanism linking cellular asymmetry to tissue reorganization.

**Friday, March 18, 2016 11:15AM - 2:15PM –**  
**Session Y1 DCMP DAMOP: Orbital Angular Momentum of Light and Matter** Ballroom I - Charles Clark, NIST

**11:15AM Y1.00001 Ghost imaging with entangled photons and orbital angular momentum**, MILES PADGETT, University of Glasgow — We utilise the position and orbital angular momentum (OAM) correlations between the signal and idler photons generated in the down-conversion process to obtain ghost images of a phase object. By using an OAM phase filter, which is non-local with respect to the object, the ghost images exhibit isotropic edge-enhancement. The strong spatial correlations between the signal and idler photons generated by spontaneous parametric downconversion have been widely utilised in many different imaging systems. The use of a scanning single element detector to recover the spatial information in the signal and idler beams fundamentally limits the detection efficiency of the imaging system to a maximum of  $1/N$  where  $N$  is the number of pixels in the image. Our approach overcomes this limitation by replacing the scanning detector by an intensified CCD camera, therefore detecting all photons irrespective of their position within the image. Using a camera in this way, coupled with the OAM edge-enhancement and image reconstruction techniques allows us to obtain images of phase objects with an average of fewer than one photon per image pixel.

**11:51AM Y1.00002 Twisting Neutron Waves<sup>1</sup>**, DMITRY PUSHIN, IQC, University of Waterloo — Most waves encountered in nature can be given a “twist”, so that their phase winds around an axis parallel to the direction of wave propagation. Such waves are said to possess orbital angular momentum (OAM). For quantum particles such as photons, atoms, and electrons, this corresponds to the particle wavefunction having angular momentum of  $L\hbar$  along its propagation axis. Controlled generation and detection of OAM states of photons began in the 1990s, sparking considerable interest in applications of OAM in light and matter waves<sup>2</sup>. OAM states of photons have found diverse applications such as broadband data multiplexing, massive quantum entanglement, optical trapping, microscopy, quantum state determination and teleportation, and interferometry. OAM states of electron beams have been used to rotate nanoparticles, determine the chirality of crystals and for magnetic microscopy. Here I discuss the first demonstration of OAM control of neutrons<sup>3</sup>. Using neutron interferometry with a spatially incoherent input beam, we show the addition and conservation of quantum angular momenta, entanglement between quantum path and OAM degrees of freedom. Neutron-based quantum information science heretofore limited to spin, path, and energy degrees of freedom, now has access to another quantized variable, and OAM modalities of light, x-ray, and electron beams are extended to a massive, penetrating neutral particle. The methods of neutron phase imprinting demonstrated here expand the toolbox available for development of phase-sensitive techniques of neutron imaging.

<sup>1</sup>Financial support provided by the NSERC Create and Discovery programs, CERC and the NIST Quantum Information Program is acknowledged.

<sup>2</sup>“Orbital angular momentum: origins, behavior and applications,” A. M. Yao and M. J. Padgett, *Adv. Opt. Photonics* **3**, 161 (2011)

<sup>3</sup>“Controlling neutron orbital angular momentum,” C. W. Clark, *et al.*, *Nature* **525**, 504 (2015)

**12:27PM Y1.00003 INVITED ABSTRACT WITHDRAWN –**

**1:03PM Y1.00004 Creating High-Harmonic Beams with Controlled Orbital Angular Momentum**, ROBERT W. BOYD, University of Ottawa — A beam of light with an angle-dependent phase  $\Phi = \ell\phi$ , where  $\phi$  is the azimuthal coordinate, about the beam axis carries an orbital angular momentum (OAM) of  $\ell\hbar$  per photon. Such beams have been exploited to provide superresolution in visible-light microscopy. The ability to create extreme ultraviolet or soft-x-ray beams with controllable OAM would be a critical step towards extending superresolution methods to extremely small feature size. Here we show that OAM is conserved during the process of high-harmonic generation (HHG). Experimentally, we use a fundamental beam with  $\ell = 1$  and interferometrically determine that the  $q$ -th harmonic has an OAM quantum number  $\ell$  equal to its harmonic order  $q$ . We also show theoretically how to couple an arbitrary low value of the OAM quantum number  $\ell$  to any harmonic order  $q$  in a controlled manner. Our results open a route to microscopy on the molecular, or even submolecular, scale.

Reference: G. Gariépy, J. Leach, K.T. Kim, T. J. Hammond, E. Frumker, R.W. Boyd, and P. B. Corkum, *Phys. Rev. Lett.* **113**, 153901 (2014).

**1:39PM Y1.00005 Unveiling orbital angular momentum and acceleration of light beams and electron beams<sup>1</sup>**, ADY ARIE, Tel-Aviv University — Special beams, such as the vortex beams that carry orbital angular momentum (OAM) and the Airy beam that preserves its shape while propagating along parabolic trajectory, have drawn significant attention recently both in light optics and in electron optics experiments. In order to utilize these beams, simple methods are needed that enable to easily quantify their defining properties, namely the OAM for the vortex beams and the nodal trajectory acceleration coefficient for the Airy beam. Here we demonstrate a straightforward method to determine these quantities by astigmatic Fourier transform of the beam. For electron beams in a transmission electron microscope, this transformation is easily realized using the condenser and objective stigmators, whereas for light beam this can be achieved using a cylindrical lens. In the case of Laguerre-Gauss vortex beams, it is already well known that applying the astigmatic Fourier transformation converts them to Hermite-Gauss beams. The topological charge (and hence the OAM) can be determined by simply counting the number of dark stripes of the Hermite-Gauss beam. We generated a series of electron vortex beams and managed to determine the topological charge up to a value of 10. The same concept of astigmatic transformation was then used to unveil the acceleration of an electron Airy beam. The shape of astigmatic-transformed depends only on the astigmatic measure and on the acceleration coefficient. This method was experimentally verified by generating electron Airy beams with different known acceleration parameters, enabling direct comparison to the deduced values from the astigmatic transformation measurements. The method can be extended to other types of waves. Specifically, we have recently used it to determine the acceleration of an optical Airy beams and the topological charge of so-called Airy-vortex light beam, i.e. an Airy light beam with an embedded vortex.

<sup>1</sup>This work was supported by DIP and the Israel Science Foundation

**Friday, March 18, 2016 11:15AM - 1:39PM –**  
**Session Y2 DCMF DMP GMAG: Spin and Valley Pseudo-Spin Transport in Strongly Spin-Orbit Coupled Systems** Ballroom II - Kin Fai Mak, Pennsylvania State University

**11:15AM Y2.00001 Transport measurements of MoS<sub>2</sub> using a van der Waals heterostructure device platform**, JAMES HONE, Columbia University — No abstract available.

**11:51AM Y2.00002 Theory of classical and quantum transport in monolayers of MoS<sub>2</sub><sup>1</sup>**, SHAFFIQUE ADAM, Yale-NUS College, 16 College Avenue West, Singapore 138527, Singapore — From the family of new van der Waals materials, the class of layered transition metal dichalcogenides has emerged as a particularly interesting system due to the inherent spin and valley degrees of freedom. In this talk we focus on the interplay between these degrees of freedom and the different types of disorder in monolayers of molybdenum disulphide. Within the semiclassical Drude-Boltzmann formalism, treating the screening of impurities with the random phase approximation, we demonstrate that different scattering mechanisms such as charged impurity scattering, intervalley scattering, and phonons provide different signatures in electronic transport. This allows us to conclude, for example, that in CVD-grown monolayers of MoS<sub>2</sub>, intervalley scattering dominates over other mechanisms at low temperatures [1]. Interestingly, charged impurities generate spatial inhomogeneity in the carrier density that results in a classical disorder-induced magnetoresistance that can be observed at room temperature [2]. However, at lower temperatures, in this regime of strong intervalley scattering, we predict that the quantum phase-coherent corrections to the conductivity results in a one-parameter crossover from weak localization to weak anti-localization as a function of magnetic field, where this crossover is determined only by the spin lifetime. By comparing with available experimental data [3], we show that this combined framework allows for a novel way to measure the spin-relaxation in monolayers of MoS<sub>2</sub>. We find that the spin scattering arises from the Dyakonov-Perel spin-orbit scattering mechanism with a conduction band spin-splitting of about 4 meV, consistent with calculations using density functional theory. REFERENCES: [1] “*Transport Properties of Monolayer MoS<sub>2</sub> Grown by Chemical Vapor Deposition*”, H. Schmidt, S. Wang, L. Chu, M. Toh, R. Kumar, W. Zhao, A. H. Castro Neto, J. Martin, S. Adam, B. Özyilmaz, and G. Eda, *Nano Lett.* **14**, 1909 (2014); [2] “*Disorder induced magnetoresistance in a two dimensional electron system*”, J. Ping, I. Yudhistira, N. Ramakrishnan, S. Cho, S. Adam, M. S. Fuhrer, *Phys. Rev. Lett.* **113**, 047206 (2014); [3] “*Quantum transport and observation of Dyakonov-Perel spin-orbit scattering in monolayer MoS<sub>2</sub>*”, H. Schmidt, I. Yudhistira, L. Chu, A. H. Castro Neto, B. Özyilmaz, S. Adam, G. Eda, arXiv:1503.00428, (2015).

<sup>1</sup>Work done in collaboration with Indra Yudhistira and the experimental groups of Goki Eda (NUS), Michael Fuhrer (Monash) and Roland Kawakami (Ohio State), and funded by Singapore National Research Foundation and Ministry of Education.

**12:27PM Y2.00003 Optical imaging of the valley Hall effect in MoS<sub>2</sub> transistors**, JIEUN LEE, Penn State University — The newly emerged two-dimensional (2D) transition metal dichalcogenides (TMDs) with nonequivalent K and K' valleys have provided an ideal laboratory for exploring the valley degree of freedom of electrons, as well as their potential applications for information processing. Valley Hall effect (VHE), in which a transverse valley current is formed under a longitudinal electrical bias in the absence of a magnetic field, has been predicted in 2D TMDs with broken inversion symmetry. The effect has recently been demonstrated in monolayer MoS<sub>2</sub> through a photo-induced anomalous Hall effect, which uses circularly polarized light to preferentially excite electrons into a specific valley. In this talk, we will present our recent results on the development of Kerr rotation microscopy to image the VHE. The valley polarizations of opposite sign accumulated on two opposing edges of MoS<sub>2</sub> transistors from the VHE are measured directly. We will also discuss the possibility of electrical control of the VHE in bilayer MoS<sub>2</sub>, which possesses inversion symmetry. An application of a vertical electric field breaks the inversion symmetry and consequently yields the VHE.

**1:03PM Y2.00004 Breaking time reversal symmetry, quantum anomalous Hall state and dissipationless chiral conduction in topological insulators<sup>1</sup>** , JAGADEESH MOODERA<sup>2</sup>, MIT — Breaking time reversal symmetry (TRS) in a topological insulator (TI) with ferromagnetic perturbation can lead to many exotic quantum phenomena exhibited by Dirac surface states including the quantum anomalous Hall (QAH) effect and dissipationless quantized Hall transport. The realization of the QAH effect in realistic materials requires ferromagnetic insulating materials and topologically non-trivial electronic band structures. In a TI, the ferromagnetic order and TRS breaking is achievable by conventional way, through doping with a magnetic element, or by ferromagnetic proximity coupling. Our experimental studies by both approaches will be discussed. In doped TI van Vleck ferromagnetism was observed. The proximity induced magnetism at the interface was stable, beyond the expected temperature range. We shall describe in a hard ferromagnetic TI system a robust QAH state and dissipationless edge current flow is achieved,<sup>1,2</sup> a major step towards dissipationless electronic applications with no external fields, making such devices more amenable for metrology and spintronics applications. Our study of the gate and temperature dependences of local and nonlocal magnetoresistance, may elucidate the causes of the dissipative edge channels and the need for very low temperature to observe QAH. In close collaboration with: CuiZu Chang,<sup>2,3</sup> Ferhat Katmis, <sup>1,2,3</sup> Peng Wei, <sup>1,2,3</sup>; From Nuclear Eng. Dept. MIT, M. Li, J. Li; From Penn State U, W-W. Zhao, D. Y. Kim, C-x. Liu, J. K. Jain, M. H. W. Chan; From Oakridge National Lab, V. Lauter; From Northeastern U., B. A. Assaf, M. E. Jamer, D. Heiman; From Argonne Lab, J. W. Freeland; From Ruhr-Universitaet Bochum (Germany), F. S. Nogueira, I. Eremin; From Saha Institute of Nuclear Physics (India), B. Satpati. References:

1. P. Wei et al., Phys. Rev. Lett. 110, 186807 (2013)
2. C-Z Chang et al., Nat. Matl 13, 473 (2015), Phys. Rev. Lett. 115, 057206 (2015)

<sup>1</sup>Work supported by NSF Grant DMR-1207469, the ONR Grant N00014-13-1-0301, and the STC Center for Integrated Quantum Materials under NSF grant DMR-1231319.

<sup>2</sup>Physics Department, <sup>2</sup>Francis Bitter Magnet Lab, <sup>3</sup>Plasma Science and Fusion Center

## Friday, March 18, 2016 11:15AM - 1:39PM –

Session Y3 DCMP GMAG: Skyrmions in Chiral Magnets Ballroom III - Nandini Trivedi, Ohio State University

### 11:15AM Y3.00001 INVITED ABSTRACT WITHDRAWN –

**11:51AM Y3.00002 Experimental Studies of Berry Phase Effects and Collective Excitations in Skyrmion Materials** , CHRISTIAN PFLEIDERER, Physik-Department, Technische Universität München, D-85748 Garching, Germany — The emergence, stability and decay of skyrmions in chiral magnets and the associated emergent electrodynamics are reviewed. The non-zero topological winding, which corresponds to precisely one quantum of emergent magnetic flux, mediates an extremely efficient coupling between the conduction electrons and the magnetic properties. This emergent flux leads to a topological Hall signal, spin transfer torques at ultra-low current densities and emergent electric fields. Additionally skyrmions are characterised by an exceptional stability, which cannot be simply suppressed under large hydrostatic pressures or doping. In fact, measurements of the Hall effect suggest the survival of non-trivial topological winding akin that of the skyrmion lattice in a non-Fermi liquid regime at high pressures, where neutrons scattering suggests the absence of long-range magnetic order. The topological unwinding of skyrmions, which involves emergent magnetic monopoles, may be at the heart of the loss of long-range order.

**12:27PM Y3.00003 Skyrmions in chiral magnets with Rashba and Dresselhaus Spin-Orbit Coupling<sup>1</sup>** , MOHIT RANDERIA, The Ohio State University — Studies of skyrmions in chiral magnets have focused largely on systems with broken bulk inversion and a Dzyaloshinskii-Moriya interaction (DMI) of the Dresselhaus form. The skyrmion crystal is then stable only in a small regime with easy-axis anisotropy. I will show how skyrmion crystal phases can be stabilized over a much larger region of field and anisotropy down to zero temperature in systems with a Rashba DMI that break surface inversion or mirror symmetry [1,2]. Increasing the ratio of Rashba to Dresselhaus DMI leads to a progressively larger domain of stability for skyrmions, especially in the easy-plane anisotropy regime. The spin texture and topological charge density then develop nontrivial spatial structures, different from conventional skyrmions, with a quantized topological charge given by a Chern number. Our theoretical results predict how tuning the Rashba spin orbit coupling and magnetic anisotropy can help stabilize skyrmion phases in thin films, surfaces, interfaces and bulk magnets with broken mirror symmetry. [1] J. Rowland, S. Banerjee, and M. Randeria, arXiv:1509.07508v2. [2] S. Banerjee, J. Rowland, O. Erten, and M. Randeria, PRX 4, 031045 (2014).

<sup>1</sup>Supported by the NSF grant DMR-1410364 and by the CEM, an NSF MRSEC, under grant DMR-1420451.

**1:03PM Y3.00004 Skyrmions in frustrated magnets<sup>1</sup>** , SHIZENG LIN, Los Alamos Natl Lab — A skyrmion in magnets or magnetic skyrmion is a stable spin texture with nontrivial topology and behaves like a particle at mesoscale. To stabilize a skyrmion, it is required to have a characteristic length scale, which can be introduced by competing interactions. Recently skyrmion lattice has been observed experimentally in chiral magnets without inversion symmetry, where the skyrmions are stabilized by the competition between the exchange and Dzyaloshinskii-Moriya interactions. The skyrmions in chiral magnets have been studied actively and have been demonstrated to be promising for applications. These skyrmions share qualitatively similar properties in metals, semiconductors and insulators and can be described by a simple universal Hamiltonian. Skyrmions can also be stabilized in frustrated magnets with inversion symmetry. In the talk, we will present a general Ginzburg-Landau theory for the skyrmions in the frustrated magnets. We will discuss their unusual properties in comparison to those in chiral magnets. Finally we will also discuss the conditions for the stabilization of skyrmions.

<sup>1</sup>This work was carried out under the auspices of the NNSA of the US DOE at LANL under Contract No. DE-AC52-06NA25396, and was supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering.

## Friday, March 18, 2016 11:15AM - 1:03PM –

Session Y4 FIP: Physics and Physicists in Cuba Ballroom IV - Mria Spiropulu, California Institute of Technology

**11:15AM Y4.00001 The Role of Science Cooperation in World-Wide Social Progress** , DAVID GROSS, Univ of California - Santa Barbara — No abstract available.

**11:51AM Y4.00002 Physics & Physicists in Cuba** , FIDEL CASTRO DAZ-BALART, Vice-president of the Academy of Sciences of Cuba — No abstract available.

**12:27PM Y4.00003 Science and Technology Diplomacy with Cuba**, FRANCES COLON, US Department of State — President Obama's announcement of U. S. policy change toward Cuba and increased freedom of interaction with the Cuban people opens unprecedented and long-awaited opportunities for the scientific and engineering communities in the U. S. and in Cuba to establish and expand collaborative efforts that will greatly advance U.S. and Cuba science and technology agendas. New rules for export of donated-only items for scientific use will bring researchers closer to the level of their professional peers around the world. Increasing Cubans' access to information will result in greater interactions between scientific communities and enable the sharing of ideas and discoveries that can fuel entrepreneurship on the island. The scientific community has expressed an extraordinary level of interest in the wide range of scientific opportunities that the new policy presents, in collaborating with their Cuban counterparts, and in supporting the development of scientific capacity in Cuba. In response to numerous expressions of interest and inquiries from the scientific community, the Office of the Science and Technology Adviser to the Secretary of State (STAS) has engaged in public outreach to inform the U.S. science and technology community of the implications of the new policy for collaborative research, emerging scientific opportunities, and the standing limitations for engagement with the people of Cuba.

**Friday, March 18, 2016 11:15AM - 2:03PM** —

**Session Y5 GMAG DMP FIAP: Semiconductor Spin Qubits** 301 - Igor Zutic, University at Buffalo

**11:15AM Y5.00001 Microscopic origin of the prolonged coherence in 4H-SiC divacancy spin qubits<sup>1</sup>**, HOSUNG SEO, ABRAM FALK, PAUL KLIMOV, DAVID CHRISTLE, DAVID AWSCHALOM, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago — Long coherence times of quantum bits (qubits) is a key prerequisite for quantum computing and quantum metrology. Recently, electronic spin qubits localized to divacancies in 4H-SiC were found to have a long spin coherence time ( $T_2$ ) exceeding 1 ms, which is longer than that of the nitrogen-vacancy (NV) center in chemically but not isotopically purified diamond. In this talk, we discuss the microscopic origin behind the prolonged divacancy coherence. By using optically detected magnetic resonance (ODMR), we show that the divacancy  $T_2$  rapidly increases as a function of magnetic field, saturating at 1.3 ms at  $T = 20$  K. We used a quantum-bath model combined with a cluster correlation expansion technique to calculate the divacancy coherence function and found an excellent agreement between theory and experiment. We show that an effective decoupling of the  $^{29}\text{Si}$  and  $^{13}\text{C}$  nuclear spins due to their gyromagnetic ratio difference is one of the key reasons responsible for suppressing the decoherence of the divacancy qubits in SiC under magnetic fields larger than 100G.

<sup>1</sup>We gratefully acknowledge financial support from the National Science Foundation through the University of Chicago MRSEC under award number DMR-1420709.

**11:27AM Y5.00002 Coherent population trapping of a nitrogen vacancy center induced by optical and surface acoustic waves**, THEIN OO, ANDREW GOLTER, HAILIN WANG, University of Oregon — We report experimental demonstration of coherent population trapping (CPT) driven by resonant optical and mechanical coupling in a nitrogen vacancy (NV) center in diamond. A surface acoustic wave (SAW) is generated with an inter-digital transducer fabricated on a ZnO layer sputtered on diamond surface. The SAW couples resonantly to a transition between two excited states of the NV center, while a laser field couples to a corresponding resonant optical transition. The combined optical and mechanical coupling to the lambda- or ladder- type three-level system leads to CPT of the NV center. These studies open the door to exploiting strong excited-state electron-phonon coupling for applications such as laser cooling of a mechanical resonator and mechanically-mediated spin entanglement.

**11:39AM Y5.00003 Quantum Control of a Nitrogen-Vacancy Center using Surface Acoustic Waves in the Resolved Sideband Limit**, DAVID GOLTER, THEIN OO, MAIRA AMEZCUA, HAILIN WANG, University of Oregon — Micro-electromechanical systems research is producing increasingly sophisticated tools for nanophononic applications. Such technology is well-suited for achieving chip-based, integrated acoustic control of solid-state quantum systems. We demonstrate such acoustic control in an important solid-state qubit, the diamond nitrogen-vacancy (NV) center. Using an interdigitated transducer to generate a surface acoustic wave (SAW) field in a bulk diamond, we observe phonon-assisted sidebands in the optical excitation spectrum of a single NV center. This exploits the strong strain sensitivity of the NV excited states. The mechanical frequencies far exceed the relevant optical linewidths, reaching the resolved-sideband regime. This enables us to use the SAW field for driving Rabi oscillations on the phonon-assisted optical transition. These results stimulate the further integration of SAW-based technologies with the NV center system.

**11:51AM Y5.00004 Development of single-crystal diamond scanning probes with nitrogen-vacancy centers for cryogenic magnetometry with nanoscale spatial resolution**, ALEC JENKINS, MATTHEW PELLICIONE, PREETI OVARTCHAIYAPONG, CHRISTOPHER REETZ, ANIA BLESZYNSKI JAYICH, University of California, Santa Barbara — Scanning probes based on the nitrogen-vacancy (NV) defect center in diamond are powerful tools for imaging magnetic phenomena at the nanoscale. In particular, extending the operation of these probes to cryogenic temperatures opens up a wide range of condensed matter systems that can be studied. In this talk, we demonstrate a variable temperature NV scanning magnetometer consisting of an atomic-force microscope housed in a closed-cycle cryostat integrated with custom confocal optics. With this microscope we have observed 6-nm spatial resolution and  $3 \mu\text{T}/\sqrt{\text{Hz}}$  sensitivity at  $T = 6$  K. The single-crystal diamond scanning probes that contain shallow and coherent NV centers are critical to the performance of the microscope. The probes are designed with the aim of reducing the NV-sample separation and increasing collection of NV fluorescence, both while maintaining the spin coherence properties of the defects. We describe the fabrication of these probes as well as ongoing efforts to improve their sensitivity and spatial resolution.

**12:03PM Y5.00005 Scanned probe imaging of nanoscale magnetism at cryogenic temperatures with a single-spin quantum sensor**, MATTHEW PELLICIONE, ALEC JENKINS, PREETI OVARTCHAIYAPONG, CHRISTOPHER REETZ, University of California, Santa Barbara, EVE EMMANUELIDU, NI NI, University of California, Los Angeles, ANIA BLESZYNSKI JAYICH, University of California, Santa Barbara — The nitrogen vacancy (NV) defect in diamond has emerged as a promising candidate for high resolution magnetic imaging based on its atomic size and quantum-limited sensing capabilities afforded by long spin coherence times. Although the NV center has been successfully implemented as a nanoscale scanning magnetic probe at room temperature, it has remained an outstanding challenge to extend this capability to cryogenic temperatures, where many solid-state systems exhibit non-trivial magnetic order. In this talk, we present NV magnetic imaging at  $T = 6$  K, first benchmarking the technique with a magnetic hard disk sample, then utilizing the technique to image vortices in the iron pnictide superconductor  $\text{BaFe}_2(\text{As}_{0.7}\text{P}_{0.3})_2$  with  $T_c = 30$  K. In addition, we discuss other candidate solid-state systems that can benefit from the high spatial resolution and field sensitivity of the scanning NV magnetometer.

**12:15PM Y5.00006 Coupling a driven magnetic vortex to individual nitrogen-vacancy spins for fast, nanoscale addressability and coherent manipulation<sup>1</sup>**, MICHAEL WOLF, ROBERT BADEA, JESSE BEREZOVSKY, Case Western Reserve University — The core of a ferromagnetic (FM) vortex domain creates a strong, localized magnetic field which can be manipulated on nanosecond timescales using small magnetic fields, or electrical currents. These capabilities present opportunities for nanoscale spin-based devices. Here, we demonstrate how these FM vortex properties can be used in a room temperature, integrated device by coupling a FM vortex to nitrogen-vacancy (NV) center spins in diamond [1]. Measurements are carried out using a combined magneto-optical microscopy and optically-detected spin resonance technique. We show that the FM vortex can be driven into proximity with an NV, inducing significant NV spin splitting and sufficiently large magnetic field gradient to address spins separated by nanometer length scales. By applying a microwave-frequency magnetic field, we drive both the vortex and the NV spins, resulting in enhanced coherent rotation of the spin state. Finally we demonstrate that by driving the vortex on fast timescales, sequential addressing and coherent manipulation of spins is possible on 100 ns timescales, while driving on faster timescales results in non-trivial coherent dynamics of the coupled vortex/NV system. [1] Wolf, M.S., Badea, R., and Berezovsky, J., cond-mat/1510.07073, (2015)

<sup>1</sup>We acknowledge the DOE award DE-SC008148

**12:27PM Y5.00007 Navigating the vortex pinning landscape for bistable coupling of a ferromagnetic vortex to individual nitrogen vacancy spins<sup>1</sup>**, JESSE BEREZOVSKY, MICHAEL WOLF, ROBERT BADEA, Case Western Reserve University — A ferromagnetic (FM) vortex coupled to nitrogen-vacancy (NV) spins in diamond provides an integrated platform for fast, nanoscale addressability of coherent spins [1]. The vortex moves in a complex effective potential landscape set by the geometry of the disk and the defects present in the material. As the vortex moves through this landscape, the coupling to a proximal NV varies. We use differential magneto-optical microscopy to extract the effective potential through which the vortex moves [2], and optically-detected magnetic resonance to study the coupling of the vortex to an adjacent NV spin. When multiple local minima are present in the vortex potential, the vortex/NV coupling displays bistability. We switch between these bistable states with short magnetic field pulses. This allows an NV spin transition to be switched between on-resonance and off-resonance with a driving field with the same set of external parameters, and also yields information about the mechanisms of vortex/NV coupling. [1] M.S. Wolf, R. Badea, J. Berezovsky, arXiv:1510.07073, 2015 [2] R. Badea, J. Berezovsky, arXiv:1510.07059, 2015.

<sup>1</sup>We acknowledge support from US Department of Energy, award DE-SC008148

**12:39PM Y5.00008 Phonon induced two-electron relaxation in two donor qubits in silicon**, YULING HSUEH, ARCHANA TANKASALA, YU WANG, GERHARD KLIMECK, Purdue University, MICHELLE SIMMONS, University of New South Wales, RAJIB RAHMAN, Purdue University — An atomistic method of calculating two-electron spin-lattice relaxation times ( $T_1$ ) is presented for two donor qubits in silicon. The singlet-triplet two-electron states are calculated from full-configuration interaction (FCI) method with one-electron basis states obtained from the tight-binding Hamiltonian including spin-orbit interaction. The FCI solution enables the investigation of various regimes of donor separations, including very closely separated donor pairs in which rearrangement of excited bonding and anti-bonding states change the wavefunction symmetries. Hyperfine mixing from the nuclear spins is included perturbatively into the two-electron states. To calculate the  $T_1$  times, the electron-phonon Hamiltonian is evaluated from the strain-dependent tight-binding Hamiltonian. The results show how the  $T_1$  times in donor qubits vary with magnetic field and donor separation for each of the three triplets. Moreover, the variation of  $T_1$  with the electric field controlled exchange coupling is also investigated.

**12:51PM Y5.00009 Pauli spin blockade in CMOS silicon double dots probed by dual gate reflectometry<sup>1</sup>**, DHARMRAJ KOTEKAR PATIL, CEA-INAC and Universit Grenoble Alpes, 17 Rue des Martyrs, F-38000 Grenoble, France, ALESSANDRO CRIPPA, Laboratorio MDM, CNR-IMM, ROMAIN MAURAND, ANDREA CORNA, CEA-INAC and Universit Grenoble Alpes, ROMAIN LAVIEVILLE, LOUIS HUTIN, SYLVAIN BARRAUD, CEA, LETI, MINATEC Campus, ALEXEI ORLOV, University of Notre Dame, Notre Dame, SILVANO DE FRANCESCHI, MARC SANQUER, XAVIER JEHL, CEA-INAC and Universit Grenoble Alpes, TEAM TEAM, COLLABORATION COLLABORATION, COLLABORATION COLLABORATION, TEAM TEAM, COLLABORATION COLLABORATION — Silicon quantum dots are attractive candidates for the development of scalable spin-based qubits. The Pauli spin blockade effect in double quantum dots can provide an efficient, temperature-independent mechanism for qubit readout. Here we report the observation of Pauli blockade in silicon double quantum dots defined in double-gate nanowire transistors fabricated using silicon-on-insulator CMOS technology. Each of the two gates is connected to an LC resonator to perform radio-frequency reflectometry. This powerful technique allows high-sensitivity detection of charge transitions in the double quantum dot down to the few-electron regime. We find evidence of Pauli spin blockade and study the magnetic-field dependence of the underlying singlet-triplet states.

<sup>1</sup>SIAM, SiSPIN

**1:03PM Y5.00010 Direct observation of long-distance coherent superexchange spin coupling in a quantum dot array**  
**Spin Exchange oscillations between distant quantum dots**, TAKAFUMI FUJITA, TIM BAART, Delft University of Technology, CHRISTIAN REICHL, WERNER WEGSCHEIDER, ETH Zurich, LIEVEN VANDERSYPEN, Delft University of Technology — Interactions mediated by long-range quantum coherence lie at the heart of important phenomena in many different fields. Charge transfer during oxidative stress in DNA [1], reactions in photosynthetic molecules [2], and behaviour of cuprate superconductors [3] are all described by tunnelling via virtual hopping. Such mechanism may also provide new ways of using quantum dots for fault tolerant quantum information processing [4]. In the presence of long-range tunnel coupling mediated by virtual occupation of intermediate levels, superexchange interactions can induce coherent oscillations between two distant electron spins. We implement this scheme in a linear array of three quantum dots with one electron on each of the outer dots. We observe coherent exchange oscillations between the two spins, and the oscillation frequency is controlled by the detuning of the electrochemical potential of the dot in between. Spin exchange at a distance may provide a new route for scaling up electron spin qubits using quantum dots. [1] B. Giese, et al, Nature 412, 318-320 (2001). [2] X.F. Wang, et al, Phys. Rev. Lett. 97,106602 (2006). [3] C. Kim, et al, Phys. Rev. Lett. 80, 4245 (1998). [4] F. Braakman, et al, Nature Nano. 8, 432-437 (2013).

**1:15PM Y5.00011 Decoherence of an electron spin qubit in an optically active quantum dot**, FUXIANG LI, Theoretical Division and CNLS, LANL, ALEXANDER BECHTOLD, DOMINIK RAUCH, TOBIAS SIMMET, PER-LENNART ARDELT, ARMIN REGLER, KAI MULLER, Walter Schottky Institut, Technische Universitat Munchen, 85748 Garching, Germany, NIKOLAI SINITSYN, Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA, JONATHAN FINLEY, Walter Schottky Institut, Technische Universitat Munchen, 85748 Garching, Germany — Understanding the spin dynamics in quantum dot, especially its detailed decoherence and relaxation is not only of theoretical interests, but also a crucial problem towards the application of quantum dot as a solid-state quantum qubit. From the phenomenological models of decoherence developed more than a decade ago, it has been now fairly accepted that the spin dynamics undergoes two stages, first a fast ensemble dephasing due to the coherent precession of spin qubit around nearly static but randomly distributed hyperfine fields ( $\sim 2$  ns) and then a much slower relaxation process ( $> 1\mu$  s) due to dynamics of the nuclear spin bath induced by complex many-body interaction effects. However, this characteristics has never been verified in the experiment, until the recent experiment breakthrough I'm going to talk about. What's more interesting is that, the experiment unambiguously shows a more complex picture, in which two dips rather than one, develops, which can be attributed to the effect of the comparatively strong quadruple field.

**1:27PM Y5.00012 Coherent control of single spins in a silicon carbide pn junction device at room temperature**, SANG-YUN LEE, MATTHIAS WIDMANN, 3rd Institute of Physics, University of Stuttgart, IAN BOOKER, Department of Physics, Chemistry and Biology, Linköping University, MATTHIAS NIETHAMMER, 3rd Institute of Physics, University of Stuttgart, TAKESHI OHSHIMA, Japan Atomic Energy Agency, ADAM GALL, Wigner Research Centre for Physics, Hungarian Academy of Sciences, NGUYEN T. SON, ERIK JANZÉN, Department of Physics, Chemistry and Biology, Linköping University, JOERG WRACHTRUP, 3rd Institute of Physics, University of Stuttgart — Spins in single defects have been studied for quantum information science and quantum metrology. It has been proven that spins of the single nitrogen-vacancy (NV) centers in diamond can be used as a quantum bit, and a single spin sensor operating at ambient conditions. Recently, there has been a growing interest in a new material in which color centers similar to NV centers can be created and whose electrical properties can also be well controlled, thus existing electronic devices can easily be adapted as a platform for quantum applications. We recently reported that single spins of negatively charged silicon vacancies in SiC can be coherently controlled and long-lived at room temperature<sup>1</sup>. As a next step, we isolated single silicon vacancies in a SiC pn junction device and investigated how the change in Fermi level, induced by applying bias, alters the charge state of silicon vacancies, thus affects the spin state control. This study will allow us to envision quantum applications based on single defects incorporated in modern electronic devices.

<sup>1</sup>M. Widmann, et al., Nat Mater 14, 164 (2015)

**1:39PM Y5.00013 Optical and Spin Signatures of Transition Metal Impurities in Silicon Carbide**<sup>1</sup>, WILLIAM KOEHL, SAMUEL J. WHITELY, BERK DILER, ALEXANDRE BOURASSA, DAVID D. AWSCHALOM, Institute for Molecular Engineering, University of Chicago, NGUYEN TIEN SON, Department of Physics, Chemistry and Biology, Linköping University, Sweden — Point defects and impurities are increasingly viewed as an important resource for solid-state implementations of quantum information technologies. Electronic spins bound to point defects like the nitrogen vacancy center in diamond and divacancy in silicon carbide are especially attractive because they function as long-lived qubit states that can be controlled optically at the single-site level. These capabilities have generated a growing interest in identifying other classes of point defect with similar properties, since discovery of such systems might allow for new ranges of functionality in solid-state quantum device design. Transition metal ions are a promising area for exploration, since they often introduce isolated electronic levels within the bandgaps of semiconductors and possess a wide variety of magnetic and optical properties. Here we describe recent experimental studies of the optical and spin properties of transition metal impurities in silicon carbide. Using ensemble spectroscopies, we evaluate their potential for use as optically-controllable spin states within this industrially-important, wide-bandgap, optoelectronic material.

<sup>1</sup>This work supported by the AFOSR, NSF MRSEC, and Argonne LDRD Program.

**1:51PM Y5.00014 Measurement of Spin Coherence Times in Proton Irradiated 4H-SiC**, JACOB EMBLEY, JOHN COLTON, Brigham Young University, SAM CARTER, Naval Research Lab, KYLE MILLER, Brigham Young University, MARGARET MORRIS, Brandeis University — Silicon vacancy defects in silicon carbide (SiC) have potential for use in spintronic devices. We used optically detected magnetic resonance and a spin echo technique to measure  $T_2$  spin coherence times for electrons in 4H-SiC. These experiments were performed at a magnetic field strength of 0.371 T and a resonant microwave frequency of 10.5 GHz. Each sample contained silicon vacancy defects that were formed through irradiation with 2 MeV protons at unique fluences ( $10^{13}$  and  $10^{14}$  cm<sup>-2</sup>). Measurements for each sample were made across a range of temperatures, from 8 K to room temperature. While we generally observed a decrease in spin coherence time with temperature, we also observed a range of temperatures (from 60 K to 160 K) for which the overall trend was reversed.

**Friday, March 18, 2016 11:15AM - 2:03PM –**

**Session Y6 GMAG DMP: Magnetic Complex Oxides II** 302 - Antia Botana, Argonne National Laboratory

**11:15AM Y6.00001 The extreme quantum limit in lightly-doped SrTiO<sub>3</sub>**<sup>1</sup>, ANAND BHATTACHARYA, Materials Science Division and Nanoscience and Technology Division, Argonne National Laboratory, Lemont IL, BRIAN SKINNER, Materials Science Division, Argonne National Laboratory, Lemont IL, GURU KHALSA, CNST, National Institute of Standards and Technology, Gaithersburg MD, ALEXEY SUSLOV, National High Magnetic Field Laboratory, Tallahassee FL — When a three dimensional electron gas is placed in a sufficiently strong magnetic field, it is said to be in the quantum limit when the cyclotron energy  $\hbar\omega_c > \epsilon_F \gg kT$ , and all of the electrons occupy the lowest Landau level. Achieving this limit in a material requires a small Fermi energy relative to the applied magnetic field, and a weak disorder potential such that magnetic freeze-out is avoided. We present an experimental study of lightly-doped single crystals of SrTiO<sub>3</sub>, which remain good bulk conductors in temperatures down to 25 mK and magnetic fields up to 45 T. Our measurements probe deep into the quantum limit, where  $\hbar\omega_c \gg \epsilon_F$  and theory has long predicted that electron-electron interactions can drive the system into a charge density wave or Wigner crystal like state. A number of interesting features arise in electrical transport in this regime, including a striking re-entrant nonlinearity in the current-voltage characteristics. We discuss these features in the context of possible correlated electron states, and present a picture based on magnetic field induced puddling of electrons in a disorder potential landscape.

<sup>1</sup>U.S. DOE, BES contract No. DE-AC02-06CH11357; NIST CNST; US NSF Cooperative Agreement No. DMR-1157490; State of Florida.

**11:27AM Y6.00002 Phonon-induced ultrafast band gap control in LaTiO<sub>3</sub>**<sup>1</sup>, MINGQIANG GU, JAMES M. RONDINELLI, Northwestern University — We propose a route for ultrafast band gap engineering in correlated transition metal oxides by using optically driven phonons. We show that the  $\Gamma$ -point electron band energies can be deterministically tuned in the nonequilibrium state. Taking the Mott insulator LaTiO<sub>3</sub> as an example, we show that such phonon-assisted processes dynamically induce an indirect-to-direct band gap transition or even a metal-to-insulator transition, depending on the electron correlation strength. We explain the origin of the dynamical band structure control and also establish its generality by examining related oxides. Lastly, we describe experimental routes to realize the band structure control with impulsive stimulated Raman scattering.

**11:39AM Y6.00003 Tuning the magnetic ordering in EuTiO<sub>3</sub> through doping**, ZHIGANG GUI, ANDERSON JANOTTI, Univ of Delaware — EuTiO<sub>3</sub> (ETO) is a complex oxide that displays strong spin-lattice coupling, large magnetoelectric effects, and undergoes a series of structural and magnetic phase transitions when subjected to pressure or epitaxial strain. ETO adopts a cubic structure and is paramagnetic at high temperatures, while at very low temperatures it transforms to an antiferrodistortive tetragonal structure with a G-type antiferromagnetic (AFM) ordering. Several approaches have been presented to tune the magnetic ordering from the G-type antiferromagnetism to the F-type ferromagnetism, often relying on external pressure or epitaxial strain. Doping through substitution of trivalent species on the europium sites or creation of oxygen vacancies have also been proposed to lead to ferromagnetism. However, the fundamental mechanism by which excess electrons from impurities or defects lead to ferromagnetic ordering is unclear. In this study, we explore the effects of doping on the magnetic ordering in EuTiO<sub>3</sub> through first-principles calculations. We show how itinerant carriers in the Ti-*d*-derived conduction-band states interact with europium *f* states, inducing an alignment of the large moments on the europium ions. The effects of doping of different types of magnetic ordering are considered, a

**11:51AM Y6.00004 Point defects, impurities, and small hole polarons in  $\text{GdTiO}_3$** , LARS BJAALIE, University of California, Santa Barbara, ANDERSON JANOTTI, University of Delaware, KARTHIK KRISHNASWAMY, CHRIS G. VAN DE WALLE, University of California, Santa Barbara —  $\text{GdTiO}_3(\text{GTO})$  has become the focus of great interest because of its use in complex-oxide heterostructures that display two-dimensional electron gases with unprecedented high densities. GTO is a Mott insulator, with a band gap arising within the partially filled Ti 3d band due to strong electron-electron interactions. GTO often displays hole conductivity, likely attributed to defects or impurities, yet the cause of this unintentional conductivity has not yet been explored. We therefore used density functional theory with a hybrid functional to study their electronic structure. Among native defects, the cation vacancies have the lowest formation energies in oxygen-rich conditions, and oxygen vacancies have the lowest formation energy in oxygen-poor conditions. Among the impurities,  $\text{r}_{\text{Gd}}$ ,  $\text{H}_i$  and  $\text{C}_\text{O}$  have the lowest formation energies. The defects and impurities are intrinsically stable only in a single “natural” charge state, to which various numbers of hole polarons can be bound, which explains the frequent observation of *p*-type hopping conductivity in the rare-earth titanates. These small hole polarons also lead to optical absorption and act as electron traps in devices. Work supported by NSF and by the LEAST Center.

**12:03PM Y6.00005 Low-energy dispersion of dynamic charge stripes in  $\text{La}_{1.75}\text{Sr}_{0.25}\text{NiO}_4$  observed with inelastic neutron scattering**<sup>1</sup>, RUIDAN ZHONG, JOHN TRANQUADA, GENDA GU, Brookhaven Natl Lab, DMITRY REZNIK, University of Colorado, BARRY WINN, Oak Ridge Natl Lab — The dynamic stripe correlations have been the subject of intense research, owing to the possible links with high- $T_c$  superconductivity. In light of a recently published, direct observation of charge-stripe fluctuations in  $\text{La}_{2-x}\text{Sr}_x\text{NiO}_4$  using inelastic neutron scattering<sup>2</sup>, we did a follow-up neutron experiment on a  $x=0.25$  sample to characterize the low-energy dispersion of these dynamic charge stripes using the HYSPEC instrument at the Spallation Neutron Source. The scattering signals are collected in the vicinity of a charge-order peak with a large wave vector (4.4, 3, 0), where dynamic spin-stripe correlations are negligible. Mapping the low-energy charge-stripe fluctuations in a wide temperature range, we observe a finite dispersion along the stripe-modulation direction at  $T \geq 160\text{K}$  where the charge stripes become disordered, while the steep dispersion in the orthogonal direction is not resolved.

<sup>1</sup>Work at BNL supported by Office of Basic Energy Sciences, US DOE, under Contract No. DE-SC00112704.

<sup>2</sup>S. Anissimova, *et al.*, Nat. Commun. 5, 3467 (2014)

**12:15PM Y6.00006 Ultrafast Dynamics of the Symmetry Breaking in Charge-ordered  $\text{La}_{1.75}\text{Sr}_{0.25}\text{NiO}_4$  Single Crystals.**<sup>1</sup>, GIACOMO COSLOVICH, Lawrence Berkeley National Lab, SLAC National Accelerator Lab, ALEXANDER F. KEMPER, Lawrence Berkeley National Lab, North Carolina State University, SASCHA BEHL, BERNHARD HUBER, Lawrence Berkeley National Lab, HANS A. BECHTEL, Advanced Light Source, Lawrence Berkeley National Lab, TAKAO SASAGAWA, Tokyo Institute of Technology, MICHAEL C. MARTIN, Advanced Light Source, Lawrence Berkeley National Lab, ROBERT A. KAINDL, Lawrence Berkeley National Lab — We report equilibrium and ultrafast optical pump-THz probe spectroscopy of the stripe-phase rare-earth nickelate compound  $\text{La}_{1.75}\text{Sr}_{0.25}\text{NiO}_4$ , unveiling the ultrafast dynamics of the crystal symmetry breaking and of local electronic arrangements. At low temperatures the folding of finite momenta vibrations due to symmetry breaking lead to the appearance of new IR-active resonances, particularly around the phonon bending mode frequency ( $\approx 11\text{ THz}$ ). Ultrafast experiments in the multi-THz spectral range show sharp THz reflectivity modulations associated with the phonon zone-folding dynamics, while the background conductivity is reminiscent of the opening of the mid-IR pseudogap. We combine experimental data with DFT calculations of the phonon dispersion to reveal the distinct dynamics of the LO and TO phonon modes at finite momenta. This work provides new insight in the role of polar electron-phonon coupling and symmetry breaking in charge-ordered systems.

<sup>1</sup>This work was supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering

**12:27PM Y6.00007 Single crystal preparation and long-range charge fluctuations in the square-planar nickelate  $\text{La}_4\text{Ni}_3\text{O}_8$ .**<sup>1</sup>, JUNJIE ZHANG, Argonne National Laboratory, YU-SHENG CHEN, Argonne National Laboratory/The University of Chicago, HONG ZHENG, DANIEL PHELAN, JOHN MITCHELL, Argonne National Laboratory — Since the discovery of high- $T_c$  superconductivity in cuprates, intensive effort has been focused on a search for superconductivity in related materials, with particular attention on nickelates. Bulk nickelates containing square-planar coordinated  $\text{Ni}^{2+}$  are of interest because  $\text{Ni}^{1+}$  is isoelectronic with  $\text{Cu}^{2+}$ , the building block of high- $T_c$  cuprates. Here we report the first single crystal synthesis of  $\text{La}_4\text{Ni}_3\text{O}_8$ , a layered nickelate containing square-planar coordinated  $\text{Ni}^{2+}$  with crystallographic and electronic structure related to that of cuprates. Magnetic susceptibility, resistivity, and heat capacity measurements confirm the reported phase transition at  $\sim 105\text{ K}$ [1]. Long-range charge fluctuations with  $q \sim (1/3, 1/3, L)$  was observed for the first time through synchrotron X-ray single crystal diffraction. Our results challenge the current understanding of the origin of the phase transition. Availability of bulk  $\text{La}_4\text{Ni}_3\text{O}_8$  single crystals is also of significant importance for unraveling its ambiguous ground-state magnetic structure, the spin state of the Ni ion, and potential for superconductivity in nickelates involving  $\text{Ni}^{2+}$  in a square-planar coordination. [1] Poltavets, V. V. et al. PRL 2010, 104, 206403.

<sup>1</sup>Work in the Materials Science Division at Argonne National Laboratory was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Division of Materials Science and Engineering.

**12:39PM Y6.00008 Cooperative phonon effects in the metal-insulator transitions of manganite and nickelate perovskites**, RICHARD T. BRIERLEY, Yale University, GIAN G. GUZMAN VERRI, Universidad de Costa Rica and Argonne National Laboratory, PETER B. LITTLEWOOD, Argonne National Laboratory and The University of Chicago — Metal-insulator transitions in manganite and nickelate perovskites depend on the competition between the electron kinetic energy, which favors the metallic phase, and the electron-phonon coupling and Coulomb interaction, which favor localization. The size of the A-site cation controls the relative rotation of the octahedral structural units of the perovskite in the range of  $0 - 15^\circ$ . This is accompanied by changes in the metal-insulator transition temperature from  $0 - 600\text{K}$ . This effect is commonly attributed to modification in the electron bandwidth from changes in orbital overlap. Although previous theoretical studies of these materials include the electron-phonon interaction, they typically do not consider cooperative phonon effects. Using a phenomenological model of the perovskite structure, we show that the long-range anisotropic forces arising from inter-site phonon interactions are modulated by changes in the octahedral rotation. We demonstrate using statistical mechanical calculations that these changes in the strain interaction can capture the variation in transition temperature with tolerance factor observed in both the manganites and nickelates.

**12:51PM Y6.00009 Direct proof of static charge stripe correlations in  $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$** <sup>1</sup>, X M CHEN, V THAMPY, C MAZZOLI, A BARBOUR, G GU, J P HILL, J M TRANQUADA, M P M DEAN, S B WILKINS, Brookhaven National Laboratory — The nature of charge stripe order in the cuprates, and in particular whether the stripes are static or dynamic, is a key issue in understanding the relationship between stripes and superconductivity. In  $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$  (LBCO) a low temperature structural distortion is widely believed to pin stripes into fixed, static domains, but such an assertion has never been directly verified. We performed resonant soft x-ray photon correlation spectroscopy (XPCS) to probe the charge order Bragg peak of 1/8 doped LBCO. At low temperatures, we observe time-independent x-ray speckle patterns persisting for more than three hours, proving the static nature of the stripes and we go on to discuss how stripe order melts with increasing temperature. Our results demonstrate that the combination of XPCS with diffraction limited light sources such as the National Synchrotron Light Source II can probe the dynamics of even subtle order parameters such as stripes in the cuprates.

<sup>1</sup>Work performed at Brookhaven National Laboratory was supported by the US Department of Energy, Division of Materials Science, under Contract No.DE-AC02-98CH10886. Use of the National Synchrotron Light Source II was supported under Contract No DE-SC0012704

**1:03PM Y6.00010 Quasi-static magnetoelectric quadrupoles as the order parameter for the pseudo-gap phase in cuprate superconductors**, MICHAEL FECHNER, MERLIN J. A. FIERZ, FLORIAN THÖLE, Materials Theory, ETH Zurich, Wolfgang-Pauli-Strasse 27, 8093 Zurich, URS STAUB, Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI, NICOLA A. SPALDIN, Materials Theory, ETH Zurich, Wolfgang-Pauli-Strasse 27, 8093 Zurich — A characteristic of ferroic materials is the emergence of a temporally static finite expectation value of an order parameter. Here, we introduce a new mechanism [1] for ferroic order, in which a non-zero quasi-static magnetoelectric quadrupolar order appears due to the coupling of fluctuating spin magnetic dipole moments and polar optical phonons. Using first-principles calculations within the LSDA+*U* method of density functional theory, we calculate the magnitude of the effect for the prototypical cuprate superconductor,  $\text{HgBa}_2\text{CuO}_{4+\delta}$ . We show that our proposed mechanism is consistent, to our knowledge, with many experimental observations for the onset of the pseudo-gap phase and therefore propose the quasi-static magnetoelectric quadrupole as a possible pseudo-gap order parameter. Finally, we show that our mechanism embraces some key aspects of previous theoretical models, in particular the description of the pseudo-gap phase in terms of orbital currents. [1] M. Fechner, M. J. A. Fierz, F. Thöle, U. Staub, and N. A. Spaldin, arXiv 1510.04844, (2015).

**1:15PM Y6.00011 Quantum oscillations in a bilayer with broken mirror symmetry: a minimal model for  $\text{YBa}_2\text{Cu}_3\text{O}_{6+\delta}$** <sup>1</sup>, AKASH MAHARAJ, YI ZHANG, Stanford University, BRAD RAMSHAW, National High Magnetic Field Laboratory, Los Alamos National Laboratory,, STEVEN KIVELSON, Stanford University — Using an exact numerical solution and semiclassical analysis, we investigate quantum oscillations (QOs) in a model of a bilayer system with an anisotropic (elliptical) electron pocket in each plane. Key features of QO experiments in the high temperature superconducting cuprate YBCO can be reproduced by such a model, in particular the pattern of oscillation frequencies (which reflect “magnetic breakdown” between the two pockets) and the polar and azimuthal angular dependence of the oscillation amplitudes. However, the requisite magnetic breakdown is possible only under the assumption that the horizontal mirror plane symmetry is spontaneously broken and that the bilayer tunneling,  $t_{\perp}$ , is substantially renormalized from its ‘bare’ value. Under the assumption that  $t_{\perp} = \tilde{Z}t_{\perp}^{(0)}$ , where  $\tilde{Z}$  is a measure of the quasiparticle weight, this suggests that  $\tilde{Z} \sim 1/20$ . Detailed comparisons with new  $\text{YBa}_2\text{Cu}_3\text{O}_{6.58}$  QO data, taken over a very broad range of magnetic field, confirm specific predictions made by the breakdown scenario.

<sup>1</sup>Supported in part by the US DOE, Office of Basic Energy Sciences under contract DE-AC02-76SF00515 (A.V.M.), the US DOE Office of Basic Energy Sciences “Science at 100 T,” (B.J.R.) and the National Science Foundation Grant No. DMR 1265593 (S.A.K., YZ)

**1:27PM Y6.00012 Controlling Spin Ordering in Rare-Earth Perovskite Vanadates**, NICHOLAS WAGNER, JAMES RONDINELLI, Northwestern University — We investigate the role and influence of local structure distortions on the antiferromagnetic spin ordering temperatures for large *A*-site radii *RVO3* perovskites (*R*=Yb-La) using a combination of data analytics (DA) and density functional theory (DFT). First, mode crystallography is used to parameterize the structural phase space. Next, we identify the important local structural features that correlate strongly with the Néel temperatures ( $T_N$ ) using Pearson correlation coefficients. From this data, we then formulate a regression model using gradient boosted decision trees (GBDT) that returns the relative importance of each feature in predicting  $T_N$ . Our analysis indicates that the amplitude of the subtle Jahn-Teller active mode, which leads to variations in the V-O bond lengths and angles, could be used as an effective structural control parameter to modify the spin ordering temperature. We then validate this data-driven structure-property relationship in artificial vanadate structures using  $T_N$  based on both our GBDT model and a model Hamiltonian using DFT energies. This combined approach allows us to gauge the accuracy of existing physical models for the antiferromagnetic ordering in vanadates and opens possible strategies to design materials with targeted  $T_N$ .

**1:39PM Y6.00013 Giant Magnetocaloric Effect in the Double-perovskite  $\text{Gd}_2\text{NiMnO}_6$** <sup>1</sup>, JAE YOUNG MOON, MI KYUNG KIM, DONG KUN OH, SANG HYUP OH, NARA LEE, YOUNG JAI CHOI, Yonsei Univ — We have synthesized single crystal of  $\text{Gd}_2\text{NiMnO}_6$  (GNMO) by the Bi-flux method and investigated magnetocaloric effect in them by magnetic measurements. Magnetic susceptibility of GNMO increases smoothly as temperature decrease and ferromagnetic order occurs below 135 K, and additional anomaly show at low temperature, indicative of the onset of  $\text{Gd}^{3+}$  spin arrangement. At the temperature, magnetic entropy change,  $-\Delta S_M$ , with the field changes of 0-9 T, calculated from isothermal *M*(*H*) data using Maxwell relation, exhibits sharp peak. This peak is gigantic and cryogenic, these make GNMO promising cryogenic magnetic refrigerant materials.

<sup>1</sup>Giant Magnetocaloric Effect in the Double-perovskite  $\text{Gd}_2\text{NiMnO}_6$

**1:51PM Y6.00014 ABSTRACT WITHDRAWN —**

**Friday, March 18, 2016 11:15AM - 1:51PM —**

**Session Y7 DCMP: Superconductivity: Devices, Vortex Dynamics, and Conductors** 303 - Lei Wang, University of South Carolina

**11:15AM Y7.00001 Silicon superconducting quantum interference device**, ANAS FRANCHETEAU, JEAN-EUDES DUVAUCHELLE, CHRISTOPHE MARCENAT, CEA Grenoble, FRANCESCA CHIODI, DOMINIQUE DBARRE, IEF Orsay, KLAUS HASSELBACH, Institut Néel CNRS Grenoble, J.R. KIRTLEY, Stanford University California, FRANOIS LEFLOCH, CEA Grenoble — We have studied a Superconducting Quantum Interference SQUID device made from a single layer thin film of superconducting silicon. The superconducting layer is obtained by heavily doping a silicon wafer with boron atoms using the Gas Immersion Laser Doping (GILD) technique. The SQUID device is composed of two nano-bridges (Dayem bridges) in a loop and shows magnetic flux modulation at low temperature and low magnetic field. The overall behavior shows very good agreement with numerical simulations based on the Ginzburg-Landau equations.

**11:27AM Y7.00002 Waveguide-integrated NbTiN superconducting nanowire single-photon detector with ultralow jitter**, RISHENG CHENG, XIAOSONG MA, Department of Electrical Engineering, Yale University, PRASANA RAVINDRAN, JOSEPH BARDIN, Department of Electrical and Computer Engineering, University of Massachusetts Amherst, HONG TANG, Department of Electrical Engineering, Yale University — We demonstrate NbTiN superconducting nanowire single-photon detectors (SNSPDs) integrated with Si<sub>3</sub>N<sub>4</sub> waveguides for counting visible and infrared photons. The nanowires with different width (30-90 nm) and length (40-80  $\mu$ m) are patterned into U-shapes on 200nm-thick Si<sub>3</sub>N<sub>4</sub> waveguides, and the photons travelling along the waveguides could be efficiently absorbed by the nanowires via evanescent coupling. With the use of high-speed SiGe cryogenic amplifier, which operates together with the detector chip at the temperature of 1.7K, the jitter of the detection system is measured to be only 19 ps due to the improved signal-to-noise ratio (SNR), compared to 48 ps measured with room-temperature amplifiers. By investigating the background noise level and the pulse shape of the output signal from the detector, we determine the contribution of the noise to the final system jitter is less than 3ps, indicating that our results are very close to the intrinsic jitter of the detector.

**11:39AM Y7.00003 A Superconducting Ion Detection Scheme for Atom Probe Tomography**, JOSEPH SUTTLE, University of Wisconsin–Madison, THOMAS KELLY, Cameca Instruments Inc., ROBERT MCDERMOTT, University of Wisconsin–Madison — Superconducting detectors are a promising avenue for improving the performance of Atom Probe Microscopes. Many types of superconducting detectors have been developed within the past several decades, each with its own strengths and weaknesses. Many of these detectors are inherently slow, bulky, require complex multiplexing schemes to attain position sensitivity, or require complex read-out electronics. In response to the rigorous demands of atom probe technology, and with the goal of developing an elegant, simple to use solution, we have developed a novel superconducting delay line detector. The principal of detection is to use the kinetic energy of incoming ions to generate excess quasiparticles in a superconducting stripline. These quasiparticles generate a measurable signal which propagates along the delay line. By measuring the timing of the output signals from this delay line, we are able to measure the time of flight for the ion and the position of its impact on the detector. We will be presenting on the performance of this detector as measured in a Field Ion Microscope.

**11:51AM Y7.00004 Highly flexible, mechanically robust superconducting wire consisting of NbN-carbon-nanotube nanofibril composites**, JEONG-GYUN KIM, CINAP, IBS, DOES, Sungkyunkwan Univ, HAEYONG KANG, DOES, Sungkyunkwan Univ, JOONGGYU KIM, YOUNG HEE LEE, DONGSEOK SUH, CINAP, IBS, DOES, Sungkyunkwan Univ — A flexible superconducting fiber is prepared by twisting carbon nanotube (CNT) sheets coated with sputter-deposited niobium nitride (NbN) layer to form the shape of yarn. Twisted CNT yarn, which has been extensively studied due to its high flexibility as well as excellent mechanical properties, and NbN, which is a superconducting material with high transition temperature ( $T_c$ ) and critical magnetic field ( $H_c$ ), are combined together by the deposition of NbN layer on free-standing CNT-sheet substrate followed by the biscrolling process. We tried many experimental conditions to investigate the superconducting properties of NbN-CNT yarn as a function of NbN thickness and number of CNT-sheet layers, and found out that the superconducting property of NbN on CNT-sheet can be comparable to that of NbN thin film on the normal solid substrate. In addition, the superconducting property survived even under the condition of severe mechanical deformation such as knotting. These results show the potential application of this technology as a large-scale fabrication method of flexible, mechanically robust, high performance superconducting wire. This work is supported by the Institute for Basic Science (IBS-R011-D1), and by the National Research Foundation (BSR-2013R1A1A1076063) funded by the Ministry of Science, ICT & Future Planning, Republic of Korea.

**12:03PM Y7.00005 Development of semi-rigid cables for low temperature superconducting detectors**, AKIHIRO KUSHINO, Kurume University, SOICHI KASAI, COAX CO., LTD. — We are developing semi-rigid cables for accurate readout of superconducting radiation/particle detectors and other low temperature experiments. The center conductor with a diameter of 0.86 mm is separated with seamless metal outer conductor by dielectric material, polytetrafluoroethylene. We used various metal materials with low thermal conductivity for the electrical conductors such as stainless-steel, cupro-nickel, brass, beryllium-copper, phosphor-bronze, niobium-titanium, and niobium. In addition to the conventional semi-rigid cables, low-pass-filter type cables were manufactured and evaluated to cut the high frequency noise into superconducting detectors. We measured their low thermal conductance and attenuation property up to 10 GHz below the liquid helium temperature.

**12:15PM Y7.00006 Understanding and eliminating the fast creep problem in Fe-based superconductors**, LEONARDO CIVALE, SERENA ELEY, BORIS MAIOROV, Materials Physics and Applications Division, Los Alamos National Laboratory, Los Alamos, USA, MASASHI MIURA, Graduate School of Science & Technology, Seikei University, Tokyo, Japan — One surprising characteristic of Fe-based superconductors is that they exhibit flux creep rates ( $S$ ) as large as, or larger than, those found in oxide high temperature superconductors (HTS). This very fast vortex dynamics appears to be inconsistent with the estimate of the influence of the thermal fluctuations as quantified by the Ginzburg number ( $Gi$ ), which measures the ratio of the thermal energy to the condensation energy in an elemental superconducting volume. In particular, compounds of the  $AFe_2As_2$  family ("122") have  $Gi \sim 10^{-5}$  to  $10^{-4}$ , so  $S$  could be expected to lie between that of low  $T_c$  materials (where typically  $Gi \sim 10^{-8}$ ) and HTS such as  $YBa_2Cu_3O_7$  ( $Gi \sim 10^{-2}$ ), as indeed occurs in other superconductors with intermediate fluctuations, such as  $MgB_2$  ( $Gi \sim 10^{-6}$  to  $10^{-4}$ ). We have found the solution to this puzzle: the fast creep rates in 122 compounds are due to non-optimized pinning landscapes. Initial evidence comes from our previous studies showing that the introduction of additional disorder by irradiation decreases creep significantly in 122 single crystals, although still remaining well above the ideal limit. We now have new evidence from 122 thin films demonstrating that  $S$  can be reduced to the lower limit set by  $Gi$  by appropriate engineering of the pinning landscape.

**12:27PM Y7.00007 Tuning Vortex Creep in Irradiated  $YBa_2Cu_3O_{7-\delta}$  Coated Conductors**, SERENA ELEY, Los Alamos National Laboratory, KAREN KIHLLSTROM, SIGRID HOLLEIS, MAXIME LEROUX, Argonne National Laboratory, MARTIN RUPICH, American Superconductor Corporation, DEAN MILLER, Argonne National Laboratory, ASGHAR KAYANI, Western Michigan University, ULRICH WELP, WAI-KWONG KWOK, Argonne National Laboratory, LEONARDO CIVALE, Los Alamos National Laboratory —  $YBa_2Cu_3O_{7-\delta}$  coated conductors (CCs) show non-monotonic changes in the temperature-dependent creep rate,  $S(T)$ , due to mixed pinning landscapes comprised of twin boundaries, planar defects, point defects, and nanoparticle precipitates. Notably, in low fields, there is a conspicuous dip in  $S$  as  $T$  increases from  $\sim 20$ K to  $\sim 65$ K. The source of this dip is poorly understood. Moreover, pinning landscapes that are favorable for high critical currents,  $J_c$ , are not necessarily optimal for low  $S$ . We have found that, though oxygen irradiation introduces few-nm-sized defects that result in significant increases in  $J_c$ , it is detrimental to creep, increasing  $S$  (reducing the dip depth) for  $T > 20$ K. Understanding the source of this dip is crucial to engineering pinning landscapes that concurrently promote high  $J_c$  and low  $S$ . To this end, we study changes in  $S(T)$  as we tune the ratio of smaller (point to few-nm-sized) defects to larger nanoparticles in an oxygen-irradiated CC by annealing in  $O_2$  at 250C to 600C. We observe a steady decrease in  $S(T > 20$ K) with increasing annealing temperature. This suggests that pre-existing nanoparticle precipitates are likely responsible for the dip in  $S(T)$ , and underlines the fact that the effects of defects are not additive, but rather can be competitive.

**12:39PM Y7.00008 Enhancement of critical current through compound defect with proton irradiation and heavy ion irradiation in YBCO coated conductors and  $\text{FeSe}_x\text{Te}_{1-x}$  crystals<sup>1</sup>**, KAREN KIHLMSTROM, Argonne National Lab and University of Illinois at Chicago, MAXIME LEROUX, Argonne National Lab, SIGRID HOLLEIS, Atominstut TU Wien, DANIELLE HARRIS, Grand Valley State University, ULRICH WELP, HELMUT CLAUS, Argonne National Lab, ASGHAR KAYANI, Western Michigan University, GENDA GU, Brookhaven National Lab, MARTY RUPCH, SRIVATSAN SATHYAMURTHY, STEVEN FLESHLER, American Superconductor Corp, FRANCESCO LAVIANO, LAURA GOZZELINO, ROBERTO GERBALDO, GIANLUCA GHIGO, Politecnico di Torino, WAI-KWONG KWOK, Argonne National Lab — We investigate the enhancement of vortex pinning by both point and columnar defects and compare the results in 2G YBCO coated conductors (CC), with  $T_c$  90K, and in  $\text{FeSe}_x\text{Te}_{1-x}$  single crystals with  $T_c$  14K. Both samples were irradiated with 250 MeV Au ions to a dose-matching field of 1T. The samples were then irradiated with 4 MeV protons to a dose of  $4 \times 10^{16}$  p/cm<sup>2</sup> and  $8 \times 10^{16}$  p/cm<sup>2</sup> in the CC and single crystal, respectively. The major effect of compound particle irradiation in both samples resulted in a synergetic enhancement of the critical current across a wide field range, beyond the enhancement from either individual irradiation type.

<sup>1</sup>This work supported by the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the U.S. D.O.E., Office of Science, Office of Basic Energy Sciences. The work in Italy was supported by the INFN-TERASPARC project.

**12:51PM Y7.00009 Critical Current by Design Through Large-scale Simulations<sup>1</sup>**, ANDREAS GLATZ, ALEX KOSHELEV, IVAN SADOVSKYY, GEORGE CRABTREE, Argonne National Laboratory — Understanding the dynamic behavior of vortex matter in complicated pinning landscapes is a major challenge for both fundamental science and energy applications. In particular, optimizing type, size and density of pinning centers can significantly enhance the critical current. Based on the time-dependent Ginzburg-Landau equation, we developed a numerical approach towards finding these optimal pinning configurations. I will give an overview of this new paradigm, called Critical Current by Design.

*References:*

[1] I. A. Sadovskyy, A. E. Koshelev, C. L. Phillips, D. A. Karpeev, A. Glatz, J. of Comp. Phys. **294**, 639 (2015).

[2] A. E. Koshelev, I. A. Sadovskyy, C. L. Phillips, A. Glatz, arXiv:1509.04212 (2015).

[3] Ivan A. Sadovskyy, Ying Jia, Maxime Leroux, Jihwan Kwon, Hefei Hu, Lei Fang, Carlos Chaparro, Shaofei Zhu, Ulrich Welp, Jianmin Zuo, Venkat Selvamannickam, George W. Crabtree, Alexei E. Koshelev, Andreas Glatz, and Wai-Kwong Kwok, arXiv:1509.06446 (2015).

<sup>1</sup>Work was supported by the Scientific Discovery through Advanced Computing (SciDAC) program funded by U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Sciences.

**1:03PM Y7.00010 Simulation of the vortex dynamics in a real pinning landscape of  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  coated conductors<sup>1</sup>**, IVAN SADOVSKYY, ALEXEI KOSHELEV, ANDREAS GLATZ, Argonne Natl Lab, VOLKAN ORTALAN, Purdue University, MARTIN RUPICH, American Superconductor, MAXIME LEROUX, Argonne Natl Lab — We present a critical current analysis of a real high-temperature superconducting (HTS) sample in a magnetic field by combining state-of-the-art large-scale Ginzburg-Landau simulations with reconstructive three-dimensional scanning transmission electron microscopy tomography of the pinning landscape in Dy-doped  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ . This methodology provides a unique look at the vortex dynamics in the presence of a complex pinning landscape, responsible for the high current-carrying capacity characteristic of commercial HTS wires. Our method demonstrates very good functional and quantitative agreement of the critical current between simulation and experiment, providing a new predictive tool for HTS wires design.

<sup>1</sup>Work was supported by the Scientific Discovery through Advanced Computing (SciDAC) program funded by U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Sciences.

**1:15PM Y7.00011 Rapid Doubling of the Critical Current of  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  Coated Conductors.**, U. WELP, M. LEROUX, K. J. KIHLMSTROM, Argonne National Laboratory, S. HOLLEIS, Technische Universitaet Wien, Austria, M. W. RUPICH, S. SATHYAMURTHY, S. FLESHLER, American Superconductor Corp., H. P. SHENG, D. J. MILLER, Argonne National Laboratory, S. ELEY, L. CIVALE, Los Alamos National Laboratory, P. M. NIRLAULA, A. KAYANI, Western Michigan University, W. K. KWOK, Argonne National Laboratory — We demonstrate the doubling of the critical current density of production-line REBCO coated conductors (CCs) in fields of 6 T ||c at 27 K by irradiation with a 3.5-MeV oxygen ion beam. This doubling of  $J_c$  is achieved within one second or less opening an industrially viable approach to address a persisting challenge, namely the greatly reduced performance of CCs in even modest applied magnetic fields. TEM images reveal that the enhanced critical current is due to finely dispersed small clusters approximately 5 nm in diameter. The major effect of the irradiation-induced defects is the reduction of the field-dependence of  $J_c$ , which we attribute to the mixed pinning landscape composed of strong pre-existing pin sites and the finely dispersed irradiation-induced defects. Work supported by the Center for Emergent Superconductivity, an EFRC funded by the U.S. Department of Energy, Office of Basic Energy Sciences. Patterning and microstructural characterization were performed at the Center for Nanoscale Materials, an Office of Science user facility, supported by the Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

**1:27PM Y7.00012 Numerical optimization methods for critical currents in superconductors<sup>1</sup>**, GREGORY KIMMEL, IVAN SADOVSKYY, ALEX KOSHELEV, ANDREAS GLATZ, Argonne National Laboratory — In this work, I present optimization methods for maximizing the critical current in high-temperature superconductors for energy applications. The critical current in the presence of an external magnetic field is mostly defined by the pinning landscape (pinscape) within the superconductor, which prevents magnetic vortices from moving and, therefore, increases its critical current. Our approach is to generate different pinscapes and obtain the resulting critical current by large-scale time-dependent Ginzburg-Landau equations [J. Comp. Phys. **294**, 639 (2015)]. Pinning centers could be any combination of defects, including spherical and columnar defects. The parameters controlling the pinscape are adaptively adjusted in order to find the optimal parameter set, which maximizes the critical current. Here, we compare different optimization methods and discuss their performance.

<sup>1</sup> Work was supported by the Scientific Discovery through Advanced Computing (SciDAC) program funded by U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Sciences.

**1:39PM Y7.00013 Probing Topological Matter with Sound<sup>1</sup>**, DAVID SCHMELTZER, City College of New York — We introduce a microscopic formulation to identify the stress in a quantum fluid to compute the stress viscosity with sound waves. The viscosity stress tensor is used to determine, e.g. the ultrasound attenuation in superconductors. When an Abrikosov lattice is formed on the surface of a Topological Insulator in a external magnetic field, Majorana modes form dispersive bands. We show that the ultrasound attenuation is modified by the Majorana modes offering a novel method to identify Topological Superconductors. Moreover we compute the stress tunneling which uses Majorana modes and represent the sound analogue of the Andreev crossed reflection. We check the violation of the sound momentum conservation of systems which only exists on the boundary of a higher dimensional system, e.g. a 1D chiral fermion which can exist at the boundary of a 2D Quantum Hall system.

<sup>1</sup>Doe-Los Alamos National Laboratory

**Friday, March 18, 2016 11:15AM - 2:15PM –**

**Session Y11 DCMP DMP: Tunneling in Superconductors: Spectroscopy, Andreev Reflection, and Nanowires** 307 - Igor Fridman, Quasar, Inc.

**11:15AM Y11.00001 Pulsed tunneling spectroscopy of strongly correlated phases in 2D electronic systems** , JOONHO JANG, BENJAMIN HUNT, Massachusetts Institute of Technology, LOREN PFEIFFER, KENNETH WEST, Princeton University, RAYMOND ASHOORI, Massachusetts Institute of Technology — We used the pulsed tunneling spectroscopy to reveal the well-defined magnophonon modes of the magnetic-field-induced Wigner crystalline phase in a GaAs 2D QW. The strong evidence of the distinctive characteristics of the phonon mode such as the power laws and mass-independence is demonstrated. In the later part of the talk, I will also present the newly-developed momentum resolved tunneling spectroscopy, which utilizes the in-plane magnetic fields to tune the momentum of tunneling electrons. Using this technique, we successfully measured the energy-momentum dispersion curve of electrons embed in a 2D heterostructure.

**11:27AM Y11.00002 Fingerprints of the superconducting pairing glue via inelastic tunneling spectroscopy** , PATRIK HLOBIL, JRG SCHMALIAN, JASMIN JANDKE, WULF WULFHEKEL, Karlsruhe Institute of Technology — In the past, tunneling spectroscopy has been interpreted as a direct probe of the fermionic density of states in superconductors. However, in this talk we discuss the impact of inelastic tunneling on tunnel spectra and show that depending on the actual system these interpretations have to be revisited. We show how such inelastic tunneling processes can occur in bulk systems and how they affect the analysis of the experimental data. Considering the spin-gap for spin excitations in the high- $T_c$  superconductors we can trace back the peak-dip-hump features observed in many unconventional superconductors to the shift of the spin spectral weight to higher energies below the critical temperature  $T_c$ .

**11:39AM Y11.00003 Planar junction tunneling study of single-crystal eutectic phases of  $\text{Sr}_2\text{RuO}_4/\text{Sr}_3\text{Ru}_2\text{O}_7$**  , XINXIN CAI, BRIAN ZAKRZEWSKI, Pennsylvania State University, H. WANG, Zhejiang University, C. ANDREOU, Pennsylvania State University, D. SCHLOM, Cornell University, Z.-Q. MAO, Tulane University, R. J. CAVA, Princeton University, YING LIU, Pennsylvania State University, Shanghai Jiao Tong University — Despite of intensive study of many years, the precise value of the superconducting energy gap of the odd-parity superconductor  $\text{Sr}_2\text{RuO}_4$  has not been fully settled. Many complications exist. The band dependence of superconductivity makes the results from a bulk measurement of the gap difficult to interpret quantitatively. Surface based measurements such as scanning tunneling spectroscopy have to deal with the suppression of the superconducting energy gap on the cleaved *ab* surface due to surface reconstruction. We performed quasi-particle tunneling measurements of the superconducting energy gap in planar junctions prepared on naturally cleaved edges of a  $\text{Sr}_2\text{RuO}_4$  crystal found in the eutectic phase of  $\text{Sr}_2\text{RuO}_4/\text{Sr}_3\text{Ru}_2\text{O}_7$ . Cleaving of such eutectic crystals exposes thin  $\text{Sr}_2\text{RuO}_4$  plates inserted in a  $\text{Sr}_3\text{Ru}_2\text{O}_7$  bulk crystal with the *c* axis along that of the  $\text{Sr}_3\text{Ru}_2\text{O}_7$  bulk, as shown by X-ray diffraction data. Results obtained on  $\text{Au-Sr}_2\text{RuO}_4/\text{Sr}_3\text{Ru}_2\text{O}_7$  tunnel junctions suggest that superconductivity survives on the surface of the plates, showing a gap value of 0.2 meV, close to the BCS value for weak-coupling superconductors. Experiments on tunnel junctions made on cleaved crystals of a mesoscopic size are underway.

**11:51AM Y11.00004 Tunneling in Al/ $\text{Al}_2\text{O}_3$ /Al junctions and its direct link with energy gap and tunneling time across the barrier.** , EDGAR PATINO , NEELIMA KELKAR, Universidad de los Andes — Quantum tunneling has been widely used in order to investigate the density of states of the materials across the barrier and magnetoresistance in magnetic tunnel junctions (MTJs). In spite of the possible applications there is no clear understanding of the barrier parameters as a function of temperature. Measurements of current-voltage (*I-V*) characteristics of a high quality Al/ $\text{Al}_2\text{O}_3$ /Al junction at temperatures ranging from 3.5 K to 300 K have been used to extract the barrier properties. Fitting results using Simmons model led to a constant value of barrier width  $s \sim 20.8$  Å and a continuous increase in the barrier height with decreasing temperature. The latter is used to determine the energy band gap temperature dependence and average phonon frequency  $\omega = 2.05 \times 10^{13} \text{ sec}^{-1}$  in  $\text{Al}_2\text{O}_3$ . Finally from the experimentally extracted barrier height and width parameters we calculate the tunneling time for a solid state tunnel junction. The order of magnitude of this time corresponds to the one obtained in sophisticated experiments. The barrier parameters are used to extract the temperature dependent dwell times in tunneling ( $\tau_D = 3.6 \times 10^{-16} \text{ sec}$  at mid-barrier energies) and locate resonances above the barrier.

**12:03PM Y11.00005 Low temperature tunneling transport in van der Waals contacted superconductor/semiconductor Schottky barriers<sup>1</sup>** , ANG LI, ARTHUR HEBARD, University of Florida — We present a comparative study over a large temperature range (2.5-300K) of Schottky barriers formed either by evaporation of normal metals (Au, Al) or by van der Waals contact of mechanically exfoliated under-doped high- $T_c$  Bi-2212 flakes onto moderately doped n-type GaAs and p-type Si semiconductor substrates. Our modified barrier-inhomogeneity model applied to the thermionic emission equation [1] gives a good description of the temperature evolution of barrier parameters, such as the zero-bias Schottky barrier height  $\Phi_{SB}^0(T)$ , the ideality factor  $\eta(T)$  and the flat band barrier height, as the temperature is lowered from high temperatures where thermionic emission dominates to lower temperatures where thermal field emission and field emission (direct tunneling) dominate. At low temperatures for all barriers studied, both  $\Phi_{SB}^0(T)$  and  $\eta^{-1}(T)$  are linear in temperature with zero intercepts. Direct tunneling is verified in the Bi-2212/n-GaAs barriers by the appearance of superconducting density of states curves along with an energy gap  $2\Delta = 65 \text{ meV}$  in good agreement with ARPES and scanning tunneling microscope results by other investigators.

[1] Jurgen H Werner and Herbert H Guttler, Journal of Applied Physics 69, 1522 (1991).

<sup>1</sup>Work supported by NSF DMR #1305783

**12:15PM Y11.00006 Current-phase relations in epitaxial Al/InAs nanowire Josephson junctions** , ERIC SPANTON, Stanford Institute for Materials and Energy Sciences, MINGTANG DENG, PETER KROGSTROP, THOMAS JESPERSEN, JESPER NYGRD, CHARLES MARCUS, University of Copenhagen, KATHRYN MOLTER, Stanford Institute for Materials and Energy Sciences — Current-phase relations (CPRs) are a fundamental property of Josephson junctions, and in superconductor-normal-superconductor (SNS) junctions they can deviate from sinusoidal behavior at low temperatures. For short junctions, the shape and amplitude of the CPR is directly related to the properties of the Andreev bound states in the junction. Understanding the proximity effect, which is mediated by Andreev reflections, is particularly important in high spin-orbit and topological materials, where proximity-induced topological superconductivity is highly sought after. We used scanning superconducting quantum interference device microscopy to measure the CPR in many epitaxial Al/InAs nanowire junctions. We found CPRs that were very forward-skewed at low temperatures, indicating highly transmitting junctions. We will discuss the temperature, low magnetic field, and gate dependence of the CPRs, and the applicability of the short-junction theory to our junctions.

**12:27PM Y11.00007 Enhanced crossed Andreev reflection in a superconducting ladder<sup>1</sup>**, ABHIRAM SOORI, International Centre for Theoretical Sciences, TIFR, Bengaluru, SUBROTO MUKERJEE, Indian Institute of Science, Bangalore — Andreev reflection is a process that happens at the junction of a normal metal (NM) and a superconductor(SC), where the Cooper-pair current in the superconductor gets equal contributions from the electron and hole channels of the normal metal. Crossed Andreev reflection (cAr) is a related process that happens in a system of two NM's independently connected to a SC when the current in the electron channel of the first NM and the current in the hole channel of the second NM together contribute to the Cooper-pair current in the SC. A typical experimental set-up to investigate cAr consists of two ferromagnetic metal leads connected to an s-wave superconductor. We propose an alternative mesoscopic set-up that enhances cAr which contains no ferromagnetic parts. Instead, our set-up consists of two NM's coupled to a superconducting ladder. We calculate the currents in the different channels and demonstrate enhanced cAr.

<sup>1</sup>AS thanks ICTS-TIFR, Bengaluru for the financial support.

**12:39PM Y11.00008 Spin polarization measurements of ferromagnetic atomic chains on a superconductor: Part I<sup>1</sup>**, YONGLONG XIE, SANGJUN JEON, ILYA DROZDOV, JIAN LI, ANDREI BERNEVIG, ALI YAZDANI, Princeton Univ — Introduction of magnetic defects in superconductors gives rise to spin polarized in-gap Shiba states. Recently chains of magnetic atoms, which give rise to a band of Shiba states, have been proposed as a platform for topological superconductivity. Spectroscopic evidence for in-gap Shiba states and Majorana end mode has been reported in previous studies of self-assembled chains of ferromagnetic Fe atoms on the surface of Pb[1]. In this talk, we introduce the technique of spin-polarized scanning tunneling microscopy and spectroscopy (SP-STM) and discuss how we prepare tips that can show spin contrast at zero magnetic field, without disrupting superconductivity on the Pb surface. We use this technique, combined with the use of a vector magnet to orient the tip magnetization to probe the spin polarization of the Shiba states induced by the Fe atomic chains onto the Pb surface. A key to interpreting such experiments with spin-polarized STM tip is to understand the role of spin-polarization in the setpoint effect, which will be discussed in the next talk. [1] S. Nadj-Perge, I.K. Drozdov, J. Li, H. Chen, S. Jeon, J. Seo, A.H. MacDonald, B.A. Bernevig, A. Yazdani, Science **346**,602 (2014)

<sup>1</sup>Work supported by ONR and Moore Foundation

**12:51PM Y11.00009 Spin Polarization Measurements of Ferromagnetic Atomic Chains on a Superconductor: Part II<sup>1</sup>**, SANGJUN JEON, YONGLONG XIE, ILYA K. DROZDOV, JIAN LI, B. ANDREI BERNEVIG, ALI YAZDANI, Princeton University — A key property of the Majorana fermions edge mode when realized at the edge of a topological superconductor is their spin. Unlike other low energy excitation in a conventional superconductor, which are made up of time-reverse partners of up and down spin, Majorana is expected to have a definite spin orientation. We utilize the technique of spin-polarized STM as described in the last talk to probe the nature of Majorana excitations in chains of Fe atoms on the surface of Pb. Previous effort on this system has detected signature of Majorana as a zero bias peak at end of such chains [1]. While this previous study shows evidence of ferromagnetism and spin-orbit coupling in such atomic chains on Pb, they did not probe the spin properties of the end mode specifically. We describe energy-resolved spin-polarized STM experiments designed to probe whether the previously reported zero energy end modes are spin-polarized or not. [1] Stevan Nadj-Perge, Ilya K. Drozdov, Jian Li, Hua Chen, Sangjun Jeon, Jungpil Seo, Allan H. MacDonald, B. Andrei Bernevig and Ali Yazdani, Science, 346, 602 (2014)

<sup>1</sup>Work supported by ONR and the Moore Foundation.

**1:03PM Y11.00010 Conductance and shot noise in ferromagnet-superconductor epitaxial tunnel junctions**, FARKHAD ALIEV, ISIDORO MARTINEZ, JUAN PEDRO CASCALES, Universidad Autonoma de Madrid, Spain, CORIOLAN TIUSAN, Technical University of Cluj-Napoca, Romania, MICHEL HEHN, Universit de Lorraine, Nancy, France — Recently ferromagnet/superconductor hybrids have attracted attention due to the possibility of inducing p-wave superconductivity and of creating novel superconducting-spintronic devices. Most of these devices have a lateral configuration and are non-epitaxial, so they could not provide coherent electron tunneling over the interfaces. Here we investigate the conductance and shot noise in fully epitaxial Fe/MgO/V/MgO/Fe, Fe/MgO/Fe/MgO/V and Fe/MgO/V tunnel junctions with 40 nm thick Vanadium and 2nm thick MgO as a function of the applied bias, temperature (down to 0.3K) and magnetic state. All junctions show presence of finite subgap conductance indicating coherent two-electron transport over the barrier. Moreover, we observe conductance anomalies above the gap suppressed at temperature exceeding critical temperature, which may imply quasiparticle interference effects. High crystalline quality of the MgO barriers is confirmed by the fact that the above gap shot noise is Poissonian (direct tunneling with single barrier) or sub-Poissonian (sequential tunneling over two barriers) and is magnetic state dependent in the last case. The subgap Fano factor shows strong increase supporting multiple Andreev reflections as a possible source of excess subgap conductance.

**1:15PM Y11.00011 Supercurrents and Andreev bound states in a superconducting/strained/superconducting silicene junction**, HAI LI, Univ of Houston, CHIN-SEN TING, Department of Physics and Texas Center for Superconductivity, University of Houston, Houston, Texas 77004, USA — Based on the Dirac-Bogoliubov-de Gennes equation, we investigated strain effects on the supercurrent and Andreev bound states (ABSs) in a superconducting/strained/superconducting silicene junction. Owing to the novel buckled structure of silicene, the supercurrent and ABS configurations can be effectively controlled by a perpendicular electric field. It was found that the supercurrent strongly depends on the direction of the strain, and the supercurrent exhibits a on/off effect under certain strains. It was demonstrated that the spin-valley symmetry of silicene can induce a spin-valley polarized supercurrent, even though the strength of the supercurrent is strongly modulated by the strain. These findings would potentially provide some intriguing insights into the correlation transport in strained silicene-based superconducting hybrid structures.

**1:27PM Y11.00012 Over-bias Light Emission due to Higher Order Quantum Noise of a Tunnel Junction**, WOLFGANG BELZIG, University of Konstanz, FEI XU, University of Konstanz, Konstanz, Germany, CECILIA HOLMQVIST, Norwegian University of Science and Technology, Trondheim, Norway — Understanding tunneling from an atomically sharp tip to a metallic surface requires to account for interactions on a nanoscopic scale. Inelastic tunneling of electrons generates emission of photons, whose energies intuitively should be limited by the applied bias voltage. However, experiments [Phys. Rev. Lett. 102, 057401 (2009)] indicate that more complex processes involving the interaction of electrons with plasmon polaritons lead to photon emission characterized by over-bias energies. We propose a model of this observation in analogy to the dynamical Coulomb blockade, originally developed for treating the electronic environment in mesoscopic circuits. We explain the experimental finding quantitatively by the correlated tunneling of two electrons interacting with an LRC circuit modeling the local plasmon-polariton mode. To explain the over-bias emission, the non-Gaussian statistics of the tunneling dynamics of the electrons is essential. Reference: F. Xu, C. Holmqvist, and W. Belzig Phys. Rev. Lett. 113, 066801 (2014)

### 1:39PM Y11.00013 Enhanced superconductivity at the interface of W/Sr<sub>2</sub>RuO<sub>4</sub> point contact<sup>1</sup>

JIAN WEI, HE WANG, WEIJIAN LOU, JIAWEI LUO, Peking Univ, YING LIU, Pennsylvania State University, J.E. ORTMANN, Z.Q. MAO, Tulane University — Differential resistance measurements are conducted for point contacts (PCs) between the Sr<sub>2</sub>RuO<sub>4</sub> (SRO) single crystal and the tungsten tip. Since the tungsten tip is hard enough to penetrate through the surface layer, consistent superconducting features are observed. Firstly, with the tip pushed towards the crystal, the zero bias conductance peak (ZBCP) due to Andreev reflection at the normal-superconducting interface increases from 3% to more than 20%, much larger than previously reported, and extends to temperature higher than the bulk transition temperature. Reproducible ZBCP within 0.2 mV may also help determine the gap value of SRO, on which no consensus has been reached. Secondly, the logarithmic background can be fitted with the Altshuler-Aronov theory of electron-electron interaction for tunneling into quasi two dimensional electron system. Feasibility of such fitting confirms that spectroscopic information like density of states is probed, and electronic temperature retrieved from such fitting can be important to analyse the PC spectra. Third, at bias much higher than 0.2 mV there are conductance dips due to the critical current effect and these dips persist up to 6.2 K. For more details see Phys. Rev. B 91, 184514 (2015).

<sup>1</sup>National Basic Research Program of China (973 Program) through Grant No. 2011CBA00106 and No. 2012CB927400.

### 1:51PM Y11.00014 Point contact spectroscopy on materials with high spin-orbit coupling

GOUTAM SHEET, Indian Institute of Science Education and Research — We will discuss the results of our point-contact spectroscopy experiments on a number of systems with high spin-orbit coupling, including topological insulators and Dirac semimetals. Such materials sometimes give rise to exotic phases of matter like unconventional superconductivity under normal metallic point contacts. On the other hand, the special spin properties of the surface of such materials can be probed using point contacts with superconducting tips. The role of special symmetry-protected properties of the surface states of such systems on Andreev reflection can also be probed. We will also discuss that point contact spectroscopy can be used as an extremely powerful tool for investigating topological systems.

### 2:03PM Y11.00015 Fabrication and measurement of multi-terminal mesoscopic Josephson junctions.<sup>1</sup>

NATALYA SOLOVYEVA, Univ of Maryland-College Park, MISHIMA TETSUYA, MICHAEL SANTOS, Homer L. Dodge Department of Physics and Astronomy, University of Oklahoma, 440 West Brooks, Norman, Oklahoma 73019-3151, JAVAD SHABANI, Physics Department, City College of New York, New York, 10031, VLADIMIR MANUCHARYAN, Univ of Maryland-College Park — We present fabrication and characterization of 3- and 4-terminal mesoscopic Josephson junctions involving InAs quantum well heterostructures [1] and superconducting Al contacts. A cross-shaped nanowire junction region with dimensions of order a few 100 nm is dry-etched in the 2DEG, followed by deposition of superconducting contacts and gating electrodes. These novel 0D devices have been recently predicted to have topological features in their Andreev spectra and finite-bias transport [2]; they may also be useful in efforts towards observation and braiding of Majorana fermions in the solid state [3]. // References: [1] J. Shabani et al. arXiv:1408.1122; [2] R-P Riwar et al. arXiv:1503.06862; B. van Heck et al. Phys. Rev. B 90, 155450 (2014); [3] S. Plissard et al. Nature Nanotechnology 8, 859 (2013)

<sup>1</sup>This material is based upon work supported by the NSF under Grant No. DMR-1207537

## Friday, March 18, 2016 11:15AM - 2:15PM —

### Session Y12 GSNP: Inference in Complex Networks 308 - Adilson Motter, Northwestern University

#### 11:15AM Y12.00001 Physics of Inference<sup>1</sup>, ZOLTAN TOROCZKAI<sup>2</sup>, Department of Physics, University of Notre Dame, USA

— Jaynes maximum entropy method provides a family of principled models that allow the prediction of a systems properties as constrained by empirical data (observables). However, their use is often hindered by the degeneracy problem characterized by spontaneous symmetry breaking, where predictions fail. Here we show that degeneracy appears when the corresponding density of states function is not log-concave, which is typically the consequence of nonlinear relationships between the constraining observables. We illustrate this phenomenon on several examples, including from complex networks, combinatorics and classical spin systems (e.g., Blume-Emery-Griffiths lattice-spin models). Exploiting these nonlinear relationships we then propose a solution to the degeneracy problem for a large class of systems via transformations that render the density of states function log-concave. The effectiveness of the method is demonstrated on real-world network data. Finally, we discuss the implications of these findings on the relationship between the geometrical properties of the density of states function and phase transitions in spin systems.

<sup>1</sup>Supported in part by grant No. FA9550-12-1-0405 from AFOSR/DARPA and by grant No. HDTRA 1-09-1-0039 from DTRA.

<sup>2</sup>Co-author: Szabolcs Horvat, Department of Physics, University of Notre Dame, USA and INSERM U846, Bron, France.

#### 11:51AM Y12.00002 Nonparametric inference of network structure and dynamics, TIAGO P.

PEIXOTO, University of Bremen — The network structure of complex systems determine their function and serve as evidence for the evolutionary mechanisms that lie behind them. Despite considerable effort in recent years, it remains an open challenge to formulate general descriptions of the large-scale structure of network systems, and how to reliably extract such information from data. Although many approaches have been proposed, few methods attempt to gauge the statistical significance of the uncovered structures, and hence the majority cannot reliably separate actual structure from stochastic fluctuations. Due to the sheer size and high-dimensionality of many networks, this represents a major limitation that prevents meaningful interpretations of the results obtained with such nonstatistical methods. In this talk, I will show how these issues can be tackled in a principled and efficient fashion by formulating appropriate generative models of network structure that can have their parameters inferred from data. By employing a Bayesian description of such models, the inference can be performed in a nonparametric fashion, that does not require any *a priori* knowledge or *ad hoc* assumptions about the data. I will show how this approach can be used to perform model comparison, and how hierarchical models yield the most appropriate trade-off between model complexity and quality of fit based on the statistical evidence present in the data. I will also show how this general approach can be elegantly extended to networks with edge attributes, that are embedded in latent spaces, and that change in time. The latter is obtained via a fully dynamic generative network model, based on arbitrary-order Markov chains, that can also be inferred in a nonparametric fashion. Throughout the talk I will illustrate the application of the methods with many empirical networks such as the internet at the autonomous systems level, the global airport network, the network of actors and films, social networks, citations among websites, voting correlations among politicians, co-occurrence of disease-causing genes and others.

#### 12:27PM Y12.00003 Identification of dynamical models of chemical reaction networks<sup>1</sup>, ALEK-

SANDAR HABER, Northwestern University — Current first-principles models of complex chemistry, such as combustion reaction networks, often give inaccurate predictions of the time variation of chemical species. Moreover, the high complexity and dimensionality of these models render them impractical for real-time prediction and control of chemical network processes. These limitations have motivated us to search for an alternative paradigm that is able to both identify the correct model from the observed dynamical data and reduce complexity while preserving the underlying network structure. In this talk, I will present one such modeling paradigm under the scenarios of complete and incomplete observability of the dynamics. The proposed approach is applicable to combustion chemistry and a range of other chemical reaction networks.

<sup>1</sup>Research supported by ARO grant W911NF-14-1-0359.

**1:03PM Y12.00004 Infering Networks From Collective Dynamics<sup>1</sup>** , MARC TIMME, Network Dynamics, Max Planck Society — How can we infer direct physical interactions between pairs of units from only knowing the units' time series? Here we present a dynamical systems' view on collective network dynamics, and propose the concept of a *dynamics' space* to reveal interaction networks from time series. We present two examples: one, where the time series stem from standard ordinary differential equations, and a second, more abstract, where the time series exhibits only partial information about the units' states. We apply the latter to neural circuit dynamics where the observables are spike timing data, i.e. only a discrete, state-dependent outputs of the neurons. These results may help revealing network structure for systems where direct access to dynamics is simpler than to connectivity, cf. [1,2,3].

This is work with Jose Casadiego, Srinivas Gorur Shandilya, Mor Nitzan, Hauke Haehne and Dimitra Maoutsa.

[1] M. Timme, Phys. Rev. Lett. 98:224101 (2007). <http://dx.doi.org/10.1103/PhysRevLett.98.224101>

[2] S.G. Shandilya & M. Timme, New J. Phys. 13, 013004 (2011). <http://dx.doi.org/10.1088/1367-2630/13/1/013004>

[3] M. Timme & J. Casadiego, Phys. Rev. A 47:343001 (2014) - Invited Review. <http://dx.doi.org/10.1088/1751-8113/47/34/343001>

<sup>1</sup>Supported by grants of the BMBF (Future Compliant Power Grids - CoNDyNet) and by the Max Planck Society to MT.

**1:39PM Y12.00005 Clustering means geometry in networks** , DMITRI KRIOUKOV, Northeastern University — Using maximum-likelihood estimation techniques, any real network data can be fit to essentially any network model, inferring the most likely values of the model parameters for the network. However there is one caveat. The results of such fitting are not spurious but meaningful and predictive, only if the network is a typical network in the unbiased ensemble of random graphs with the inferred values of model parameters. Therefore, given a particular combination of a real network and a model, the first question one has to answer is what structural properties of the network ensure that this network is a typical element in the ensemble of random graphs defined by the model. This question is usually highly intractable, explaining why it is almost never answered before the fitting/inference task is performed. Inspired by recent observations that random geometric graphs reproduce many structural and dynamical properties of a variety of real networks, we find the network structural properties that guarantee that networks that have these properties are in fact geometric, meaning that latent space network models are their true models. Specifically we prove that peculiar organization of clustering observed in real networks is one of the main such properties. In other words, maximum-entropy random graphs with specific clustering properties, which are quite different from the clustering properties of random graphs in the Strauss model, are actually soft random geometric graphs with a specific form of the connection probability function. Using this function we can then infer the coordinates of nodes in a latent space for any given network, and reliably check if the network is a typical network in the resulting ensemble of soft random geometric graphs. If it is, then the inferred coordinates are meaningful and real, and can be used for prediction tasks with proved guarantees that the results of such predictions are reliable and not just transient artifacts.

## Friday, March 18, 2016 11:15AM - 2:15PM –

Session Y13 DBIO: Beyond Darwin: Evolution in Single Cells 309 - Robert Austin, Princeton University

**11:15AM Y13.00001 Mutation Hotspots in Single Cells** , SUSAN ROSENBERG, Baylor College of Medicine — No abstract available.

**11:51AM Y13.00002 Unraveling the genetic driving forces enabling antibiotic resistance at the single cell level.** , JULIA BOS, Princeton University — Bacteria are champions at finding ways to quickly respond and adapt to environments like the human gut, known as the epicentre of antibiotic resistance. How do they do it? Combining molecular biology tools to microfluidic and fluorescence microscopy technologies, we monitor the behavior of bacteria at the single cell level in the presence of non-toxic doses of antibiotics. By tracking the chromosome dynamics of *Escherichia coli* cells upon antibiotic treatment, we examine the changes in the number, localization and content of the chromosome copies within one cell compartment or between adjacent cells. I will discuss how our work pictures the bacterial genomic plasticity as a driving force in evolution and how it provides access to the mechanisms controlling the subtle balance between genetic diversity and stability in the development of antibiotic resistance.

**12:27PM Y13.00003 Collective Functionality through Bacterial Individuality** , MARTIN ACKERMANN, ETH Zurich and Eawag — According to the conventional view, the properties of an organism are a product of nature and nurture - of its genes and the environment it lives in. Recent experiments with unicellular organisms have challenged this view: several molecular mechanisms generate phenotypic variation independently of environmental signals, leading to variation in clonal groups. My presentation will focus on the causes and consequences of this microbial individuality. Using examples from bacterial genetic model systems, I will first discuss different molecular and cellular mechanisms that give rise to bacterial individuality. Then, I will discuss the consequences of individuality, and focus on how phenotypic variation in clonal populations of bacteria can promote interactions between individuals, lead to the division of labor, and allow clonal groups of bacteria to cope with environmental uncertainty. Variation between individuals thus provides clonal groups with collective functionality.

**1:03PM Y13.00004 Longitudinal expression of the genome of a single cell** , NADER POURMAND, University of California Santa Cruz — No abstract available.

**1:39PM Y13.00005 Single Cell Oncogenesis.** , XIN LU, University of Texas MD Anderson Cancer Center — Cancer originates from a single cell that has gone through generations of evolution of genetic and epigenetic changes that drive the cell to become malignant. In some cancers such as various types of leukemia, cancer is clonal. Yet in other cancers like glioblastoma (GBM), that is likely to be caused by simultaneous evolution of multiple subclones within the same tissue. It is obvious that a single cell can evolve into a clonal tumor upon genetic alterations, at molecular and cellular levels, holds the key to the real appreciation of cancer biology and therapeutics. Surprisingly very little is known about the process of spontaneous tumorigenesis from single cells in human. The main reason is the lack of technology to track the natural process of single cell changes from a homeostatic state to a malignant state. We developed a patented compound, photoactivatable ("caged") tamoxifen analogue 4-OHC and associated techniques (photo-switch), which we believe opens the opportunity to address this urgent biological as well as clinical question about cancer. We are using genetically engineered mouse models of head and neck squamous cell carcinoma and high grade astrocytoma (in which the tumor cells, when transformed through acute loss of tumor suppressor genes PTEN and TP53 and gain of oncogenic KRAS, can drive tumorigenesis) and molecular heterogeneity in these tissues.

Single Cells” 3/18/2016 11:15 AM.

**Friday, March 18, 2016 11:15AM - 2:15PM –**

**Session Y14 DCOMP: Progress Towards a Solution of the Hubbard Model** 310 - Emanuel Gull, University of Michigan

**11:15AM Y14.00001 Tensor network studies of the two-dimensional t-J and Hubbard models**, PHILIPPE CORBOZ, Institute for Theoretical Physics, University of Amsterdam — Tensor networks are a class of variational wave functions enabling an efficient representation of quantum many-body states, where the accuracy can be systematically controlled by the bond dimension of the tensors. A well-known example are matrix product states, the underlying ansatz of the density matrix renormalization group (DMRG) method, which has become the state-of-the-art tool to study (quasi-) 1D systems. Progress in quantum information theory, in particular a better understanding of entanglement in quantum many-body systems, has led to the development of 2D tensor networks, including projected entangled-pair states (PEPS) or the 2D multi-scale entanglement renormalization ansatz (MERA). These methods provide one of the most promising routes for the simulation of strongly correlated systems in 2D, in particular models where Quantum Monte Carlo fails due to the negative sign problem. In this talk I report on recent progress in simulating the 2D t-J and Hubbard models with infinite PEPS (iPEPS) which is a tensor network ansatz for a 2D wave function in the thermodynamic limit. Our results reveal an extremely close competition between a uniform d-wave superconducting state and different types of stripe states, where iPEPS yields better variational energies than other state-of-the-art variational methods for large 2D systems.<sup>1</sup> The stripes are site-centered with coexisting charge-, spin-, and superconducting order, where stripes with in-phase d-wave order have an equal or only slightly lower energy than stripes with anti-phase d-wave order. Finally, a nematic anisotropy reduces the pairing amplitude and the energies of stripe states are lowered relative to the uniform state with increasing nematicity.

<sup>1</sup>P. Corboz, T. M. Rice, and M. Troyer, Phys. Rev. Lett. 113, 046402 (2014); P. Corboz, arXiv:1508.04003.

**11:51AM Y14.00002 Solutions of the Two Dimensional Hubbard Model: Benchmarks and Results from a Wide Range of Numerical Algorithms**, JAMES LEBLANC, Univ of Michigan - Ann Arbor — In this talk we present numerical results for ground state and excited state properties (energies, double occupancies, and Matsubara-axis self energies) of the single-orbital Hubbard model on a two-dimensional square lattice. In order to provide an assessment of our ability to compute accurate results in the thermodynamic limit we employ numerous methods including auxiliary field quantum Monte Carlo, bare and bold-line diagrammatic Monte Carlo, method of dual fermions, density matrix embedding theory, density matrix renormalization group, dynamical cluster approximation, diffusion Monte Carlo within a fixed node approximation, unrestricted coupled cluster theory, and multireference projected Hartree-Fock. We illustrate cases where agreement between different methods is obtained in order to establish benchmark results that should be useful in the validation of future results.

**12:27PM Y14.00003 Mott physics and spin fluctuations: A unified framework**, OLIVIER PARCOLLET, Institute of Theoretical Physics, IPHT, CEA-Saclay, France — I will present the "TRILEX" formalism for strongly correlated electron systems and its application to the Hubbard model. TRILEX is designed to unify Dynamical Mean Field Theory (DMFT) and spin fluctuation approaches close to the Mott transition in a minimal way. It is based on a local approximation of the dynamical three-leg interaction vertex and solved using a self-consistent local quantum impurity model. It allows to address simultaneously the Mott physics à la DMFT and the effect of long range antiferromagnetic fluctuations. While its computational cost is comparable to a single site Extended-DMFT computation, the self-energy is momentum-dependent. Moreover TRILEX is the starting point of a systematic and controlled method based on clusters. I will discuss the application of TRILEX to the Hubbard model on a two-dimensional square lattice. As interactions are increased towards the Mott insulating state, the local vertex acquires a strong frequency dependence, driving the system to a Mott transition, while at low enough temperatures the momentum dependence of the self-energy is enhanced due to large spin fluctuations. Upon doping, a Fermi arc is found in the one-particle spectral function, which is one signature of the pseudogap state.

**1:03PM Y14.00004 Dynamical Vertex Approximation for the Hubbard Model**, ALESSANDRO TOSCHI, Institute of Solid State Physics, TU Wien, Vienna (Austria) — A full understanding of correlated electron systems in the physically relevant situations of three and two dimensions represents a challenge for the contemporary condensed matter theory. However, in the last years considerable progress has been achieved by means of increasingly more powerful quantum many-body algorithms, applied to the basic model for correlated electrons, the Hubbard Hamiltonian. Here, I will review the physics emerging from studies performed with the dynamical vertex approximation [1], which includes diagrammatic corrections to the local description of the dynamical mean field theory (DMFT). In particular, I will first discuss [2] the phase diagram in three dimensions with a special focus on the commensurate and incommensurate magnetic phases, their (quantum) critical properties, and the impact of fluctuations on electronic lifetimes and spectral functions. In two dimensions, the effects of non-local fluctuations beyond DMFT grow enormously, determining the appearance of a low-temperature insulating behavior for all values of the interaction in the unfrustrated model [3]: Here the prototypical features of the Mott-Hubbard metal-insulator transition, as well as the existence of magnetically ordered phases, are completely overwhelmed by antiferromagnetic fluctuations of exponentially large extension, in accordance with the Mermin-Wagner theorem. Eventually, by a fluctuation diagnostics [4] analysis of cluster DMFT self-energies, the same magnetic fluctuations are identified as responsible for the pseudogap regime in the hole-doped frustrated case, with important implications for the theoretical modeling of the cuprate physics.

[1] A. Toschi, A.A. Katanin, and K. Held, "Dynamical vertex approximation: A step beyond dynamical mean-field theory", Phys. Rev. B **75**, 045118 (2007).

[2] G. Rohringer, A. Toschi, A. Katanin, and K. Held, "Critical Properties of the Half-Filled Hubbard Model in Three Dimensions", Phys. Rev. Lett. **107**, 256402 (2011).

[3] T. Schäfer, F. Geles, D. Rost, G. Rohringer, E. Arrigoni, K. Held, N. Blümer, M. Aichhorn, and A. Toschi, "Fate of the false Mott-Hubbard transition in two dimensions", Phys. Rev. B **91**, 125109 (2015).

[4] O. Gunnarsson, T. Schäfer, J.P.F. LeBlanc, E. Gull, J. Merino, G. Sangiovanni, G. Rohringer, and A. Toschi, "Fluctuation Diagnostics of the Electron Self-Energy: Origin of the Pseudogap Physics", Phys. Rev. Lett. **114**, 236402 (2015).

**1:39PM Y14.00005 Density matrix embedding theory studies of the two-dimensional Hubbard model<sup>1</sup>**, BO-XIAO ZHENG, Princeton University — Density matrix embedding theory (DMET) provides a quantum embedding framework to compute the electronic structure in strongly correlated lattice systems. It has been applied to various model Hamiltonians and *ab initio* systems. In this talk, I will review the results obtained in the two-dimensional one-band Hubbard model using DMET. Over the last years, we mapped a calibrated ground-state phase diagram of the two-dimensional Hubbard model, concerning magnetic, superconducting and various inhomogeneous phases. Based on the results from this work, as well as the consistent data from other numerical methods, we are able to conclude that many parts of the Hubbard phase diagram is already settled up to an accurate energy scale of 0.001t. Recently, by using large-scale auxiliary-field quantum Monte Carlo (AFQMC) in the impurity problem, we are able to treat much larger embedded clusters at half-filling (and with the constrained path approximation at non-half-filling), which provides a deeper understanding on the finite-size effects of energy and observables in both quantum embedding and finite cluster numerical methods. Finally, we systematically investigated the putative inhomogeneous phases in the underdoped, strong coupling Hubbard model, proposing new inhomogeneous patterns as strong candidates for the ground state. Reference: [1] Bo-Xiao Zheng, Garnet K.-L. Chan, arXiv:1504.01784 [2] J.P.F. Leblanc, Andrey E. Antipov, et al., arXiv:1505.02290

<sup>1</sup>We acknowledge funding from the US Department of Energy, Office of Science, through DE-SC0008624 and DE-SC0010530. This work was also performed as part of the Simons Collaboration on the Many Electron Problem, sponsored by the Simons Foundation.

**Friday, March 18, 2016 11:15AM - 2:03PM** —  
**Session Y15 DMP: 2D Materials: Superconductivity and Correlations III** 314 - Walter Lambrecht, Case Western Reserve University

**11:15AM Y15.00001 Superconductivity in monolayer FeSe and quantum Griffiths singularity in 2D superconductors<sup>1</sup>**, JIAN WANG, Peking University — By direct transport and magnetic measurements, we provide first direct evidence for high temperature superconductivity in monolayer FeSe films on insulating SrTiO<sub>3</sub> (STO) substrates with the onset T<sub>c</sub> and critical current density much higher than those for bulk FeSe [1]. Besides, the thickness dependent superconductivity in ultrathin FeSe films on STO has been investigated [2,3]. By both in situ scanning tunneling microscopy/spectroscopy and ex situ transport and magnetization measurements, we find that the two-atomic-layer Ga film with graphene-like structure on wide band-gap semiconductor GaN is superconducting with T<sub>c</sub> up to 5.4 K [4]. Furthermore, in three-atomic-layer Ga films, we observe for the first time the quantum Griffiths singularity of superconductor-metal transition in two dimensional (2D) superconductors [5]. References: 1. Chin. Phys. Lett. 31, 017401 (2014) (Editors' choice in Science 343, 230 (2014)) 2. Scientific Reports 4, 6040 (2014) 3. arXiv:1507.08431 (accepted by 2D Materials) 4. Physical Review Letters 114, 107003 (2015) (Editors' Suggestion) 5. Science 350, 542 (2015) (accompanied with a perspective paper: Science 350, 509)

<sup>1</sup>Supported by the National Basic Research Program of China (Nos. 2013CB934600 & 2012CB921300), the National Natural Science Foundation of China (Nos. 11222434 & 11174007), and the Research Fund for the Doctoral Program of Higher Education (RFDP) of China.

**11:51AM Y15.00002 High-T<sub>c</sub> superconductivity at 40 K emerged in ultrathin FeSe electric-double-layer transistors**, SHIOGAI JUNICHI, YUKIHIRO ITO, TOSHIKI MITSUHASHI, TSUTOMU NOJIMA, ATSUSHI TSUKAZAKI, Institute for Materials Research, Tohoku University — A few unit-cell (UC) FeSe films on SrTiO<sub>3</sub> substrates have recently attracted much attentions owing to emergence of high temperature superconductivity (high-T<sub>c</sub>) about 65 K compared to the bulk value of 8 K. Modulation of electronic structure, charge transfer from SrTiO<sub>3</sub>, and electron-phonon coupling between the film and substrate are proposed as possible origins for high-T<sub>c</sub>. Although the in-situ scanning tunneling and photoemission spectroscopies have been intensively studied [1], systematic thickness, carrier density and substrate material dependences of electrical measurements have been limited so far. Here we report on high-T<sub>c</sub> in FeSe films on SrTiO<sub>3</sub> and MgO in electric-double-layer transistor (EDLT) [2]. Both the film thickness and electric field can be tuned by electrochemical etching and electrostatic doping in EDLT. The systematic thickness dependences reveal that the onset T<sub>c</sub> of 40 K appears from around 10 nm to 1 UC under the electric field while the initial 18-nm-thick FeSe shows no high-T<sub>c</sub>. Our results point out the importance of electron accumulation or electronic band modulation for high-T<sub>c</sub> in FeSe rather than electron-phonon coupling. [1] Q. Y. Wang et al., Chin. Phys. Lett. 29, 037402 (2012). [2] J. Shiogai et al., Nature Physics (2015).

**12:03PM Y15.00003 Ferromagnetism and d+id superconductivity in 1/2 doped correlated systems on triangular lattice**, BING YE, ANDREJ MESAROS, YING RAN, Boston Coll — We investigate the quantum phase diagrams of t-J model on triangular lattice at 1/2 doping with various lattice sizes by using a combination of density matrix renormalization group (DMRG), variational Monte Carlo and quantum field theories. To sharply distinguish different phases, we calculated the symmetry quantum numbers of the ground state wave functions, and the results are further confirmed by looking into correlation functions. Our results show there is a first order phase transition from ferromagnetism to d+id superconductor, with the transition taking place at  $J/t = 0.4 \pm 0.2$ .

**12:15PM Y15.00004 Topological superconductivity in magnetic adatom chains on a superconductor- multiple topological phases and disorder**, TEEMU OJANEN, KIM PYHNEN, ALEX WESTSTRM, Department of applied physics, School of Science, Aalto University — Recent experimental efforts to realize topological superconductors and Majorana bound states in magnetic chains on top of a superconductor has stimulated lots of associated theory work. In this talk I will present recent results on topological superconductivity in dilute ferromagnetic chains on a superconducting surface with a Rashba spin-orbit coupling. We develop a theoretical framework that allows us to study the properties of magnetic chains at arbitrary subgap energies. Our analysis reveals that the system can support at least five distinct topological phases within realistic parameter regime. Our findings also show that the isolated bound-state energies do not need to be fine-tuned close to the gap centre and that the topological phases may be surprisingly robust towards various sources of disorder.

**12:27PM Y15.00005 Iron-Based Superconductors as topological matter**, JIANGPING HU, purdue univeristy & Institute of physics, cas — We show the existence of non-trivial topological properties in Iron-based superconductors. Several examples are provided, including (1) the single layer FeSe grown on SrTiO<sub>3</sub> substrate, in which an topological insulator phase exists due to the band inversion at M point; (2) CaFeAs<sub>2</sub>, a staggered intercalation compound that integrates both quantum spin hall and superconductivity in which the nontrivial topology stems from the chain-like As layers away from FeAs layers; (3) the Fe(Te,Se) thin films in which the nontrivial Z<sub>2</sub> topological invariance originates from the parity exchange at  $\Gamma$  point that is controlled by the Te(Se) height; (4) nontrivial topology that is driven by the nematic order in FeSe. These results lay ground for integrating high T<sub>c</sub> superconductivity with topological properties to realize new emergent phenomena, such as majorana particles, in iron-based high temperature superconductors Reference: (1) NingNing Hao and Jiangping Hu, Topological phases in the Single Layer FeSe"; Phys. Rev. X 4, 031053 (2014). (2) X Wu, C Le, Y Liang, S Qin, H Fan and J. P. Hu Effect of As-chain layers in CaFeAs<sub>2</sub>" Phys. Rev. B 89 205102 (2014) (3) X. Wu, S. Qin, Y. Liang, C. Le, H. Fan, and J. Hu, CaFeAs<sub>2</sub>: a Staggered Intercalation of Quantum Spin Hall and High Temperature Superconductivity," Physics. Rev. B (Rapid Communication), 91, 081111 (2015) (4) X Wu, Y Liang and JP Hu, unpublished.

**1:03PM Y15.00006 Supercurrent in the quantum Hall regime: part I**, CHUNG-TING KE, Duke University, FRANCOIS AMET, Appalachian state university, IVAN BORZENETS, University of Tokyo, JIYINGMEI WANG, Duke University, KEJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, RUSSELL DEACON, Center for Emergent Matter Science, RIKEN, MICHIIHISA YAMAMOTO, University of Tokyo, YURIY BOMZE, Duke University, SEIGO TARUCHA, University of Tokyo, GLEB FINKELSTEIN, Duke University — The remarkable electronic quality of graphene/boron nitride heterostructures makes them an ideal medium to study induced superconductivity. Our Josephson junctions are made of encapsulated graphene demonstrate ballistic superconducting transport at the micron scale. In the hole-doped regime, a Fabry-Perot resonator is formed by PN junctions close to superconducting contacts, which causes quantum interference of the critical current. We study variations of the Fraunhofer pattern (I.C vs. B) thought the gate voltage range. At higher magnetic fields, superconducting transport across the junctions becomes profoundly non-periodic. Despite demonstrating strong fluctuations as a function of density and magnetic field, we find that supercurrent persists in a wide range of parameters.

**1:15PM Y15.00007 Supercurrent in the quantum Hall regime, part II**, FRANCOIS AMET, Appalachian State University, CHUNG TING KE, Duke University, IVAN BORZENETS, University of Tokyo, JIYINGMEI WANG, Duke University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, RUSSEL DEACON, Center for Emergent Matter Science, RIKEN, MICHIIHISA YAMAMOTO, University of Tokyo, YURIY BOMZE, Duke University, SEIGO TARUCHA, University of Tokyo, GLEB FINKELSTEIN, Duke University — A novel promising route for creating topological states and excitations is to combine superconductivity and the quantum Hall effect. Despite this potential, signatures of superconductivity in the quantum Hall regime remain scarce, and a superconducting current through a Landau-quantized two-dimensional electron gas has so far eluded experimental observation. High-mobility graphene/BN heterostructures exhibit the quantum Hall effect at relatively low field and are therefore particularly suitable to study the fate of the Josephson effect in that regime. Here, we report the observation of a superconducting current through graphene at fields as high as 2 Tesla. In that regime, the normal-state resistance is quantized but pockets of superconductivity still persist at small current bias. We will describe their bias and temperature dependence. Magnetic field interference patterns in the supercurrent inform on possible mechanisms mediating this supercurrent.

**1:27PM Y15.00008 Complex Stoichiometry reordering of PTCDA on Ag(111) upon K Inter-calation**, G.P. BRIVIO, A. BABY, Univ. Milano-Bicocca (Italy), C. ZWICK, M. GRUENEWALD, R. FORKER, T. FRITZ, Univ. Jena (Germany), G. FRATESI, Univ. Milano (Italy), O.T. HOFMANN, E. ZOJER, Graz Univ. Technology (Austria) — Alkali metal atoms are a simple yet efficient n-type dopant of organic semiconductors. However, the molecular crystal structures need be controlled and well understood in order to optimize the electronic properties (charge carrier density and mobility) of the target material. Here, we report that potassium intercalation into PTCDA monolayer domains on a Ag(111) substrate induces distinct stoichiometry-dependent structural reordering processes, resulting in highly ordered and large K<sub>x</sub>PTCDA domains. The emerging structures are analyzed by low temperature scanning tunneling microscopy (STM), scanning tunneling hydrogen microscopy (STHM), and low-energy electron diffraction (LEED) as a function of the stoichiometry and by density functional theory (DFT) calculations. Large stable monolayer domains are found for x=2,4. The epitaxy types for all intercalated stages are determined as point-on-line. The K atoms adsorb in the vicinity of the oxygen atoms of the PTCDA molecules, and their positions are determined with sub-Angstrom precision. This is a crucial prerequisite for the prospective assessment of the electronic properties of such composite films, as they depend on the mutual alignment between donor atoms and acceptor molecules.

**1:39PM Y15.00009 Uncovering fermionic zero-energy modes through a boundary-matrix approach**, ABHIJEET ALASE, Graduate Student, EMILIO COBANERA, Postdoctoral researcher, GERARDO ORTIZ, LORENZA VIOLA, Professor — Given a non-interacting fermionic lattice system with arbitrary boundary conditions, we show how the problem of diagonalizing the single-particle Hamiltonian can be split into suitably defined bulk and boundary problems. Following this exact separation, a boundary matrix may be constructed, which contains complete information about the emergence and nature of zero-energy modes, even in the thermodynamic limit. Our approach is applicable to model Hamiltonians in arbitrary space dimensions of relevance to topological quantum matter. As a concrete illustration, we show how to correctly describe the zero-energy Majorana modes of a time-reversal-invariant two-band s-wave topological superconductor in a Josephson ring configuration, and also provide physical insight into the predicted unconventional Josephson effect.

**1:51PM Y15.00010 Interaction-driven strong topology on the boundary of a weak topological superconductor**, DANIEL MENDLER, Inst. für theo. Festkörperphysik, Inst. of Nanotechnology, Karlsruhe Inst. of Technology, PANAGIOTIS KOTETES, Center for Quantum Devices, Niels Bohr Inst., U. of Copenhagen/Inst. für theo. Festkörperphysik, Karlsruhe Inst. of Technology, GERD SCHÖN, Inst. für theo. Festkörperphysik, Inst. of Nanotechnology, Karlsruhe Inst. of Technology — We focus on a class of topological superconductors (TSCs) which exhibit a bulk energy gap and support Majorana flat bands (MFBs) on the surface. In contrast to previous proposals relying on strong TSCs with nodal bandstructure, here MFBs are solely protected by a weak topological invariant reflecting a global or local strong anisotropy. In the present case interactions play a dual role, on one hand driving the spontaneous symmetry breaking to an anisotropic superconducting phase and on the other, gapping out the arising MFBs yielding a strong topological phase on the boundary. The prototype system showing this kind of behavior is the nematic *p<sub>z</sub>*-superconductor, which supports surface MFBs. While the interactions stabilize the *p<sub>z</sub>*-SC phase in the bulk and induce the MFBs, suppressed bulk p-wave pairing terms occur on the surface, thus lifting the MFB-degeneracy. A similar situation can take place if the nematic features are only local, a scenario which is realizable in a heterostructure consisting of a conventional superconductor in proximity to a topological insulator surface with intrinsic magnetic order.

**Friday, March 18, 2016 11:15AM - 2:15PM –**

**Session Y16 DMP: Silicene, Germanene, and Beyond** 315 - Sufe Shi, Rensselaer Polytechnic Institute

**11:15AM Y16.00001 Graphene challengers: silicene, germanene and stanene, group IV elemental synthetic electronic materials.**, GUY LE LAY, Retired — Silicene, germanene and stanene, graphene's group IV elemental cousins, have attracted considerable interest since the birth of silicene in 2012 [1]. These novel synthetic two-dimensional (2D) Si, Ge and Sn allotropes are artificially created in situ under ultra high vacuum, since, at variance with graphene, which descends from graphite, they have no parent crystal in nature. They are considered as promising candidates for ultimate scaling of nanoelectronic devices [2,3]. Indeed, the recent fabrication of the first silicene field effect transistors with ambipolar characteristics operating at room temperature demonstrates their potential as emerging 2D electronic materials [4]. In this invited talk, I will present the archetype 3x3 silicene phase formed on a silver (111) substrate [1], its sister phases and the growth of multilayer silicene, which hosts Dirac fermions and which is stable in ambient air, protected by its ultra-thin native oxide [5]. The recent synthesis of single layer germanene [6,7] and stanene [8], near room temperature 2D topological insulators will be also presented, while multilayer germanene will be further addressed. Challenging graphene, silicene, germanene and stanene, which are directly compatible with the current semiconductor industry, could lead to the development of a new class of low energy consumption nanoelectronic devices. 1. P. Vogt et al., Phys. Rev. Lett., 108, 155501 (2012). 2. A. Dimoulas, Microelectronic Engineering, 131, 68 (2015). 3. G. Le Lay, Nature Nanotechnology, 10, 202 (2015). 4. Li Tao et al., Nature Nanotechnology, 10, 227 (2015). 5. P. De Padova et al., 2D Mater., 1, 021003 (2014). 6. M.E. Davila et al., New J. Phys., 16, 095002 (2014). 7. M. Derivaz et al. Nano Lett., 15, 2510 (2015). 8. Feng-feng Zhu et al., Nature Mater., 14, 1020 (2015).

**11:51AM Y16.00002 Prediction of a quantum anomalous Hall state in Co-decorated silicene.**, THANESHWOR KALONI, GEORG SCHRECKENBACH, University of Manitoba, MICHAEL FREUND, FTI — Based on first-principles calculations, we demonstrate that Co-decorated silicene can host a quantum anomalous Hall state. The exchange field induced by the Co atoms combined with the strong spin-orbit coupling of the silicene opens a nontrivial band gap at the K point. As compared to other transition metals, Co-decorated silicene is unique in this respect, since usually hybridization and spin-polarization induced in the silicene suppress a quantum anomalous Hall state.

**12:03PM Y16.00003 Ordered structure upon deposition of Ge on the monolayer silicene on Ag(111)**, HAN-DE CHEN, DENG SUNG LIN, Department of Physics, National Tsing Hua University — The growth of monolayer silicene on Ag (111) has been a hot research in recent years. The akin structure of the same group IV element: Germanene, has also been grown successfully on different metal substrates. In this investigation, Ge has been deposited by molecular beam epitaxy on the monolayer-thick silicene grown on Ag(111). Low-temperature scanning tunneling microscopy (LT-STM) has been employed to observe the surface morphology and atomic structure. On the  $(3 \times 3)$ Si phase, only one Ge adatom is found on each  $(3 \times 3)$ Si unit cell on two different sites, A and B. The deposited Ge adatoms prefer to settle around a unit cell that has already incorporated one Ge adatom, thereby forming two domains  $(3 \times 3)$ A and  $(3 \times 3)$ B. Results on  $(7 \times 7)$ Si superstructure showing local ordering will also be presented.

**12:15PM Y16.00004 Germanene-like defects in Reverse Monte Carlo model of amorphous germanium revealed through new visualization method**, AL RAHEMTULLA, Univ of Guelph, BRUNO TOMBERLI, Capilano University, EDWARD KIM, University of Guelph, SJOERD ROORDA, Université de Montreal, STEFAN KYCIA, University of Guelph — High Resolution x-ray diffraction experiments of amorphous germanium (a-Ge) revealed structural differences that cannot be reconciled with accepted theoretical models. An intuitive computational technique has been developed to construct 3D statistical density maps to directly resolve local atomic structure of a-Ge. A reverse monte carlo routine is used to compare the continuous random network model to the experimental model of a-Ge. Undercoordination in the refined model is shown to exist bimodally, as a 4-coordinated tetrahedron and a buckled 3-coordinated structure similar to germanene. These structures account for 95.7% of the total atoms in an approximate 5:2 ratio respectively.

**12:27PM Y16.00005 Room Temperature Silicene Field-Effect Transistors<sup>1</sup>**, DEJI AKINWANDE, The University of Texas - Austin — Silicene, a buckled Si analogue of graphene, holds significant promise for future electronics beyond traditional CMOS. In our predefined experiments via encapsulated delamination with native electrodes approach, silicene devices exhibit an ambipolar charge transport behavior, corroborating theories on Dirac band in Ag-free silicene. Monolayer silicene device has extracted field-effect mobility within the theoretical expectation and ON/OFF ratio greater than monolayer graphene, while multilayer silicene devices show decreased mobility and gate modulation. Air-stability of silicene devices depends on the number of layers of silicene and intrinsic material structure determined by growth temperature. Few or multi-layer silicene devices maintain their ambipolar behavior for days in contrast to minutes time scale for monolayer counterparts under similar conditions. Multilayer silicene grown at different temperatures below 300°C possess different intrinsic structures and yield different electrical property and air-stability. This work suggests a practical prospect to enable more air-stable silicene devices with layer and growth condition control, which can be leveraged for other air-sensitive 2D materials. In addition, we describe quantum and classical transistor device concepts based on silicene and related buckled materials that exploit the 2D topological insulating phenomenon. The transistor device physics offer the potential for ballistic transport that is robust against scattering and can be employed for both charge and spin transport.

<sup>1</sup>This work was supported by the ARO.

**1:03PM Y16.00006 Nearest Neighbor Hopping conduction observed with ionic liquid induced silicon surface states<sup>1</sup>**, JJ NELSON, K. V. REICH, M. SAMMON, B. I. SHKLOVSKII, A. M. GOLDMAN, University of Minnesota — A two-dimensional hole gas can be created on the surface of a bulk Si wafer by using an ionic liquid in an electric double layer transistor configuration (EDLT). EDLTs are useful in observing metal to insulator and superconductor to insulator transitions due to record high carrier densities of  $10^{15} \text{ cm}^{-2}$  that can be achieved. In some cases the high carrier densities are due in part to oxidation of the sample surface. With an EDLT configuration we have observed a 2D insulator-to-metal transition with low mobility Si at the highest reported critical carrier density. [J. Nelson and A. M. Goldman Phys. Rev. B 91, 241304(R) (2015)] The experiment reported here is designed to promote electrostatic carrier induction over electrochemical reactions and is focused on carrier densities near  $10^{11} \text{ cm}^{-2}$ . At such a low densities we observe nearest neighbor hopping conduction on the surface of Si.[J. Nelson et al., Phys. Rev. B 92, 085424 (2015)] This observation suggests that the ionic liquid covering the surface should be treated as a series of discrete charges that can act as a platform to better understand EDLT physics at higher carrier densities.

<sup>1</sup>This work was supported in part by the National Science Foundation under grant NSF-1263316.

**1:15PM Y16.00007 Gapped Dirac cone in silicene and germanene on  $\text{Al}_2\text{O}_3(0001)$** , MINGXING CHEN, MICHAEL WEINERT, Univ of Wisconsin, Milwaukee — Developing guidelines to find promising substrates that can stabilize the monolayer honeycomb structures of silicene and germanene while simultaneously preserving the Dirac-electron-driven properties is of practical importance for applications. From first-principles calculations, we find that silicene on Al-terminated  $\text{Al}_2\text{O}_3(0001)$  retains the main structural profile of the ideal low-buckled silicene with a binding energy comparable to that of silicene on Ag(111). Unfolded  $k$ -projected bands reveal that a gapped Dirac cone is formed at the K point. The underlying mechanism is that the substrate has a large energy gap and the workfunctions are such that there is little direct bonding of between the silicene Dirac states and the substrate, which further guides us to find gapped Dirac states in germanene on  $\text{Al}_2\text{O}_3(0001)$ .

**1:27PM Y16.00008 Single and Few Layer Silicene: Structural, Electronic and Transport Properties<sup>1</sup>**, J DAVID CAREY, NATHANAEEL ROOME, University of Surrey — Single layer silicene has weaker  $\pi$  bonding that graphene resulting in buckling of the Si atoms in different sub-lattices. Despite the loss of planarity, a linear bandstructure emerges where we find a Fermi velocity of about  $5.3 \times 10^5 \text{ m/s}$ . Determination of the phonon dispersion characteristics reveals a  $\Gamma$  point optical phonon with an energy of 69 meV and a K point optical phonon with an energy of 62 meV. In graphene these phonons play important role in scattering electrons, and in Raman spectroscopy, but have larger energies of 194 and 166 meV, respectively. The lower phonon energies in silicene, arising from the higher atomic masses, would be expected to scatter carriers efficiently and limit carrier mobility. We have calculated, however, that the electron-optical phonon coupling matrix elements are about a factor of 25 times smaller than in graphene and this important result will help with the further development of silicene based devices due to reduced phonon scattering. The two stable stacking configurations of bilayer silicene, AA and AB, now have to account of the position of the atomic buckling in the two layers, leading to four possible atomic configurations with the buckling between the layers being in- or out-of-phase with each other. We find that in contrast to graphene, the two stable configurations are based on AA type stacking being about 70 meV per atom more stable than AB stacking. The potential for elemental layered materials beyond graphene for device applications will also be discussed.

<sup>1</sup>Single and Few Layer Silicene: Structural, Electronic and Transport Properties

**1:39PM Y16.00009 Two-dimensional group-IV monochalcogenides: structural, electronic and optical properties.**<sup>1</sup>, LIDIA GOMES, ALEXANDRA CARVALHO, A. H. CASTRO NETO, National University of Singapore — Two-dimensional materials have attracted a massive attention of the scientific and industrial communities due to their unusual and interesting properties. The layered group-IV monochalcogenides-SnS, SnSe, GeS and GeSe- has gained attention as a promising group with potentially useful applications in diverse fields. The bulk SnS, a naturally occurring mineral, has been considered as an alternative to be used in film PV cells, due to its electronic and optical properties. We use first principles calculations to explore structural, electronic and optical properties of this group, with focus in their two-dimensional forms. We show that all those binary compounds are semiconducting, with bandgap energies covering most of the visible range. They have multiple valleys in the valence and conduction bands, with spin-orbit splitting of the order of 19-86 meV. An enhanced static dielectric permittivity is found for the monolayers. Structural analysis shows that the 2D form of these materials presents very high piezoelectric constants, exceeding values recently observed for other 2D-systems. The existence of a negative Poisson ratio is predicted for the GeS compound.

<sup>1</sup>We acknowledge the NRF-CRP award "Novel 2D materials with tailored properties: beyond graphene" (R-144-000-295-281).

**1:51PM Y16.00010 Scattering mechanisms in shallow undoped Si/SiGe quantum wells**, DOMINIQUE LAROCHE, Sandia Natl Labs, SHIH-HSIEN HUANG, National Taiwan University and National Nano Device Laboratories, ERIK NIELSEN, Sandia Natl Labs, YEN CHUANG, JIUN-YUN LI, CHIH-WEN LIU, National Taiwan University and National Nano Device Laboratories, TZU-MING LU, Sandia Natl Labs — We report the magneto-transport and scattering mechanism analysis of a series of increasingly shallow Si/SiGe quantum wells with the shallowest 2DEG located only  $\sim 10$  nm away from the surface. The peak mobility increases with increasing depth, suggesting that charge centers near the oxide/semiconductor interface is the main source of disorder. The power-law exponent of the mobility versus density curve,  $\mu \propto n^\alpha$ , is extracted as a function of the depth. At intermediate densities, the power-law dependence is characterized by  $\alpha \sim 2.3$  while at the highest achievable densities for devices with intermediate depth, an exponent  $\alpha \sim 5$  is observed. We propose, and show by simulations, that this increase in  $\alpha$  is explained by a non-equilibrium model where electrons migrating to the surface smooth out the potential landscape seen by the 2DEG. This work has been supported by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, U.S. Department of Energy (DOE). Sandia National Laboratories is a multi program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. DOE's National Nuclear Security Administration under contract DE-AC04-94AL

**2:03PM Y16.00011 Silicene-type Surface Reconstruction on C40 Hexagonal Silicides**, CAMERON VOLDERS, PETRA REINKE, Univ of Virginia — Silicene has emerged as the next two-dimensional material possessing a Dirac type electronic structure making it a prime candidate for integration in electronic devices. The study of silicene is relatively new and many aspects have yet to be fully understood. Here we present a scanning tunneling microscopy (STM) study of a Silicene-type surface reconstruction observed on nanometer scale hexagonal-MoSi<sub>2</sub> crystallites. This surface reconstruction is specific to the C40 structure of h-MoSi<sub>2</sub> and can initially be defined as a geometric silicene while the coupling between the silicene surface and the silicide bulk is under investigation. The lateral dimensions correspond to a superstructure where the silicene hexagons are slightly buckled and two of the six Si atoms are visible in the STM images creating a honeycomb pattern. The local electronic structure of the silicene is currently being studied with ST spectroscopy and the impact of confinement will be addressed. These results open an alternative route to Silicene growth by using surface reconstructions on metallic and semiconducting C40 silicide structures, which is promising for direct device integration on Si-platforms.

**Friday, March 18, 2016 11:15AM - 2:15PM –**  
**Session Y17 DMP: 2D Semiconductor Physics IV** 316 - Liping Yu, Temple University

**11:15AM Y17.00001 Engineering excitonic properties and valley polarization in transition metal dichalcogenide monolayers**<sup>1</sup>, BERNHARD URBASZEK, CNRS-Toulouse University — Binary Transition metal dichalcogenide (TMDC) monolayer (ML) materials MoS<sub>2</sub>, MoSe<sub>2</sub>, WSe<sub>2</sub>, WS<sub>2</sub> and MoTe<sub>2</sub> share common properties such as a direct optical bandgap, Spin-Orbit splittings of hundreds of meV and coupled spin-valley states. Optical absorption and emission are dominated by robust excitons, whose resonances also strongly influence Raman scattering amplitudes [1] and second harmonic generation efficiency [2]. Important differences in opto-electronic properties between these materials depend on whether the exciton ground state is optically bright or dark. This order will depend on the conduction band Spin-Orbit splitting and the electron-hole Coulomb interaction and will have strong influence on the light emission yield of the TMDC MLs. In this talk we discuss Spin-Orbit engineering in Mo(1-x)W(x)Se<sub>2</sub> alloy monolayers [3]. We probe the impact of the tuning of the conduction band Spin-Orbit spin splitting on the bright versus dark exciton population. For MoSe<sub>2</sub> monolayers the PL intensity decreases as a function of temperature by an order of magnitude (T=4-300 K), whereas for WSe<sub>2</sub> we measure surprisingly an order of magnitude increase. The ternary material shows a trend between these two extreme behaviors. In addition we show a non-linear increase of the optically generated valley polarization as a function of tungsten (W) concentration. Tuning the optical properties in applied external fields will be discussed. [1] G. Wang et al, PRL 115, 117401 (2015) [2] G. Wang et al, 2D Mater. 2, 045005 (2015) [3] G. Wang et al, Nature Comms. (in press, arxiv 1506.08114)

<sup>1</sup>We acknowledge funding from ERC Grant No 306719 and ANR MoS<sub>2</sub>ValleyControl

**11:51AM Y17.00002 Hybrid interlayer excitons with tunable dispersion relation**, BRIAN SKINNER, Massachusetts Institute of Technology — When two semiconducting materials are layered on top of each other, interlayer excitons can be formed by the Coulomb attraction of an electron in one layer to a hole in the opposite layer. The resulting exciton is a composite boson with a dispersion relation that is a hybrid between the dispersion relations of the electron and the hole separately. In this talk I show how such hybridization is particularly interesting when one layer has a Mexican hat-shaped dispersion relation and the other has a conventional parabolic dispersion. In this case the interlayer exciton can have a range of qualitatively different dispersion relations, which can be continuously altered by an external field. This tunability in principle allows one to continuously tune a collection of interlayer excitons between different quantum many-body phases, including Bose-Einstein condensate, Wigner crystal, and fermion-like moat band phases.

**12:03PM Y17.00003 Electric Field Dependent Photoluminescence in Atomically Thin Transition Metal Dichalcogenides van der Waals Heterostructures.**, LUIS A. JAUREGUI, ALEX A. HIGH, ALAN DIBOS, ANDREW JOE, ELGIN GULPINAR, HONGKUN PARK, PHILIP KIM, Harvard University, Department of Physics — Jauregui, Alex A. High, Alan Dibos, Andrew Joe, Elgin Gulpinar, Hongkun Park, Philip Kim Harvard University, Physics Department -abstract- Single layer transition metal dichalcogenides (TMDC) are 2-dimensional (2D) semiconductors characterized by a direct optical bandgap and large exciton binding energies ( $>100$  meV). We fabricate CQW heterostructures made of 2D TMDCs with hexagonal Boron nitride (BN) as atomically thin barrier and gate dielectric, with top and bottom gate electrodes. We study the evolution of photoluminescence (PL) spectrum with varying BN barrier thickness, electric field, temperature and polarization. Our measured low-temperature (T = 3K) PL peaks show full width at half maxima on the order of  $\sim 3$ meV. We identify the photoluminescence peaks, corresponding to the charged exciton emission, which red shifts and its brightness increases while the neutral exciton emission becomes darker for increasing electric field.

**12:15PM Y17.00004 Giant and tunable valley degeneracy splitting in  $\text{MoTe}_2$**  , XIAO LI, The University of Texas at Austin, JINGSHAN QI, Jiangsu Normal University, QIAN NIU, The University of Texas at Austin, JI FENG, Peking University — Valleys in monolayer transition-metal dichalcogenides seamlessly connect two basic carriers of quantum information, namely, the electron spin and photon helicity. Lifting the valley degeneracy is an attractive route to achieve further optoelectronic manipulations. However, the magnetic field only creates a very small valley splitting. We propose a strategy to create giant valley splitting by the proximity-induced Zeeman effect. Our first principles calculations of monolayer  $\text{MoTe}_2$  on a  $\text{EuO}$  substrate show that valley splitting over 300 meV can be generated. Interband transition energies become valley dependent, leading to selective spin-photon coupling by optical frequency tuning. The valley splitting is also continuously tunable by rotating the substrate magnetization. The giant and tunable valley splitting adds a different dimension to the exploration of unique optoelectronic devices based on magneto-optical coupling and magnetoelectric coupling.

**12:27PM Y17.00005 Tunable optical second-harmonic generation from bilayer  $\text{MoS}_2$  by controlled inversion symmetry breaking** , CLAUDIA RUPPERT, TU Dortmund/Columbia Univ., YILEI LI, Stanford Univ./Columbia Univ., LEI WANG, Cornell Univ./Columbia Univ., EN-MIN SHIH, JAMES HONE, Columbia Univ., TONY HEINZ, Stanford Univ./Columbia Univ. — Due to the presence of a center of inversion, optical second-harmonic generation (SHG) from an unperturbed bilayer  $2\text{H-MoS}_2$  crystal is strongly suppressed compared to the non-centrosymmetric monolayer. In this paper, we show that SHG from bilayer  $\text{MoS}_2$  is enhanced when it is supported on a fused silica substrate. This enhancement originates from lifting of inversion-symmetry induced by substrate interactions. Further, by applying an out-of-plane electrostatic field in a back-gating geometry, we demonstrate highly tunable SH radiation from supported  $\text{MoS}_2$  bilayers. Complementing recent work on bilayer  $\text{WSe}_2$  [1], where the sample is primarily studied in the hole-doped regime, the bilayer  $\text{MoS}_2$  samples in our study are shown to be in the electron-doped regime. Through a comparison of the field-induced change in the second-order nonlinear susceptibilities of monolayer and bilayer  $\text{MoS}_2$ , we identify the importance of interlayer coupling in the tunable SHG from bilayer  $\text{MoS}_2$ . [1] Huakang Yu, Deep Talukdar, Weigao Xu, Jacob B. Khurgin, and Qihua Xiong, Nano Lett. 15 5653 (2015)

**12:39PM Y17.00006 Strain-induced topological quantum phase transition in phosphorene oxide** , SEOUNG-HUN KANG, JEJUNE PARK, Kyung Hee University, SUNGJONG WOO, Korea Institute for Advanced Study, YOUNG-KYUN KWON, Kyung Hee University — Using *ab initio* density functional theory, we investigate the structural stability and electronic properties of phosphorene oxides ( $\text{PO}_x$ ) with different oxygen compositions  $x$ . A variety of configurations are modeled and optimized geometrically to search for the equilibrium structure for each  $x$  value. Our electronic structure calculations on the equilibrium configuration obtained for each  $x$  reveal that the band gap tends to increase with the oxygen composition of  $x \downarrow 0.5$ , and then to decrease with  $x \downarrow 0.5$ . We further explore the strain effect on the electronic structure of the fully oxidized phosphorene,  $\text{PO}$ , with  $x = 1$ . At a particular strain without spin-orbit coupling (SOC) is observed a band gap closure near the  $\Gamma$  point in the  $k$  space. We further find the strain in tandem with SOC induces an interesting band inversion with a reopened very small band gap ( $\sim 5$  meV), and thus gives rise to a topological quantum phase transition from a normal insulator to a topological insulator. Such a topological phase transition is confirmed by the wave function analysis and the band topology identified by the  $Z_2$  invariant calculation.

**12:51PM Y17.00007 Electronic and structural phase transitions induced by uniaxial strains in monolayer  $\text{SnSe}$**  , YABEI WU, Shanghai University; University at Buffalo, SUNY, WEIWEI GAO, University at Buffalo, SUNY, PEIHONG ZHANG, Shanghai University; University at Buffalo, SUNY, WEI REN, Shanghai University — Two dimensional (2D) materials have attracted unprecedented research interest owing to their unique properties that are suitable for various applications. Recent research has started to explore 2D materials beyond graphene; examples include transition metal dichalcogenides and black phosphorus. Bulk  $\text{SnSe}$  is a layered semiconductor which exists in two phases. The low temperature  $\text{Pnma}$  phase has an indirect band gap of 0.89 eV and a direct band gap of 1.3 eV, while the high temperature  $\text{Cmcm}$  phase is stabilized at  $T > 800$  K. In this talk, we will present first-principles investigations of the effects of strains on the electronic and structural properties of  $\text{SnSe}$ . We find that uniaxial strains are an effective means to tune the properties single layer  $\text{SnSe}$ , and may also induce phase transitions in this system.

**1:03PM Y17.00008 Strain Engineering of Transition Metal Dichalcogenides** , ALI DADGAR, ABHAY PASUPATHY, IRVING HERMAN, DENNIS WANG, Columbia University, KYUNGNAM KANG, EUI-HYEOK YANG, Stevens Institute of Technology — The application of strain to materials can cause changes to bandwidth, effective masses, degeneracies and even structural phases. In the case of the transition metal dichalcogenide (TMD) semiconductors, small strain (around 1 percent) is expected to change band gaps and mobilities, while larger strains are expected to cause phase changes from the triangular  $2\text{H}$  phase to orthorhombic  $1\text{T}'$  phases. We will describe experimental techniques to apply small and large (around 10 percent) strains to one or few layer samples of the TMD semiconductors, and describe the effect of the strain using optical (Raman, photoluminescence) and cryogenic transport techniques.

**1:15PM Y17.00009 Simultaneous tunability of electronic and phononic gap in  $\text{SnS}_2$  under normal compressive strain** , BABU RAM<sup>1</sup>, AADITYA MANJANATH<sup>2</sup>, Ph.D student , ABHISHEK KUMAR SINGH<sup>3</sup>, Assistant Professor — Ever since the discovery of graphene, 2D materials have emerged as an attractive field of research. Here, using density functional theory based calculations, we show tunability in the electronic structure of mono to multilayered  $\text{SnS}_2$  under biaxial tensile (BT), biaxial compressive (BC), and normal compressive (NC) strains. We obtain a reversible semiconductor to metal (S-M) transition in mono to multilayered  $\text{SnS}_2$  without changing the nature of the band gap (i.e. indirect). For the stability analysis with applied strain, we use bilayer (2L-)  $\text{SnS}_2$  as our prototype system. Surprisingly, under a high NC strain, 2L- $\text{SnS}_2$  does not exhibit unstable modes. The phonon spectra of 2L- $\text{SnS}_2$  shows a gap in the optical region, which, most interestingly, increases with applied NC strain. Such a simultaneous tunability of the electronic as well as phononic properties of  $\text{SnS}_2$  under applied strain can be exploited in many applications such as pressure sensors, micromechanical resonators, frequency filters, and in many other multi-physics devices.

<sup>1</sup>Materials Research Centre , Indian Institute of Science , Bangalore, India

<sup>2</sup>Materials Research Centre and Centre for Nanoscience and Engineering, Indian Institute of Science, Bangalore, India

<sup>3</sup>Materials Research Centre, Indian Institute of Science, Bangalore, India

**1:27PM Y17.00010 Using dispersive medium to control excitons in 2D materials.** , ANDREY KLOTS, Vanderbilt University, KIRILL I. BOLOTIN, Vanderbilt University; Freie University — Excitons in 2D materials (2DMs) are known to be sensitive to the surrounding environment. This makes it possible to modify 2D excitons by depositing materials with controlled dielectric constant on top of 2DMs. This possibility becomes especially interesting if we consider materials with dielectric permittivity  $\epsilon$  that depends both on wavevector  $k$  (this happens if the medium is spatially non-uniform) and frequency  $\omega$ . Here, we develop platforms to control  $\epsilon(k, \omega)$  and explore resulting changes in light-matter interactions of 2DMs. To examine the effect of wavevector-dependent permittivity of the medium, we study absorption/photoluminescence of graphene and  $\text{MoS}_2$  in the vicinity of highly non-uniform medium - an array of metal nanoparticles, 3-5 nm in diameter. In this case absorption of light can lead to creation of excitons with non-zero momentum. These dark states are not accessible via regular absorption spectroscopy. We study the case of frequency-dependent permittivity by surrounding  $\text{MoS}_2$  by a highly-dispersive media (e.g. dielectric liquids, graphene and  $\text{VO}_2$ ). We demonstrate non-trivial frequency-dependent renormalization of the quasiparticle bandgap and exciton binding energies.

**1:39PM Y17.00011 Functional polymers for electronic-structure modulation of MoS<sub>2</sub>** , ASHWIN RAMASUBRAMANIAM, Department of Mechanical and Industrial Engineering, University of Massachusetts Amherst, RYAN SELHORST, EGGLE PUODZIUKY-NAITE, JEFFREY DEWEY, Department of Polymer Science and Engineering, University of Massachusetts Amherst, PEIJIAN WANG, MICHAEL BARNES, Department of Chemistry, University of Massachusetts Amherst, TODD EMRICK, Department of Polymer Science and Engineering, University of Massachusetts Amherst — Two-dimensional semiconductors based on the Mo and W family of transition metal dichalcogenides (TMDCs) are emerging as an important class of materials with unique optoelectronic properties. However, there remain challenges associated with precise control over carrier doping and work functions that need to be overcome for device applications. We report the synthesis of new tetrathiafulvalene (TTF)-based polymers that provide enhanced solution stabilization of MoS<sub>2</sub> nanosheets while simultaneously modulating their electronic structure through robust, non-covalent interactions. Kelvin probe force microscopy (KPFM) imaging of TTF-polymer functionalized 2H MoS<sub>2</sub> nanosheets confirms n-doping of the MoS<sub>2</sub> with an accompanying reduction in the work function. Density functional theory calculations provide insight into the TTF-MoS<sub>2</sub> interfacial interactions and provide a theoretical basis for modulation of electronic properties of MoS<sub>2</sub> via charge-transfer interactions. These combined results illustrate the potential for polymer doping of TMDCs as a viable and scalable approach for synthesis of new hybrid materials for optoelectronics.

**1:51PM Y17.00012 Electronic and magnetic engineering of transition metal dichalcogenides** , YOUJIAN TANG, VINCENT CRESPI, Penn State Univ. Physics Dept, VINCENT CRESPI GROUP TEAM — Transition metal dichalcogenides (TMDs) have moderate bandgaps and great potential in electronic and optoelectronic applications. We show that by intercalation and compensated doping of transition metal ions, we could generate a “half-semiconductor”, half-metal or doped magnetic semiconductor. We will also show that covalently connecting a single layer of WS<sub>2</sub> to a small aromatic molecule with appropriate electronegativity, it is possible to align the molecular energy levels with the WS<sub>2</sub> conduction band edge, yielding an electronic structure of potential interest for thermoelectric applications, and covalently connecting single-layer WS<sub>2</sub> to magnetic coordination compounds could introduce magnetization into the WS<sub>2</sub> layer.

**2:03PM Y17.00013 Electronic states at transition metal dichalcogenide lateral heterointerfaces<sup>1</sup>** , OSCAR AVALOS-OVANDO, Ohio University, DIEGO MASTROGIUSEPPE, Instituto de Física Rosario, SERGIO ULLOA, Ohio University — Materials with different band gaps are typically used to create heterostructures that enable band sculpting, depending on different shape and boundaries of the systems. These are used in diode lasers and high-speed transistors devices. Potential material candidates for such heterostructures at the monolayer level are the family of transition-metal dichalcogenides, MX<sub>2</sub> (with M=Mo,W and X=S,Se), especially interesting materials with strong spin-orbit coupling and valley degrees of freedom. We consider lateral interfaces between pairs of these materials, and study the effect of different boundary geometries, motivated by recent experimental reports of the growth of such interfaces with different geometries [2,3]. Using an effective 3-orbital tight-binding model [1], we focus our attention on monolayer ribbons and triangular flakes. We analyze the formation of edge/interface states for different gap nesting materials. We study the spatial distribution and orbital character of the wave functions throughout, as well as their dependence on interface termination. [1] G. B. Liu et al., PRB 88, 085433 (2013). [2] C. Huang et al., Nat. Mat. 13, 1096 (2014). [3] Y. Gong et al., Nat. Mat. 13, 1135 (2014).

<sup>1</sup>Supported by NSF DMR-1508325

## Friday, March 18, 2016 11:15AM - 2:15PM –

Session Y18 GMAG DMP: Frustrated Magnetism: Pyrochlore and Kagome Lattices 317 - Lucile Savary, MIT

**11:15AM Y18.00001 Quantum spin ices and magnetic states from dipolar-octupolar doublets on the pyrochlore lattice** , GANG CHEN<sup>1</sup>, Fudan Univ, Perimeter Institute for Theoretical Physics — We consider a class of electron systems in which dipolar-octupolar Kramers doublets arise on the pyrochlore lattice. In the localized limit, the Kramers doublets are described by the effective spin1/2 pseudospins. The most general nearest-neighbor exchange model between these pseudospins is the XYZ model. In addition to dipolar ordered and octupolar ordered magnetic states, we show that this XYZ model exhibits two distinct quantum spin ice (QSI) phases, that we dub dipolar QSI and octupolar QSI. These two QSIs are distinct symmetry enriched U(1) quantum spin liquids, enriched by the lattice symmetry. Moreover, the XYZ model is absent from the notorious sign problem for a quantum Monte Carlo simulation in a large parameterspace. We discuss the potential relevance to real material systems such as Dy<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>, Nd<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub>, Nd<sub>2</sub>Hf<sub>2</sub>O<sub>7</sub>, Nd<sub>2</sub>Ir<sub>2</sub>O<sub>7</sub>, Nd<sub>2</sub>Sn<sub>2</sub>O<sub>7</sub> and Ce<sub>2</sub>Sn<sub>2</sub>O<sub>7</sub>.

<sup>1</sup>chggst@gmail.com, Refs: Y-P Huang, G Chen, M Hermele, Phys. Rev. Lett. 112, 167203 (2014).

**11:51AM Y18.00002 Layered kagome spin ice** , JAMES HAMP, SIAN DUTTON, University of Cambridge, MARTIN MOURIGAL, Georgia Tech, PAROMITA MUKHERJEE, University of Cambridge, JOSEPH PADDISON, Georgia Tech, HARAPAN ONG, CLAUDIO CASTELNOVO, University of Cambridge — Spin ice materials provide a rare instance of emergent gauge symmetry and fractionalisation in three dimensions: the effective degrees of freedom of the system are emergent magnetic monopoles, and the extensively many ‘ice rule’ ground states are those devoid of monopole excitations. Two-dimensional (kagome) analogues of spin ice have also been shown to display a similarly rich behaviour. In kagome ice however the ground-state ‘ice rule’ condition implies the presence everywhere of magnetic charges. As temperature is lowered, an Ising transition occurs to a charge-ordered state, which can be mapped to a dimer covering of the dual honeycomb lattice. A second transition, of Kosterlitz-Thouless or three-state Potts type, occurs to a spin-ordered state at yet lower temperatures, due to small residual energy differences between charge-ordered states. Inspired by recent experimental capabilities in growing spin ice samples with selective (layered) substitution of non-magnetic ions, in this work we investigate the fate of the two ordering transitions when individual kagome layers are brought together to form a three-dimensional pyrochlore structure coupled by long range dipolar interactions. We also consider the response to substitutional disorder and applied magnetic fields.

**12:03PM Y18.00003 Theory of quantum kagome ice<sup>1</sup>** , YI-PING HUANG, MICHAEL HERMELE, Department of Physics, University of Colorado Boulder — Some pyrochlore oxides realize novel dipolar-octupolar (DO) doublets on the sites of the pyrochlore lattice of corner-sharing tetrahedra. With magnetic field along the (111) direction, such systems can approximately be described as decoupled layers of a  $S = \frac{1}{2}$  XYZ model on Kagome planes, with perpendicular magnetic field. A recent quantum Monte Carlo study found a zero temperature disordered phase in this model, dubbed quantum kagome ice, and proposed that it is a type of  $Z_2$  quantum spin liquid (J. Carrasquilla, Z. Hao and R. G. Melko, *Nat. Comm.*, **6**, 7421). We will describe an effective theory for this putative  $Z_2$  spin liquid, and present results on its symmetry fractionalization and resulting properties that may be tested in future numerical simulations.

<sup>1</sup>the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES) under Award DE-SC0014415

**12:15PM Y18.00004 Dynamics of quantum excitations in square ice<sup>1</sup>**, CLAUDIO CASTELNOVO, TCM group, Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK, STEFANOS KOURTIS, Department of Physics, Princeton University, Princeton, NJ 08544, USA — The study of emergent excitations in classical spin ice has culminated in the discovery of a condensed-matter realization of magnetic monopoles. In spin-ice materials where quantum fluctuations play an important role, excitations acquire quantum properties that promote them to more complicated and exciting objects. To understand these quantum excitations better in a relatively simple context, we construct a toy model of excited square ice and solve it both exactly by tuning it to a Rokhsar-Kivelson point and numerically for small clusters. We furthermore numerically evaluate the dynamic spin structure factor and compare it to effective free-particle theories. Our results offer a useful point of comparison for further theoretical and experimental work.

<sup>1</sup>Supported by ICAM branch contributions, EPSRC Grant No. EP/G049394/1, the Helmholtz Virtual Institute New States of Matter and Their Excitations and the EPSRC NetworkPlus on Emergence and Physics far from Equilibrium

**12:27PM Y18.00005 Magnetic monopoles in quantum spin ice**, OLGA PETROVA, RODERICH MOESSNER, Max Planck Institute for the Physics of Complex Systems, SHIVAJI SONDHI, Princeton University — Typical spin ice materials can be modeled using classical Ising spins. The geometric frustration of the pyrochlore lattice causes the spins to satisfy ice rules, whereas a violation of the ice constraint constitutes an excitation. Flipping adjacent spins fractionalizes the excitation into two monopoles. Long range dipolar spin couplings result in Coulombic interactions between charges, while the leading effect of quantum fluctuations is to provide the monopoles with kinetic energy. We study the effect of adding quantum dynamics to spin ice, a well-known classical spin liquid, with a particular view of how to best detect its presence in experiment. For the weakly diluted quantum spin ice, we find a particularly crisp phenomenon, namely, the emergence of hydrogenic excited states in which a magnetic monopole is bound to a vacancy at various distances [1].

[1] O. Petrova, R. Moessner, S. L. Sondhi, Phys. Rev. B **92**, 100401 (2015)

**12:39PM Y18.00006 Spinon walk in quantum spin ice**, YUAN WAN, JUAN CARRASQUILLA, ROGER MELKO, Perimeter Institute for Theoretical Physics — Quantum spin ice is a novel family of spin ice magnets that possess substantial quantum fluctuations. The fractional excitations are spinons, which are quantum analog of the monopoles in classical spin ice. The spinon propagates in quantum spin ice via quantum tunnelling. As opposed to a conventional quantum particle, the spinon moves in a background of disordered spins. The orientation of background spins controls the spinon motion, whereas the spinon motion in turn alters the spin background. One may naturally ask what a suitable framework for understanding the dynamics of spinon is in quantum spin ice, and furthermore, whether the spinon propagation is coherent. In this talk, we address these issues by investigating a minimal model that captures the essential features of single spinon dynamics in quantum spin ice. We demonstrate that the spinon motion can be thought of as a quantum walk with entropy-induced memory. Our numerical simulation shows that the simple quasi-particle behaviour emerges out of the intricate interplay between the spinon and the background spins.

**12:51PM Y18.00007 Neutron scattering in  $Er_{2-x}Y_xTi_2O_7$** , JONATHAN GAUDET, ALANNAH HALLAS, DALINI MAHARAJ, EDWIN KERMARREC, McMaster Univ, NICHOLAS P. BUTCH, NIST Center for Neutron Research, HANNA DABOWSKA, BRUCE GAULIN, McMaster Univ —  $Er_2Ti_2O_7$  (ETO) is a strong candidate for ground state selection via the order by disorder mechanism. A  $\psi_2$  magnetic ground state appears below  $T_N=1.2$  K, where  $\psi_2$  and  $\psi_3$  are the two basis states of the irreducible representation  $\Gamma_5$ . No sample dependence has been observed in the thermodynamics properties of ETO at low temperature, and in particular on its phase transition to long range magnetic order. ETO's ordered Neel state has been shown to be robust even to a relatively high level of magnetic dilution, as occurs with non-magnetic  $Y^{3+}$  substitution of  $Er^{3+}$ . However, recently two theoretical studies have predicted that ETO's  $\psi_2$  ground state should be unstable to formation of the  $\psi_3$  state, in the presence of such disorder. To explore this possibility, we grew single crystals of  $Er_{2-x}Y_xTi_2O_7$  (EYTO) with  $x = 0, 0.2$  and  $0.4$  and performed a systematic inelastic neutron scattering studies using the Disk Chopper time-of-flight spectrometer (DCS) at the National Institute of Standards and Technology (NIST). We will show elastic and inelastic neutron scattering at low temperatures and as a function of applied magnetic field for all three samples and discuss the role of such quenched disorder on the spin dynamics of EYTO.

**1:03PM Y18.00008 Semi-classical Theory of Quantum Spin Ice**, MICHAL KWASIGROCH, CLAUDIO CASTELNOVO, University of Cambridge — The low temperature properties of quantum spin ice compounds  $Yb_2Ti_2O_7$  and  $Pr_2Zr_2O_7$  are described by spin-1/2 degrees of freedom associated with magnetic Yb or Pr atoms residing on vertices of corner-sharing tetrahedra. Strong Ising exchange enforces the well-known 2-in-2-out rules for each tetrahedron at low temperatures. These describe the macroscopically degenerate spin ice configurations. Recently, it has been shown [Phys. Rev. B **69**, 064404 (2004)] that the addition of weak easy-plane exchange can lead to hybridisation of the classically allowed spin-ice configurations and the emergence of a gapless quantum spin liquid. We show that a semi-classical treatment of this U(1) liquid phase captures the QED-like physics and we derive quantitative estimates of the low-energy dispersion and the dynamic structure factor. These compare well with the existing Monte Carlo simulations.

**1:15PM Y18.00009 From pinch points to pinch lines: a new spin liquid on the pyrochlore lattice**, OWEN BENTON, LUDOVIC JAUBERT, HAN YAN, NIC SHANNON, Okinawa Inst of Sci & Tech — One of the most fascinating discoveries in the study of spin liquids has been the existence of emergent gauge fields arising out of a disordered magnetic ground state. The best known example is provided by the spin ice pyrochlores  $Ho_2Ti_2O_7$  and  $Dy_2Ti_2O_7$ , whose underlying gauge structure is revealed by the presence of pinch-point singularities in the neutron scattering response. Here we report the discovery of a new spin liquid on the pyrochlore lattice, the low temperature fluctuations of which are naturally described by the fluctuations of a tensor field with a continuous gauge freedom. This gauge structure underpins a novel form of spin correlations, giving rise to “pinch-line” singularities- line-like analogues of the pinch-point singularity extending along the  $\langle 111 \rangle$  directions of reciprocal space. Remarkably, our theory reproduces several otherwise unaccounted for features of neutron scattering experiments on  $Tb_2Ti_2O_7$ .

**1:27PM Y18.00010 Numerical evidence for a chiral spin liquid in the XXZ model on the kagome lattice in a magnetic field<sup>1</sup>**, HITESH CHANGLANI, KRISHNA KUMAR, BRYAN CLARK, EDUARDO FRADKIN, University of Illinois Urbana Champaign — Frustrated spin systems in two dimensions provide a fertile ground for discovering exotic states of matter, often with topologically non-trivial properties. In this work, we investigate the possible existence of a chiral spin liquid state in the spin 1/2 XXZ model on the frustrated kagome lattice in the presence of a magnetic field. This model is equivalent to a hard-core bosonic one with density-density interactions at finite filling fraction. Motivated by previous field theoretic predictions utilizing a Chern-Simons theory adapted for this lattice [1,2], we focus our attention to understanding the XY limit for the 2/3 magnetization plateau (equivalent to a system of hard-core bosons at 1/6 filling with weak nearest-neighbor repulsive interactions). Performing exact or accurate numerical computations, and based on energetics and construction of minimally entangled states and associated modular matrices, we provide evidence for such a spin liquid. We study the nature of this phase and examine its stability to additional interactions. [1] K. Kumar, K. Sun, and E. Fradkin, Phys. Rev. B **90**, 174409 (2014) [2] K. Kumar, K. Sun, and E. Fradkin, Phys. Rev. B **92**, 094433 (2015)

<sup>1</sup>We acknowledge support from the SciDAC program under award number DE-FG02-12ER46875.

**1:39PM Y18.00011 Spin liquids on an anisotropic kagome lattice**, ROBERT SCHAFFER, KYUSUNG HWANG, YEJIN HUH, YONG BAEK KIM, Univ of Toronto — Much recent theoretical and experimental effort has been devoted to the search for quantum spin liquids, which arise in the presence of strong frustration of magnetic interactions. Motivated by recent experiments on the vanadium oxyfluoride material DQVOF, we examine possible spin liquid phases on an anisotropic kagome lattice of  $S = 1/2$  spins, in which the  $C_6$  symmetry is broken to  $C_3$ . Using the projective symmetry group analysis, we determine the possible phases for both bosonic and fermionic  $Z_2$  spin liquids on this lattice. Using VMC, we study the Heisenberg model on this lattice, and show that a  $Z_2$  spin liquid emerges as the ground state in the presence of this anisotropy.

**1:51PM Y18.00012 Classification of  $Z_2$  spin liquids in a hyperkagome lattice by projective symmetry groups**, BIAO HUANG, Ohio State Univ - Columbus, YONG BAEK KIM, University of Toronto; Korea Institute for Advanced Study, YUAN-MING LU, Ohio State Univ - Columbus — Being a rare candidate material supporting 3D spin liquid states,  $\text{Na}_4\text{Ir}_3\text{O}_8$  has attracted much theoretical and experimental interest in the past decade. Propelled by such developments, we give a complete classification of  $Z_2$  spin liquid states in the hyperkagome lattice formed by  $\text{Ir}^{4+}$  ions in the projective symmetry group approach. A list of mean field states with different fractional quasi-particle excitations are correspondingly given, and their excitation gaps are analyzed. The effects of spin-orbit coupling due to the 5d electrons in Ir are also discussed. This work paves the way for further variational Monte-Carlo study of the spin liquid physics in hyperkagome lattices.

**2:03PM Y18.00013  $Z_2$  gauge theory for valence bond solids on the kagome lattice**, KYUSUNG HWANG, YEJIN HUH, YONG BAEK KIM, Department of Physics and Centre for Quantum Materials, University of Toronto, Toronto, Ontario M5S 1A7, Canada — We present an effective  $Z_2$  gauge theory that captures various competing phases in spin-1/2 kagome lattice antiferromagnets: the topological  $Z_2$  spin liquid (SL) phase, and the 12-site and 36-site valence bond solid (VBS) phases. Our effective theory is a generalization of the recent  $Z_2$  gauge theory proposed for SL phases by Wan and Tchernyshyov. In particular, we investigate possible VBS phases that arise from vison condensations in the SL. In addition to the 12-site and 36-site VBS phases, there exists 6-site VBS that is closely related to the symmetry-breaking valence bond modulation patterns observed in the recent density matrix renormalization group simulations. We find that our results have remarkable consistency with a previous study using a different  $Z_2$  gauge theory. Motivated by the lattice geometry in the recently reported vanadium oxyfluoride kagome antiferromagnet, our gauge theory is extended to incorporate lowered symmetry by inequivalent up- and down-triangles. We investigate effects of this anisotropy on the 12-site, 36-site, and 6-site VBS phases. Particularly, interesting dimer melting effects are found in the 36-site VBS. We discuss the implications of our findings and also compare the results with a different type of  $Z_2$  gauge theory used in previous studies.

## Friday, March 18, 2016 11:15AM - 2:15PM —

Session Y19 GMAG DCMF: Correlated Electron Magnetism 318 - Steven Disseler, NIST

**11:15AM Y19.00001 Orbital Delocalization and Enhancement of Magnetic Interactions in Perovskite Oxyhydrides**, KAI LIU, YUSHENG HOU, XINGAO GONG, HONGJUN XIANG, Fudan University, CCMG TEAM — Recent experiments showed that some perovskite oxyhydrides have surprisingly high magnetic-transition temperature. In order to unveil the origin of this interesting phenomenon, we investigate the magnetism in  $\text{SrCrO}_2\text{H}$  and  $\text{SrVO}_2\text{H}$  on the basis of first-principles calculations and Monte Carlo simulations. Our work indicates that the Cr-O-Cr superexchange interaction in  $\text{SrCrO}_2\text{H}$  is unexpectedly strong. Different from the previous explanation in terms of the  $\text{H}^-$  ion substitution induced increase of the Cr-O-Cr bond angle, we reveal instead that this is mainly because the 3d orbitals in perovskite oxyhydrides becomes more delocalized since  $\text{H}^-$  ions have weaker electronegativity and less electrons than  $\text{O}^{2-}$  ions. The delocalized 3d orbitals result in stronger Cr-O interactions and enhance the magnetic-transition temperature. This novel mechanism is also applicable to the case of  $\text{SrVO}_2\text{H}$ . Furthermore, we predict that  $\text{SrFeO}_2\text{H}$  will have unprecedented high Neel temperature because of the extraordinarily strong Fe-H-Fe  $\sigma$ -type interactions. Our work suggests the anion substitution can be used to effectively manipulate the magnetic properties of perovskite compounds.

**11:27AM Y19.00002 Understanding the magnetoelastic behavior of pure and Co substituted  $\text{GdNi}^1$** , DURGA PAUDYAL, Y. MUDRYK, The Ames Laboratory, Iowa State University, Ames, IA 50011, V. K. PECHARSKY, K. A. GSCHNEIDNER, JR., The Ames Laboratory and Department of Materials Science and Engineering, Iowa State University, Ames, IA 50011 — Total-energy calculations employing local spin density approximation including Hubbard  $U$  (onsite electron correlation) parameter and temperature and magnetic field dependent x-ray diffraction experiments show large anisotropic shifts in lattice parameters and a giant linear magnetostriction without a structural transformation and a negligible volume magnetostriction in  $\text{GdNi}$ . In agreement with the magnetization and heat-capacity experiments, the total-energy and band splitting results confirm that the anisotropic shape changes in  $\text{GdNi}$  are associated with the second-order ferromagnetic to paramagnetic transformation. When the band splitting due to the ferromagnetic ordering of the 4f moments increases, the concomitant anisotropic changes in the lattice minimize the total free energy of the crystal indicating an unusual interplay between magnetism and crystal structure. The positive formation energy at 0K and the nature of the density of states at the Fermi level confirm an unstable equiatomic Gd compound when Ni is fully substituted by Co. However, the enhanced effective exchange interactions with small Co substitutions increase the Curie temperature without losing the chemical stability.

<sup>1</sup>The Ames Laboratory is operated for the US DOE by Iowa State. This work was supported by the DOE, Office of Basic Energy Sciences, Materials Sciences Division under contract No. DE-AC02-07CH11358.

**11:39AM Y19.00003 Direct observation of a helical magnetic order near the superconducting state of  $\text{MnP}$  under pressure**, YISHU WANG, California Institute of Technology, YEJUN FENG, Argonne National Lab, J.-G. CHENG, Chinese Academy of Sciences, T. F. ROSENBAUM, California Institute of Technology — A recent high-pressure electrical transport study of the 3d transition metal compound  $\text{MnP}$  manifested a complex pressure-temperature phase diagram of different types of magnetism and superconductivity. However, the nature of the high-pressure magnetic phase proximate to the superconducting state was not determined. We use non-resonant X-ray magnetic diffraction to probe the magnetic order in  $\text{MnP}$  under pressure. We discover incommensurate helical order in a confined region under high pressure, and ascertain the phase boundary through the pressure evolution of the lattice. Although the antiferromagnetic and superconducting phases are separated, there is no signature of a strong first-order phase transition between them. We discuss how our direct observation of a helimagnetic order in  $\text{MnP}$  helps to better understand aspects of magnetically-mediated superconductivity.

**11:51AM Y19.00004 Neutron scattering study on the magnetic and superconducting phases of MnP**, SHINICHIRO YANO, NSRRC, DIANE LANCON, HENRIK RONNOW, EPFL, THOMAS HANSEN, ILL, JASON GARDNER, NSRRC — We have performed series of neutron scattering experiments on MnP. MnP has been investigated for decades because of its rich magnetic phase diagram. The magnetic structure of MnP is ferromagnetic (FM) below  $T_C = 291$  K. It transforms into a helimagnetic structure at  $T_S = 47$  K with a propagation vector  $q = 0.117a^*$ . Superconductivity was found in MnP under pressures of 8 GPa with a  $T_{SC}$  around 1 K by J.-G. Cheng. Since Mn-based superconductors are rare, and the superconducting phase occurs in the vicinity of FM, new magnetic and helimagnetic phases, there is a need to understand how the magnetism evolves as one approach the superconducting state. MnP is believed to be a double helix magnetic structure at  $T_S = 47$  K. We observed new  $2\delta$  and  $3\delta$  satellite peaks whose intensity are  $200 \sim 1000$  times smaller than these of  $1\delta$  satellite peaks on the cold triple axis spectrometer SIKA under zero magnetic fields. We also found the periods of helimagnetic structure changes as a function of temperature. If time permits, we will discuss recent experiments under pressure. However, we have complete picture of magnetic structure of this system with and without applied pressure, revealing the interplay between the magnetic and superconducting phases.

**12:03PM Y19.00005 Unusual behavior of uranium dioxide at high magnetic fields. Part I<sup>1</sup>**, K. GOFRYK, Idaho National Laboratory, M. JAIME, V. ZAPF, N. HARRISON, Los Alamos National Laboratory, A. SAUL, Aix-Marseille University, France, G. RADTKE, University of Paris 06, CNRS, France, J. C. LASHLEY, Los Alamos National Laboratory, M. SALAMON, University of Texas, Dallas, A. D. ANDERSSON, C. STANEK, T. DURAKIEWICZ, J. L. SMITH, Los Alamos National Laboratory —  $UO_2$  is a Mott-Hubbard insulator with well-localized  $5f$ -electrons and its crystal structure is the face-centered-cubic fluorite. It experiences a first-order antiferromagnetic phase transition at 30.8 K to a non-collinear antiferromagnetic structure that remains a topic of debate. It is believed that the first order nature of the transition results from the competition between the exchange interaction and the Jahn-Teller distortion of oxygen atoms. Despite extensive experimental and theoretical efforts the nature of the competing degrees of freedom and their couplings (such as spin-phonon coupling) are still unclear. Here we present results of our extensive thermodynamic investigations, on well-characterized and oriented single crystals of  $UO_2$ , focusing on magnetization  $M(T,H)$  measurements in DC and pulsed magnetic fields to up 65 T at the NHMFL.

<sup>1</sup>Work supported by the Department of Energy, Office of Basic Energy Sciences, Materials Sciences, and Engineering Division. The NHMFL Pulsed Field Facility is supported by the NSF, the U.S. D.O.E., and the State of Florida through NSF cooperative grant DMR

**12:15PM Y19.00006 Unusual behavior of uranium dioxide at high magnetic fields. Part II\***, M. JAIME, LANL, K. GOFRYK, INL, V. ZAPF, N. HARRISON, LANL, A. SAUL, Aix-Marseille Univ., G. RADTKE, Univ. Paris, J.C. LASHLEY, LANL, M. SALAMON, UT Dallas, A.D. ANDERSSON, C. STANEK, T. DURAKIEWICZ, J.L. SMITH, LANL — More than 65 years worth of unrelenting experimental and theoretical research on seemingly uncomplicated  $UO_2$ , a Mott-Hubbard insulator with well-localized  $5f$ -electrons and a fluorite  $fcc$  crystal structure, have not been able to elucidate some important questions such as the detailed nature of the low temperature AFM state, or the reasons behind unusual lattice properties that severely hinder the ability of this important nuclear material to transport heat. The high thermal conductivity shown by its non-magnetic counterpart,  $ThO_2$ , has hinted to the notion that unusual spin-lattice coupling is behind the crippled thermal behavior of  $UO_2$ . Here we present results of our thermodynamic investigations, on well-characterized and oriented single crystals, focusing on fiber Bragg grating magnetostriction measurements in pulsed magnetic fields to 90T at the NHMFL PFF. Our data support a multidomain non-collinear 3-k AFM order below 30.8K, coupled to an oxygen-cage trigonal distortion that breaks time reversal symmetry. \*Work supported by the US DOE BES, Mat. Sci., and Eng. Div. The NHMFL PFF is supported by the NSF, the U.S. DOE., and the State of Florida through NSF coop. grant DMR-1157490. Work at LANL was supported by the U.S. DOE BES project "Science at 100 Tesla".

**12:27PM Y19.00007 Modulated magnetism in the ferromagnet PrPtAl : clear experimental evidence of the 'order by disorder' theory.**, J.-PH. REID, Univ. of St. Andrews, CHRIS O'NEILL, Univ. of Edinburgh, ALEX WALKER, Univ. of St. Andrews, CALUM LITHGOW, GINO ABDUL-JABBAR, Univ. of Edinburgh, EDWARD YELLAND, Univ of St Andrews, DMITRY A. SOKOLOV, ANDREW D. HUXLEY, Univ. of Edinburgh — The ferromagnet PrPtAl is unlike any other. At the phase boundary between paramagnetism and ferromagnetism the fluctuations of the order parameter are so strong that energetically favourable phases of novel modulated magnetism emerge. In fact, its lack of order (the disorder) that is pivotal to promote a new order. This mechanism is referred to as order by disorder and is the centre of numerous theoretical studies [2,3]. In this seminar, following an introduction on the topic of ferromagnetic materials, I will show how we can use both electrical and thermal conductivities to learn everything about these phases of modulated magnetism and to validate the predictions of the order by disorder theory. [1] G. Abdul-Jabbar et al. Nat. Phys. 11, 321327 (2015). [2] G. J. Conduit et al. Phys. Rev. Lett. 103, 207201 (2009). [3] U. Karahasanovic et al. Phys. Rev. B 85, 165111 (2012).

**12:39PM Y19.00008 Unexpected magnetism, and transport properties in mixed lanthanide compound.**<sup>1</sup>, ARJUN PATHAK, KARL GSCHNEIDNER, JR, VITALIJ PECHARSKY, Ames Laboratory, US DOE, AMES LABORATORY TEAM — For intelligent materials design it is desirable to have compounds which have multiple functionalities such as a large magnetoresistance, ferromagnetic and ferimagnetic states, and field-induced first-order metamagnetic transitions. Here, we discuss one such example where we have combined two lanthanide elements Pr and Er in  $Pr_{0.6}Er_{0.4}Al_2$ . This compound exhibits multiple functionalities in magnetic fields between 1 and 40 kOe. It undergoes only a trivial ferrimagnetism to paramagnetism transition in a zero magnetic field, but  $Pr_{0.6}Er_{0.4}Al_2$  exhibits a large positive magnetoresistance (MR) for  $H \geq 40$  kOe, a small but non negligible negative MR for  $H \leq 30$  kOe, and a clear Griffiths-like phase behavior at  $< 1$  kOe. The compound also exhibits an asymmetry of hysteresis loop, or exchange bias (EB) effect after field cooling from the paramagnetic state. These phenomena are attributed to the competition between single-ion anisotropies of Pr and Er ions coupled with the opposite nearest-neighbor and next-nearest-neighbor exchange interactions.

<sup>1</sup>This work was supported by the US Department of Energy, Office of Basic Energy Science, Division of Material Sciences and Engineering. The research was performed at the Ames Laboratory. The Ames Laboratory is operated by Iowa State University for the US D

**12:51PM Y19.00009 Magnetic and Metal-Insulator Transition in natural Transition Metal Sulfides**, RENXIONG WANG, TRISTIN METZ, I-LIN LIU, KEFENG WANG, XIANGFENG WANG, Department of Physics, University of Maryland College Park, J.R JEFFRIES, Lawrence Livermore National Laboratory, S.R. SAHA, R.L. GREENE, J. PAGLIONE, Department of Physics, University of Maryland College Park, C. C. SANTELLI, J. POST, Department of Mineral Sciences, Smithsonian Museum of Natural History — In collaboration with the Smithsonian Institution's National Museum of Natural History, we present detailed studies of a class of natural minerals with potential to harbor correlated behavior. Transition metal sulfide minerals, such as Bornite ( $Cu_5FeS_4$ ), are an important family of compounds known for their thermoelectric properties. We will present low temperature experimental studies of magnetic transitions and focus on a compound that exhibits a metal to insulator transition coincident with entrance to an antiferromagnetic ground state, suggesting a potentially interesting system with promise for realizing new correlated states of matter in a naturally occurring mineral.

**1:03PM Y19.00010 Emergent triangular structure in doped extended honeycomb Hubbard model**, LUCA F. TOCCHIO, Consiglio Nazionale delle Ricerche (CNR) and International School for Advanced Studies (SISSA), RYUI KANEKO, ROSER VALENTI, Goethe-Universität Frankfurt, FEDERICO BECCA, Consiglio Nazionale delle Ricerche (CNR) and International School for Advanced Studies (SISSA), CLAUDIUS GROS, Goethe-Universität Frankfurt — We investigate the extended honeycomb Hubbard model at  $3/4$  filling. By using the mean-field approximation, we find a transition from a normal metal to a ferromagnetic metal at large Coulomb interaction  $U$ , and a transition to a charge ordered metal at large nearest-neighbor Coulomb interaction  $V$ . In the presence of both  $U$  and  $V$ , we find a metal-insulator transition, where the insulating state possesses charge and magnetic orders. The charge rich sites are nearly fully occupied, while the charge poor sites form a triangular lattice at nearly half filling. We also apply the variational Monte Carlo method to take into account quantum fluctuations beyond the mean-field treatment, and find this charge ordered state to be stable at sufficiently large  $U$  and  $V$ .

**1:15PM Y19.00011 Mechanisms of finite-temperature magnetism in the three-dimensional Hubbard model**, DANIEL HIRSCHMEIER, Institut für Theoretische Physik, Universität Hamburg,, HARTMUT HAFERMANN, Mathematical and Algorithmic Sciences Lab, France Research Center, Huawei Technologies Co, EMANUEL GULL, Department of Physics, University of Michigan, ALEXANDER I. LICHTENSTEIN, Institut für Theoretische Physik, Universität Hamburg,, ANDREY E. ANTIPOV, Department of Physics, University of Michigan — We examine the nature of the transition to the antiferromagnetically ordered state in the half-filled three-dimensional Hubbard model using the dual-fermion multiscale approach. Consistent with analytics, in the weak-coupling regime we find that spin-flip excitations across the Fermi surface are important, and that the strong coupling regime is described by Heisenberg physics. In the intermediate interaction, strong correlation regime we find aspects of both local and non-local correlations. We analyze the critical exponents of the transition in the strong coupling regime and find them to be consistent with Heisenberg physics down to an interaction of  $U/t=10$ .

**1:27PM Y19.00012 Quantum Monte Carlo study of magnetism in the Lieb Lattice**, NATANIEL COSTA, TIAGO SANTOS<sup>1</sup>, THEREZA PAIVA, RAIMUNDO DOS SANTOS, Universidade Federal do Rio de Janeiro, RICHARD SCALETTAR, UC Davis — The Hubbard model on the 'Lieb lattice' provides an important example of how flat band systems may lead to ferromagnetism: at half filling Lieb proved that a ferrimagnetic ground state *can* be achieved. Since a rigorous proof that long range order does indeed emerge is still lacking, here we report Determinant Quantum Monte Carlo (DQMC) simulations for this model. We found that the spin correlation between nearest neighbors are always antiferromagnetic, and that for small  $U$  ferromagnetic long range order does set in in the ground state. However, spatial spin correlations weaken as  $U$  is increased, and we established that long range order is suppressed above  $U_c \approx 4.5$ . We obtain the dependence of the magnetization with the on-site repulsion  $U$ , and show that it displays a maximum at  $U \approx 3$ . The behavior of the compressibility and of the double occupancy across this transition is also discussed.

<sup>1</sup>Also at Department of Physics, UC Davis

**1:39PM Y19.00013 Using dephasing to distinguish composite and elementary particles**, LEONID P. PRYADKO, University of California, Riverside, CLAUDIO CASTELNOVO, University of Cambridge, MARK I. DYKMAN, Michigan State University, RODERICH MOESSNER, Max-Planck-Institut für Physik komplexer Systeme, Dresden, VADIM N. SMELYANSKIY, Google — Many-body topological excitations like domain walls in 1D can be treated quantum mechanically as particles. We establish limits on such a description in the presence of weak dephasing. Specifically, we compare dynamics of a particle in a tight-binding model with weak on-site dephasing, and that of a kink separating two locally distinguishable domains. In the latter case, dephasing rate of the off-diagonal matrix elements  $\rho_{ab}$  of the density matrix is proportional to the distance  $|a - b|$  from the diagonal, compared to a constant dephasing rate of such matrix elements for a single particle. We show that in a transport setting (quantum diffusion), with small density gradients, the dynamics of these two systems is nearly identical. The difference can only be seen when far off-diagonal matrix elements are important, as in the formation of a bound state, or in a two-path interferometer. We analyze the spectroscopic signature of a bound state of a domain wall, and suggest possible experimental signatures in spin chains.

**1:51PM Y19.00014 Spontaneous symmetry breaking in correlated wave functions**, RYUI KANEKO, Goethe-Universität Frankfurt, LUCA F. TOCCHIO, Consiglio Nazionale delle Ricerche (CNR) and International School for Advanced Studies (SISSA), ROSER VALENTI, Goethe-Universität Frankfurt, FEDERICO BECCA, Consiglio Nazionale delle Ricerche (CNR) and International School for Advanced Studies (SISSA), CLAUDIUS GROS, Goethe-Universität Frankfurt — We show that Jastrow-Slater wave functions, in which a density-density Jastrow factor is applied onto an uncorrelated fermionic state, may possess long-range order even when all symmetries are preserved in the wave function. This fact is mainly related to the presence of a sufficiently strong Jastrow term (also including the case of full Gutzwiller projection, suitable for describing spin models). Selected examples are reported, including the spawning of Néel order and dimerization in spin systems, and the stabilization of density and orbital order in itinerant electronic systems. [1] Ryui Kaneko, Luca F. Tocchio, Roser Valentí, Federico Becca, and Claudius Gros, arXiv:1510.08653.

**2:03PM Y19.00015 On the magnetic structure and band gap of the double perovskite Ba<sub>2</sub>CuOsO<sub>6</sub>: Density functional analysis<sup>1</sup>**, CHANGHOON LEE, JISOOK HONG, JI HOON SHIM, Pohang University of Science and Technology, MYUNG-HWAN WHANGBO, North Carolina State University — The ordered double-perovskite Ba<sub>2</sub>CuOsO<sub>6</sub>, consisting of 3d and 5d transition-metal magnetic ions (Cu<sup>2+</sup> and Os<sup>6+</sup>, respectively), is a magnetic insulator. It obeys the Curie-Weiss law with  $\theta = -13.3$  K. We evaluated the spin exchange interactions of Ba<sub>2</sub>CuOsO<sub>6</sub> by performing energy-mapping analysis based on DFT+U calculations and determined the band gap of Ba<sub>2</sub>CuOsO<sub>6</sub> by DFT+U and DFT+U+SOC calculations. The antiferromagnetic ordering of Ba<sub>2</sub>CuOsO<sub>6</sub> is due largely to the spin exchange interactions between Cu<sup>2+</sup> ions, which are enhanced by the empty eg orbitals of the intervening Os<sup>6+</sup> ions. Both electron correlation and spin-orbit coupling are necessary to open a band gap for Ba<sub>2</sub>CuOsO<sub>6</sub>.

<sup>1</sup>2013R1A1A2060341

**Friday, March 18, 2016 11:15AM - 2:15PM** —  
Session Y20 DMP: Correlations and Superconductivity in Fe-chalcogenides III 319 - Robert Moore, SLAC

**11:15AM Y20.00001 Unraveling the electron pairing mechanism of FeSe by MBE and STM<sup>1</sup>**, CANLI SONG, Tsinghua University — Studies of high-transition-temperature superconductivity usually suffer from various imperfections in materials. Here we apply the state-of-the-art molecular beam epitaxy (MBE) to prepare controllably high-quality FeSe films on various substrates, and explore their superconducting properties using cryogenic scanning tunneling microscope [1,2]. Single impurities, twin boundaries as well as strain are found in the MBE-grown FeSe films on graphene, and invariably suppress the superconductivity [1, 3, 4]. Meanwhile, electronic nematicity and signatures of a bosonic mode, whose energy also decreases with strain [4], were identified. More significantly, we observed two disconnected superconducting domes at alkali-metal potassium (K)-dosed FeSe surface, stepping towards the mechanistic understanding of superconductivity in FeSe-derived superconductors. Our results are clarifying the secret of high-T<sub>c</sub> superconductivity in FeSe-related superconductors, and by implications, in other unconventional superconductors, and guiding how to enhance T<sub>c</sub> by interface engineering. References: [1] Can-Li Song et al., Science 332, 1410 (2011). [2] Q. Y. Wang et al., Chin. Phys. Lett. 29, 037402 (2012). [3] C. L. Song et al., Phys. Rev. Lett. 109, 137004 (2012). [4] C. L. Song et al., Phys. Rev. Lett. 112, 057002 (2014).

<sup>1</sup>This work was nancially supported by National Science Foundation and Ministry of Science and Technology of China.

**11:51AM Y20.00002 In-plane Resistivity Anisotropy in Mechanically De- twinned Single Crystals FeSe**, ERIK TIMMONS, MAKARIY TANATAR, The Ames Laboratory and Iowa State University, ANNA BOHMER, The Ames Laboratory, GIL DRACHUCK, Iowa State University, VALENTIN TAUFOR, SERGEY BUD'KO, PAUL CANFIELD, RUSLAN PROZOROV, The Ames Laboratory and Iowa State University, MICHAEL SCHUETT, RAFAEL FERNANDES, University of Minnesota, RUSLAN PROZOROV GROUP TEAM, PAUL CANFIELD GROUP TEAM, RAFAEL FERNANDES GROUP TEAM — The in-plane resistivity anisotropy was studied in stress-detwinned vapor transport grown single crystals of FeSe, which exhibit the tetragonal-orthorhombic structural transition temperature at  $T_s \sim 90$  K in unstrained samples, but no long-range magnetic order. Direct transport and elastoresistivity measurements show a significant in-plane resistivity anisotropy above  $T_s$  induced by a very moderate mechanical stress. This anisotropy peaks slightly below  $T_s$  and decreases to nearly zero on cooling to base temperature, while the degree of orthorhombic distortion grows monotonically before saturating at low temperatures. We explain the non-monotonic temperature dependence of the resistivity anisotropy as a result of the inelastic scattering of electrons by anisotropic spin fluctuations. Experimental work was supported by the U.S. DOE/OS/MSED and was performed at the Ames Laboratory, Iowa State University under contract DE-AC02-07CH11358. M.S. acknowledges the support from the Humboldt Foundation. R.M.F. is supported by the U.S. DOE, Office of Science, Basic Energy Sciences, under Award No. DE-SC0012336.

**12:03PM Y20.00003 Nematic quantum criticality in FeSe<sub>1-x</sub>S<sub>x</sub> revealed by elastoresistance measurements**, SUGURU HOSOI, KOHEI MATSUURA, HAO WANG, KOUSUKE ISHIDA, YUTA MIZUKAMI, Department of Advanced Materials Science, University of Tokyo, Kashiwa, Chiba 277-8561, Japan, TATSUYA WATASHIGE, SHIGERU KASAHARA, YUJI MATSUDA, Department of Physics, Kyoto University, Sakyo-ku, Kyoto 606-8502, Japan, TAKASADA SHIBAUCHI, Department of Advanced Materials Science, University of Tokyo, Kashiwa, Chiba 277-8561, Japan — Electronic nematicity and its connection to the high-temperature superconductivity is one of the central issues in iron-based superconductors. Among them, FeSe is unique in that it exhibits a tetragonal-to-orthorhombic structural transition but no antiferromagnetic order, which enables us to study the nematicity without the effect of magnetism. Here we report on elastoresistance measurements in FeSe<sub>1-x</sub>S<sub>x</sub> evidencing a nonmagnetic nematic quantum critical point near  $x \sim 0.2$ . When the Se site is substituted by the isovalent S, the structural transition temperature is reduced gradually and it vanishes above  $x \sim 0.2$ . From the changes in in-plane resistivity induced by anisotropic strain, we evaluate the nematic susceptibility which shows Curie-Weiss-like temperature dependence. We find that with increasing  $x$  the Weiss temperature changes its sign indicating a quantum critical point, while there is no sign of antiferromagnetism for all samples. The superconducting transition temperature does not show a significant change with S concentration, suggesting that the nonmagnetic nematic quantum criticality does not help to enhance superconductivity in this system.

**12:15PM Y20.00004 Nematic magnetoelastic effect contrasted between Ba(Fe<sub>1-x</sub>Co<sub>x</sub>)<sub>2</sub>As<sub>2</sub> and FeSe**, YUWEN HU<sup>1</sup>, XIAO REN, Peking University, China, RUI ZHANG, Rice University, USA, HUIQIAN LUO, Chinese Academy of Sciences, China, SHIGERU KASAHARA, TATSUYA WATASHIGE, Kyoto University, Japan, TAKASADA SHIBAUCHI, University of Tokyo, Japan, PENGCHENG DAI, Rice University, USA, YAN ZHANG, Peking University, China; Collaborative Innovation Center of Quantum Matter, China, YUJI MATSUDA, Kyoto University, Japan, YUAN LI, Peking University, China; Collaborative Innovation Center of Quantum Matter, China — Whether the nematic order ubiquitously found in Fe-based superconductors is driven by the spin or the charge or orbital degree of freedom is currently under heated debate. To elucidate its microscopic origin, we report a Raman scattering study of lattice dynamics, which quantify the extent of  $C_4$ -symmetry breaking, in BaFe<sub>2</sub>As<sub>2</sub> and FeSe. FeSe possesses a nematic ordering temperature  $T_s$  and orbital-related band-energy split below  $T_s$  that are similar to those in BaFe<sub>2</sub>As<sub>2</sub>, but unlike BaFe<sub>2</sub>As<sub>2</sub> it has no long-range magnetic order. We find that the  $E_g$  phonon-energy split in FeSe sets in only well below  $T_s$ , and its saturated value is substantially smaller than that in BaFe<sub>2</sub>As<sub>2</sub>. Together with reported results for the Ba(Fe<sub>1-x</sub>Co<sub>x</sub>)<sub>2</sub>As<sub>2</sub> family, the data suggest that magnetism exerts a major influence on the lattice.

<sup>1</sup>Present address: Princeton University, USA

**12:27PM Y20.00005 Berry's phase observed in the ordered state of Fe(Se,S)**, SHIGERU KASAHARA, T. YAMASHITA, Y. SHIMOYAMA, T. WATASHIGE, Y. MATSUDA, Kyoto University, J. BÉARD, M. NARDONE, W. KNAFO, LNCMI-Toulouse, M.D. WATSON, N.R. DAVIS, A.I. COLDEA, Univ. of Oxford, M. SUZUKI, R. ARITA, RIKEN, H. IKEDA, Ritsumeikan Univ., T. SHIBAUCHI, The Univ. of Tokyo — Among iron-based superconductors, FeSe offers a unique platform in that it exhibits a nematically ordered phase without long-range magnetic ordering. Several experiments have shown that the low-temperature Fermi surface of FeSe consists only of very small, shallow pockets [1-3]. Tuning the ground state via isoelectronic chemical substitution provides an ideal way to solve the puzzles regarding the nematic ordering in this material. Here, by using ultra-high magnetic fields up to  $\sim 90$  T, we report observations of Shubnikov-de Haas (SdH) oscillations in isoelectronically substituted Fe(Se,S). For the smallest pocket of  $\sim 0.2\%$  of the Brillouin-zone, we observe non-zero  $\pi$  Berry's phase shift in the SdH oscillations. Our results indicate presence of Dirac cone, which would be a key to understand the mechanism of the nematic ordering in this system.

[1] S. Kasahara *et al.*, Proc. Natl. Acad. Sci. U. S. A. 111, 16309 (2014).

[2] T. Terashima *et al.*, Phys. Rev. B 90, 144517 (2014).

[3] M.W. Watson *et al.*, Phys. Rev. Lett. 115, 027006 (2015).

### 12:39PM Y20.00006 Nematicity in FeSe single crystals probed by pump-probe spectroscopy<sup>1</sup>

, C. W. LUO, P. C. CHENG, K. H. WU, J. Y. JUANG, Department of Electrophysics, National Chiao Tung University, Hsinchu 300, Taiwan, S.-H. WANG, J.-C. CHIANG, J.-Y. LIN, Institute of Physics, National Chiao Tung University, Hsinchu 300, Taiwan, D. A. CHAREEV, Institute of Experimental Mineralogy, Chernogolovka, Moscow Region, 142432, Russia, O. S. VOLKOVA, A. N. VASILIEV, Low Temperature Physics and Superconductivity Department, Moscow State University, 119991 Moscow, Russia — The anisotropic quasiparticle dynamics in FeSe single crystals have been studied by polarized pump-probe spectroscopy. Two distinguishable relaxation components were unambiguously observed in transient reflectivity changes ( $\Delta R/R$ ). The orientation-dependent fast component with the timescale of 0.1-1.5 ps associated with the electronic structure clearly shows two-fold symmetry, which further reveals the gap opening along  $k_y$  below the temperature of structure phase transition ( $T_s$ ) and the electronic nematicity can persist up to 200 K. For the slow component with the timescale of 8-25 ps, it is assigned to the energy relaxation through spin sub-system and also shows a two-fold symmetry below  $T_s$ . However, this two-fold symmetry is dramatically weakened above  $T_s$  and surprisingly persists up to at least 200 K. Consequently, the high-temperature nematic fluctuations in FeSe may be driven by the order parameters which associated with both charge (orbital) and spin sub-systems.

<sup>1</sup>This project is financially sponsored by the MOST, Taiwan, (Grants No. 103-2923-M-009-001-MY3) and the MOE-ATU plan at NCTU

### 12:51PM Y20.00007 Nematic quantum paramagnet and possible application to FeSe , FA WANG,

Peking Univ, STEVEN A. KIVELSON, Stanford University, DUNG-HAI LEE, UC Berkeley — The nematic phases in iron pnictides are in close proximity to the stripe antiferromagnetic order, suggesting that magnetism is the driving force for the spontaneous 4-fold crystal rotation symmetry breaking. In contrast, bulk FeSe shows a nematic phase below 90K at ambient pressure, but has no magnetic long range order down to very low temperature. This prompts suggestions that the nematicity in FeSe is driven by some other mechanism. We argue that magnetic correlation can still drive nematic order in the absence of magnetic order. By field theoretical considerations and exact diagonalization results on finite size lattices, we conclude that the paramagnetic phase in frustrated spin-1  $J_1$ - $J_2$  models on square lattice is such a "nematic quantum paramagnet", which breaks only the crystal 4-fold rotation symmetry. The prototype wavefunctions of such quantum ground states are horizontal(vertical) aligned spin-1 AKLT chains. We suggest that the local spins in FeSe may form this phase due to strong frustration. One unique consequence of this proposal is that the nematic paramagnetic phase will be close to both stripe and Neel antiferromagnetic order, and will thus host low but finite energy spin fluctuations at both ordering wavevectors.

### 1:03PM Y20.00008 Sign-Reversing Orbital Polarization in FeSe Driven by the Nematic Symmetry Breaking Self-Energy , SEIICHIRO ONARI, Okayama University, YOUICHI YAMAKAWA, HIROSHI KONTANI, Nagoya University —

Novel  $k$ -dependence of the orbital polarization in the orthorhombic phase in FeSe has been observed by the ARPES measurement [1], where the sign-reversal of the orbital splitting appears between hole pockets and electron pockets. We analyze the multi-orbital Hubbard models in the orbital-ordered state by extending the orbital-spin fluctuation theory [2]. The present theory describes the spontaneous symmetry breaking with respect to the orbital polarization and spin susceptibility self-consistently. In the orbital-ordered state, we obtain the two Dirac cone Fermi pockets in addition to the sign-reversing orbital polarization, consistently with experiments. The orbital-order originates from the strong orbital-spin interplay due to the Aslamazov-Larkin processes. [1] Y. Suzuki *et al.*, arXiv:1504.00980. [2] S. Onari, Y. Yamakawa, and H. Kontani, arXiv:1509.01172.

### 1:15PM Y20.00009 Nematicity and magnetism in FeSe and other families of Fe-based superconductors , YOUICHI YAMAKAWA, Nagoya university, SEIICHIRO ONARI, Okayama university, HIROSHI KONTANI, Nagoya university —

We investigate the emergence of the nematic orbital order ( $n_{xz} \neq n_{yz}$ ) in various Fe-based superconductors based on the first-principles Hubbard models [1]. In Fe-based superconductors, spin-fluctuation-mediated large orbital-fluctuations appear because of the strong orbital-spin interplay due to the many-body effect. This effect is very significant in FeSe due to the small ratio between the Hund's and Coulomb interactions ( $J/\bar{U}$ ) and large  $d_{xz}$ ,  $d_{yz}$ -orbitals weight at the Fermi level. For this reason, in FeSe, orbital order is established by weak spin fluctuations, so the magnetism is absent. In contrast, in LaFeAsO, the magnetic order appears just below the structural transition temperature both experimentally and theoretically. Thus, the orbital-spin interplay is the key ingredient of the wide variety of the normal-state phase diagram in Fe-based superconductors. [1] Y. Yamakawa, S. Onari, and H. Kontani, arXiv:1509.01161.

### 1:27PM Y20.00010 Determinant Quantum Monte Carlo Study of a Multi-orbital Electronic Model: Application to Nematic and Superconducting Order in FeSe , PHILIPP DUMITRESCU, MAKSYM SERBYN,

University of California, Berkeley, RICHARD SCALETTAR, University of California, Davis, ASHVIN VISHWANATH, University of California, Berkeley — The iron chalcogenide FeSe has attracted much recent interest due to a high superconducting transition in monolayer samples. In bulk samples, nematic order is seen without the presence of magnetic order, hinting at the importance of nematic order in determining the monolayer properties. We study an effective two band model of the iron-pnictides with interactions that capture the nematic ordering arising from spontaneous symmetry breaking between the two orbitals. These models are sign-problem free and can be simulated in an unbiased fashion using Determinant Quantum Monte Carlo. We find a variety of unexpected orders and consider the effects of the nematic fluctuations on superconductivity.

### 1:39PM Y20.00011 Alternating-Sign S-Wave Superconductivity in Single-Layer FeSe from the Local Moment Limit<sup>1</sup> , JOSE RODRIGUEZ, California State University at Los Angeles —

We obtain the exact low-energy spectrum of two mobile electrons roaming over a 4 by 4 lattice of iron atoms governed by a t-J model for a monolayer of FeSe. Each iron atom contains the minimum  $d_{xz}$  and  $d_{yz}$  orbitals. The hopping parameters (t) account only for electron bands centered at wave vectors  $(\pi, 0)$  and  $(0, \pi)$ , while the Heisenberg exchange parameters (J) imply a quantum-critical point (QCP) at half-filling that separates a commensurate spin-density wave (cSDW) at strong Hund coupling from a hidden-order antiferromagnet at weak Hund coupling. The hidden-order antiferromagnet has ordering wavevector  $(\pi, \pi)$ . After tuning the Hund coupling near the QCP, we find an  $S^{+-}$  ground state and a  $D^{+-}$  excited state that are separated in energy from the edge of a quasi-particle continuum. Both bound states alternate in sign between electron pairs at cSDW momenta and electron pairs at emergent electronic structure with zero 2D momentum. Exact calculations for a single electron with the same t-J model parameters find that the emergent electronic structure at zero 2D momentum moves off the Fermi level as Hund coupling weakens below the QCP. We therefore suggest that the above  $S^{+-}$  groundstate describes Coopers pairs in a monolayer of FeSe.

<sup>1</sup>Research supported in part by AFOSR grant no. FA9550-13-1-0118

### 1:51PM Y20.00012 Comparing the anomalous phonons in Fe(Te,Se) and (Fe,Ni)(Te,Se) via neutron scattering , JOHN SCHNEELOCH, Brookhaven National Laboratory, ZHIJUN XU, University of California, Berkeley, GENDA GU, IGOR ZALIZNYAK, Brookhaven National Laboratory, BARRY WINN, Oak Ridge National Laboratory, JOSE RODRIGUEZ-RIVERA, National Institute of Standards and Technology, ROBERT BIRGENEAU, University of California, Berkeley, GUANGYONG XU, JOHN TRANQUADA, Brookhaven National Laboratory —

We studied the anomalous acoustic-type phonons in the Fe(Te,Se) iron-based superconductor family that arise from the (100) Bragg peak, which is forbidden according to the reported crystal structure for these materials. Inelastic neutron scattering was performed on superconducting and non-superconducting crystals of various compositions. The (100) phonons were much weaker in a non-superconducting nickel-doped crystal than in a superconducting crystal with similar selenium fraction, but comparison with another non-superconducting crystal suggests the difference is not simply related to superconductivity. This composition dependence was observed for both transverse and longitudinal phonons. The temperature dependences of the (100) phonons resembled those of conventional phonons. We will discuss these results and possible explanations for the relation between composition and lattice dynamics in this system.

**2:03PM Y20.00013 Elucidating the magnetic and superconducting phases in  $\text{Rb}_x\text{Fe}_y\text{Se}_{2-z}\text{S}_z$ .** , MENG WANG, MING YI, University of California, Berkeley, WEI TIAN, Oak Ridge National Laboratory, EDITH BOURRET-COURCHESNE, Lawrence Berkeley National Laboratory, ROBERT BIRGENEAU, University of California, Berkeley — The complex interdigitated phases have greatly frustrated attempts to document the basic features of the superconductivity in the  $A_x\text{Fe}_y\text{Se}_{2-z}\text{S}_z$  ( $A$  = alkali metals) system. We have employed elastic neutron scattering, energy-dispersive x-ray spectroscopy, and resistivity measurements to elucidate the relations of these phases in  $\text{Rb}_x\text{Fe}_y\text{Se}_{2-z}\text{S}_z$ . We find: i) the iron content is the driving parameter in stabilizing the structural separated phases; ii) the existence of the 245 antiferromagnetic phase stabilizes the iron vacancy free phase; iii) the sulfur substitutions progressively tune the iron vacancy free phase from a superconductor in  $\text{Rb}_x\text{Fe}_2\text{Se}_2$  to a metallic phase in  $\text{Rb}_x\text{Fe}_2\text{S}_2$ . Several phase diagrams as functions of the iron content and the Se:S ratio will be provided.

**Friday, March 18, 2016 11:15AM - 2:15PM –**

**Session Y21 GSCCM DCOMP DMP: Materials in Extremes: Metals at High Strain Rates II**  
320 - Ramon Ravelo, University of Texas, El Paso

**11:15AM Y21.00001 The relaxation of shear stress in a metal alloys with a wide grain size distribution under shock loadings** , EVGENIYA G. SKRIPNYAK, VLADIMIR V. SKRIPNYAK, National Research Tomsk State University, NATALIYA V. SKRIPNYAK<sup>1</sup>, National Research Tomsk State University — The influence of a grain size distribution on the relaxation of shear stress in the metal alloys under shock wave loading was investigated by numerical simulation. The model takes into account the influence of a grain size distribution and a precipitation concentration on the kinetics of shear stress relaxation. The relaxation rate of shear stress in shock waves depends on the specific volume of nano- and ultra-fine grains in the FCC and HCP metal alloys. A wide distribution of grain size reduces the relaxation rate of elastic precursor in HCP alloys. The relaxation of the elastic precursor depends on size and volume concentration of precipitates in metal alloys. Results of simulation show that the rate of plastic deformation in the shock wave exceeds significantly that of the elastic precursor at the same value of shear stresses.

<sup>1</sup>Linköping University, Sweden

**11:27AM Y21.00002 Strain Functionals for Characterizing Atomistic Geometries** , EDWARD KOBER, SVEN RUDIN, Los Alamos National Laboratory — The development of a set of strain tensor functionals that are capable of characterizing arbitrarily ordered atomistic structures is described. This approach defines a Gaussian-weighted neighborhood around each atom and characterizes that local geometry in terms of  $n$ -th order strain tensors, which are equivalent to the moments of the neighborhood. Fourth order expansions can distinguish the cubic structures (and deformations thereof), but sixth order expansions are required to fully characterize hexagonal structures. Other methods used to characterize atomic structures, such as the Steinhardt parameters or the centrosymmetry metric, can be derived from this more general approach. These functions are continuous and smooth and much less sensitive to thermal fluctuations than other descriptors based on discrete neighborhoods. They allow material phases, deformations, and a large number of defect structures to be readily identified and classified. Applications to the analysis of shock-loaded samples of Cu, Ta and Ti will be presented. This strain functional basis can also then be used for developing interatomic potential functions, and an initial application to Cu will be presented.

**11:39AM Y21.00003 Dual Domain Material Point Method for Materials in Extreme<sup>1</sup>** , DUAN ZHANG, TILAK DHAKAL, Los Alamos National Laboratory — Dual domain material point method is the latest version of the material point method designed to overcome many numerical difficulties of the original material point method with an increased numerical accuracy. In this talk, after reviewing the numerical theory of the method, we apply this method to cases involving extreme material deformation, shock propagation, and pulverization based on continuum theories. We will compare this method to other similar particle methods, and then examine the applicability and needed modification of the continuum theory for cases involving strong thermodynamic non-equilibrium. The history of the material deformation is often important in such systems. We will explore the Lagrangian capability brought by the use of particles in the dual domain material point method and introduce a multiscale scheme taking advantages of the particle-mesh communications in the method to study history dependent thermodynamically non-equilibrium systems, caused by extreme material deformations, such as hypervelocity impact and shock loading. We will also discuss the history tracking capability, analyze numerical advantages and difficulties, and show the results obtained from this numerical scheme.

<sup>1</sup>Work supported by ASC project of LANL

**11:51AM Y21.00004 Multiscale Modeling using Molecular Dynamics and Dual Domain Material Point Method<sup>1</sup>** , TILAK DHAKAL, DUAN ZHANG, Los Alamos National Laboratory — For problems with very large material deformation rate, the time scale of material deformation can be shorter than the time that the material takes to reach a thermodynamic equilibrium. In these situations constitutive relation for the material becomes difficult to obtain. Furthermore, for these non-equilibrium problems, the history dependency of the material becomes important. A numerical method capable of tracking material deformation history is needed in a numerical simulation effort. In this work we use the dual domain material point (DDMP) method, which uses Lagrangian material points to track the history of the material where as Eulerian grids are used to calculate the gradients in continuum level. Molecular dynamics (MD) calculations are performed in the material points to calculate the closure quantities such as stress bypassing the need for a constitutive relation. Since the material points do not need to directly communicate among each other, the MD calculations can be done in parallel. In this work, GPUs are used to accelerate MD calculations. Examples of shock wave propagation in monoatomic gas and in Cerium metal are presented.

<sup>1</sup>Work supported by ASC project of LANL.

**12:03PM Y21.00005 Study on the oblique perforation of thin steel plates by flat and ogival projectiles** , ZITAO GUO, School of Civil engineering & urban construction, Jiujiang University, WEI ZHANG, PENG REN, Hypervelocity Impact Research Center, Harbin Institute of Technology, HYPERVELOCITY IMPACT RESEARCH CENTER COLLABORATION — This paper presents a numerical study on the oblique perforation of thin steel plates. Numerical simulations of 1 mm single A3 steel plates impacted by flat and ogival projectiles at 0, 15, 30, 45 and 60 angles over a range of velocities from 50 to 250 m/s were performed using the finite element code ABAQUS, where a modified versions of the J-C constitutive relation and fracture criterion based on a series of quasi-static and dynamic tensile tests with smooth and notched axisymmetric specimens were adopted to approximate behaviors of target material. Corresponding oblique perforation experiments were also conducted in order to be compared and calibrated. Initial-residual velocity curves and ballistic limits of targets under different angle impact were determined and compared, and the effects of projectile nose shape and obliquity on the ballistic resistance and failure models of targets were investigated. Results show that the nose shape of the projectile and oblique angles severely affected both the energy absorption and the failure mode of the target plate during perforation. Good agreement is found between the numerical simulations and experimental results.

**12:15PM Y21.00006 Ductility of metal alloys with grain size distribution in a wide range of strain rates**, VLADIMIR V. SKRIPNYAK, NATALIYA V. SKRIPNYAK<sup>1</sup>, EVGENIYA G. SKRIPNYAK, National Research Tomsk State University — Ductility of ultrafine grained (UFG) metal alloys with a distribution of grain size was investigated in wide loading conditions by numerical simulation. The multiscale models with a unimodal and a bimodal grain size distributions were developed using the data of structure research of hexagonal close packed and face center cubic UFG alloys. Macroscopic fracture is considered as a result of the formation of percolation clusters of damage at the mesoscopic level. The critical fracture strain of UFG alloys on the mesoscale level depends on the relative volumes of coarse grains. The nucleation of damages at quasi-static and dynamic loading is associated with strain localization in UFG partial volumes with bimodal grain size distribution. The concentration of damages arise in the vicinity of the boundaries of coarse and ultrafine grains. The occurrence of a bimodal grain size distributions causes the increase of UFG alloys' ductility, but decrease of their tensile strength.

<sup>1</sup>Linköping University, Sweden

**12:27PM Y21.00007 Experimental analysis of quasi-static and dynamic fracture initiation toughness of gy4 armor steel material<sup>1</sup>**, PENG REN, Jiangsu University of Science and Technology, ZITAO GUO, Jiujiang University — Quasi-static and dynamic fracture initiation toughness of gy4 armour steel material are investigated using three point bend specimen. The modified split Hopkinson pressure bar (SHPB) apparatus with digital image correlation (DIC) system is applied to dynamic loading experiments. Full-field deformation measurements are obtained by using DIC to elucidate on the strain fields associated with the mechanical response. A series of experiments are conducted at different strain rate ranging from 10<sup>-3</sup> s<sup>-1</sup> to 10<sup>3</sup> s<sup>-1</sup>, and the loading rate on the fracture initiation toughness is investigated. Specially, the scanning electron microscope imaging technique is used to investigate the fracture failure micromechanism of fracture surfaces. The gy4 armour steel material fracture toughness is found to be sensitive to strain rate and higher for dynamic loading as compared to quasi-static loading.

<sup>1</sup>This work is supported by National Nature Science Foundation under Grant 51509115

**12:39PM Y21.00008 Lithium Melt Line Determined using the Z Method**, MARVIN ZOCHER, LEONID BURAKOVSKY, Los Alamos National Laboratory — The Z method is a numerical procedure that can be used for the construction of phase diagrams. In the present work the method is discussed and its use is demonstrated through a determination of the melt line for lithium.

**12:51PM Y21.00009 A fitting empirical potential for NiTi alloy and its application.**, GUOWU REN, TIEGANG TANG, Institute of Fluid Physics, Chinese Academy of Engineering Physics, Mianyang, 621999, HUSEYIN SEHITOGLU, Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801 — Due to its superelastic behavior, NiTi shape memory alloy receives considerable attentions over a wide range of industrial and commercial applications. Limited to its complex structural transformation and multiple variants, semiempirical potentials for performing large-scale molecular dynamics simulations to investigate the atomistic mechanical process, are very few. In this work, we construct a new interatomic potential for the NiTi alloy by fitting to experimental or ab initio data. The fitting potential correctly predicts the lattice parameter, structural stability, equation of state for cubic B2(austenite) and monoclinic B19'(martensite) phases. In particular the elastic properties( three elastic constants for B2 and thirteen ones for B19') are in satisfactory agreement with the experiments or ab initio calculations. Furthermore, we apply this potential to conduct the molecular dynamics simulations of the mechanical behavior for NiTi alloy and the results capture its reversible transformation.

**1:03PM Y21.00010 Highly Accurate Calculations of the Phase Diagram of Cold Lithium**, LUKE SHULENBURGER<sup>1</sup>, ANDREW BACZEWSKI, Sandia National Laboratories — The phase diagram of lithium is particularly complicated, exhibiting many different solid phases under the modest application of pressure. Experimental efforts to identify these phases using diamond anvil cells have been complemented by ab initio theory, primarily using density functional theory (DFT). Due to the multiplicity of crystal structures whose enthalpy is nearly degenerate and the uncertainty introduced by density functional approximations, we apply the highly accurate many-body diffusion Monte Carlo (DMC) method to the study of the solid phases at low temperature. These calculations span many different phases, including several with low symmetry, demonstrating the viability of DMC as a method for calculating phase diagrams for complex solids. Our results can be used as a benchmark to test the accuracy of various density functionals. This can strengthen confidence in DFT based predictions of more complex phenomena such as the anomalous melting behavior predicted for lithium at high pressures.

<sup>1</sup>Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. DOE's National Nuclear Security Administration under contract DE-AC04-94AL85000

**1:15PM Y21.00011 Cold melting of Li under pressure: Perspectives from first-principles molecular dynamics simulations<sup>1</sup>**, WEIYI XIA, WEIWEI GAO, Department of Physics, University at Buffalo, SUNY, Buffalo, NY 14260, USA, XIANG GAO, Beijing Computational Science Research Center, Beijing, China, 100084, PEIHONG ZHANG, Department of Physics, University at Buffalo, SUNY, Buffalo, NY 14260, USA — Despite much work (experiment and theory), the pressure-dependent melting temperature of Li is still under debate. In particular, there is still controversy and significant uncertainty in determining the melting temperature of Li at pressures around 50 GPa. An earlier report [1] suggests that Li melts at as low as 190 K between 40 and 64 GPa. Such a low melting temperature is not likely unless quantum effects of lattice vibration play a significant role. Later experiment [2], on the other hand, reports that Li melts above 300 K under pressured up to 64 GPa and does not seem to support the view that lattice quantum effects to play any important role. In this talk, we will present results from large-scale (large systems and long simulation times) first-principles molecular dynamics simulations and phonon free energy calculations, aiming at resolving some of the issues. [1] C.L. Guillaume et al, Nature Phys. 7, 211 (2011). [2] A. M. J. Schaeffer et al, Phys. Rev. Lett. 109, 185702 (2012). [3] F.A. Gorelli et al, Phys. Rev. Lett. 108, 055501 (2012).

<sup>1</sup>This work is supported by US NSF under Grant No. DMR-0946404 and DMR-1506669. Work at Beijing CSRC is supported by the National Natural Science Foundation of China (Grant No. 11328401).

**1:27PM Y21.00012 Nuclear quantum and electronic exchange-correlation effects on the high pressure phase diagram of lithium**, RAYMOND CLAY, Univ of Illinois - Urbana, MIGUEL MORALES, STANIMIR BONEV, Lawrence Livermore National Laboratory — Lithium at ambient conditions is the simplest alkali metal and exhibits textbook nearly-free electron character. However, increased core/valence electron overlap under compression leads to surprisingly complex behavior. Dense lithium is known to possess a maximum in the melting line, a metal to semiconductor phase transition around 80 GPa, reemergent metallicity around 120 GPa, and low coordination solid and liquid phases. In addition to its complex electronic structure at high pressure, the atomic mass of lithium is low enough that nuclear quantum effects could have a nontrivial impact on its phase diagram. Through a combination of density functional theory based path-integral and classical molecular dynamics simulations, we have investigated the impact of both nuclear quantum effects and anharmonicity on the melting line and solid phase boundaries. Additionally, we have determined the robustness of previously predicted tetrahedral clustering in the dense liquid to the inclusion of nuclear quantum effects and approximate treatment of electronic exchange-correlation effects.

**1:39PM Y21.00013 Nature of Pressure-induced Insulating States in Simple Metals**, IVAN NAUMOV, RUSSELL HEMLEY, Carnegie Institution of Washington — As experimentally established, all the alkali metals and heavy alkaline earth metals (Ca, Sr and Ba) become progressively less conductive on compression, at least up to some critical limit over a broad pressure range. Of these metals, Li and Na clearly undergo pressure-induced metal-insulator transitions, which may also be called reverse Mott transitions. Here, using group theory arguments and first-principles calculations, we show that such transitions can be understood in terms of band representations introduced by Zak. The valence bands in the insulating states are described by simple and composite band representations constructed from localized Wannier functions centered on points unoccupied by atoms [1]. The character of the Wannier functions is closely related to the degree of s-p(-d) hybridization and reflects multi-center chemical bonding in these insulating states. The conditions under which an insulating state is allowed for structures having an integer number of atoms per primitive unit cell as well as re-entrant (i.e., metal-insulator-metal) transition sequences are detailed, resulting in predictions of semimetallic phases with flat surface states. The general principles developed are tested and applied to the alkali and alkaline earth metals, including elements where high-pressure insulating phases have been identified or reported (e.g., Li, Na, and Ca). This research was supported by EFree, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award DESC0001057. [1] I. I. Naumov and R. J. Hemley, PRL, **114**, 156403 (2015).

**1:51PM Y21.00014 Simulation texture development of polycrystalline aluminum under dynamic loading**, XIAOMIAN HU, HAO PAN, ZIHUI WU, Institute of Applied Physics and Computational Mathematics, Beijing — Effect of texture to dynamic response of polycrystalline metals under dynamic loading attracted much attention because of interesting phenomena and great challenges to experiment and simulation. This paper uses a crystal plasticity finite element method (CPFEM) with a dislocation based hardening law to model the texture development of polycrystalline aluminum under simple compression, uniaxial strain ramp loading and shock wave loading. Strain hardening under the three compression conditions is also compared. The simulation results show that the preferred orientation during of the polycrystalline aluminum under the three compression conditions has some different. It caused normalized stress-strain profiles of state of 1D stress and 1D strain are different when strain is over 5% and strain rate is same.

**2:03PM Y21.00015 Cooling rates dependence of medium range order development in metallic glasses**<sup>1</sup>, C. Z. WANG, Y. ZHANG, F. ZHANG, M. I. MENDELEV, M. J. KRAMER, K. M. HO, Ames Laboratory, Iowa State University — Rapid cooling from metallic liquids is a widely used approach to synthesize novel alloys with desirable properties because such rapid cooling drives phase selection away from equilibrium phases resulting in new metastable phases and morphologies. However, molecular dynamics simulation of such rapid solidifications faces a well-known time-scale challenge that the cooling rate is several orders of magnitude faster than experiments. We propose an efficient cooling strategy in which most of the computer time is spent on a prolonged isothermal process slightly below the glass-transition temperature  $T_g$ . Such a sub- $T_g$  annealing reduces the effective cooling rates in MD simulations to  $\sim 10^7$  K/s. The effects of lowering cooling rates on the evolution of short-range and medium-range orders are investigated. The glassy samples prepared in this way demonstrate significant energetic stability, slow dynamics, and well-developed short-range and medium-range orders.

<sup>1</sup>Work supported by DOE-BES under Contract No. DE-AC02-07CH11358.

## Friday, March 18, 2016 11:15AM - 1:39PM –

Session Y22 DMP: Van der Waals Bonding in Advanced Materials: Methods 321 - John Singleton, Los Alamos National Laboratory

**11:15AM Y22.00001 Quasi-local approximation of non-local exchange-correlation kernels in the adiabatic-connection fluctuation-dissipation theorem**<sup>1</sup>, DEYU LU, Brookhaven National Laboratory — The adiabatic-connection fluctuation-dissipation theorem (ACFDT) is a formal theoretical framework to treat van der Waals (vdW) dispersion interactions. Under the random phase approximation (RPA), it yields the correct asymptotic behavior at large distances, but the short-range correlation is overestimated. It has been demonstrated that non-local exchange-correlation kernels can systematically correct the errors of RPA for homogenous electron gas. However, direct extension of non-local kernels derived from the electron gas model to inhomogeneous systems raises several issues. In addition to the high computational expense, the non-local kernels worsen the rare gas dimer binding curve as compared to RPA. In this study, we propose a quasi-local approximation of the non-local kernel in order to address these issues.

<sup>1</sup>This research used resources of the Center for Functional Nanomaterials, which is a U.S. DOE Office of Science Facility, at Brookhaven National Laboratory under Contract No. DE-SC0012704.

**11:27AM Y22.00002 The Connection between Diagrams and Electrodynamics in the Long-Range Dispersion Energy**, RAHUL MAITRA, ROBERT DISTASIO, Cornell University — In this talk, we will discuss the different avenues that lead to the complete treatment of the long-range dispersion interaction energy between isolated fragments that are located outside the area of orbital (or electron density) overlap. By analyzing the higher-order terms in the perturbative expansion of the dispersion energy *via* a dipole response function formalism, we show that each of these terms can be expressed as physically meaningful quantities in classical electrodynamics. Based on this approach, we generalize the connection between the higher-order perturbative contributions to the dispersion energy, the different classes of diagrams (e.g. rings, ladders, etc.), and the aforementioned electrodynamic response functions.

**11:39AM Y22.00003 A fully consistent spin formalism for the nonempirical van der Waals density functional vdW-DF**<sup>1</sup>, T. THONHAUSER, S. ZULUAGA, C. ARTER, Wake Forest University, K. BERLAND, University of Oslo, E. SCHRÖDER, P. HYLDGAARD, Chalmers University of Technology — We present a proper nonempirical spin-density formalism for the van der Waals density functional (vdW-DF) method. We show that this generalization, termed svdW-DF, is firmly rooted in the single-particle nature of exchange and we test it on a range of spin systems. We investigate in detail the role of spin in the van der Waals driven adsorption of H<sub>2</sub> and CO<sub>2</sub> in the linear magnets Mn-MOF74, Fe-MOF74, Co-MOF74, and Ni-MOF74. In all cases, we find that spin plays a significant role during the adsorption process despite the general weakness of the molecular-magnetic responses. The case of CO<sub>2</sub> adsorption in Ni-MOF74 is particularly interesting, as the inclusion of spin effects results in an increased attraction, opposite to what the diamagnetic nature of CO<sub>2</sub> would suggest. We explain this counter-intuitive result, tracking the behavior to a coincidental hybridization of the O *p* states with the Ni *d* states in the down-spin channel. More generally, by providing insight on van der Waals interactions in concert with spin effects, our nonempirical svdW-DF method opens the door for a deeper understanding of weak nonlocal magnetic interactions.

<sup>1</sup>Work supported by DOE DE-FG02-08ER46491 and NSF DMR-1145968.

**11:51AM Y22.00004 Dispersion Interactions in High-Density Molecular Crystals**, PETER CSERNICA, RAHUL MAITRA, ROBERT DISTASIO, Cornell University — Dispersion interactions are ubiquitous quantum mechanical phenomena arising from correlated electron density fluctuations in molecules and materials. As a key component of non-bonded interactions, dispersion forces play a critical role in determining the structure and stability of molecular crystals. Due to the relative intermolecular separation in high-density molecular crystals, an accurate description of these non-bonded interactions requires the inclusion of terms beyond the asymptotic induced-dipole–induced-dipole ( $C_6/R^6$ ) contribution. In this work, we have developed a first principles based approach within the framework of Density Functional Theory (i.e., that only depends on the charge density  $n(\mathbf{r})$ ) for capturing the higher-order induced multipolar contributions to the correlation energy. As a first application of this method, we have investigated the structure and stability of the high-density ice molecular crystal polymorphs at the ice VI—ice VII—ice VIII triple point (278K, 2.1GPa) using *ab-initio* molecular dynamics in the isobaric-isothermal ( $NpT$ ) ensemble.

**12:03PM Y22.00005 On the pseudopotential approximation in the van der Waals density functional calculations**, IKUTARO HAMADA, MARTIN CALLSEN, National Institute for Materials Science — The van der Waals density functional (vdW-DF)[1,2] is a density functional that is able to describe van der Waals and covalent interactions in a seamless fashion, and has been applied to a variety of systems. In practical calculations, the pseudopotential (PP) approximation has been employed, for which the PPs should be generated consistently for the chosen exchange correlation XC functional. However, usually PPs generated with a generalized gradient approximation (GGA) XC functional are used and the effect of the approximation to the XC functional applied in the PP generation is scarcely discussed. In this work, we discuss the appropriate XC functionals in the PP generation for the vdW-DF calculations. Furthermore, we compare the vdW-DF results for several systems using the PP's generated with appropriate XC and those with GGA XC[3].

[1] M. Dion *et al.* Phys. Rev. Lett. **92**, 246401 (2004).

[2] K. Berland, *et al.*, Rep. Prog. Phys. **78**, 066501 (2015).

[3] M. Callsen and I. Hamada, Phys. Rev. B **91**, 195103 (2015).

**12:15PM Y22.00006 Van der Waals Interactions Between Subsystems with Overlapping Electron Density**, MICHELE PAVANELLO, Rutgers University — We claim that a subsystem formulation of Density-Functional Theory (DFT) can simplify both the theoretical framework and the computational effort for calculating the electronic structure of condensed phase systems. In addition, the naturally subsystem-like form of molecular aggregates makes subsystem DFT a better descriptor of the underlying physics than regular DFT of the supersystem. As an example, we present a novel van der Waals theory based on subsystem DFT which can treat seamlessly non-overlapping as well as overlapping subsystem electron densities. The theory is amenable to sensible approximations, such as RPA, and offers natural algorithms to fold in post-RPA corrections. Application of the theory to the computation of binding energies of dimers in the S22 set, and computation of selected potential energy surfaces is presented. [1] “FDE-vdW: A van der Waals Inclusive Subsystem Density-Functional Theory”, J. Chem. Phys., **141**, 044127 (2014) [2] “Exact Kinetic Energy Enables Accurate Evaluation of Weak Interactions by the FDE-vdW Method”, J. Chem. Phys., **143**, 084120 (2015) [3] “Subsystem Density-Functional Theory as an Effective Tool for Modeling Ground and Excited States, their Dynamics, and Many-Body Interactions”, J. Phys.: Condens. Matter, **27**, 183202 (2015)

**12:27PM Y22.00007 The Dipole Polarizability of a Water Molecule *in* Liquid Water**, ROBERT DISTASIO, RAHUL MAITRA, Cornell University — The dipole polarizability,  $\alpha$ , provides a measure of the tendency of a molecule or material to deform (or polarize) in the presence of an electric field. Within the framework of density functional theory (DFT), we present a hierarchy of first principles based approaches for computing  $\alpha$  of a molecule located in the condensed phase. This hierarchy includes a successive treatment of both short-range (hybridization, Pauli exchange-repulsion, etc.) and long-range (Coulomb) electrodynamic response screening in the computation of  $\alpha$ , while simultaneously accounting for the surrounding condensed-phase environment. Utilizing highly accurate liquid water configurations generated from van der Waals inclusive hybrid DFT based *ab initio* molecular dynamics, we computed  $\alpha$  for a given water molecule *in* liquid water as a first application of this approach. Our findings will be compared and contrasted with  $\alpha$  computed for an isolated gas-phase water molecule.

**12:39PM Y22.00008 Study of correlations from Ab-Initio Simulations of Liquid Water<sup>1</sup>**, ADRIAN SOTO, MARIVI FERNANDEZ-SERRA, Stony Brook University, DEYU LU, SHINJAE YOO, Brookhaven National Laboratory — An accurate understanding of the dynamics and the structure of H<sub>2</sub>O molecules in the liquid phase is of extreme importance both from a fundamental and from a practical standpoint. Despite the successes of Molecular Dynamics (MD) with Density Functional Theory (DFT), liquid water remains an extremely difficult material to simulate accurately and efficiently because of fine balance between the covalent O-H bond, the hydrogen bond and the attractive van der Waals forces. Small errors in those produce dramatic changes in the macroscopic properties of the liquid or in its structural properties. Different density functionals produce answers that differ by as much as 35% in ambient conditions, with none producing quantitative results in agreement with experiment at different mass densities [J. Chem Phys. **139**, 194502(2013)]. In order to understand these differences we perform an exhaustive scanning of the geometrical coordinates of MD simulations and study their statistical correlations with the simulation output quantities using advanced correlation analyses and machine learning techniques.

<sup>1</sup>This work was partially supported by DOE Award No. DE-FG02-09ER16052, by DOE Early Career Award No. DE-SC0003871, by BNL LDRD 16-039 project and BNL Contract No. DE-SC0012704.

**12:51PM Y22.00009 The Role of Anharmonicity and Nuclear Quantum Effects in the Pyridine Molecular Crystal: An *ab initio* Molecular Dynamics Study<sup>1</sup>**, HSIN-YU KO, Princeton University, ROBERT A. DISTASIO JR., Cornell University, BISWAJIT SANTRA, ROBERTO CAR, Princeton University — Molecular crystal structure prediction has posed a substantial challenge to first-principles methods and requires sophisticated electronic structure methods to determine the stabilities of nearly degenerate polymorphs [1,2,3]. In this work, we demonstrate that the anharmonicity from van der Waals interactions is relevant to the finite-temperature structures of pyridine and pyridine-like molecular crystals. Using such an approach, we find that the equilibrium structures are well captured with classical *ab initio* molecular dynamics (AIMD), despite the presence of light atoms such as hydrogen. Employing path integral AIMD simulations, we demonstrate that the success of classical AIMD results from a separation of nuclear quantum effects between the intermolecular and intramolecular degrees of freedom. In this separation, the quasiclassical and anharmonic intermolecular degrees of freedom determine the equilibrium structure, while the quantum and harmonic intramolecular degrees of freedom are averaging to the correct intramolecular structure. [1] M A Neumann, F J J Leusen, and J Kendrick, Angew. Chem. Int. Ed. **47**, 2427 (2008). [2] A Otero-de-la-Roza and E R Johnson, J. Chem. Phys. **137**, 054103 (2012). [3] A M Reilly and A Tkatchenko, J. Phys. Chem. Lett. **4**, 1028 (2013).

<sup>1</sup>This work has been supported by the Department of Energy under Grants No. DE-FG02-05ER46201 and DE-SC0008626

**1:03PM Y22.00010 Phonon dispersion in acene molecular crystals using van der Waals density functionals**, FLORIAN BROWN-ALTVATER, University of California, Berkeley, TONATIUH RANGEL, Lawrence Berkeley National Laboratory, JEFFREY B. NEATON, University of California, Berkeley; Lawrence Berkeley National Laboratory — Much progress has been made of late in understanding the fundamental processes in optoelectronic materials. An ongoing challenge is the accurate inclusion of nuclear motion and to go beyond the Born-Oppenheimer approximation. Especially in materials like molecular crystals, where van der Waals (vdW) forces dominate the cohesive energy and the electronic structure is very sensitive to intermolecular geometry, phonons can be an important facilitator and dissipation mechanism. Thus there is a need to assess and understand the efficacy of existing approaches for phonon dispersions in vdW-bound solids. In this work we use a vdW density functional to calculate the phonon dispersion of members of the acene family. We establish the accuracy of the method using naphthalene, obtaining excellent agreement with experimental results, and in a further step, we explore the strength of the electron-phonon coupling across the Brillouin zone. Taken all together, our calculations illustrate the potential for quantitative prediction of vibrational properties of weakly-bound organic crystals over the entire Brillouin zone from first principles.

**1:15PM Y22.00011 Ligand control of magnetic ordering temperature in copper-pyrazine square lattice antiferromagnets<sup>1</sup>**, JOHN SINGLETON, National High Magnetic Field Laboratory, Los Alamos, P. GODDARD, Warwick University, UK, I. FRANKE, J. MOELLER, S. BLUNDELL, A. STEELE, C. TOPPING, University of Oxford, T. LANCASTER, Durham University, UK, C. BAINES, Paul Scherrer Institute, Switzerland, J. BENDIX, University of Copenhagen, R. MCDONALD, National High Magnetic Field Laboratory, Los Alamos, J. BRAMBLEBY, M. LEES, Warwick University, UK, S. LAPIDUS, P. STEPHENS, SUNY, Stony Brook, B. TRAMLEY, University of Idaho, K. FUNK, M. CONNER, J. CORBEY, H. TRAN, Eastern Washington University, J. SCHLUETER, Argonne National Laboratory, J. MANSON, Eastern Washington University — Using a mixed-ligand synthetic scheme, we create a family of quasi-two-dimensional (Q2D) antiferromagnets:  $[\text{Cu}(\text{HF}_2)(\text{pyz})_2]\text{ClO}_4$  [pyz = pyrazine],  $[\text{Cu}L_2(\text{pyz})_2](\text{ClO}_4)_2$  [ $L$  = pyO = pyridine-N-oxide and 4-phpyO = 4-phenylpyridine-N-oxide]. These possess equivalent 2D  $[\text{Cu}(\text{pyz})_2]^{2+}$  nearly square layers, but show interlayer spacings from 6.57 Å to 16.78 Å, dictated by the axial ligands. Structural and magnetic properties are derived from x-ray diffraction, ESR, pulsed-field magnetometry and muon-spin rotation, and compared to those of the prototypical 2D magnetic polymer  $\text{Cu}(\text{ClO}_4)_2(\text{pyz})_2$ . We find that the 2D exchange coupling remains largely unaffected by the axial ligand substitution, while the magnetic ordering temperature decreases slowly with increasing layer separation. Experimental data are compared to theory, including DFT.

<sup>1</sup>Supported by NSF, DoE, the State of Florida and EPSRC (UK)

**1:27PM Y22.00012 UNUSUALLY LARGE YOUNG'S MODULI OF AMINO ACID MOLECULAR CRYSTALS\***, IDO AZURI, ELENA MEIRZADEH, DAVID EHRE, Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth, Israel, SIDNEY R. COHEN, Chemical Research Support, Weizmann Institute of Science, Rehovoth, Israel, ANDREW M. RAPPE, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, Philadelphia, PA, USA, MEIR LAHAV, IGOR LUBOMIRSKY, LEEOR KRONIK, Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth, Israel — Young's moduli of selected amino acid molecular crystals were studied both experimentally and computationally using nanoindentation and dispersion-corrected density functional theory. The Young modulus is found to be strongly facet-dependent, with some facets exhibiting exceptionally high values (as large as 44 GPa). The magnitude of Young's modulus is strongly correlated with the relative orientation between the underlying hydrogen-bonding network and the measured facet. Furthermore, we show computationally that the Young modulus can be as large as 70-90 GPa if facets perpendicular to the primary direction of the hydrogen-bonding network can be stabilized. This value is remarkably high for a molecular solid and suggests the design of hydrogen-bond networks as a route for rational design of ultra-stiff molecular solids. \*Angew. Chem. Int. Ed.. doi: 10.1002/anie.201505813

**Friday, March 18, 2016 11:15AM - 2:15PM –**  
**Session Y23 DMP GERA FIAP: Thermoelectrics, Low Dimensional Materials** 322 - Zhiting Tian,  
 Virginia Tech

**11:15AM Y23.00001 Optimizing Thermoelectric Properties in Composites**, MICHAEL J. ADAMS, HYUNGYU JIN, JOSEPH P. HEREMANS, The Ohio State University — Here we consider semiconductor composites as a way to yield high thermoelectric figure of merit. Effective medium theory limits the figure of merit of a composite made from two non-interacting materials, A and B, to the larger of the two [1, 2]. In previous work, we describe a mechanism that can lift this limitation by treating charge and heat flux separately. Silica beads coated with a conducting shell are inserted into a thermoelectric host. Thermal conductivity decreases with insulating material added, but electrical conductivity is maintained via locally conducting surfaces. We apply the theory to p-type (Bi,Sb)2Te3 host material. Several permutations are possible: Te-coated beads in Sb-rich material, or Sb-coated beads in Te-rich material. First, we review data for varying bead coatings and heat treatments, followed by varying stoichiometry in the host. New data considers an additional parameter of varying bead diameter, as well as optimizing these parameters simultaneously to enhance thermoelectric performance. References: [1] David J. Bergman and Ohad Levy, J. Appl. Phys. 70 6821 (1991) [2] David J. Bergman and Leonid G. Fel, J. Appl. Phys. 85 8205 (1999)

**11:27AM Y23.00002 High thermoelectric figure-of-merit in Sb<sub>2</sub>Te<sub>3</sub>/Ag<sub>2</sub>Te bulk composites as Pb-free p-type thermoelectric materials**, MINHOO LEE, JONG-SOO RHYEE, Kyung Hee Univ - Suwon Campus, SU-DONG PARK, Korea Electrotechnology Research Institute — We investigated thermoelectric properties of the Sb<sub>2</sub>Te<sub>3</sub>/Ag<sub>2</sub>Te (ST/AT) composites with molar ratios of ST/AT = 1/1, 2/1, 4/1, 8/1, 16/1, and 32/1. The extrinsic composites, synthesized by wet ball milling of two separate powders of Sb<sub>2</sub>Te<sub>3</sub> and Ag<sub>2</sub>Te, are differentiated with intrinsic composites by high temperature phase separation in that it is low temperature synthesis process. The thermoelectric properties of the composites show systematic behaviour of decreased electrical and thermal conductivities with increasing Ag<sub>2</sub>Te dispersion concentration. The ST/AT = 1/1 composite exhibits extremely low lattice thermal conductivity with high power factor over a wide temperature range, resulting in high ZT value 1.5 at 700 K, which is the significantly enhanced value of ZT compared with other Pb-free p-type chalcogenide thermoelectric materials.

**11:39AM Y23.00003 Coupled improvement between thermoelectric and piezoelectric materials**, DAVID MONTGOMERY, COREY HEWITT, CHAOCHAO DUN, DAVID CARROLL, Wake Forest University — A novel coupling effect in a thermoelectric and piezoelectric meta-structure is discussed. Thermo-piezoelectric generators (TPEGs) exhibit a synergistic effect that amplifies output voltage, and has been observed to increase piezoelectric voltages over 500% of initial values a time dependent thermoelectric/pyroelectric effect. The resulting improvement in voltage has been observed in carbon nanotubes as well as inorganics such as two-dimensional Bismuth Selenide platelets and Telluride nanorods thin-film thermoelectrics. TPEGs are built by integrating insulating layers of polyvinylidene fluoride (PVDF) piezoelectric films between flexible thin film p-type and n-type thermoelectrics. The physical phenomena arising in the interaction between thermoelectric and piezoelectrics is discussed and a model is presented to quantify the expected coupling voltage as a function of stress, thermal gradient, and different thermoelectric materials. TPEG are ideal to capture waste heat and vibrational energy while creating larger voltages and minimizing space when compared with similar thermoelectric or piezoelectric generators.

**11:51AM Y23.00004 Thermomagnetic transport properties of ferromagnetic MnBi**, STEPHEN BOONA, JOSEPH HEREMANS, Ohio State University — Spin-dependent transport phenomena such as the spin Seebeck effect and magnon drag offer intriguing new possibilities for tuning the thermoelectric properties of magnetically ordered materials. One particularly interesting approach is to examine magnetic materials that are expected to display large intrinsic spin orbit coupling, such as MnBi. In spite of this material's popularity as a candidate for rare-earth free permanent magnets, no studies have been published so far concerning its Seebeck or Nernst coefficients. This talk will discuss our recent measurements of the thermomagnetic properties of high purity polycrystalline MnBi between 2K and 385K and in magnetic fields up to 7T. Our measurements reveal the existence of a substantial anomalous Nernst effect (ANE) from 382K down to the spin reorientation temperature of 90K, while the other transport phenomena show relatively weak magnetic field dependence at all temperatures. We also observe that the Seebeck and ANE coefficients display strikingly similar temperature dependence, with the former peaking at approximately  $-10 \mu\text{V/K}$  and the latter at approximately  $-2.5 \mu\text{V/K/T}$ , hinting at the important role of spin-dependent processes in determining the transport properties of this material.

**12:03PM Y23.00005 Integration of 2-Dimensional Materials for Thermoelectric Power Generation**, FADHEL ALSAFFAR, ABDULRAHMAN AL HUSSAIN, MOH. R. AMER, None, CENTER OF EXCELLENCE FOR GREEN NANOTECHNOLOGIES COLLABORATION, DEPARTMENT OF ELECTRICAL ENGINEERING (UCLA) COLLABORATION — Recent developments in nanomaterial research have significantly progressed the performance of thermoelectric devices. Theoretical investigations of the thermoelectric properties of 2-Dimensional monolayers demonstrate a high figure of merit (ZT) [1, 2]. Here, we investigate the integration of these 2-Dimensional materials for power generation applications using solar heat. We show that using black phosphorus monolayer (phosphorene) as the *p*-type material, and Molybdenum disulfide ( $\text{MoS}_2$ ) monolayers as the *n*-type material, we get an effective figure of merit (ZT) at least (1.5) with a conversion efficiency of 13% at 280°C. Our results suggest that the integration of various 2-Dimensional materials is a promising approach for commercial thermoelectric power generation applications. **References:** [1] W. Huang, X. Luo, C. K. Gan, S. Y. Quek, and G. Liang, "Theoretical study of thermoelectric properties of few-layer  $\text{MoS}_2$  and  $\text{WSe}_2$ ," *Physical Chemistry Chemical Physics*, vol. 16, pp. 10866-10874, 2014. [2] R. Fei, A. Faghaninia, R. Soklaski, J.-A. Yan, C. Lo, and L. Yang, "Enhanced thermoelectric efficiency via orthogonal electrical and thermal conductances in phosphorene," *Nano Letters*, vol. 14, pp. 6393-6399, 2014.

**12:15PM Y23.00006 First-Principles Study on Thermoelectric Performance of Phosphorene and Phosphorene Oxide**, SEUNGJUN LEE, JEJUNE PARK, SEOUNG-HUN KANG, YOUNG-KYUN KWON, Department of Physics and Research Institute for Basic Sciences, Kyung Hee University, Seoul, 130-701, Korea — Using first-principles density functional theory, we studied thermoelectric properties of phosphorene and its oxidized structure called phosphorene oxide (PO). Using the identified stable configurations and electronic structures of phosphorene and PO, we solved the Boltzmann transport equation to evaluate their electrical conductivity, Seebeck coefficient, and thermal conductivity contributed from both electrons and phonons. In order to correctly estimate the thermoelectric figure of merit or ZT values, it is indispensable to determine the relaxation time, which can be estimated by applying the deformation potential theory. We observe that the electrical conductivity of phosphorene is higher along the armchair direction than along the zigzag direction, while the thermal conductivity shows an opposite behavior. Because of such an orthogonal relation between the electrical and thermal conductivities, phosphorene exhibits quite a large ZT value along the armchair direction. It is, on the other hand, calculated that PO has electrical conductivity similar to phosphorene, however its thermal conductivity is significantly smaller than phosphorene, resulting in larger ZT values. We expect that PO can be utilized for a high performance thermoelectric application.

**12:27PM Y23.00007 Understanding phonon transport in thermoelectric materials using *ab initio* approaches**, DAVID BROIDO, Boston College — Good thermoelectric materials have low phonon thermal conductivity,  $k_{ph}$  [1]. Accurate theories to describe  $k_{ph}$  are important components in developing predictive models of thermoelectric efficiency that can help guide synthesis and measurement efforts. We have developed *ab initio* approaches to calculate  $k_{ph}$ , in which phonon modes and phonon scattering rates are computed using interatomic force constants determined from density functional theory, and a full solution of the Boltzmann transport equation for phonons is implemented [2-5]. A recent approach to calculate interatomic force constants using *ab initio* molecular dynamics [6] has yielded a good description of the thermal properties of  $\text{Bi}_2\text{Te}_3$ . But, the complexity of new promising candidate thermoelectric materials introduces computational challenges in assessing their thermal properties. An example is germanane, a germanium based hydrogen-terminated layered semiconductor [7], which we will discuss in this talk. [1] H. J. Goldsmid, *Thermoelectric Refrigeration* (Plenum, New York, 1964); [2] D. A. Broido et al, *Appl. Phys. Lett.*, 91, 231922 (2007); [3] A. Kundu et al, *Phys. Rev. B*, 84, 125426 (2011); [4] W. Li et al, *Phys. Rev. B* 86, 174307 (2012); [5] Olle Hellman and I. A. Abrikosov, *Phys. Rev. B* 88, 144301 (2013); [6] O. Hellman and D. A. Broido, *Phys. Rev. B* 90, 134309 (2014); [7] E. Bianco, et al., *ACS Nano* 7, 4414 (2013).

**1:03PM Y23.00008 Ab initio theory of thermal properties of germanane**, MATTHEW HEINE, Boston College, LUCAS LINDSAY, Oak Ridge National Lab, JESÚS CARRETE, NATALIO MINGO, LITEN, CEA-Grenoble, OLLE HELLMAN, Linköping University, DAVID BROIDO, Boston College — Germanane(GeH) is a germanium based hydrogen-terminated multi-layered graphene analogue semiconductor, which may be a promising thermoelectric due to its high electron mobility and the capability to tune its transport properties [1]. We have performed first principles calculations of the thermal properties of germanane. Harmonic and anharmonic interatomic force constants are calculated within the framework of density functional theory, from which phonon dispersions, specific heat, thermal expansion are obtained. The phonon Boltzmann equation is solved to obtain the lattice thermal conductivity. The disparity in constituent masses in GeH gives phonon modes that are distinctly Ge or H in character and causes the specific heat not to saturate until much higher temperatures than in bulk Ge. Weak interlayer bonding and strong phonon-phonon scattering result in highly anisotropic and quite low intrinsic lattice thermal conductivity compared to Ge. [1] E. Bianco et. al., *ACS Nano* 7, 4414-4421 (2013).

**1:15PM Y23.00009 Thermal Conductance at the 2D  $\text{MoS}_2$ -hexagonal Boron Nitride Interface**, YI LIU, Natl Univ of Singapore, KEDAR HIPPALGAONKAR, Institute of Materials Research and Engineering, A\*STAR, ZHUN YONG ONG, Institute of High Performance Computing, A\*STAR, JOHN TL THONG, CHENGWEI QIU, Natl Univ of Singapore — In recent years, a number of 2D heterostructure devices have emerged, including graphene/hexagonal boron nitride (*h*-BN), graphene/ $\text{MoS}_2$  and  $\text{MoS}_2$ /*h*-BN. Among them,  $\text{MoS}_2$ /*h*-BN field-effect transistors with  $\text{MoS}_2$  channels and *h*-BN dielectric have been reported to have higher carrier mobility and reduced hysteresis compared to  $\text{MoS}_2$  on  $\text{SiO}_2$ . Despite relatively high in-plane thermal conductivity of  $\text{MoS}_2$  and *h*-BN, heat dissipation from these 2D devices is mainly limited by heat transfer in the vertical direction. Consequently, their operating temperatures are strongly influenced by the interface thermal conductance. In this work, we demonstrate the measurement of interface thermal conductance between  $\text{MoS}_2$  and *h*-BN. This is realized by electrically heating  $\text{MoS}_2$  and monitoring their temperatures through Raman spectroscopy. The obtained interface thermal conductance between  $\text{MoS}_2$  and *h*-BN is  $1.77 \text{ MW/m}^2\text{K}$ , smaller than the reported value for the graphene/*h*-BN interface, due to the weak coupling of phonon modes between  $\text{MoS}_2$  and *h*-BN based on our NEGF calculation. The low interface thermal conductance value suggests this interface is not favorable for heat dissipation, and should be considered carefully for the design of electronic and optoelectronic devices based on  $\text{MoS}_2$ /*h*-BN heterostructures.

**1:27PM Y23.00010 Maximizing the thermoelectric performance of topological insulator  $\text{Bi}_2\text{Te}_3$  films in the few-quintuple layer regime**, HUIJUN LIU, JINGHUA LIANG, LONG CHENG, JIE ZHANG, Wuhan University, ZHENYU ZHANG, University of Science and Technology of China — Using first-principles calculations and Boltzmann theory, we explore the feasibility to maximize the thermoelectric figure of merit ( $ZT$ ) of topological insulator  $\text{Bi}_2\text{Te}_3$  films in the few-quintuple layer regime. We discover that the delicate competitions between the surface and bulk contributions, coupled with the overall quantum size effects, lead to a novel and generic non-monotonous dependence of  $ZT$  on the film thickness. In particular, when the system crosses into the topologically non-trivial regime upon increasing the film thickness, the much longer surface relaxation time associated with the robust nature of the topological surface states results in a maximal  $ZT$  value, which can be further optimized to  $\sim 2.0$  under physically realistic conditions. We also reveal the appealing potential of bridging the long-standing  $ZT$  asymmetry of  $p$ - and  $n$ -type  $\text{Bi}_2\text{Te}_3$  systems. These findings help to establish intricate connections between the thermoelectric materials and topological insulators.

**1:39PM Y23.00011 Temperature sensing and real-time two-dimensional mapping at the micro-scale**, XIAOYE HUO, GANG LI, ZHENHAI WANG, XINYU MAO, SHENGYONG XU, Key Laboratory for Physics and Chemistry of Nanodevices, Department of Electronics, Peking University — To sense temperature at micro/nano scales and obtain its detailed distribution in space and in time remains a technical challenge in many cases. We observed an unexpected thermoelectric size effect, where the absolute Seebeck coefficient of metallic thin film stripes (e.g. Ni, Cr, Pd, W, Bi, Sc, etc.) decreased with the stripe width from  $100\mu\text{m}$  down to  $100\text{nm}$ . This phenomenon was utilized in micro/nano-stripe-based thin film temperature sensors. By using an array of such sensors, two-dimensional temperature distribution at the micro-scale could be precisely mapped. Small temperature sensors with a total width less than  $1\mu\text{m}$  and a sensitivity of  $0.5\text{--}2.2\mu\text{V/K}$  were fabricated, showing a potential for monitoring temperatures at submicro-scales. By using a special multiplexer and software, nearly real-time 2D temperature mapping was performed, demonstrating 2D thermal history of target surface with a delay of less than one minute. These thin film sensors were also fabricated on flexible Parylene-C substrates for application in flexible electronic devices, temperature monitoring of cell culturing, and heat transfer between Au nanoparticles and metallic stripes due to plasmonic excitation under laser radiation.

**1:51PM Y23.00012 Engineering Group-IV Monochalcogenides by Doping and Alloying**, HANSIKA SIRIKUMARA, TREVOR FITZPATRICK, THUSHARI JAYASEKERA, Southern IL Univ-Carbondale — Group-IV monochalcogenides,  $\text{MX}$  ( $\text{M}=\text{Sn, Ge}$  and  $\text{X}=\text{S, Se}$ ) have shown to be promising materials for thermoelectric and photovoltaic applications. These properties can be further engineered by substitutional doping and alloying. Using the results from *ab initio* Density Functional Theory calculations, we identified a series of new class of monochalcogenide alloys in the form  $\text{Ge}(1-x)\text{Sn}_x\text{S}$ ,  $\text{Ge}(1-x)\text{Sn}_x\text{Se}$ ,  $\text{GeS}_x\text{Se}(1-x)$ ,  $\text{SnS}_x\text{Se}(1-x)$ . Stability of their two-dimensional counterparts will also be discussed in this presentation.

**2:03PM Y23.00013 Thermal conductivity behavior of superatom molecular crystals**, WEE-LIAT ONG, Columbia University / Carnegie Mellon University, EVAN OBRIEN, Columbia University, PATRICK DOUGHERTY, JILLIAN EPSTEIN, C. FRED HIGGS, ALAN MCGAUGHEY, Carnegie Mellon University, XAVIER ROY, Columbia University, JONATHAN MALEN, Carnegie Mellon University — The room temperature thermal conductivity of several superatom molecular crystals (SMCs) are measured and found to be below  $0.3\text{ W/mK}$ . The trend of room temperature thermal conductivity of the different crystals agree well with their sound speeds obtained independently using nano-indentation. These crystals, however, can exhibit non-crystalline thermal conductivity behavior depending on their constituent elements. A superatom is a cluster of atoms that acts as a stable entity [e.g., fullerenes ( $\text{C}_{60}$ )]. By careful mixing and assembling these nano-sized superatoms, the resulting superatom-assembled materials hold promises for improving various technological devices. Organic-inorganic superatoms can assemble into unary SMCs or co-crystallized with  $\text{C}_{60}$  superatoms into binary SMCs. Thermal transport is of considerable interest with possible new physics in these hierarchically atomic precise crystals in the low temperature regime. The thermal conductivity of the SMCs are measured using the frequency domain thermoreflectance setup. Unary SMCs exhibit an almost invariant thermal conductivity down to a temperature of  $150\text{ K}$ . Binary SMCs, however, can either show a crystalline-like increase or an amorphous-like decrease with decreasing temperature.

## Friday, March 18, 2016 11:15AM - 2:15PM –

Session Y25 DCMP: Superconductivity: Theory III 324 - Khadijah Najafi, Georgetown

**11:15AM Y25.00001 Valence Bond Theory of Correlated-Electron Superconductivity<sup>1</sup>**, TIRTHANKAR DUTTA, SUMIT MAZUMDAR, Univ of Arizona, TORSTEN CLAY, Mississippi State Univ — Whether or not the weakly doped Mott-Hubbard semiconductor is superconducting remains controversial. We present a new valence bond theory of correlated-electron superconductivity, that has overlap with the original RVB approach, and yet is substantively different. Superconductivity within the theory emerges from a correlated-electron state in which there is a strong tendency to spin-singlet formation, and where the bandwidth due to pair-tunneling is very large. We show that such a situation occurs far away from the  $1/2$ -filled band, at or near banfilling of  $1/4$ . In the presence of electron-phonon interactions the  $1/4$ -filled band can form a spin-paired CDW state that we have called a paired-electron crystal, and that is a Wigner crystal of pairs. In the presence of frustration the spin-paired bonds become mobile to give a paired-electron liquid, which is a precursor to superconductivity. The superconducting state here is reached from a co-operative effect between electron-electron and electron-phonon interactions, and the theory thus has overlap also with the bipolaron theory of superconductivity. We will present exact numerical calculations on a  $4\times 4$  lattice using the valence bond basis to substantiate our conjectures.

<sup>1</sup>Supported by DOE Grant DE-FG02-06ER46315 and NSF-CHE-151475

**11:27AM Y25.00002 Retarded VS instantaneous : not so conflicting views on the pairing dynamics of the extended Hubbard model<sup>1</sup>**, A. REYMBAUT, M. FELLOUS ASIANI, Université de Sherbrooke, L. FRATINO, Royal Holloway, U. London, M. CHARLEBOIS, S. VERRET, Université de Sherbrooke, G. SORDI, Royal Holloway, U. London, D.. SÉNÉCHAL, A.-M. S. TREMBLAY, Université de Sherbrooke — While most experimental and theoretical clues lean towards a magnetic origin for the pairing mechanism of high temperature superconductors, the question of its degree of retardation in the strong correlation regime remains highly controversial [1-5]. Part of the answer to this question lies in the frequency dependence of the anomalous spectral function of doped Mott insulators. That spectral function is associated with the Gorkov function and can be extracted at finite temperature using the MaxEntAux method for analytic continuation [6]. Using Cellular Dynamical Mean-Field Theory for the Hubbard model with nearest-neighbor repulsion, we show that the retarded contribution coming from the anomalous spectral function is accompanied by a contribution to the real part of the anomalous self-energy at infinite frequency. This contribution suggests the emergence of a "mixed" pairing mechanism, mostly retarded, slightly instantaneous. [1] P. W. Anderson, Science 316 (5832), 1705 (2007) [2] D. J. Scalapino, E-letter resp. to Science 316, 1705 (2007) [3] T. A. Maier, et al., PRL 100, 237001 (2008) [4] D. Sénéchal, et al., PRB 87, 075123 (2013) [5] E. Gull and A. Millis, PRB 90, 041110(R) (2014) [6] A. Reymbaut, et al., PRB 92, 060509(R) (2015)

<sup>1</sup>Supported by NSERC, CIFAR, and the Tier I Canada Research Chair

**11:39AM Y25.00003 Crucial Role of Internal Collective Modes in Underdoped Cuprates<sup>1</sup>**, AABHAAS V. MALLIK, UMESH K. YADAV, Indian Institute of Science Bangalore, AMAL MEDHI, Indian Institute of Science Education and Research Thiruvananthapuram, H. R. KRISHNAMURTHY, VIJAY B. SHENOY, Indian Institute of Science Bangalore — The enigmatic cuprate superconductors have attracted resurgent interest with several recent reports and discussions of competing orders in the underdoped side. Motivated by this, here we address the natural question of frailty of the  $d$ -wave superconducting state in underdoped cuprates. Using a combination of theoretical approaches we study a  $t - J$  like model. We report an – as yet unexplored – instability that is brought about by an “internal” fluctuation (anti-symmetric mode) of the  $d$ -wave state. This new theoretical result helps in understanding recent ARPES and STM studies. We also suggest further experiments to uncover this physics.

<sup>1</sup>Work supported by CSIR, UGC, DST and DAE

**11:51AM Y25.00004 Competition between antiferromagnetism and superconductivity: a quantum Monte Carlo study**, TIANXING MA, 1, Department of Physics, Beijing Normal University, Beijing 100875, China 2, Department of Physics, University of California, San Diego, California, DA WANG, School of Physics, Nanjing University, Nanjing, 210093, China, CONJUN WU, Department of Physics, University of California, San Diego, California 92093, USA — Among correlated materials, the vicinity between various magnetic orders and superconductivity is one of the most notorious issues, which is present in high temperature superconductors like doped cuprates and ironpnictides, as well as in organic superconductors. In a multi-band Hubbard model, or, equivalently, a large-spin Hubbard model, it has been shown that the sign problem of quantum Monte Carlo simulations can be removed at arbitrary fillings in a wide parameter regime, which offers the unique opportunity to perform a detailed unbiased analysis of the competition between antiferromagnetism and superconductivity. Within this framework, we performed QMC simulations to investigate the phase diagram as doping and interaction strength, and our nonbiased numerical results reveal that the antiferromagnetic long-range order can be realized around doping  $0.06$ , and the maximal superconducting pairing correlation is brought by doping, which occurs around the optimal doping  $0.30$ , and then decreases in both the underdoped and overdoped regimes.

**12:03PM Y25.00005 Superconducting Fluctuations in the Normal State of the Two-Dimensional Hubbard Model**, XI CHEN, JAMES LEBLANC, EMANUEL GULL, University of Michigan — The dynamical mean field theory and its cluster extensions, such as the dynamical cluster approximation, are effective and accurate methods for solving the 2D Hubbard model. Progress is limited by exponential scaling, especially for quantities relevant to superconducting correlations. In this work, we demonstrate how the vertex contribution to the pairing susceptibility can be used as an indicator of the proximity to the superconducting transition temperature. This allows us to analyze a wider region of parameter space at a higher (numerically accessible) temperature in the normal state. The optimal interaction strength, doping and next-nearest hopping for  $d_{x^2-y^2}$  superconductivity are located. We conclude that optimal transition temperature occurs at intermediate coupling strength, electron-doped side. This approach is systematically extended to other superconducting symmetries as well. A change in sign of the vertex contribution to  $d_{xy}$  superconductivity from repulsive near half filling to attractive at large doping is discovered.

**12:15PM Y25.00006 Strongly enhanced superconductivity in coupled  $t$ - $J$  segments**, SAHINUR REJA, JEROEN VAN DEN BRINK, SATOSHI NISHIMOTO, IFW Dresden — The  $t$ - $J$  Hamiltonian is one of the cornerstones in the theoretical study of strongly correlated copper-oxide based materials. Using the density matrix renormalization group method we calculate the phase diagram of the one-dimensional (1D)  $t$ - $J$  chain in the presence of a periodic hopping modulation, as a prototype of coupled-segment models. While in the uniform 1D  $t$ - $J$  model near half-filling superconducting (SC) state dominates only at unphysically large values of the exchange coupling constant  $J/t > 3$ , we show that a small hopping and exchange modulation very strongly reduces the critical coupling to be as low as  $J/t \sim 1/3$  – well within the physical regime. The phase diagram as a function of the electron filling also exhibits metallic, insulating line phases and regions of phase separation. We suggest that a SC state is easily stabilized if  $t$ - $J$  segments creating local spin-singlet pairing are coupled to each other – another example is ladder system.

**12:27PM Y25.00007 Cluster dynamic mean-field study on the superconductivity in doped honeycomb lattice Hubbard model**, XIAO YAN XU, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, HUNG T. DANG, STEFEN WESSEL, Institute for Theoretical Solid State Physics, JARA-FIT and JARA-HPC, RWTH Aachen University, 52056 Aachen, Germany, ZI YANG MENG, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — The issue of superconductivities emerging from doped honeycomb lattice Mott insulator remains inconclusive. Existing proposals, such as  $p$ - $ip$  triplet pairing driven by ferromagnetic fluctuations,  $d$ - $id$  singlet pairing driven by antiferromagnetic fluctuations or van Hove singularities in the band structure, are not compatible. This is mainly due to the limitation of various approximated techniques employed in addressing such question with inherent strongly correlated nature. Trying to clarify the situation, we perform large-scale cluster dynamic mean-field simulations to explore the superconductivity instabilities in the doped honeycomb lattice Hubbard model, from medium to strong coupling. To benchmark, we make use of both interaction- and hybridization-expansion continuous time quantum Monte Carlo methods to exactly solve the quantum cluster embedded in self-consistently determined mean-field bath. Temperature dependence of various superconducting susceptibilities are calculated, hence, we provide the least biased results of the competition of the superconductivity in different channels in the phase diagram spanned by doping and electronic interaction.

**12:39PM Y25.00008 Charge dynamics in doped cuprates<sup>1</sup>**, MACIEJ MASKA, MARCIN MIERZEJEWSKI, University of Silesia, Poland, EVGENY KOCHETOV, Joint Institute for Nuclear Research, Russia, JANEZ BONCA, University of Ljubljana, Slovenia — It has recently been suggested that contrary to common belief, the quantum spin fluctuations of the antiferromagnetic background may not be crucial in explaining the dynamical properties of quasiparticles in strongly correlated systems near half-filling (see H. Ebrahimnejad, *et al.* Nature Physics **10**, 951 (2014)). In accordance with this suggestion, we demonstrate that the  $t$ - $J$  model even without the transverse spin components reproduces many of the ARPES results, provided that the three-site term, usually neglected in calculations, is properly taken into account. The dynamical properties of doped charges are calculated with the help of the Monte Carlo method combined with exact diagonalization. The validity of neglecting the spin-flip processes in the Ising version of the  $t$ - $J$  model is checked by a comparison with results of a fully quantum approach based on exact diagonalization in the limited functional space (EDLFS). Our method allows us to show how the spectral properties of doped holes change for a wide range of the doping level. We also demonstrate that the effective model reveals a tendency towards formation of charge density waves.

<sup>1</sup>This work was supported by the Polish National Science Centre (NCN) grant DEC-2013/11/B/ST3/00824

**12:51PM Y25.00009 Controllable electron interactions in quantum dots coupled to nanowires**, ALEXANDRE TACLA, Department of Physics and SUPA, University of Strathclyde, GUANGLEI CHENG, MICHELLE TOMCZYK, JEREMY LEVY, Department of Physics and Astronomy, University of Pittsburgh, ANDREW DALEY, Department of Physics and SUPA, University of Strathclyde, DAVID PEKKER, Department of Physics and Astronomy, University of Pittsburgh — We theoretically study transport properties in quantum dot devices proximity coupled to superconducting nanowires. In particular, we investigate the controllable transition from resonant pair tunneling to Andreev bound states, which has been recently observed in nanodevices fabricated at the interface of the oxide heterostructure  $\text{LaAlO}_3/\text{SrTiO}_3$ . We show that such a transition in transport features can signify a Lifshitz transition, at which electron interactions change from attractive to repulsive. We also discuss an alternate description in terms of magnetic impurities.

**1:03PM Y25.00010 Spontaneously broken time-reversal symmetry in high-temperature cuprate superconductors.** , MIKAEL FOGELSTROM, MIKAEL HAKANSSON, TOMAS LOFWANDER, Chalmers — Conventional superconductors are strong diamagnets that through the Meissner effect expel magnetic fields. It would therefore be surprising if a superconducting ground state would support spontaneous magnetic fields. Such time-reversal symmetry broken states have been proposed for the high-temperature superconductors, but their identification remains experimentally controversial. Here we show a route to a low-temperature superconducting state with broken time-reversal symmetry that may accommodate currently conflicting experiments. This state is characterised by an unusual vortex pattern in the form of a necklace of fractional vortices around the perimeter of the material, where neighbouring vortices have opposite current circulation. This vortex pattern is a result of a spectral rearrangement of current carrying states near the edges. Ref. M. Håkansson, T. Löfwander, and M. Fogelström, Nature Phys.11 755, (2015)

**1:15PM Y25.00011 Searching for stripe order in the Hubbard model** , EDWIN HUANG, CHRISTIAN MENDEL, HONGCHEN JIANG, SHENXIU LIU, YVONNE KUNG, SLAC National Accelerator Laboratory and Stanford University, BRIAN MORITZ, SLAC National Accelerator Laboratory, STEVEN JOHNSTON, University of Tennessee, Knoxville, THOMAS DEVEREAUX, SLAC National Accelerator Laboratory and Stanford University — The existence of stripe ordering in doped cuprates is well-established experimentally, but the microscopic mechanisms of their formation and their relation to superconductivity remain open questions. Previous density-matrix renormalization group (DMRG) studies on t-J and Hubbard ladders, in the parameter regimes relevant to cuprates, have suggested the presence of charge and spin stripes in the ground states of these microscopic models. To further investigate these tendencies towards stripe formation, we perform determinant quantum Monte Carlo (DQMC) and DMRG simulations for the single-band and three-band Hubbard models on identical rectangular lattice geometries. For both methods, upon hole doping, we find the spontaneous formation of domain walls in the spin correlation function, characterized by a  $\pi$ -phase shift of the antiferromagnetic ordering upon traversing a domain wall. We compare and contrast the results from the single-band and three-band Hubbard models using both techniques.

**1:27PM Y25.00012 Theory of dirty Rashba superconductivity in ultrathin Pb films<sup>1</sup>** , HUA CHEN, HYOUNGDO NAM, CHIH-KANG SHIH, ALLAN MACDONALD, The University of Texas at Austin — Pb is a typical s-wave superconductor and also has strong atomic spin-orbit coupling. In Pb thin films inversion symmetry breaking combined with the large atomic spin-orbit coupling will split the otherwise spin-degenerate bands of Pb, an effect which can be roughly accounted for by Rashba spin-orbit coupling. Motivated by a recent experiment, we used a 2D model involving Rashba spin-orbit coupling and s-wave pairing to study the influence of the former on the superfluid density, parallel critical field, and the resistive transition to the superconducting phase. We found that in both the clean and the dirty limits, Rashba spin-orbit coupling has little influence on the superfluid density and the Kosterlitz-Thouless transition temperature. However, in the dirty limit the Rashba spin-orbit coupling can significantly enhance the parallel critical field, making the Clogston-Chandrasekhar limit inapplicable. The strong suppression of the spin pair-breaking effect of a parallel magnetic field by the Rashba spin-orbit coupling and impurity scattering can make the orbital pair-breaking effect dominant again even in ultrathin films. Finally, we propose and examine a number of mechanisms that can lead to a smeared resistive transition under parallel magnetic fields.

<sup>1</sup>Supported by ONR-N00014-14-1-0330

**1:39PM Y25.00013 Directionality in photonic arrays via dissipation engineering** , A. METELMANN, H. E. TÜRECI, Princeton University — Achieving control over the direction of propagation of photons in one and higher dimensional structures is of high interest in a large number of research fields, e.g. in photonic crystals, metamaterials or superconducting circuit setups. Nonreciprocal devices can act as circulators and optical isolators, but they are hard to implement on chip because they require large magnetic fields. Several proposals have been made to overcome this limitation. A possible route to achieve directional properties in an optical device without utilizing the effect of Faraday rotation, is for example via the introduction of distinct phases via external driving or dynamical modulation of the refractive index. In this talk, we follow a different route by using dissipation engineering to obtain control over the propagation direction of photons in one and two dimensional structures. Moreover, we will discuss possible implementations within a superconducting circuit architecture.

**1:51PM Y25.00014 Current Correlations in a Majorana Beam Splitter** , EREZ BERG, ARBEL HAIM, Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot, 76100, Israel, FELIX VON OPPEN, Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, YUVAL OREG, Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot, 76100, Israel — We study current correlations in a  $T$ -junction composed of a grounded topological superconductor and of two normal-metal leads which are biased at a voltage  $V$ . We show that the existence of an isolated Majorana zero mode in the junction dictates a universal behavior for the cross correlation of the currents through the two normal-metal leads of the junction. The cross correlation is negative and approaches zero at high bias voltages as  $-1/V$ . This behavior is robust in the presence of disorder and multiple transverse channels, and persists at finite temperatures. In contrast, an accidental low-energy Andreev bound state gives rise to non-universal behavior of the cross correlation. We employ numerical transport simulations to corroborate our conclusions.

**2:03PM Y25.00015 Odd-parity superconductors with two-component order parameters: nematic and chiral, gapped and nodal** , JRN W F VENDERBOS, VLADYSLAV KOZII, LIANG FU, Massachusetts Institute of Technology — Motivated by growing experimental evidence that superconductivity in the doped topological insulator  $\text{Cu}_x\text{Bi}_2\text{Se}_3$  has an odd-parity pairing with broken rotational symmetry, we study the general class of odd-parity superconductors with two-component order parameters. We address the energetics and physical properties of different superconducting phases, with special emphasis on the role of spin-orbit coupling, which is generally strong in topological insulator and related materials. We show that within the weak-coupling BCS theory, in the absence of spin-orbit coupling, isotropic superconductors are favored, which are analogs of the A- or B-phase of  $^3\text{He}$ . In the presence of spin-orbit coupling, however, we find that a nematic superconducting phase, which spontaneously breaks rotational symmetry are favored. We determine the superconducting gap structures and find, in addition to fully gapped odd-parity superconductors, nodal superconductors with Dirac and Weyl quasiparticles, which are markedly different from superfluid phases of  $^3\text{He}$ .

**Friday, March 18, 2016 11:15AM - 2:15PM –**

**Session Y26 DCMP: Electron-phonon Interactions in 2D Materials (Raman/ ARPES)** 325 - Jyoti Katoch, The Ohio State University

**11:15AM Y26.00001 Raman characterization of few-layered 1T'-MoTe<sub>2</sub><sup>1</sup>**, IRVING HERMAN, DENNIS WANG, ALI DADGAR, Columbia Univ, SANG-WOOK CHEONG, Rutgers, The State University of New Jersey, ABHAY PASUPATHY, Columbia Univ — Transition metal dichalcogenides (TMDs) exhibit a wealth of physical phenomena that have been studied via electronic transport and optical characterization because of their potential device applications in the 2-D limit. In particular, theory has predicted that a certain subset of TMDs, specifically those in the structurally distorted octahedral (1T') phase, are large-gap quantum spin Hall (QSH) insulators. Here we characterize the thickness of one such TMD, 1T'-MoTe<sub>2</sub>, down to the monolayer limit using Raman spectroscopy and compare our results to atomic force microscopy (AFM) measurements. Our goal is to determine how thinning it down via micromechanical exfoliation changes the intensities and frequencies of its Raman modes, thus enabling one to track layer dependence in a definitive yet minimally invasive manner in much the same way used for graphene and other layered materials.

<sup>1</sup>This work is supported by NSF IGERT (DGE-1069240)

## **11:27AM Y26.00002 ABSTRACT WITHDRAWN —**

**11:39AM Y26.00003 Resonant-Raman Intensities of N-layer Transition Metal Dichalcogenides from First Principles**, HENRIQUE MIRANDA, University of Luxembourg, GUILLAUME FROELICHER, ETTIENNE LORCHAT, FRANOIS FERNIQUE, IPCMS (CNRS - Universit de Strasbourg), ALEJANDRO MOLINA-SNCHEZ, University of Luxembourg, STPHANE BERCIAUD, IPCMS (CNRS - Universit de Strasbourg), LUDGER WIRTZ, University of Luxembourg — Transition metal dichalcogenides (TMDs) have interesting optical and electronic properties that make them good candidates for nano-engineering applications. Raman spectroscopy provides information about the vibrational modes and optical spectrum at the same time: when the laser energy is close to an electronic transition, the intensity is increased due to resonance. We investigate these effects combining different ab initio methods: we obtain ground-state and vibrational properties from density functional theory and the optical absorption spectrum using GW corrections and the Bethe-Salpeter equation to account for the excitonic effects which are known to play an important role in TMDs. Using a quasi-static finite differences approach [1], we calculate the dielectric susceptibility for different light polarizations and different phonon modes in order to determine the Raman tensor of TMDs, in particular of multi-layer and bulk MoTe<sub>2</sub>. We explain recent experimental results for the splitting of high-frequency modes [2] and deviations from the non-resonant Raman model. We also give a brief outlook on possible improvements of the methodology. [1] Y. Gillet et. al., Phys. Rev. B 88, 094305 (2013). [2] G. Froehlicher et. al., Nano Lett. 15, 6481 (2015).

**11:51AM Y26.00004 Raman investigation of molybdenum disulfide with different polytypes**, JAE-UNG LEE, KANGWON KIM, SONGHEE HAN, Sogang University, GYEONG HEE RYU, ZONGHOON LEE, UNIST, HYEONSIK CHEONG, Sogang University — The Raman spectra of molybdenum disulfide (MoS<sub>2</sub>) with different polytypes are investigated. Although 2H-MoS<sub>2</sub> is most common in nature, the 3R phase can exist due to a small difference in the formation energy. However, only a few studies are reported for the 3R phase, and most studies have focused on the 2H phase. We found the 2H, 3R and mixed phases of exfoliated few-layer MoS<sub>2</sub> from natural molybdenite crystals. The crystal structures of 2H- and 3R-MoS<sub>2</sub> are confirmed by the HR-TEM measurements. By using 3 different excitation energies, we compared the Raman spectra of different polytypes in detail. We show that the Raman spectroscopy can be used to identify not only the number of layers but also the polytypes of MoS<sub>2</sub>.

**12:03PM Y26.00005 Observation of anomalous Stokes versus anti-Stokes ratio in MoTe<sub>2</sub> atomic layers<sup>1</sup>**, THOMAS GOLDSTEIN, SHAO-YU CHEN, Department of Physics, University of Massachusetts Amherst, DI XIAO, Department of Physics, Carnegie Mellon University, ASHWIN RAMASUBRAMANIAM, Department of Mechanical & Industrial Engineering, University of Massachusetts Amherst, JUN YAN, Department of Physics, University of Massachusetts Amherst — We grow hexagonal molybdenum ditelluride (MoTe<sub>2</sub>), a prototypical transition metal dichalcogenide (TMDC) semiconductor, with chemical vapor transport methods and investigate its atomic layers with Stokes and anti-Stokes Raman scattering. We report observation of all six types of zone center optical phonons. Quite remarkably, the anti-Stokes Raman intensity of the low energy layer-breathing mode becomes more intense than the Stokes peak under certain experimental conditions, creating an illusion of 'negative temperature'. This effect is tunable, and can be switched from anti-Stokes enhancement to suppression by varying the excitation wavelength. We interpret this observation to be a result of resonance effects arising from the C excitons in the vicinity of the Brillouin zone center, which are robust even for multiple layers of MoTe<sub>2</sub>. The intense anti-Stokes Raman scattering provides a cooling channel for the crystal and opens up opportunities for laser cooling of atomically thin TMDC semiconductor devices.

<sup>1</sup>Supported by the University of Massachusetts Amherst, the National Science Foundation Center for Hierarchical Manufacturing (CMMI-1025020) and Office of Emerging Frontiers in Research and Innovation (EFRI-1433496).

## **12:15PM Y26.00006 ABSTRACT WITHDRAWN —**

**12:27PM Y26.00007 Magnetism and Raman Spectroscopy of Pristine and Hydrogenated TaSe<sub>2</sub> Monolayer tuned by Tensile and Pure Shear Strain**, SUGATA CHOWDHURY, The Catholic University of America, Washington DC & National Institute of Standards and Technology, MD, JEFFREY SIMPSON, Towson University, MD & National Institute of Standards and Technology, MD, T. L. EINSTEIN, Univ of Maryland-College Park, ANGELA R. HIGHT WALKER, National Institute of Standards and Technology, MD — 2D-materials with controllable optical, electronic and magnetic properties are desirable for novel nanodevices. Here we studied these properties for both pristine and hydrogenated TaSe<sub>2</sub> (TaSe<sub>2</sub>-H) monolayer (ML) in the framework of DFT using the PAW method. We considered uniaxial and biaxial tensile strain, as well as shear strain along the basal planes in the range between 1% and 16%. Previous theoretical works (e.g. APL 107, 032402 (2015)) considered only symmetrical biaxial tensile. Pristine ML is ferromagnetic for uniaxial tensile strain along  $\hat{x}$  or  $\hat{y}$ . For tensile strain in  $\hat{y}$ , the calculated magnetic moments of the Ta atoms are twice those for the same strain in  $\hat{x}$ . Under pure shear strain (expansion along  $\hat{y}$  and compression along  $\hat{x}$ ), a pristine ML is ferromagnetic, but becomes non-magnetic when the strain directions are interchanged. Due to carrier-mediated double-exchange, the pristine ML is ferromagnetic when the Se-Ta-Se bond angle is  $< 82^\circ$  and the ML thickness is  $< 3.25\text{\AA}$ . We find that all Raman-active phonon modes show obvious red-shifting due to bond elongation and the E<sub>2</sub> modes degeneracy is lifted as strain increases. For a TaSe<sub>2</sub>-H ML, the same trends were observed. Results show the ability to tune the properties of 2D-materials.

**12:39PM Y26.00008 Quantum plasmonic nano-imaging of few-layer MoS<sub>2</sub>**, DMITRI VORONINE, Texas AM University — Transition metal dichalcogenides such as MoS<sub>2</sub> are promising 2D materials with many applications. Their diffraction-limited optical characterization using Raman spectroscopy provides important structure-functional information. In this work, nanoscale tip-enhanced Raman scattering (TERS) signals of few-layer MoS<sub>2</sub> are presented and limits of signal enhancement are investigated by varying the tip-sample gap. Quantum plasmonic quenching of gold photoluminescence signals was observed for subnanometer gaps. Similar quantum plasmonic behavior was observed for more than 3 nm gaps between gold substrate and tip with few-layer MoS<sub>2</sub> junctions. These results may be used for designing new generation quantum optoelectronic devices.

**12:51PM Y26.00009 Nanoscale control of phonon excitations in graphene**, HYO WON KIM, WONHEE KO, JIYEON KU, Samsung Adv Inst of Tech, SEUNGHWA RYU, Korea Advanced Institute of Science and Technology, SUNG WOO HWANG, Samsung Adv Inst of Tech — Phonons, which are collective excitations in a lattice of atoms or molecules, play a major role in determining various physical properties of condensed matter, such as thermal and electrical conductivities. In particular, phonons in graphene interact strongly with electrons; however, unlike in usual metals, these interactions between phonons and massless Dirac fermions appear to mirror the rather complicated physics of those between light and relativistic electrons. Therefore, a fundamental understanding of the underlying physics through systematic studies of phonon interactions and excitations in graphene is crucial for realizing graphene-based devices. In this study, we demonstrate that the local phonon properties of graphene can be controlled at the nanoscale by tuning the interaction strength between graphene and an underlying Pt substrate. Using scanning probe methods, we determine that the reduced interaction due to embedded Ar atoms facilitates electron-phonon excitations, further influencing phonon-assisted inelastic electron tunneling.

**1:03PM Y26.00010 Observation of angle resolved bands of  $C_{60}$  by photoemission spectroscopy**, CLAUDIA OJEDA-ARISTIZABAL, Dept. of Physics and Astronomy California State University, DREW LATZKE, Dept. of Physics Univ. of California Berkeley, Lawrence Berkeley National Laboratory, JONATHAN DELINGER, Advanced Light Source, Lawrence Berkeley National Laboratory, ALEX ZETTL, ALESSANDRA LANZARA, Dept. of Physics Univ. of California Berkeley, Lawrence Berkeley National Laboratory — The band structure of a  $C_{60}$  thick film deposited in-situ on a crystalline surface is studied by angle resolved photoemission spectroscopy (ARPES). We observe the presence of a well-defined low energy diffraction pattern (LEED) and dispersive HOMO bands, suggesting a crystalline arrangement of the  $C_{60}$  molecules. The momentum and photon energy dependence of these bands is presented.

**1:15PM Y26.00011 Optical properties of transition metal dichalcogenide monolayers**, BENEDIKT SCHARF, State Univ of NY - Buffalo, TOBIAS FRANK, MARTIN GMITRA, JAROSLAV FABIAN, University of Regensburg, IGOR ZUTIC, State Univ of NY - Buffalo, VASIL PEREBEINOS, Skolkovo Institute of Science and Technology — In recent years, 2D materials, such as transition metal dichalcogenide (TMDCs) monolayers, have attracted a great deal of attention due to their excellent transport and optical properties. Using a tight-binding description and the Bethe-Salpeter equation, we theoretically investigate optical and excitonic properties of TMDC monolayers in different setups. Such 2D materials exhibit peculiar screening properties and excitons with large binding energies. This can also lead to important spin-based applications as the spin-orbit coupling in the valence band results in a splitting close to the K and K' points and yields spin-relaxation times orders of magnitude larger than in III-V semiconductors.

**1:27PM Y26.00012 Band Structure Studies of in situ Deposited  $C_{60}$  and the Effects of Doping**, DREW LATZKE, University of California, Berkeley and Lawrence Berkeley National Laboratory, CLAUDIA OJEDA-ARISTIZABAL, California State University Long Beach, Department of Physics and Astronomy, JONATHAN DENLINGER, Lawrence Berkeley National Laboratory, ALEX ZETTL, ALESSANDRA LANZARA, University of California, Berkeley and Lawrence Berkeley National Laboratory — We present electronic band structure studies of the unique system of in situ deposited thin film  $C_{60}$  on a bulk substrate through high-resolution angle-resolved photoemission spectroscopy (ARPES) measurements. We discuss the electronic band structure in relation to novel phenomena recently found in other low-dimensional samples. Finally, we investigate the doping dependence of the thin film  $C_{60}$  band structure as we deposit dopants on the surface in situ.

**1:39PM Y26.00013 ARPES studies of van der Waals heterostructure<sup>1</sup>**, ERYIN WANG, State Key Laboratory of Low Dimensional Quantum Physics and Department of Physics, Tsinghua University, Beijing, XIAOBO LU, Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Science, Beijing, GUORUI CHEN, State Key Laboratory of Surface Physics and Department of Physics, Fudan University, Shanghai, ALEXEI V. FEDOROV, Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, YUANBO ZHANG, State Key Laboratory of Surface Physics and Department of Physics, Fudan University, Shanghai, GUANGYU ZHANG, Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Science, Beijing, SHUYUN ZHOU, State Key Laboratory of Low Dimensional Quantum Physics and Department of Physics, Tsinghua University, Beijing — Van der Waals heterostructures are a novel class of "materials by design" which are formed by stacking different two-dimensional crystals together via van der Waals interaction. The periodic potential by the Moiré superlattice can be used as a control knob for tuning the electronic properties of two dimensional materials and can induce various novel quantum phenomena. Here we report direct electronic structure studies of a model van der Waals heterostructure using angle-resolved photoemission spectroscopy (ARPES).

<sup>1</sup>This work is supported by the National Natural Science Foundation of China and Ministry of Education of China.

**1:51PM Y26.00014 Unified Description of the Optical Phonon Modes in  $N$ -Layer  $MoTe_2$** , GUILLAUME FROELICHER, ETIENNE LORCHAT, FRANÇOIS FERNIQUE, IPCMS (CNRS - Université de Strasbourg), CHAITANYA JOSHI, ALEJANDRO MOLINA-SÁNCHEZ, LUDGER WIRTZ, University of Luxembourg, STÉPHANE BERCIAUD, IPCMS (CNRS - Université de Strasbourg) —  $N$ -layer transition metal dichalcogenides (denoted  $MX_2$ ) provide a unique platform to investigate the evolution of the physical properties between the bulk (3D) and monolayer (quasi-2D) limits. Here, we present a unified analysis of the optical phonon modes in  $N$ -layer  $2H$ - $MX_2$  [1]. The  $2H$ -phase (or hexagonal phase) is the most common polytype for semiconducting  $MX_2$  (such as  $MoS_2$ ). Using Raman spectroscopy, we have measured the manifold of low-frequency (rigid layer), mid-frequency (involving intralayer displacement of the chalcogen atoms only), and high-frequency (involving intralayer displacements of all atoms) Raman-active modes in  $N = 1$  to 12 layer  $2H$ -molybdenum ditelluride ( $MoTe_2$ ). For each monolayer mode, the  $N$ -dependent phonon frequencies give rise to fan diagrams that are quantitatively fit to a force constant model. This analysis allows us to deduce the frequencies of *all* the bulk (including silent) optical phonon modes. [1] G. Froehlicher, E. Lorchat, F. Fernique, C. Joshi, A. Molina-Sánchez, L. Wirtz, and S. Berciaud, Unified Description of the Optical Phonon Modes in  $N$ -Layer  $MoTe_2$ , Nano Letters, **15** (10), pp 6481-6489 (2015)

**2:03PM Y26.00015 Mapping wavevector dependent electron-phonon coupling and nonequilibrium phonon dynamics in thin graphite with ultrafast electron diffuse scattering**, JEAN-PHILIPPE BOISVERT, ROBERT P. CHATELAIN, MARK J. STERN, MARK SUTTON, Department of Physics, Center for the Physics of Materials, McGill University, BRADLEY J. SIWICK, Departments of Physics and Chemistry, Center for the Physics of Materials, McGill University — Radio-frequency compressed ultrafast electron diffraction has been used to probe the coherent and incoherent coupling of impulsive electronic excitation at 1.55 eV (800 nm) to optical and acoustic phonon modes directly from the perspective of the lattice degrees of freedom. Recent improvements in source brightness for ultrafast diffraction experiments are now allowing for the study of diffuse scattering signals. Here, we show that ultrafast electron diffuse scattering (UEDS) can yield time and momentum-resolved phonon population data. Beyond the possibility of directly probing the dynamics of thermalization, this can also be used to determine the wavevector dependent electron-phonon coupling strength in materials. This new information provides significant insights into the electron relaxation pathways of graphitic materials. In particular, we present the first direct measurement of the  $K$ -point phonon population dynamics after impulsive electronic excitation and maps of the phonon population in momentum-space. Finally, we propose a simple mechanism for the thermalization of graphitic materials after impulsive electronic excitation which unifies all ultrafast measurements of this process to date.

**Friday, March 18, 2016 11:15AM - 2:15PM** —

Session Y27 DCMF: Low Dimensional Correlated Systems 326 - Ben Ueland, Ames National Laboratory

**11:15AM Y27.00001 Electromagnetic response of time-reversal breaking metallic phases in two dimensions<sup>1</sup>**, VICTOR CHUA, WATHID ASSAWASUNTHONNET, EDUARDO FRADKIN, Univ of Illinois - Urbana — The electromagnetic response of models of nematic non Fermi-liquids previously proposed in Ref.[1] are re-examined using conventional many-body methods. Nematic phases of this model are described by two 2-component real vectors which express the isotropy breaking nematicity in two Fermi-surfaces. Of interest is the time-reversal symmetry breaking nematic phase with a non-vanishing unquantized spontaneous anomalous Hall effect at zero external magnetic fields, and has a geometrical description as a Berry phase. We compare and contrast our results with conventional response calculations with those predicted with the higher-dimensional bosonization method [2,3]. Finally we present preliminary results on an RG analysis of this system. [1] K Sun and E Fradkin, Phys. Rev. B 78, 245122 (2008). [2] HJ Kwon, A Houghton, and JB Marston, Phys. Rev. B 52, 8002 (1995) [3] MJ Lawler, DG Barci, V Fernandez, E Fradkin, L Oxman, Phys. Rev. B 73, 085101 (2006)

<sup>1</sup>This work was supported by the Gordon and Betty Moore Foundation

**11:27AM Y27.00002 Transport in a One-Dimensional Hyperconductor**, EUGENIU PLAMADEALA, Univ of California - Santa Barbara, MICHAEL MULLIGAN, Stanford University, CHETAN NAYAK, Univ of California - Santa Barbara, Microsoft Station Q — We define a ‘hyperconductor’ to be a material whose electrical and thermal DC conductivities are infinite at zero temperature. The low-temperature behavior of a hyperconductor is controlled by a quantum critical phase of interacting electrons that is stable to all potentially-gap-generating interactions and arbitrary potentially-localizing disorder. We compute the low-temperature DC and AC electrical and thermal conductivities in a one-dimensional hyperconductor, studied previously by the present authors, in the presence of both disorder and umklapp scattering. We identify the conditions under which the transport coefficients are finite, and exhibit examples of violations of the Wiedemann-Franz law. We show that the temperature dependence of the electrical conductivity is a power law,  $\sigma \propto 1/T^{1-2(2-\Delta_X)}$  for  $\Delta_X \geq 2$ , down to zero temperature when the Fermi surface is commensurate with the lattice. In the incommensurate case with weak disorder, such scaling is seen at high-temperatures, followed by an exponential increase of the conductivity  $\ln \sigma \sim 1/T$  at intermediate temperatures and, finally,  $\sigma \propto 1/T^{2-2(2-\Delta_X)}$  at the lowest temperatures. In both cases, the thermal conductivity diverges at low temperatures.

**11:39AM Y27.00003 Photon-dressed quasiparticle states in 1D and 2D materials: a many-body Floquet approach**, FRANCA MANGHI, MATTEO PUVIANI, University of Modena and Reggio Emilia — We study the interplay between electron-electron interactions and non-equilibrium conditions associated to time-dependent external fields. Exploring phases of quantum matter away from equilibrium may give access to regimes inaccessible under equilibrium conditions. What makes this field particularly interesting is the possibility to engineer new phases of matter by an external tunable control. We have developed a scheme that allows to treat photo-induced phenomena in the presence of electron-electron many body interactions, where both the nonlinear effects of the external field and the electron-electron correlation are treated simultaneously and in a non-perturbative way. The Floquet approach is used to include the effects of the external time periodic field, and the Cluster Perturbation Theory to describe interacting electrons in a lattice. They are merged in a Floquet-Green function method that allows to calculate photon dressed quasiparticle excitation. For 1D systems we show that an unconventional Mott insulator-to-metal transition occurs for given characteristics of the applied field (intensity and frequency). The method has also been applied to the 2D honeycomb lattice (graphene), where in the presence of realistic values of electron-electron interaction, we show that linearly polarized light may give rise to non-dissipative edge states associated to a non-trivial topological behavior.

**11:51AM Y27.00004 Composite fermions and the field-tuned superconductor-insulator transition**, SRINIVAS RAGHU, MICHAEL MULLIGAN, Stanford University — In several two-dimensional films that exhibit a magnetic field-tuned superconductor to insulator transition (SIT), stable metallic phases have been observed. Building on the ‘dirty boson’ description of the SIT, we suggest that the metallic region is analogous to the composite Fermi liquid observed about half-filled Landau levels of the two-dimensional electron gas. The composite fermions here are mobile vortices attached to one flux quantum of an emergent gauge field. The composite vortex liquid is a 2D non-Fermi liquid metal, which we argue is stable to weak quenched disorder. We describe several experimental consequences of the emergent composite vortex liquid.

**12:03PM Y27.00005 Mirror symmetry and the half-filled Landau level**, MICHAEL MULLIGAN, SHAMIT KACHRU, Stanford University, GONZALO TORROBA, Centro Atomico Bariloche and CONICET, HUAJIA WANG, University of Illinois at Champaign-Urbana — We study the dynamics of the half-filled zeroth Landau level of Dirac fermions using mirror symmetry, a supersymmetric duality between certain pairs of 2 + 1-dimensional theories. We show that the half-filled zeroth Landau level of a pair of Dirac fermions is dual to a pair of Fermi surfaces of electrically-neutral composite fermions, coupled to an emergent gauge field. Thus, we use supersymmetry to provide a derivation of flux attachment and the emergent Fermi liquid-like state for the lowest Landau level of Dirac fermions. We find that in the dual theory the Coulomb interaction induces a dynamical exponent  $z = 2$  for the emergent gauge field, making the interactions classically marginal. This enables us to map the problem of 2+1-dimensional Dirac fermions in a finite transverse magnetic field, interacting via a strong Coulomb interaction, into a perturbatively controlled model. We analyze the resulting low-energy theory using the renormalization group and determine the nature of the BCS interaction in the emergent composite Fermi liquid.

**12:15PM Y27.00006 Phase transitions induced by magnetic field in graphite**, BENOIT FAUQUE, LPEM (UPMC-CNRS), Ecole Supérieure de Physique et de Chimie Industrielles, 75005 Paris, France, DAVID LEBOEUF, Laboratoire National des Champs Magnétiques Intenses, UPR 3228, CNRS-UJF-UPS-INSA, 38042 Grenoble, France, WILLEM RISCHAU, LPEM (UPMC-CNRS), Ecole Supérieure de Physique et de Chimie Industrielles, 75005 Paris, France, WOJCIECH TABIS, BAPTISTE VIGNOLLE, CYRIL PROUST, Laboratoire National des Champs Magnétiques Intenses, CNRS, INSA, UJF, UPS, Toulouse 31400, France, KAMRAN BEHNIA, LPEM (UPMC-CNRS), Ecole Supérieure de Physique et de Chimie Industrielles, 75005 Paris, France — Graphite is compensated semi-metals characterized by a tiny three dimensional Fermi surface. A magnetic field of about 10T is large enough to confine electrons and holes to their lowest Landau levels. These are therefore ideal candidates to explore the nature of the electronic ground state of a three-dimensional electron gas pushed beyond the so-called quantum limit. Various instabilities have been predicted in this peculiar limit where electronic interactions are enhanced. We find that the magnetic field induces two successive phase transitions, made of two distinct ordered states, each restricted to a finite field window. In both states, the in-plane and out-of-plane conductivity behaves differently: not only the onset of the transition are different in both quantity but also an energy gap opens up in the out-of-plane conductivity and coexists with an unexpected in-plane metallicity for a fully gap bulk system. Such peculiar metallicity may arise as a consequence of edge-state transport expected to develop in the presence of a bulk gap.

**12:27PM Y27.00007 Exotic insulating states of  $(t_{2g})^4$  Hubbard model with spin-orbit coupling**, TOSHIHIRO SATO, RIKEN, TOMONORI SHIRAKAWA, RIKEN CEMS, SEIJI YUNOKI, RIKEN, RIKEN CEMS, RIKEN AICS — We numerically study electronic properties of a  $t_{2g}$ -orbital Hubbard model with a relativistic spin-orbit coupling (SOC) at four electrons per site. Our approach is a multi-orbital dynamical mean field theory with a continuous-time quantum Monte Carlo solver based on a strong coupling expansion. The main issue is the variation of electronic structure in the parameter space of the SOC and the Coulomb interactions at temperature fixed. For larger Coulomb interactions, a Van Vleck-type nonmagnetic insulating state with a total angular momentum  $J = 0$  is induced by the SOC. When the SOC decreases, the insulating state is magnetically ordered along with increasing the hybridization between a nonmagnetic  $J = 0$  state and an excited  $J = 1$  state. Moreover, for smaller Coulomb interactions, we demonstrate that an excitonic insulating state without magnetic order appears, in addition to metallic and band insulating states. The exciton condensation is formed by an electron-hole pairing between the local effective total angular momentum  $j = 1/2$  and  $j = 3/2$  based bands.

**12:39PM Y27.00008 Vison Condensation and Bond Density Wave Order in the Cuprates**, AAVISHKAR PATEL, ANDREA ALLAIS, DEBANJAN CHOWDHURY, SUBIR SACHDEV, Harvard Univ — We consider  $Z_2$  spin liquids on the square lattice. These can undergo a confinement transition to a valence bond solid (VBS) phase via the condensation of vortex excitations carrying  $Z_2$  magnetic flux (visons) [1]. The resulting condensed phase is described by a fully frustrated Ising model (FFIM) on the dual square lattice, with additional couplings allowed by symmetries. We argue that such a model can also apply to confinement transitions out of the fractionalized Fermi liquid (FL\*) states of doped antiferromagnets. We study the low energy states of such a model and discuss their implications for the incommensurate d-form factor bond density wave order observed in several recent experiments on the cuprate superconductors. [1] R. Jalabert and S. Sachdev, Phys. Rev. B 44, 686 (1991).

**12:51PM Y27.00009 Transition from the  $Z_2$  spin liquid to antiferromagnetic order: spectrum on the torus**, SETH WHITSITT, SUBIR SACHDEV, Harvard Univ — We study the finite-size spectrum of the quantum critical point between a  $Z_2$  spin liquid and a coplanar antiferromagnet on the torus. Due to the existence of nontrivial order on either side of this transition, this critical point cannot be described in a conventional Landau-Ginzburg framework. Instead it is described by a theory involving fractionalized degrees of freedom known as the  $O(4)^*$  model, whose spectrum is altered in a significant way by its proximity to a topologically ordered phase. We compute the spectrum by relating it to the spectrum of the  $O(4)$  Wilson-Fisher fixed point on the torus, along with a selection rule on the states, and with nontrivial boundary conditions corresponding to topological sectors in the spin liquid. The spectrum of the Wilson-Fisher fixed points is then calculated directly from the  $\epsilon$ - and large- $N$  expansions, which allows a reconstruction of the full spectrum of the  $O(4)^*$  model. This spectrum is a unique characteristic of a fractionalized quantum critical point as well as a universal signature of the existence of a proximate  $Z_2$  topological phase which can be compared with numerical computations.

(contacted membership@aps for help with logging in and waiting for reply)

**1:03PM Y27.00010 Long-range Coulomb interaction in nodal ring semi-metals**, YEJIN HUH, University of Toronto, EUN-GOOK MOON, KAIST, YONG BAEK KIM, University of Toronto — Recently there have been several proposals of materials predicted to be nodal ring semi-metals, where zero energy excitations are characterized by a nodal ring in the momentum space. This class of materials falls between the Dirac-like semi-metals and the more conventional Fermi-surface systems. As a step towards understanding this unconventional system, we explore the effects of the long-range Coulomb interaction. Due to the vanishing density of states at the Fermi level, Coulomb interaction is only partially screened and remains long-ranged. Through renormalization group and large- $N_f$  computations, we have identified a non-trivial interacting fixed point. The screened Coulomb interaction at the interacting fixed point is an irrelevant perturbation, allowing controlled perturbative evaluations of physical properties of quasiparticles. We discuss unique experimental consequences of such quasiparticles: acoustic wave propagation, anisotropic DC conductivity, and renormalized phonon dispersion as well as energy dependence of quasiparticle lifetime.

**1:15PM Y27.00011 Scaling of Greenwood Peierls conductance on a diluted square lattice**, WILLIAM SCHWALM, ALBERT SCHMITZ, Univ of North Dakota — The modified rectangle lattice of Dhar is a bond-diluted square lattice. The structure is self-similar and finitely ramified, like a fractal. Nevertheless certain discrete Schrödinger equation Green functions for the modified rectangle are known in closed form in the infinite lattice limit and the spectrum is continuous. By standard transfer matrix renormalization methods we present a study scaling properties of the Greenwood Peierls conductance distribution across the lattice with one dimensional lead wires attached as a function of lattice size and of additional disorder of several types.

**1:27PM Y27.00012 Phase coexistence in the  $O(N) \oplus O(M)$  nonlinear sigma model: a conformal bootstrap study**, CHRIS HOOLEY, SAM RIDGWAY, University of St Andrews, U.K. — The low-temperature physics of systems with competing orders is a ubiquitous topic in modern condensed matter physics. A commonly studied field theory of such systems is the  $O(N) \oplus O(M)$  nonlinear sigma model: an  $O(N+M)$  model with a mass term attached to  $N$  of the field components. Depending on the sign of the mass term, order in the  $O(N)$  sector or the  $O(M)$  sector is favored. However, the physics near the high-symmetry point is subtle, and in some cases (e.g.  $N=M=2$ ) it remains unclear whether there is a first-order spin-flop transition or a finite-width microscopic coexistence phase. In this talk, we present an analysis of the  $O(N) \oplus O(M)$  model based on the conformal bootstrap method. This allows us to classify the critical points of the models in question, and by extension determine whether a coexistence phase exists or not.

**1:39PM Y27.00013 Quantum Monte Carlo study of hard-core bosons in a pyrochlore lattice with six-site ring-exchange interactions**, CATHERINE TIEMAN, VALERY ROUSSEAU, College of Wooster — Highly frustrated quantum systems on lattices can exhibit a wide variety of phases. In addition to the usual Mott insulating and superfluid phases, these systems can also produce some so-called “exotic phases”, such as super-solid and valence-bond-solid phases. An example of particularly frustrated lattice is the pyrochlore structure, which is formed by corner-sharing tetrahedrons. Many real materials adopt this structure, for instance the crystal  $Cd_2Re_2O_7$ , which exhibits superconducting properties. However, the complex structure of these materials combined with the complexity of the dominant interactions that describe them makes their analytical study difficult. Also, approximate methods, such as mean-field theory, fail to give a correct description of these systems. In this work, we report on the first exact quantum Monte Carlo study of a model of hard-core bosons in a pyrochlore lattice with six-site ring-exchange interactions, using the Stochastic Green Function (SGF) algorithm. We analyze the superfluid density and the structure factor as functions of the filling and ring-exchange interaction strength, and we map out the ground state phase diagram.

**1:51PM Y27.00014 Phase Diagram of the  $Z_3$  Parafermionic Chain with Chiral Interactions**, YE ZHUANG, HITESH CHANGLANI, NORM TUBMAN, TAYLOR HUGHES, Univ of Illinois - Urbana — Majorana fermions and parafermions are exotic quasiparticles with non-Abelian fractional statistics that can be realized and stabilized in one-dimensional models. We study the simplest generalization of the Kitaev p-wave wire, i.e. the  $Z_3$  parafermionic chain [Phys. Rev. B 92, 035154 (2014)]. Using a Jordan-Wigner transform we focus on the equivalent three-state chiral clock model, and study its rich phase diagram using the density matrix renormalization group technique. We perform our analyses using quantum entanglement diagnostics which allow us to determine phase boundaries, and the nature of the phase transitions. In particular, we study the transition between the topological (ordered) and trivial phases (disordered), as well as to an intervening critical (incommensurate) phase which appears in a wide region of the phase diagram. The phase diagram is predicted to contain a Lifshitz type transition which we confirm using entanglement measures. We also attempt to locate and characterize a putative tricritical point in the phase diagram where the three above mentioned phases meet at a single point.

**2:03PM Y27.00015 Photon-induced phase transitions of individual electronic phase separated domains in manganites strips**, HANXUAN LIN, KAI ZHANG, HAO LIU, TIAN MIAO, YANG YU, LIFENG YIN<sup>1</sup>, JIAN SHEN<sup>2</sup>, Fudan University — Effective photosensors should be built on materials whose properties depend sensitively on light. Manganites are one of the candidates, where light can trigger resistivity change by several orders of magnitude. Such dramatic change is often associated with photoinduced phase transitions of electronic phase separated (EPS) domains in manganites. Previous studies of the light effect all use macroscopic manganite samples, which consist of large numbers of EPS domains smearing out the photon-induced phase transitions. Here, we observe the signature of individual domains' photoinduced phase transition by macroscopic transport measurement of spatially confined manganites strips. Pronounced photon-induced resistivity jumps emerge in the warming process, which reveals the dynamics of the phase transitions of individual EPS domains upon interaction with light. Magnetic force microscope (MFM) has been used to investigate the mechanism of those resistivity jumps.

<sup>1</sup>Supervisor

<sup>2</sup>Supervisor

**Friday, March 18, 2016 11:15AM - 2:15PM –**  
**Session Y28 DMP DCMP: Weyl Semimetals: Theory and New Materials** 327 - Siddharth Parameswaran, University of California, Irvine

**11:15AM Y28.00001 Prediction of an arc-tunable Weyl Fermion metallic state in  $\text{Mo}_x\text{W}_{1-x}\text{Te}_2$** , TAY-RONG CHANG, Natl Tsing Hua U., SU-YANG XU, Princeton U., GUOQING CHANG, CHI-CHENG LEE, SHIN-MING HUANG, National University of Singapore, BAOKAI WANG, Northeastern U., GUANG BIAN, HAO ZHENG, DANIEL SANCHEZ, ILYA BELOPOLSKI, NASSER ALIDOUST, MADHAB NEUPANE, Princeton U., ARUN BANSIL, Northeastern U., HORNG-TAY JENG, Natl Tsing Hua U., HSIN LIN, National University of Singapore, M. ZAHID HASAN, Princeton U. — A Weyl semimetal is a new state of matter that hosts Weyl fermions as emergent quasiparticles. The Weyl fermions correspond to isolated points of bulk band degeneracy, Weyl nodes, which are connected only through the crystals boundary by an exotic Fermi arc surface state. The length of the Fermi arc gives a measure of the topological strength, because the only way to destroy the Weyl nodes is to annihilate them in pairs in k space. To date, Weyl semimetals are only realized in the TaAs class. Here, we propose a tunable Weyl metallic state in  $\text{Mo}_x\text{W}_{1-x}\text{Te}_2$  via our first-principles calculations, where the Fermi arc length can be continuously changed as a function of Mo concentration, thus tuning the topological strength of the system [1]. Our results provide an experimentally feasible route to realizing Weyl physics in the layered compound  $\text{Mo}_x\text{W}_{1-x}\text{Te}_2$  where non-saturating magneto-resistance and pressure driven superconductivity have been observed.  
[1] T.-R. Chang et al., arXiv:1508.06723.

**11:27AM Y28.00002 Nonsymmorphic topological photonic crystal with a single surface Dirac cone**, LING LU, CHEN FANG, LIANG FU, STEVEN JOHNSON, JOHN JOANNOPOULOS, MARIN SOLJACIC, MIT, MIT COLLABORATION — We predict a realization of the nonsymmorphic topological crystalline phase: a three-dimensional (3D) photonic crystal with a single surface Dirac cone. A single Dirac cone on the surface is the hallmark of the 3D topological insulators, where the double degeneracy at the Dirac point is protected by time-reversal symmetry and the spin-splitting away from the point is provided by the spin-orbital coupling. In our 3D topological photonic crystal, the degeneracy at the Dirac point is protected by a nonsymmorphic glide reflection and the linear splitting away from it is enabled by breaking time-reversal symmetry. Such a gapless surface state is fully robust against random disorder of any type. This bosonic topological band structure is achieved by applying alternating magnetization to gap out the 3D "generalized Dirac points" discovered in the bulk of our crystal. The Z2 bulk invariant is characterized through the evolution of Wannier centers. Our proposal—readily realizable using ferrimagnetic materials at microwave frequencies—can also be regarded as the photonic analog of topological crystalline insulators, providing the first 3D bosonic symmetry-protected topological system.

**11:39AM Y28.00003 Topological semimetals with Riemann surface states<sup>1</sup>**, CHEN FANG, Institute of Physics, Chinese Academy of Sciences, LING LU, JUNWEI LIU, LIANG FU, Massachusetts Inst of Tech-MIT — Topological semimetals have robust bulk band crossings between the conduction and the valence bands. Among them, Weyl semimetals are so far the only class having topologically protected signatures on the surface known as the "Fermi arcs". Here we theoretically find new classes of topological semimetals protected by nonsymmorphic glide reflection symmetries. On a symmetric surface, there are multiple Fermi arcs protected by nontrivial  $Z_2$  spectral flows between two high-symmetry lines (or two segments of one line) in the surface Brillouin zone. We observe that so far topological semimetals with protected Fermi arcs have surface dispersions that can be mapped to noncompact Riemann surfaces representing simple holomorphic functions. We propose perovskite superlattice  $[(\text{SrIrO}_3)_{2m}, (\text{CaIrO}_3)_{2n}]$  as a nonsymmorphic Dirac semimetal.

<sup>1</sup>C.F. and L.F. were supported by the S3TEC Solid State Solar Thermal Energy Conversion Center, an Energy Frontier Research Center funded by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES), under Award No. DE-SC0001299/DE

**11:51AM Y28.00004 Type-II Weyl semimetals**, ALEXEY SOLUYANOV, DOMINIK GRESCH, ETH Zurich, ZHIJUN WANG, Princeton University, QUANSHENG WU, MATTHIAS TROYER, ETH Zurich, XI DAI, IOP, Chinese Academy of Sciences, ANDREI BERNEVIG, Princeton University — The Dirac equation of quantum field theory gives rise to massless Weyl fermions that respect Lorentz invariance. In condensed matter these fermions are realized as low energy excitations in Weyl semimetals. In these materials a topologically protected linear crossing of two bands, called a Weyl point, occurs at the Fermi level resulting in a point-like Fermi surface. Lorentz invariance, however, can be violated in condensed matter, and here we generalize the Dirac equation accordingly to obtain a fundamentally new kind of Weyl fermions. In particular, we report on a novel type of Weyl semimetal, with a new type of Weyl point that emerges at the boundary between electron and hole pockets. This node, although still a protected crossing, has an open, not point-like, Fermi surface, resulting in physical properties very different from that of standard Weyl points. We show that an established material,  $\text{WTe}_2$ , is an example of this novel type of topological semimetals.

**12:03PM Y28.00005 Topological Dirac line nodes in centrosymmetric semimetals**, YOUNGKUK KIM, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, Philadelphia, Pennsylvania 19104-6323, USA, BENJAMIN WIEDER, CHARLES KANE, Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, Pennsylvania 19104-6396, USA, ANDREW RAPPE, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, Philadelphia, Pennsylvania 19104-6323, USA, TI SEED TEAM — Dirac line nodes (DLNs) are one-dimensional lines of Dirac band-touching points, characterized by linear dispersion in only a single direction in momentum space. In the presence of inversion symmetry and time-reversal symmetry, crystals with vanishing spin-orbit coupling can host topologically protected DLNs. Recently, we have proposed and characterized a novel Z2 class of DLN semimetals [1]. We present Z2 topological invariants, dictating the presence of DLNs, based on the parity eigenvalues at the time-reversal invariant crystal momenta. Our first-principles calculations show that DLNs can be realized in  $\text{Cu}_3\text{N}$  in an anti- $\text{ReO}_3$  structure via a metal-insulator electronic transition, driven by transition metal doping. We also discuss the resultant surface states and the effects of spin-orbit coupling.

**12:15PM Y28.00006 Symmetry-protected ideal Weyl semimetal in HgTe-class materials**, SHAO-KAI JIAN, Institute for Advanced Study, Tsinghua University, Beijing 100084, China, JIAWEI RUAN, National Laboratory of Solid State Microstructures, School of Physics, Nanjing University, Nanjing 210093, China, HONG YAO, Institute for Advanced Study, Tsinghua University, Beijing 100084, China, HAIJUN ZHANG, National Laboratory of Solid State Microstructures, School of Physics, Nanjing University, Nanjing 210093, China, SHOU-CHENG ZHANG, Department of Physics, McCullough Building, Stanford University, Stanford, CA 94305-4045, USA, DINGYU XING, National Laboratory of Solid State Microstructures, School of Physics, Nanjing University, Nanjing 210093, China — Ideal Weyl semimetals with all Weyl nodes exactly at the Fermi level and no coexisting trivial Fermi surfaces in the bulk, similar to graphene, could feature deep and novel physics such as exotic transport phenomena induced by the chiral anomaly. Here, we show that HgTe and half-Heusler compounds, under a broad range of inplane compressive strain, could be the first materials in nature realizing ideal Weyl semimetals with four pairs of Weyl nodes and topological surface Fermi arcs. Generically, we find that the HgTe-class materials with nontrivial band inversion and noncentrosymmetry provide a promising arena to realize ideal Weyl semimetals. Such ideal Weyl semimetals could further provide a unique platform to study emergent phenomena such as the interplay between ideal Weyl fermions and superconductivity in the half-Heusler compound LaPtBi.

**12:27PM Y28.00007 Spin-Orbit Nodal Semimetals in the Layer Groups**, BENJAMIN WIEDER, Department of Physics and Astronomy, University of Pennsylvania, YOUNGKUK KIM, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, CHARLES KANE, Department of Physics and Astronomy, University of Pennsylvania — Recent interest in point and line node semimetals has lead to the proposal and discovery of these phenomena in numerous systems. Frequently, though, these nodal systems are described in terms of individual properties reliant on specific space group intricacies or band-tuning conditions. Restricting ourselves to cases with strong spin-orbit interaction, we develop a more general framework which captures existing systems and predicts new examples of nodal materials. In many previously proposed systems, the three-dimensional nature of the space group has obscured key generalities. Therefore, we show how within our framework one can predict and characterize a diverse set of nodal phenomena even in two-dimensional systems constructed of three-dimensional sites, known as the “Layer Groups”. Introducing a set of simple models, we characterize the allowed semimetallic structures in the layer groups and draw connections to analogous three-dimensional systems.

**12:39PM Y28.00008 Scanning Tunneling Microscopy study and unusual transport properties of the topological semimetal  $\alpha$ -Sn.**, JIAWEI RUAN, Nanjing Univ — Weyl semimetals are new states of quantum matter with topological Weyl nodes near Fermi level in the bulk and Fermi arcs at the surface, which are paid a lot attention in recently years. Herewe report another topological semimetal  $\alpha$ -Sn., which is double Weyl semimetal in the magnetic field and Dirac semimetal in an appropriate in-plane strain. By combing Landau level spectroscopy and quasiparticle interference, we obtain the linear dispersion near the Dirac point within strain while quadratic band dispersion near  $\Gamma$  point without strain. We also observe the negative longitudinal magnetoresistance (LMR) in both two system, which is caused by chiral anomaly. However ,the LMR profiles of strained  $\alpha$ -Sn have a little rise and then descend while the unstrained one drop directly, which is due to the different type of Weyl semimetal and further confirm our prediction.

**12:51PM Y28.00009 Spinless Weyl semimetals and  $Z_2$  topological crystalline insulator with glide symmetry**, HEEJAE KIM, Tokyo Institute of Technology, SHUICHI MURAKAMI, TIES, Tokyo Institute of Technology — A topological crystalline insulator (TCI) is one of the kimmy protected topological phases protected by crystalline symmetries such as rotational symmetry, mirror symmetry etc. In recent works, a new class of three-dimensional (3D)  $Z_2$  TCI with a nonsymmorphic glide plane symmetry is theoretically predicted both for spinless and spinfull systems. Our study shows that a spinless Weyl semimetal (WSM) phase always emerges between a normal insulator (NI) and TCI phases transition in general glide symmetric spinless systems. In particular, we find how the  $Z_2$  topological invariant is changed by pair creations and pair annihilations of Weyl nodes in general phase transition. To confirm this scenario, we introduce a simple spinless tight-binding model on a 3D rectangular lattice with two sublattices and two orbitals with glide plane symmetry. Using this model, we show that the spinless WSM phase emerges between the NI and TCI phases, and the changing of  $Z_2$  topological invariant comes from the behavior of Weyl nodes. Our numerical calculation also shows that surface Fermi arcs in the spinless WSM phase evolve into a surface Dirac cone in the TCI phase.

**1:03PM Y28.00010 Interacting weak topological insulators and their transition to Dirac semimetal phases<sup>1</sup>**, GIORGIO SANGIOVANNI, WERNER HANKE, Universitat Wurzburg, GANG LI, Vienna University of Technology, BJOERN TRAUZETTEL, Universitat Wurzburg — Topological insulators in the presence of strong Coulomb interaction constitute novel phases of matter. Transitions between these phases can be driven by single-particle or many-body effects. On the basis of *ab-initio* calculations, we identify a concrete material, *i.e.*  $\text{Ca}_2\text{PtO}_4$ , that turns out to be a hole-doped weak topological insulator. Interestingly, the Pt-*d* orbitals in this material are relevant for the band inversion that gives rise to the topological phase. Therefore, Coulomb interaction should be of importance in  $\text{Ca}_2\text{PtO}_4$ . To study the influence of interactions on the weak topological insulating phase, we look at a toy model corresponding to a layer-stacked 3D version of the Bernevig-Hughes-Zhang model with local interactions. For small to intermediate interaction strength, we discover novel interaction-driven topological phase transitions between the weak topological insulator and two Dirac semimetal phases. The latter correspond to gapless topological phases. For strong interactions, the system eventually becomes a Mott insulator.

<sup>1</sup>DFG Grant No. Ha 1537/23-1 within the Forschergruppe FOR 1162, SPP Grant Ha 1537/24-2, SFB 1170 “ToCoTronics”, SPP 1666, the Helmholtz Foundation (VITI), the “Elitenetzwerk Bayern” (ENB graduate school on “Topological insulators”)

**1:15PM Y28.00011 Landau levels and longitudinal magnetoresistance in generalized Weyl semimetals**, XIAO LI, BITAN ROY, Condensed Matter Theory Center and Joint Quantum Institute, University of Maryland — The notion of axial anomaly is a venerable concept in quantum field theory that has received ample attention in condensed matter physics due to the discovery of Weyl materials (WSMs). In such systems Kramers non-degenerate bands touch at isolated points in the Brillouin zone that act as (anti)monopoles of Berry flux, and the monopole number ( $m$ ) defines the topological invariant of the system. Although so far only simple WSMs (with  $m = 1$ ) has been found in various inversion and/or time-reversal asymmetric systems, generalized Weyl semimetals with  $m > 1$  can also be found in nature, for example double-Weyl semimetals in  $\text{HgCr}_2\text{Se}_4$  and  $\text{SrSi}_2$  and triple-Weyl semimetals. In this work, we demonstrate the Landau level spectrum in generalized Weyl systems and its ramification on longitudinal magnetotransport measurements. We show that in the quantum limit generalized Weyl semimetals display negative longitudinal magnetoresistance due to the chiral anomaly. Moreover, the magnetoresistance has nontrivial dependence on the relative orientation of the external fields with the crystallographic axis, stemming from underlying anisotropic quasiparticle dispersion in the pristine system. Our theory can thus provide diagnostic tools to pin the quasiparticle properties in Weyl systems.

**1:27PM Y28.00012 Magnetotransport in a Weyl semimetal**, YUYA OMINATO, MIKITO KOSHINO, Tohoku University — We studied the magnetotransport in a Weyl semimetal having the surface boundary, to investigate the effect of the topological surface states on the chiral anomaly. We Found that the conductivity behavior becomes completely different from that of the in finite system, where the surface state plays a crucial role in the relaxation of the bulk carriers.

**1:39PM Y28.00013 Cohomological Insulators**, A. ALEXANDRADINATA, Yale University, ZHIJUN WANG, B. ANDREI BERNEVIG, Princeton University — We present a cohomological classification of insulators, in which we extend crystal symmetries by Wilson loops. Such an extended group describes generalized symmetries that combine space-time transformations with quasimomentum translations. Our extension generalizes the construction of nonsymmorphic space groups, which extend point groups by real-space translations. Here, we *further* extend nonsymmorphic groups by reciprocal translations, thus placing real and quasimomentum space on equal footing. From a broader perspective, cohomology specifies not just the symmetry group, but also the quasimomentum manifold in which the symmetry acts – both data are needed to specify the band topology. In this sense, cohomology underlies band topology.

**1:51PM Y28.00014 Hourglass Fermions**, ZHIJUN WANG, A. ALEXANDRADINATA, ROBERT J. CAVA, B. ANDREI BERNEVIG, Princeton University — Spatial symmetries in crystals are distinguished by whether they preserve the spatial origin. We show how this basic geometric property gives rise to a new topology in band insulators. We study spatial symmetries that translate the origin by a fraction of the lattice period, and find that these nonsymmorphic symmetries protect a novel surface fermion whose dispersion is shaped like an hourglass; surface bands connect one hourglass to the next in an unbreakable zigzag pattern. These exotic fermions are materialized in the large-gap insulators:  $\text{KHg}X$  ( $X=\text{As, Sb, Bi}$ ), which we propose as the first material class whose topology relies on nonsymmorphic symmetries. Beside the hourglass fermion, a different surface of  $\text{KHg}X$  manifests a 3D generalization of the quantum spin Hall effect. To describe the bulk topology of nonsymmorphic crystals, we propose a non-Abelian generalization of the geometric theory of polarization. Our nontrivial topology originates not from an inversion of the parity quantum numbers, but rather of the rotational quantum numbers, which we propose as a fruitful in the search for topological materials. Finally,  $\text{KHg}X$  uniquely exemplifies a cohomological insulator, a concept that we will introduce in a companion work.

**2:03PM Y28.00015 Hourglass Fermions and Cohomological Insulators**, B ANDREI BERNEVIG, Princeton university, ARIS ALEXANDRADINATA, Yale University, ZHIJUN WANG, ROBERT CAVA, Princeton university — We present a new fermion, the Hourglass fermions, which extends the currently known Dirac, Weyl and Majorana classification. We further present a set of materials which host this particle as a surface state. The materials already exist in nature and have a large gap. The topological index involves group cohomology, and, in our particular material example, a group-extension of an already non-symmorphic group.

## Friday, March 18, 2016 11:15AM - 2:15PM –

Session Y29 DCMP DMP: Topological Insulators: Theory II 328 - Jay Sau, University of Maryland

**11:15AM Y29.00001 Gauge-discontinuity contributions to the Chern-Simons orbital magnetoelectric coupling**, JIANPENG LIU, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, DAVID VANDERBILT, Department of Physics and Astronomy, Rutgers University — We propose a new method for calculating the Chern-Simons orbital magnetoelectric coupling, conventionally parametrized in terms of a phase angle  $\theta$ . We propose to relax the periodicity condition in one direction ( $k_z$ ) so that a gauge discontinuity is introduced on a 2D  $\mathbf{k}$  plane normal to  $k_z$ . The total  $\theta$  response then has contributions from both the integral of the Chern-Simons 3-form over the 3D bulk BZ and the gauge discontinuity expressed as a 2D integral over the  $\mathbf{k}$  plane. Sometimes the boundary plane may be further divided into subregions by 1D “vortex loops” which make a third kind of contribution to the total  $\theta$ , expressed as a combination of Berry phases around the vortex loops. The total  $\theta$  thus consists of three terms which can be expressed as integrals over 3D, 2D and 1D manifolds. When time-reversal symmetry is present and the gauge in the bulk BZ is chosen to respect this symmetry, both the 3D and 2D integrals vanish; the entire contribution then comes from the vortex-loop integral, which is either 0 or  $\pi$  corresponding to the  $Z_2$  classification of 3D time-reversal invariant insulators. We demonstrate our method by applying it to the Fu-Kane-Mele model with an applied staggered Zeeman field.

**11:27AM Y29.00002 Bulk-boundary correspondence in (3+1)-dimensional topological phases**, APOORV TIWARI, XIAO CHEN, SHINSEI RYU, University of Illinois, Urbana Champaign — We discuss (2+1)-dimensional gapless surface theories of bulk (3+1)-dimensional topological phases, such as the BF theory at level K, and its generalization. In particular, we put these theories on a flat (2+1) dimensional torus  $T^3$  parameterized by its modular parameters, and compute the partition functions obeying various twisted boundary conditions. We show the partition functions are transformed into each other under  $SL(3, \mathbb{Z})$  modular transformations, and furthermore establish the bulk-boundary correspondence in (3+1) dimensions by matching the modular  $S$  and  $T$  matrices computed from the boundary field theories with those computed in the bulk. We also propose the three-loop braiding statistics can be studied by constructing the modular  $S$  and  $T$  matrices from an appropriate boundary field theory.

**11:39AM Y29.00003 Classification of interacting fermionic phases by dimensional reduction**, RAQUEL QUEIROZ, ESLAM KHALAF, Max Planck Institute for Solid State Physics, ADY STERN, Weizmann Institute of Science — Topological phases of noninteracting fermions are classified in each spatial dimension according to their symmetry class, in a periodic way [1]. When including interactions, however, this classification can be modified. It was first shown that in one-dimensional chains, the  $Z$  classification of the BDI symmetry class is reduced to  $Z_8$  [2]. That is, every group of 8 Majorana states at the edge of a BDI chain can be gapped out through a suitable interaction, despite preserving its fundamental symmetries. In this work, we present a dimensional reduction argument to derive the role of interactions in the classification of fermionic symmetry protected topological phases. For symmetry classes classified by a  $Z$  invariant in odd dimensions, we propose a general  $n$ -particle quartic interaction that renders the system topologically trivial. We argue that all phases characterized by a topological invariant smaller than  $n$  in the noninteracting limit remain topologically distinct once interactions are included, thereby reducing the noninteracting  $Z$  classification to  $Z_n$ . [1] Ryu, S., *et. al.*, NJP 12, 065010 (2010); [2] Fidkowski, L. and Kitaev, A., PRB 81, 134509 (2010).

**11:51AM Y29.00004 Dynamical Axion Field in a Magnetic Topological Insulator Superlattice<sup>1</sup>**, JING WANG, BIAO LIAN, SHOU-CHENG ZHANG, Department of Physics, Stanford University — We propose that the dynamical axion field can be realized in a magnetic topological insulator superlattice or a topological paramagnetic insulator. The magnetic fluctuations of these systems produce a pseudoscalar field which has an axionic coupling to the electromagnetic field, and thus it gives a condensed-matter realization of the axion electrodynamics. Compared to the previously proposed dynamical axion materials where a long range antiferromagnetic order is required, the systems proposed here have the advantage that only a uniform magnetization or a paramagnetic state is needed for the dynamic axion. We further propose several experiments to detect such a dynamical axion field.

<sup>1</sup>This work is supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under Contract No. DE-AC02-76SF00515.

**12:03PM Y29.00005 Surface theorem for the Chern-Simons magnetoelectric coupling**, THOMAS OLSEN, Department of Physics, Technical University of Denmark, IVO SOUZA, Centro de Física de Materiales, Universidad del País Vasco, MARYAM TAHERINEJAD, DAVID VANDERBILT, Department of Physics and Astronomy, Rutgers University — The magnetoelectric response  $\alpha_{ij} = \partial M_j / \partial \mathcal{E}_i$  of insulators has an isotropic geometric contribution,  $\alpha_{ij}^{\text{CS}} = (\theta e^2 / 2\pi h) \delta_{ij}$ . For crystals that respect neither inversion nor time-reversal symmetry the Chern-Simons (CS) axion coupling  $\theta$  can take arbitrary values, which however can only be determined modulo  $2\pi$  from bulk calculations. Once an insulating surface termination is specified it becomes possible to resolve the quantum of indeterminacy, as with the spontaneous electric polarization. We prove this "surface theorem" by considering the  $\theta$  coupling of a finite slab from the viewpoint of the hybrid Wannier representation. Each Wannier sheet carries a Chern number, and tiling up the periodic sheet structure close to the surface and counting the leftover Chern amount gives the excess quantized surface anomalous Hall conductivity (AHC). We illustrate these ideas for a tight-binding model consisting of Haldane-model layers with alternating Chern numbers. For appropriate choices of the interlayer couplings, this model realizes an adiabatic pump of CS axion coupling. Over a pumping cycle, one quantum of surface AHC gets transferred from the bottom to the top surface, changing  $\theta$  by  $2\pi$ .

**12:15PM Y29.00006 Effective hydrodynamic field theory and condensation picture of topological insulators**, ATMA CHAN, University of Illinois at Urbana-Champaign, THOMAS KVORNING, Stockholm University, SHINSEI RYU, EDUARDO FRADKIN, University of Illinois at Urbana-Champaign — While many features of topological band insulators are commonly discussed at the level of single-particle electron wave functions, such as the gapless Dirac spectrum at their boundary, it remains elusive to develop a hydrodynamic or collective description of fermionic topological band insulators in 3+1 dimensions. As the Chern-Simons theory for the 2+1-dimensional quantum Hall effect, such a hydrodynamic effective field theory provides a universal description of topological band insulators, even in the presence of interactions, and that of putative fractional topological insulators. In this paper, we undertake this task by using the functional bosonization. The effective field theory in the functional bosonization is written in terms of a two-form gauge field, which couples to a U(1) gauge field that arises by gauging the continuous symmetry of the target system (the U(1) particle number conservation). Integrating over the U(1) gauge field by using the electromagnetic duality, the resulting theory describes topological band insulators as a condensation phase of the U(1) gauge theory (or as a monopole condensation phase of the dual gauge field). The hydrodynamic description, and the implication of its duality, of the surface of topological insulators are also discussed.

**12:27PM Y29.00007 Emergence of a Chern-insulating state from a semi-Dirac dispersion**, HUAQING HUANG, Tsinghua University, ZHIRONG LIU, Peking University, HONGBIN ZHANG, Rutgers University, WENHUI DUAN, Tsinghua University, DAVID VANDERBILT, Rutgers University — By combining first-principles calculations with Wannier-based tight-binding modeling, we demonstrate that a  $\text{TiO}_2/\text{VO}_2$  heterostructure that was previously proposed as a prototypical semi-Dirac system becomes a Chern insulator (quantum anomalous Hall insulator) in the presence of spin-orbit coupling. We show that this occurs only when the semi-Dirac structure is of a special type that can be formed by the merging of three conventional Dirac points. Our results reveal how the nontrivial topology with nonzero Chern number emerges naturally from this kind of semi-Dirac structure, establishing a general scenario that provides a new route to the formation of Chern-insulating states in practical materials systems.

**12:39PM Y29.00008 Microscopic study of anomalous Hall effect edge states in topological insulator nanoribbons**, CARLO M. CANALI, ANNA PERTSOVA, Linnaeus University, ALLAN H. MACDONALD, The University of Texas at Austin — Thin films of a magnetic topological insulator (TI) support gapless chiral states on their lateral surfaces, which give rise to the quantum anomalous Hall effect (QAHE) [1,2]. Despite progress in the experimental realization of the QAHE there are many open issues which require an explanation, including remnant longitudinal resistance and relatively imprecise Hall quantization compared to the ordinary QHE in a strong perpendicular magnetic field. These features can be linked to the presence of non-chiral dissipative states on the side walls of the sample. We develop a microscopic theory of side-wall states in ribbons of a magnetic TI. We show the emergence of the chiral edge states as a function of exchange field strength and ribbon width. We demonstrate the existence of non-chiral edge states, whose number depends on the system dimensions. In contrast to previous work [3], we find that the non-chiral states are always gapped, a finding which is supported by recent experiments assessing the precision and temperature dependence of QAHE [4]. Finally, we investigate the role of chemical disorder in equilibrating edge channels and in Hall quantization accuracy. 1.Yu, Science 329, 61(2010); 2.Chang, Science 340, 167(2013); 3.Wang, PRL 111, 086803(2013); 4.Chang, PRL 115, 057206(2015).

**12:51PM Y29.00009 Universal framework for identifying topological materials and its numerical implementation in Z2Pack software package**, DOMINIK GRESCH, MATTHIAS TROYER, ALEXEY SOLUYANOV, ETH Zurich, GABRIEL AUTES, OLEG YAZYEV, EPFL, ANDREI BERNEVIG, Princeton University, DAVID VANDERBILT, Rutgers University — Band structure topology has drastic effects on many observable phenomena in solids, and thus is a fundamental characteristic of a material. We present general framework for identifying various topologies of band structures and introduce a public software package –Z2Pack – for computing the associated topological invariants. Z2Pack works with first-principles calculations, tight-binding and k.p models. It can be used to identify both topological insulators and semimetals.

**1:03PM Y29.00010 Geometric Effect on Quantum Anomalous Hall State in Magnetic Topological Insulator**, YANXIA XING, Department of Physics, Beijing Institute of Technology, Beijing 100081, China — An intriguing observation on the quantum anomalous Hall (QAH) effect in a magnetic topological insulator (MTI) is the dissipative edge states. With the aid of non-equilibrium Green's functions, the QAH effect in an MTI with a three dimensional effective tight-binding model is studied. We predict that due to geometric structure in the third dimension  $z$ , the unidirectional contact between terminal leads and central scattering region induces the backscattering in the central Hall bar, as the function of split gates. Such backscattering leads to a nonzero longitudinal resistance and quantized Hall resistance, which would explain the dissipative edge states in experiments. A further numerical simulation proves above prediction as well. These results are rewarding on future experimental observations and transport calculations based on first principle.

**1:15PM Y29.00011 Thermodynamic signatures of edge states in Topological Insulators**, ANTON QUELLE, EMILIO COBANERA, CRISTINA MORAIS SMITH, Univ of Utrecht — Topological insulators are states of matter distinguished by the presence of symmetry protected metallic boundary modes. These edge modes have been characterised in terms of transport and spectroscopic measurements, but a thermodynamic description has been lacking. The challenge arises because in conventional thermodynamics the potentials are required to scale linearly with extensive variables like volume, which does not allow for a general treatment of boundary effects. In this paper, we overcome this challenge with Hill thermodynamics. In this extension of the thermodynamic formalism, the grand potential is split into an extensive, conventional contribution, and the subdivision potential, which is the central construct of Hill's theory. For topologically non-trivial electronic matter, the subdivision potential captures measurable contributions to the density of states and the heat capacity: it is the thermodynamic manifestation of the topological edge structure. Furthermore, the subdivision potential reveals phase transitions of the edge even when they are not manifested in the bulk, thus opening a variety of new possibilities for investigating, manipulating, and characterizing topological quantum matter solely in terms of equilibrium boundary physics.

**1:27PM Y29.00012 Topological States of Heterostructures**, DEMET USANMAZ, PINKU NATH, JOSE J. PLATA, Department of Mechanical Engineering and Materials Science, Duke University, MARCO BUONGIORNO NARDELLI, Department of Physics and Department of Chemistry, University of North Texas, MARCO FORNARI, Department of Physics, Central Michigan University, STEFANO CURTAROLO, Materials Science, Electrical Engineering, Physics and Chemistry, Duke University — Topological insulators (TIs) have exotic properties, such as having insulating behavior in the bulk and metallic states at the surface<sup>[1]</sup>. Observations of metallic states rely on the spin-orbit induced band inversion in bulk materials and are protected by time-reversal symmetry or crystal symmetry<sup>[2]</sup>. These remarkable characteristics of TIs give rise to various applications from spintronics to quantum computers. In order to broaden the range of applications of TIs and make it more effective, an exploration of high quality heterostructures are required. Creating heterostructures of TIs has recently demonstrated to be advantageous for controlling electronic properties<sup>[3]</sup>. Inspired by these interesting properties, we have investigated the topological interface states of heterostructures. References [1] B. Yan, S-C. Zhang, *Rep. Prog. Phys.*, **75**, 096501 (2012). [2] Y. Ando, *J. Phys. Soc. Jpn.*, **82**, 102001 (2013). [3] K. Nakayama, K. Eto, Y. Tanaka, T. Sato, S. Souma, T. Takahashi, K. Segawa, Y. Ando, *Phys. Rev. Lett.*, **109**, 236804 (2012)

**1:39PM Y29.00013 Detecting band inversions by measuring the environment: fingerprints of electronic band topology in bulk phonon linewidths**, KUSH SAHA, University of California, Irvine, KATHERINE LEGARE, ION GARATE, University of Sherbrooke, Canada — The interplay between topological phases of matter and dissipative baths constitutes an emergent research topic with links to condensed matter, photonic crystals, cold atomic gases and quantum information. While recent studies suggest that dissipative baths can induce topological phases in intrinsically trivial quantum materials, the backaction of topological invariants on dissipative baths is overlooked. By exploring this back action for a centrosymmetric Dirac insulator coupled to phonons, we show that the linewidths of bulk optical phonons can reveal electronic band inversions. This result is the first known example where topological phases of an open quantum system may be detected by measuring the bulk properties of the surrounding environment.

**1:51PM Y29.00014 Spin Generation Via Bulk Spin Current in Three Dimensional Topological Insulators**, XINGYUE PENG, University of California, Davis - Physics Department — To date, charge transport and spin generation in three-dimensional topological insulators (3D TIs) are primarily modeled as a single-surface phenomenon. We propose a new mechanism of spin generation where the role of the insulating yet topologically non-trivial bulk becomes explicit: an external electric field creates a transverse pure spin current through the bulk of a 3D TI, which transports spins between the top and bottom surfaces and leads to spin accumulation on both. The surface spin density and charge current are then proportional to the spin relaxation time, which for a sufficiently high disorder level can be extended by nonmagnetic scattering analogous to the Dyakonov-Perel spin relaxation mechanism. This new spin generation mechanism suggests a distinct and practical strategy for the enhancement of surface spin polarization by increasing nonmagnetic impurity concentration. Numerical results obtained by coherent potential approximation (CPA) based on a 4-band lattice model confirm that this spin generation mechanism originates from the unique topological connection of the top and bottom surfaces and is absent in other two dimensional systems such as graphene, even though they possess a similar Dirac cone-type dispersion.

**2:03PM Y29.00015 Unconventional band structure for a periodically gated surface of a three dimensional Topological Insulator<sup>1</sup>**, SANKALPA GHOSH<sup>2</sup>, PUJA MONDAL<sup>3</sup>, Physics Department, IIT Delhi, New Delhi-110016, India — The surface states of the three dimensional (3D) Topological Insulators are described by two-dimensional (2D) massless Dirac equation. A gate voltage induced one dimensional potential barrier on such surface creates a discrete bound state in the forbidden region outside the Dirac cone. Even for a single barrier it is shown such bound state can create electrostatic analogue of Shubnikov de Haas oscillation which can be experimentally observed for relatively smaller size samples. However when these surface states are exposed to a periodic arrangement of such gate voltage induced potential barriers, the band structure of the same got nontrivially modified. This is expected to significantly alter the properties of macroscopic system. We also suggest that in suitable limit the system may offer ways to control electron spin electrostatically which may be practically useful

<sup>1</sup>Supported by UGC Fellowship (PM) and a UKIERI-UGC Thematic Partnership

<sup>2</sup>The first author of this work is Puja Mondal

<sup>3</sup>She is a Graduate Student

## Friday, March 18, 2016 11:15AM - 2:15PM –

Session Y30 DMP: Ionically Controlled Transport and Electrooptical Functionalities at Oxide Interfaces 329 - Juan Carlos Idrobo

**11:15AM Y30.00001 Single atom electrochemical and atomic analytics<sup>1</sup>**, RAMA VASUDEVAN<sup>2</sup>, Oak Ridge National Laboratory — In the past decade, advances in electron and scanning-probe based microscopies have led to a wealth of imaging and spectroscopic data with atomic resolution, yielding substantial insight into local physics and chemistry in a diverse range of systems such as oxide catalysts, multiferroics, manganites, and 2D materials. However, typical analysis of atomically resolved images is limited, despite the fact that image intensities and distortions of the atoms from their idealized positions contain unique information on the physical and chemical properties inherent to the system. Here, we present approaches to data mine atomically resolved images in oxides, specifically in the hole-doped manganite  $\text{La}_{5/8}\text{Ca}_{3/8}\text{MnO}_3$ , on epitaxial films studied by in-situ scanning tunnelling microscopy (STM). Through application of bias to the STM tip, atomic-scale electrochemistry is demonstrated on the manganite surface. STM images are then further analyzed through a suite of algorithms including 2D autocorrelations, sliding window Fourier transforms, and others, and can be combined with basic thermodynamic modelling to reveal relevant physical and chemical descriptors including segregation energies, existence and strength of atomic-scale diffusion barriers, surface energies and sub-surface chemical species identification. These approaches promise to provide tremendous insights from atomically resolved functional imaging, can provide relevant thermodynamic parameters, and auger well for use with first-principles calculations to yield quantitative atomic-level chemical identification and structure-property relations.

<sup>1</sup>This research was sponsored by the Division of Materials Sciences and Engineering, BES, DOE. Research was conducted at the Center for Nanophase Materials Sciences, which also provided support and is a DOE Office of Science User Facility.

<sup>2</sup>Institute for Functional Imaging of Materials, and Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

**11:51AM Y30.00002 Transport Properties of Exfoliated BSCCO on LAO/STO Heterostructures<sup>1</sup>**, SYLVIA UJWARY, University of Pittsburgh, ERIN SUTTON, MASON GRAY, KENNETH BURCH, Boston College, JEREMY LEVY, University of Pittsburgh — We investigate the interaction between high-temperature superconductor  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$  (BSCCO) flakes deposited on the oxide heterostructure  $\text{LaAlO}_3/\text{SrTiO}_3$  (LAO/STO). Conductive-atomic force microscope (c-AFM) lithography will be used to create nanowires at the LAO/STO interface that couple to the BSCCO. Through coupling of these materials, we will be able to study phenomena such as the proximity effect and coulomb drag.

<sup>1</sup>We gratefully acknowledge support from the NASA PA Space Grant Consortium (SU), and the National Science Foundation (Grant No. DMR-1410846)

**12:03PM Y30.00003 Systematic investigation of chemical substitution in  $\text{BaSnO}_3$  using the combinatorial approach<sup>1</sup>**, ICHIRO TAKEUCHI, JONGMOON SHIN, SEUNGHUN LEE, XIAOHANG ZHANG, H. M. IFTEKHAR JAIM, Dept. of Materials Science and Engineering, University of Maryland, SE-YOUNG JEONG, Dept. of Cogno-Mechatronics Eng., Pusan National University —  $\text{BaSnO}_3$  has been regarded as a possible material for photo-catalysis, dielectric capacitors, and transparent conductors. We are systematically investigating the effect of chemical substitution for A and B sites in  $\text{BaSnO}_3$  using a high-throughput methodology. We have thus far investigated the effect of substituting La and Sr for the Ba-site and Pb and Bi for the Sn-site. The composition spread films were prepared on  $\text{MgO}$ ,  $\text{SrTiO}_3$  and  $\text{LaAlO}_3$  using combinatorial pulsed laser deposition. The lattice parameters and band-gap energies were found to continually change as a function of the concentration of each substitutional dopant. We find that the band gap can be tuned from 2.8 eV for  $\text{BaSn}_{0.05}\text{Pb}_{0.95}\text{O}_3$  to 4.5 eV for  $\text{Ba}_{0.05}\text{La}_{0.95}\text{SnO}_3$ . Especially for  $\text{Ba}_{1-x}\text{La}_x\text{SnO}_3$  with x in the range of  $0.05 < x < 0.5$ , we consistently observe resistivity as low as  $0.23 \text{ m}\Omega\text{cm}$  at room temperature while maintaining optical transparency with a typical bandgap of  $\sim 4 \text{ eV}$ . The effect of crystalline defects on electrical properties will also be discussed.

<sup>1</sup>This project is funded by AFOSR.

**12:15PM Y30.00004 Correlated Heterostructures for Efficient Solar Cells**, ELIAS ASSMANN, MARKUS AICHORN, TU Graz, Austria, GIORGIO SANGIOVANNI, University of Würzburg, Germany, SATOSHI OKAMOTO, Oak Ridge National Laboratory, PETER BLAHA, SUMANTA BHANDARY, KARSTEN HELD, TU Vienna, Austria — Polar/non-polar oxide heterostructures such as  $\text{LaAlO}_3/\text{SrTiO}_3$  have become well-known for the many intriguing phenomena occurring at the interface, especially the internal potential gradient and the resulting 2d electron gas. We propose to make use of these unique systems as absorbing materials for high-efficiency solar cells [1]. In particular,  $\text{LaVO}_3/\text{SrTiO}_3$  (i) has a direct band gap  $\sim 1.1 \text{ eV}$ , nearly optimal for a solar cell; (ii) the internal potential gradient serves to efficiently separate the photo-generated electron-hole pairs and reduce recombination losses; (iii) the conducting interface offers a natural contact for charge-carrier extraction. Furthermore, (iv) oxide heterostructures afford the flexibility to combine layers with different gaps, e.g.  $\text{LaVO}_3$  with  $\text{LaFeO}_3$ , in order to achieve even higher efficiencies with band-gap graded solar cells. We use density-functional theory and dynamical mean-field theory to study this strongly correlated heterostructure.

[1] Assmann et al., PRL 110, 078701 (2013)

Experimental corroboration: Liang et al., Sci. Rep. 3, 1975 (2013); Wang et al., PR Applied 3, 064015 (2015)

**12:27PM Y30.00005 Ferroelectricity and hysterically controlled photocurrent in  $\text{NaMnF}_3$  Thin Film<sup>1</sup>**, MING YANG, AMIT KC, PAVEL BORISOV, DAVID LEDERMAN, ALDO ROMERO, CHENG CEN, West Virginia Univ — Abstract: In recent year many fascinating electron correlation phenomena have been discussed, such as two dimensional electron gas, metal-insulator transitions and multiferroic interactions. While most of the researches concentrate on complex oxides, there are strong indications that complex fluorides may have analogous, or even enhanced properties.  $\text{NaMnF}_3$  is one such example. Theoretical work predicted that  $\text{NaMnF}_3$  has multiferroic characters and strong magneto-electric coupling. Thin films of  $\text{NaMnF}_3$  with 50 nm thickness were grown on  $\text{SrTiO}_3$  substrates via molecular beam epitaxy. By performing piezoelectric force microscopy, rewritable polarizations were manipulated and stable ferroelectric switching was obtained in  $\text{NaMnF}_3$  at room temperature. At low temperatures, persistent photocurrent was observed under the illumination of 400nm laser. Amplitude and direction of such photocurrent can be hysterically controlled by external biases. This phenomenon is due to the fact that photocarriers generated in  $\text{SrTiO}_3$  are driven by the controlled built-in electric field in  $\text{NaMnF}_3$  thin film. These findings indicate great potential of complex fluorides in applications such as ferroelectric switches, photovoltaic devices and memory storages. This work is supported by DMREF-NSF 1434897.

<sup>1</sup>This work is supported by DMREF-NSF 1434897.

**12:39PM Y30.00006 Linear electro-optic effect in strained  $\text{BaTiO}_3$** , ALEX DEMKOV, KURT FREDREICKSON, The University of Texas — The nominal perovskite  $\text{ABO}_3$  structure is cubic and centro-symmetric. Therefore, by symmetry there should be no linear electro-optic (EO) effect. However, perovskites are known to experience various lattice distortions that result in reduced symmetry. The ferroelectric transition in  $\text{BaTiO}_3$  (BTO) is one obvious example. Below 393 K the cell becomes tetragonal and Ti shifts away from the center of inversion and produces a dipole moment and a robust linear EO or Pockels effect. In this talk I will discuss how the EO response in BTO can be enhanced by strain and show our recent results obtained with density functional theory. This work was supported by the Air Force Office of Scientific Research (Grant FA9550-12-1-0494)

**12:51PM Y30.00007 Build-in Electric Field Induced Mechanical Property Change**, TE-YU CHIEN, Univ of Wyoming, JIAN LIU, University of Tennessee, Knoxville, ANDREW J. YOST, University of Wyoming, JACQUES CHAKHALIAN, University of Arkansas, JOHN W. FREELAND, NATHAN P. GUISENGER, Argonne National Laboratory — Mechanical properties describe how materials respond to external stress. Microscopically, many intrinsic and extrinsic factors, such as bond length and strength (intrinsic) and grain boundaries (extrinsic), may affect the mechanical property of the materials. In this study, we observed a change of fracturing behavior of Nb-doped  $\text{SrTiO}_3$  in a Schottky barrier near the interfaces with metallic  $\text{LaNiO}_3$  films. Through cross-sectional scanning tunneling microscopy and spectroscopy (XSTM/S) experiments and theoretical analysis, the observed fractured topography could be explained by the change of the bond length caused alternation of mechanical property inside the Schottky barrier. Same model could also explain the widely observed dielectric dead layer for  $\text{SrTiO}_3$  in contact with metal electrodes.

**1:03PM Y30.00008 Ionic and electrochemical phenomena induced by structural and chemical defects in oxide thin films**, CARMELA ARUTA, National Research Council CNR-SPIN Rome, Italy — Interactions at the surfaces/interfaces between complex oxides and gaseous environment are fundamental for the efficiency of many environmental friendly systems and applications. Such interactions can be modified by the intricate interrelationship between microstructure and chemical substitution defects, being their role on functional properties, such as ionic conductivity and surface reaction rates, as particularly relevant as difficult to discriminate. New possibilities in thin film fabrication allow growth of oxide thin films with a more precise control of the structure and chemical stoichiometry, thus unveiling new perspectives in the study of electrochemical effects for physical functionalities, through nanoscale characterizations by complementary state-of-art techniques. As an example of interfacial structural defect effects, we will discuss the case of yttrium doped barium zirconate thin films, where the cation substitutions represent a viable mechanism, alternative to the formation of dislocations near the interface, to relieve the strain building up in the film growing on a highly mismatched substrate, thus providing fast transport pathways together with enhanced interface electrochemical reactivity. The effect of the chemical defects will be further presented in the case of samarium-doped ceria films with different doping concentration. We will explain the role of the trivalent doping on the conduction mechanism, i.e. proton or oxygen ion, which in turns may greatly influence the surface reactivity.

**1:39PM Y30.00009 First principles study of oxygen vacancies and iron impurities on electrical and optical properties of NiO<sup>1</sup>**, JOHN PETERSEN, TWAGIRAYEZU FIDELE, Texas State University, PABLO BORGES, Universidade Federal de Viosa, Brazil, LUISA SCOLFARO, WILHELMUS GEERTS, Texas State University — We are studying the properties of iron doped NiO by Density Functional Theory. NiO is being considered for use in RRAM, based on the reversible switching of a thin transition metal oxide (TMO) layer between a low and high resistance state using the mechanism of soft breakdown. RRAM's high integration density, its high endurance and good retention, its low energy use, and its high speed make it a potential candidate for replacing Flash memory. Switching between the high and low resistance state is inhomogeneous, and low resistance nano-filaments are formed. Fe impurities are introduced to optimize the switching properties. The effects of oxygen vacancies and iron on the electronic structure and optical properties of NiO are calculated and compared with experiment. Antiferromagnetic rhombohedral 108 atom cells with 1.85% Fe concentration are considered. Due to the highly-correlated nature of d orbitals in TMOs, a Hubbard U correction is applied to calculations in this work via the GGA + U method of DFT using VASP. Hybrid HSE06 calculations will also be considered. Localized energy levels from iron and from oxygen vacancies are identified, and their effects on dielectric permittivity are presented.

<sup>1</sup>Texas State University (Research Enhancement grant) and DOD (HBCU/MI grant W911NF-15-1-0394)

**1:51PM Y30.00010 Investigation on the Mechanism and Application of Nanoscale NiO Memristors**, ZHONG SUN, YONGGANG ZHAO, Tsinghua Univ, MIN HE, LIN GU, CHAO MA, KUIJUAN JIN, LINLIN WEI, JIANQI LI, IOP, CAS, NANNAN LUO, QINGHUA ZHANG, WENHUI DUAN, CEWEN NAN, Tsinghua Univ, DEPARTMENT OF PHYSICS TEAM, IOP, CAS COLLABORATION, SCHOOL OF MATERIALS SCIENCE AND ENGINEERING COLLABORATION — In contrast to the oxygen-vacancy-based model for the memristive *n*-type metal oxides, the coexistence of cation and anion vacancies had been suggested theoretically to be crucial to the bipolar memristive behavior of NiO. We have revealed the deterministic role of concentration surplus of cation vacancy over anion vacancy in bipolar memristive NiO, with C-AFM measuring the electrical properties, and STEM combined with EELS characterizing the ionic vacancies, giving an experimental support for the first time to the dual-defects-based model, which is of fundamental importance for the comprehensive understanding of memristor mechanisms. Furthermore, we have fabricated NiO nanodots with AAO templates, in which the intrinsically rectifying-resistive switching (IR-RS) has been observed. This is the first work studying the IR-RS in the scale of real devices, where the feasibility for selection device-free memory application has been demonstrated. The IR-RS in NiO nanodots has been ascribed exclusively to the built-in *p* – *n* homojunction, differing from previous cases dominated by the interfacial Schottky barriers.

**2:03PM Y30.00011 Nanoscale BaTiO<sub>3</sub> MOSCAP formation for ferroelectric field effect transistor application**, PATRICK PONATH, AGHAM POSADAS, Univ of Texas, Austin, MICHAEL SCHMIDT, PAUL HURLEY, RAY DUFFY, Tyndall National Institute, ALEX DEMKOV, Univ of Texas, Austin — Titanates are an important class of materials with many interesting functional properties and applications for non-volatile memory, i.e. BaTiO<sub>3</sub>, which is a promising candidate for the realization of a ferroelectric field-effect transistor. However, the difficulty of chemically etching titanates has hindered their commercial use in device manufacturing so far. Here, we report a technique to circumvent this problem. Using molecular beam epitaxy, we grew compressively strained ferroelectric BaTiO<sub>3</sub>, within photolithographically defined openings of a sacrificial SiO<sub>2</sub> layer on germanium (001) with Pt as a top electrode. Etching away the sacrificial SiO<sub>2</sub> can reveal isolated nanoscale gate stacks circumventing the need to etch the titanate thin film. Using X-ray diffraction we find that the BaTiO<sub>3</sub> film is tetragonal with the longer *c*-axis being out of plane, which is a requirement for the ferroelectric field effect transistor. The crystal quality of the BaTiO<sub>3</sub> films grown in the openings is confirmed using RHEED and cross-sectional transmission electron microscopy. Focused ion beam etching of the Pt layer is then used to electrically isolate a Pt/BaTiO<sub>3</sub>/SrTiO<sub>3</sub>/Ge stack to perform electrical measurements.

**Friday, March 18, 2016 11:15AM - 1:27PM –**

**Session Y31 DCP GSOF: Water at Biological Interfaces 331 - Douglas Tobias**

**11:15AM Y31.00001 Characterization of protein hydration by solution NMR spectroscopy**, JOSHUA WAND, Department of Biochemistry & Biophysics, University of Pennsylvania — A comprehensive understanding of the interactions between protein molecules and hydration water remains elusive. Solution nuclear magnetic resonance (NMR) spectroscopy has been proposed as a means to characterize these interactions but is plagued with artifacts when employed in bulk aqueous solution. Encapsulation of proteins in reverse micelles prepared in short chain alkane solvents can overcome these technical limitations. Application of this approach has revealed that the interaction of water with the surface of protein molecules is quite heterogeneous with some regions of the protein having long-lived interactions while other regions show relatively transient hydration. Results from several proteins will be presented including ubiquitin, staphylococcal nuclease, interleukin 1beta, hen egg white lysozyme (HEWL) and T4 lysozyme. Ubiquitin and interleukin 1beta are signaling proteins and interact with other proteins through formation of dry protein-protein interfaces. Interestingly, the protein surfaces of the free proteins show relatively slowed (restricted) motion at the surface, which is indicative of low residual entropy. Other regions of the protein surface have relatively high mobility water. These results are consistent with the idea that proteins have evolved to maximize the hydrophobic effect in optimization of binding with protein partners. As predicted by simulation and theory, we find that hydration of internal hydrophobic cavities of interleukin 1beta and T4 lysozyme is highly disfavored. In contrast, the hydrophilic polar cavity of HEWL is occupied by water. Initial structural correlations suggest that hydration of alpha helical structure is characterized by relatively mobile water while those of beta strands and loops are more ordered and slowed. These and other results from this set of proteins reveals that the dynamical and structural character of hydration of proteins is heterogeneous and complex. Supported by the National Science Foundation.

**11:51AM Y31.00002 Hydration Dynamics of Biomolecules from Co-solvents to Crowding**, KEVIN KUBARYCH, University of Michigan — Biomolecules self-assemble into complex functional structures with high fidelity largely due to interactions between the macromolecules and water. Once folded, the dynamics of water molecules in the vicinity of extended macromolecular interfaces can be altered relative to the bulk, leading to complex, heterogeneous and distance-dependent transport properties near these surfaces. Using a strategy based on transition metal carbonyl vibrational probes covalently conjugated to the protein surface, we have been able to use ultrafast two-dimensional infrared (2D-IR) spectroscopy to probe the dynamics from this most important perspective. In a series of studies, we have found these probes to be primarily sensitive to the orientational dynamics of the hydrating water molecules, and have studied both protein/water and membrane/water interfaces. Several key findings have emerged, including a modest 2-3-fold slowdown of hydration water's reorientational dynamics relative to the bulk, and a dynamical transition that occurs due to collective hydration induced by macromolecular crowding. We will summarize our progress to-date, as well as present our newest results on the effects of ions and the dynamical signatures of preferential solvation.

## **12:27PM Y31.00003 Observation of Water-Protein Interaction Dynamics with Broadband Two-Dimensional Infrared Spectroscopy**

**LUIGI DE MARCO, ANDREW HAKY, ANDREI TOKMAKOFF**, The University of Chicago — Two-dimensional infrared (2D IR) spectroscopy has proven itself an indispensable tool for studying molecular dynamics and intermolecular interactions on ultrafast timescales. Using a novel source of broadband mid-IR pulses, we have collected 2D IR spectra of protein films at varying levels of hydration. With 2D IR, we can directly observe coupling between water's motions and the protein's. Protein films provide us with the ability to discriminate hydration waters from bulk water and thus give us access to studying water dynamics along the protein backbone, fluctuations in the protein structure, and the interplay between the molecular dynamics of the two. We present two representative protein films: poly-L-proline (PLP) and hen egg-white lysozyme (HEWL). Having no N-H groups, PLP allows us to look at water dynamics without interference from resonant energy transfer between the protein N-H stretch and the water O-H stretch. We conclude that at low hydration levels water-protein interactions dominate, and the water's dynamics are tied to those of the protein. In HEWL films, we take advantage of the robust secondary structure to partially deuterate the film, allowing us to spectrally distinguish the protein core from the exterior. From this, we show that resonant energy transfer to water provides an effective means of dissipating excess energy within the protein, while maintaining the structure. These methods are general and can easily be extended to studying specific protein-water interactions.

## **12:39PM Y31.00004 Fluctuating Thermodynamics for Biological Processes<sup>1</sup>**

**SIHYUN HAM**, Sookmyung Women's University — Because biomolecular processes are largely under thermodynamic control, dynamic extension of thermodynamics is necessary to uncover the mechanisms and driving factors of fluctuating processes. The fluctuating thermodynamics technology presented in this talk offers a practical means for the thermodynamic characterization of conformational dynamics in biomolecules. The use of fluctuating thermodynamics has the potential to provide a comprehensive picture of fluctuating phenomena in diverse biological processes. Through the application of fluctuating thermodynamics, we provide a thermodynamic perspective on the misfolding and aggregation of the various proteins associated with human diseases. In this talk, I will present the detailed concepts and applications of the fluctuating thermodynamics technology for elucidating biological processes.

<sup>1</sup>This work was supported by Samsung Science and Technology Foundation under project number SSTF-BA1401-13.

## **1:15PM Y31.00005 Thermodynamic properties of water solvating biomolecular surfaces<sup>1</sup>**

**MATTHIAS HEYDEN**, Ruhr-University Bochum — Changes in the potential energy and entropy of water molecules hydrating biomolecular interfaces play a significant role for biomolecular solubility and association. Free energy perturbation and thermodynamic integration methods allow calculations of free energy differences between two states from simulations. However, these methods are computationally demanding and do not provide insights into individual thermodynamic contributions, i.e. changes in the solvent energy or entropy. Here, we employ methods to spatially resolve distributions of hydration water thermodynamic properties in the vicinity of biomolecular surfaces. This allows direct insights into thermodynamic signatures of the hydration of hydrophobic and hydrophilic solvent accessible sites of proteins and small molecules and comparisons to ideal model surfaces. We correlate dynamic properties of hydration water molecules, i.e. translational and rotational mobility, to their thermodynamics. The latter can be used as a guide to extract thermodynamic information from experimental measurements of site-resolved water dynamics. Further, we study energy-entropy compensations of water at different hydration sites of biomolecular surfaces.

<sup>1</sup>This work is supported by the Cluster of Excellence RESOLV (EXC 1069) funded by the Deutsche Forschungsgemeinschaft.

## **Friday, March 18, 2016 11:15AM - 2:15PM –**

**Session Y32 DCP: Chemical Physics of Extreme Environments III** 332 - Marsha Lester, University of Pennsylvania

## **11:15AM Y32.00001 Complexities in Pressure Dependent Kinetics Across a Wide-Range of Temperatures and Pressures**

**STEPHEN KLIPPENSTEIN**, Argonne Natl Lab — Sample ab initio transition state theory based master equation calculations will be used to illustrate interesting features of the kinetics for a variety of reactions of importance in astrochemistry, atmospheric, and combustion chemistry. The calculations will explore the role of long-range interactions, angular momentum conservation, tunneling, radiative emission, roaming processes, torsional motions, and prompt dissociation of incipient molecules. Comparisons with experiment will be presented to illustrate the current accuracy of such calculations.

## **11:51AM Y32.00002 Forming a Two-Ring Polycyclic Aromatic Hydrocarbon without a Benzene Intermediate: the Reaction of Propargyl with Acetylene**

**DAVID OSBORN**, Sandia National Laboratories, **JOHN SAVEE**, Los Gatos Research, **TALITHA SELBY**, University of Wisconsin, Washington County, **OLIVER WELZ**, BASF SE, **CRAIG TAATJES**, Sandia National Laboratories — The reaction of acetylene (HCCH) with a resonance-stabilized free radical is a commonly invoked mechanism for the generation of polycyclic aromatic hydrocarbons (PAH), which are likely precursors of soot particles in combustion. In this work, we examine the sequential addition of acetylene to the propargyl radical (H<sub>2</sub>CCCH) at temperatures of 800 and 1000 K. Using time-resolved multiplexed photoionization mass spectrometry with tunable ionizing radiation, we identified the isomeric forms of the C<sub>5</sub>H<sub>5</sub> and C<sub>7</sub>H<sub>7</sub> intermediates in this reaction sequence, and confirmed that the final C<sub>9</sub>H<sub>8</sub> product is the two-ring aromatic compound indene. We identified two different resonance-stabilized C<sub>5</sub>H<sub>5</sub> intermediates, with different temperature dependencies. Furthermore, the C<sub>7</sub>H<sub>7</sub> intermediate is the tropylium radical (c-C<sub>7</sub>H<sub>7</sub>), not the benzyl radical (C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>), as is usually assumed in combustion environments. These experimental results are in general agreement with the latest electronic structure / master equation results of da Silva et al. This work shows a pathway for PAH formation that bypasses benzene / benzyl intermediates.

**12:03PM Y32.00003 TBA**, **JOHN STANTON**, Univ of Texas, Austin — No abstract available.

## **12:39PM Y32.00004 Threshold collision induced dissociation experiment for azobenzene and its derivatives.**

**MOHAMMADREZA REZAEI**, Physics Department, University of Tennessee, Knoxville; The Department of Physics and Astronomy; **TEXAS AM UNIVERSITY**, **ROBERT COMPTON**, Physics Department, University of Tennessee, Knoxville; Chemistry Department, University of Tennessee, Knoxville — In this study we investigated protonated azobenzene cation and properties of trans 2,2',6,6'-tetrafluoroazobenzene anion using the collision induced dissociation method and the results are compared with the results from ab initio electronic structure calculations. We measured the bond dissociation energies experimentally and found which theoretical quantum chemistry methods yield best results. Several high accuracy multi-level calculations such as CBS-QB3, G3 and G4 had been carried out to obtain reliable thermochemical information for azobenzene and several of its derivatives and their anion or cation. We also performed other experiments such as Raman spectroscopy to study these light sensitive molecules with promising applications such as photo-switching.

**12:51PM Y32.00005 TBA**, **JUDIT ZADOR**, CRF-Sandia National Lab — No abstract available.

**1:27PM Y32.00006 A Compressed Sensing Approach to Select Optimal Atom-Centered Basis Functions for DFT and Beyond**, CHENCHEN WANG, Fritz Haber Institute, NIKLAS MENZEL, TU Berlin, LUCA M. GHIRINGHELLI, Fritz Haber Institute, GITTA KUTYNIOK, TU Berlin, MATTHIAS SCHEFFLER, Fritz Haber Institute — The choice of the basis sets is one of the most important factors in quantum chemical calculations. It is particularly challenging for functionals that treat electron correlations. Commonly used basis sets for advanced exchange-correlation functionals are not sufficiently accurate. This leads to extended basis set, such as the most famous correlation-consistent basis sets by Dunning. However, such basis sets have been so far widely used mainly for light atoms and their molecules, since they are too expensive for transition metals. We have developed a new approach to select basis functions based on compressed sensing (CS), a recently developed signal processing technique. CS provides a simple and efficient framework for basis selection based on  $l_1$  norm regularization techniques. As introductory example, we select via our CS-based approach Gaussian basis functions (GTO) from a large pool of various GTOs, in order to fit to the reference atomic orbitals. We calculate the total energy for atoms from H to O, and then extend to molecules, e.g.,  $H_2$ ,  $N_2$ , and  $O_2$ . For H, He, and Li, our total-energy results are within 0.05% compared with STO-6G energies. Starting from Be, CS selected basis set provide significantly better results than STO-6G, even when only 5 GTOs are considered. Our new approach enables us to determine optimal basis sets for heavier atoms and molecules.

**1:39PM Y32.00007 Accurately Predicting Complex Reaction Kinetics from First Principles**, WILLIAM GREEN, Massachusetts Institute of Technology — Many important systems contain a multitude of reactive chemical species, some of which react on a timescale faster than collisional thermalization, i.e. they never achieve a Boltzmann energy distribution. Usually it is impossible to fully elucidate the processes by experiments alone. Here we report recent progress toward predicting the time-evolving composition of these systems a priori: how unexpected reactions can be discovered on the computer, how reaction rates are computed from first principles, and how the many individual reactions are efficiently combined into a predictive simulation for the whole system. Some experimental tests of the a priori predictions are also presented.

## Friday, March 18, 2016 11:15AM - 2:15PM –

**Session Y33 FIAP: Organic Electronics and Photonics - Spin Transport and Photophysics** 336  
- Bryan Boudouris, Purdue University

**11:15AM Y33.00001 Engineering of spin injection and spin transport in organic spin valves using  $\pi$ -conjugated polymer brushes.**<sup>1</sup>, RUGANG GENG, ANANDI ROY, RAM SUBEDI, JASON LOCKLIN, THO NGUYEN, University of Georgia, WENBO ZHAO, XIAOGUANG LI, University of Science and Technology of China — Charge transport in amorphous organic semiconductors is governed by carriers hopping between localized states with small spin diffusion length. Furthermore, the spin interfacial resistance of organic spin valves (OSVs) is poorly controlled resulting in controversial reports of the magnetoresistance response. Here, we used surface initiated Kumada transfer polycondensation to covalently graft  $\pi$ -conjugated poly(3-methylthiophene) brushes from the  $La_{0.67}Sr_{0.33}MnO_3$  (LSMO) bottom electrode. The covalent attachment along with the brush morphology allows for more control over the LSMO/brush interfacial resistance and large spacer mobility. Remarkably, with 15 nm brush spacer layer, we observed an optimum magnetoresistance (MR) effect of 70% at cryogenic temperatures and a MR of 2.7% at 280K. The temperature dependence of the MR is nearly an order of magnitude weaker than that found in control OSVs made from spin-coated poly(3-hexylthiophene). Using a variety of different brush layer thicknesses, the thickness dependent MR at 20K was investigated. A spin diffusion length of 20 nm at 5 mV junction voltage rapidly increases to 55 nm at -280 mV.

<sup>1</sup>We acknowledge NSF (CHE 1412714 and DMR 0953112) (J.L.), the UGA start-up funds and Faculty Research Grant (T.N.), NSFC and NBRPC (2012CB922003 and 2015CB921201, X.G.L.) for funding this work.

**11:27AM Y33.00002 Intrinsic spin and momentum relaxation in organic single-crystalline semiconductors probed by ESR and Hall measurements**<sup>1</sup>, JUNTO TSURUMI, ROGER HUSERMANN, SHUN WATANABE, CHIKAHIKO MITSUI, TOSHIHIRO OKAMOTO, HIROYUKI MATSUI, JUN TAKEYA, Univ of Tokyo — Spin and charge momentum relaxation mechanism has been argued among organic semiconductors with various methods, devices, and materials. However, little is known in organic single-crystalline semiconductors because it has been hard to obtain an ideal organic crystal with an excellent crystallinity and controllability required for accurate measurements. By using more than 1-inch sized single crystals which are fabricated via contentious edge-casting method developed by our group, we have successfully demonstrated a simultaneous determination of spin and momentum relaxation time for gate-induced charges of 3,11-didecyldinaphtho[2,3-*d*:2',3'-*d'*]benzo[1,2-*b*:4,5-*b'*]dithiophene, by combining electron spin resonance (ESR) and Hall effect measurements. The obtained temperature dependences of spin and momentum relaxation times are in good agreement in terms of power law with a factor of approximately -2. It is concluded that Elliott-Yafet spin relaxation mechanism can be dominant at room temperature regime (200 – 300 K). Probing characteristic time scales such as spin-lattice, spin-spin, and momentum relaxation times, demonstrated in the present work, would be a powerful tool to elucidate fundamental spin and charge transport mechanisms.

<sup>1</sup>We acknowledge the New Energy and Industrial Technology Developing Organization (NEDO) for financial support.

**11:39AM Y33.00003 Vast Hole- and Electron-Polaron Spatial Extent in Oligomeric  $\pi$ -Conjugated Porphyrin Arrays**, PAUL ANGIOLILLO, Saint Joseph's University, JEFF RAWSON, MICHAEL THERIEN, Duke University — *meso*-Ethyne bridged  $\pi$ -conjugated zinc porphyrin oligomers ( $PZn_n$  compounds) have been demonstrated to evince lowest excited singlet states that are globally delocalized. It has also previously been shown that hole-polaron states of these oligomers exhibit delocalization lengths that mirror the molecular spatial dimension, 7.5 nm in the case of the heptamer. Here we demonstrate that the electron-polaron states in  $PZn_n$  compounds also feature vast areal delocalization. This finding is evidenced by concurrent optical and electron spin resonance measurements, coupled with electronic structure calculations that suggest atypically small reorganization energies for one-electron reduction of these materials. These results are buttressed by electron spin relaxation measurements of  $PZn_n$  electron polarons that show that both  $T_1$  and  $T_2$  relaxation times are unusually large, on the order of  $10^3$  ns and  $10^2$  ns, respectively. Since rapid charge delocalization defines an important mechanism that mitigates Coulombic stabilization of photogenerated electron-hole pairs to create separated free charge carriers, and spin polarization lifetimes feature prominently in spin currents, these findings identify conjugated materials with exceptional optical, electronic, and spintronic properties.

**11:51AM Y33.00004 Magnetization Dynamics of Organic-based Magnetic Heterostructures**, MICHAEL CHILCOTE, YU LU, HAILONG WANG, FENGYUAN YANG, EZEKIEL JOHNSTON-HALPERIN, Dept. of Physics, The Ohio State University — We present temperature dependent ferromagnetic resonance measurements of both isolated magnetic films and bilayers, including all organic and organic/inorganic hybrid magnetic heterostructures. These results establish organic magnetic heterostructures as an exciting new materials platform for the exploration of the fundamental mechanisms driving magnetic ordering in organic-based materials and promise the extension of organic spintronics into the regime of dynamically-driven spin currents, such as those found in spin pumping. The low cost, low-temperature conformal deposition of organic-based thin film magnets makes them an attractive class of materials for device applications. For example, they offer the potential for novel applications in high frequency magnetoelectronics on flexible substrates. Our materials are of the form  $M[\text{Acceptor}]_x$  ( $M$  = transition metal,  $x \approx 2$ ), exhibit room temperature magnetic ordering, and provide the opportunity to tailor magnetic properties through the selection of the transition metal ions and organic ligands. In particular, we focus on ferrimagnetic films and heterostructures where  $M$  = vanadium and the organic ligands are tetracyanoethylene (TCNE), ethyl tricyanoethylene carboxylate (ETCEC), and methyl tricyanoethylene carboxylate (MeTCEC).

**12:03PM Y33.00005 Large Magnetoresistance at High Bias Voltage in Double-layer Organic Spin Valves<sup>1</sup>**, R. C. SUBEDI, S. H. LIANG, R. GENG, Department of Physics & Astronomy, University of Georgia, Athens, GA 30602, USA, Q.T. ZHANG, L. LOU, J. WANG, School of Materials Science and Engineering, Nanyang Technological University, Singapore 639798, Singapore, X. F. HAN, Beijing National Laboratory of Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, T. D. NGUYEN, Department of Physics & Astronomy, University of Georgia, Athens, GA 30602, USA — We report studies of magnetoresistance (MR) in double-layer organic spin valves (DOSV) using tris (8-hydroxyquinolino) aluminum ( $\text{Alq}_3$ ) spacers. The device exhibits three distinct resistance levels depending on the relative magnetizations of the ferromagnetic electrodes. We observed a much weaker bias voltage dependence of MR in the device compared to that in the conventional organic spin valve (OSV). The MR magnitude reduces by the factor of two at 0.7 V bias voltage in the DOSV compared to 0.02 V in the conventional OSV. Remarkably, the MR magnitude reaches 0.3% at 6 V bias in the DOSVs, the largest MR response ever reported in OSVs at this bias. Our finding may have a significant impact on achieving high efficient bipolar OSVs strictly performed at high voltages.

<sup>1</sup>University of Georgia start-up fund, Ministry of Education, Singapore, National Natural Science Foundation of China

**12:15PM Y33.00006 Multi-scale modeling of spin transport in organic semiconductors**, SHAYAN HEMMATIYAN, Department of Physics, Texas AM University, College Station, Texas 77843, USA/Institut für Physik, Johannes Gutenberg Universität Mainz, Germany, AMAURY SOUZA, Institut für Physik, Johannes Gutenberg Universität Mainz, D-55099 Mainz, Germany, PASCAL KORDT, Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany, ERIK MCNELLIS, Institut für Physik, Johannes Gutenberg Universität Mainz, D-55099 Mainz, Germany, DENIS ANDRIENKO, Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany, JAIRO SINOVA, Institut für Physik, Johannes Gutenberg Universität Mainz, D-55099 Mainz, Germany — In this work, we present our theoretical framework to simulate simultaneously spin and charge transport in amorphous organic semiconductors. By combining several techniques e.g. molecular dynamics, density functional theory and kinetic Monte Carlo, we are able to study spin transport in the presence of anisotropy, thermal effects, magnetic and electric field effects in a realistic morphologies of amorphous organic systems. We apply our multi-scale approach to investigate the spin transport in amorphous  $\text{Alq}_3$  (Tris(8-hydroxyquinolino)aluminum) and address the underlying spin relaxation mechanism in this system as a function of temperature, bias voltage, magnetic field and sample thickness.

**12:27PM Y33.00007 Chromophoric disorder in conjugated polymers: the curious case of P3HT**, LENA SIMINE, Rice University, PETER ROSSKY, Dept. of Chemistry, Rice University — The origin of the broad absorption spectrum of conjugated polymers is discussed. Motivated by the open questions posed in the recent experimental literature, we investigate theoretically the chromophoric disorder in single molecule poly(3hexyl)thiophene (P3HT) at the atomic level using quantumclassical simulations. We reproduce the absorption spectrum and confirm qualitatively the prediction of simplified models the localization length of the first excited state decreases with increasing temperature. Counter to expectation, the same trend is observed for the average energy of the chromophore: in spite of a shorter localization length, the spectrum of the hot chromophore is redshifted with respect to its cold counterpart. We trace this peculiarity to the anharmonicity of the underlying torsional potential which allows preferential access to more planar interring conformations at high temperature. The contributions of bending to the transitional energies, the origin of inhomogeneous broadening and the possibility of classification of the chromophore as planar/twisted/bent at low and high temperatures are discussed.

**12:39PM Y33.00008 Varying the apparent conduction mechanism in polymer semiconductors**, EMILY G. BITTLE, HYUN WOOK RO, JAMES I. BASHAM, DEAN DELONGCHAMP, DAVID GUNDLACH, Natl Inst of Stds & Tech, OANA JURCHESCU, Wake Forest University — The weak van der Waals inter-molecular interactions in organic semiconductors (OSCs) result in large variations in transport behavior ranging from hopping to band-like. Accurately measuring and modelling charge transport is a prerequisite to establishing robust transport-microstructure correlations and developing predictive structure-function relationships for optimized materials design and processing. Field-effect transistors have become a favored test structure for parameterizing and benchmarking the electronic properties of OSCs due to their ease of fabrication, measurement, and possible use in commercial applications. However, correctly analyzing transistor current-voltage measurements to extract material properties has proven difficult, as parasitic effects influence the device electrical properties and mask intrinsic material properties. Here, we use impedance spectroscopy to evaluate the effects of contacts on device operation and extract the properties of the channel which we compare with conventional DC measurements. We apply this approach to model systems of the widely studied polymer regioregular poly(3-hexylthiophene-2,5-diyl) which we engineer through different solidification kinetics to achieve distinct, well characterized degrees of molecular order. When increasing the order we find that the transport changes from field enhanced to field independent. This study addresses the origins of transport behavior seen in OSCs while discerning non-linear contact effects from field dependent transport.

**12:51PM Y33.00009 Suppression of molecular vibrations in strained organic semiconductors**, TAKAYOSHI KUBO, ROGER HUSERMANN, JUNTO TSURUMI, JUNSHI SOEDA, YUGO OKADA, YU YAMASHITA, CHIKAHICO MITSUI, TOSHIHIRO OKAMOTO, HIROYUKI MATSUI, JUN TAKEYA, Univ of Tokyo, SUSUMU YANAGISAWA, Univ of the Ryukyus, NORIHISA AKAMATSU, ATSUSHI SHISHIDO, Tokyo Tech — The inherent softness of organic semiconductors, which makes them totally suited for flexible applications, also offers us an idea on the modulation of the charge transport in largely strained crystal structure. Here, solution-processed single crystal of 3,11-didecyldinaphtho[2,3-*d*:2',3'-*d'*]benzo[1,2-*b*:4,5-*b'*]dithiophene ( $\text{C}_{10}$ -DNBDT-NW)<sup>1</sup> is uniaxially and compressively strained for 3% simply by bending the flexible substrate. With this strain, the field-effect mobility increases dramatically from 9.7  $\text{cm}^2/\text{Vs}$  to 16.5  $\text{cm}^2/\text{Vs}$  by up to 70%, which is reversible and repeatable for successive bending. Combined with X-ray diffraction and low temperature measurement, a series of calculations based on density functional theory reveal the origin of the enhanced charge transport to be the suppression of the thermal fluctuation of the molecules rather than the slight change of the band structure. Our work shows that compression of the crystal structure directly hinders molecular vibrations and thus leads to the suppression of dynamic disorder, which is a unique mechanism in soft organic semiconductors.

<sup>1</sup>C. Mitsui, *Adv. Mater.* 6, 4546

**1:03PM Y33.00010 Illumination of Conjugated Polymer in Solution Alters its Conformation and Thermodynamics: The Role of Incident Light Intensity, Wavelength and Exposure Time**, BRIAN MORGAN, University of Tennessee, MARK DADMUN, University of Tennessee, Oak Ridge National Laboratory — The importance of chain structure in conjugated polymer-based material active layers and its relation to device efficiencies in OPVs, organic field transistors, and OLEDs, has been well established. However the influence of light absorption on the conjugated polymer structure is not well understood. We have employed small angle neutron scattering to investigate structural changes occurring in solutions of poly(3-hexylthiophene-2,5-diyl) with exposure to white light. Our previous results indicate significant change in the structure of the polymer upon illumination, an effect we attribute to an alteration in the thermodynamic interactions of the polymer with the surrounding solvent. In order to further our understanding of this phenomenon, we have studied the modulation of these light/dark structural changes as a function of solvent choice, incident light intensity, illumination wavelength, and light exposure duration. Analysis of this data allows refinement and increased control of these light-initiated effects, moving our efforts closer to the development of a powerful, non-destructive, and tunable method for controlling polymer conformation in solution and novel light-responsive materials.

**1:15PM Y33.00011 Real-time charge carrier motion in P3HT studied with Kelvin Probe Microscopy<sup>1</sup>**, CHLOE CASTANEDA, ALYINA ZAIDI, JASON MOSCATELLO, KATHERINE AIDALA, Mount Holyoke College — We have developed a technique that uses scanning probe microscopy (SPM) to study the real-time injection and extraction of charge carriers in organic semiconductor devices. We investigate P3HT (full name) in an inverted field effect transistor geometry with gold electrodes. By positioning the SPM tip at an individual location and using Kelvin probe microscopy to record the potential over time, we can record how the charge carriers respond to changing the backgate voltage while the source and drain electrodes are grounded. We see relatively fast screening for negative backgate voltages because holes are quickly injected into the P3HT film. The screening is slower for positive gate voltages, because some of these holes are trapped and therefore less mobile. We compare P3HT transistors with different fabrication procedures that are expected to change the trap distribution: no silanization of the oxide and no annealing, silanization and no annealing, and both silanization and annealing. By incrementally stepping the gate voltage, we probe different trap depths. The recorded change in potential over time is best fit by a double exponential, suggesting two physical mechanisms involved in screening.

<sup>1</sup>This work is supported by NSF grant DMR-0955348, and the Center for Hierarchical Manufacturing at the University of Massachusetts, Amherst (NSF CMMI-1025020).

**1:27PM Y33.00012 Spatially resolved charge transport study in discotic liquid crystalline organic semiconductors**, SANJOY PAUL, Department of Physics, Kent State University, ALEXANDER SEMYONOV, Department of Chemistry and Biochemistry, Kent State University, NATHAN J. DAWSON, KENNETH D. SINGER, Department of Physics, Case Western Reserve University, ROBERT J. TWIEG, Department of Chemistry and Biochemistry, Kent State University, BRETT ELLMAN, Department of Physics, Kent State University — Spatially resolved time-of-flight photogeneration and mobility have been measured on a discotic liquid crystalline organic semiconductor using scanning time-of-flight microscopy (STOFm). STOFm simultaneously obtains time-of-flight transients and polarized transmittance across the sample. Various shapes in time-of-flight transients were observed and extracted charge transport parameters such as photogeneration efficiency, mobility, and trapping show significant spatial variation. In some cases these can be linked to electrode surface inhomogeneities. Detailed measurement methodology, experimental results and challenges in their analysis will be discussed.

**1:39PM Y33.00013 The Effects of Stoichiometry on the Optical Properties of PTZ-TCNQ Charge Transfer Crystals**, IRIS STONE, JAYDEEP JOSHI, George Mason University, ROBERT SMITH, SCOTT MELIS, EDWARD VAN KEUREN, Georgetown University, PATRICK VORA, George Mason University — Charge transfer (CT) crystals are two-component organic materials formed by stacked pairs of donor and acceptor molecules. Depending on the choice of donor and acceptor molecules it is possible to achieve semiconducting, insulating, or metallic characteristics, making the CT crystal platform potentially transformative for applications in low-cost flexible electronics. The use of phenothiazine (PTZ) donors and tetracyanoquinodimethane (TCNQ) acceptors is predicted to result in a semiconducting state with high electron and hole mobilities, properties that are ideal for ambipolar transistors. Here, we seek to understand the effect of stoichiometry on the optical and electronic properties of PTZ:TCNQ CT crystals by comparing nanowires with 1:1 stoichiometry to a novel 3:1 stoichiometry using temperature-dependent optical spectroscopy. Ensemble photoluminescence and absorption measurements indicate that a CT state forms in the 1:1 sample, whereas the 3:1 sample exhibits weaker coupling between TCNQ and PTZ. These results support a strong correlation between stoichiometry and optical properties. Our observations give important insight into how the intermolecular coupling varies with stoichiometry and are crucial to future efforts to realize an organic ambipolar transistor.

**1:51PM Y33.00014 Quantitative Probes of Electron-Phonon Coupling in an Organic Charge-Transfer Material**, AARON RURY, SHAYNE SORENSON, ERIC DRISCOLL, JAHAN DAWLATY, University of Southern California — While organic charge transfer (CT) materials may provide alternatives to inorganic materials in electronics and photonics applications, properties central to applications remain understudied in these organic materials. Specifically, electron-phonon coupling plays a pivotal role in electronic applications yet this coupling in CT materials remains difficult to directly characterize. To better understand the suitability of organic CT materials for electronic applications, we have devised an experimental technique that can directly assess electron-phonon coupling in a model organic CT material. Upon non-resonant interaction with an ultrafast laser pulse, we show that coherent excitation of Raman-active lattice vibrations of quinhidrone, a 1:1 co-crystal of the hydroquinone and p-benzoquinone, modulates the energies of electronic transitions probed by a white light pulse. Using a well-established theoretical framework of vibrational quantum beat spectra across the probe bandwidth, we quantitatively extract the parameters describing these electronic transitions to characterize electron-phonon coupling in this material. In conjunction with temperature-dependent resonance Raman measurements, we assess the hypothesis that several sharp transitions in the near-IR correspond to previously unknown excitonic states of this material. These results and their interpretation set the foundation for further elucidation of the one of the most important parameters in the application of organic charge-transfer materials to electronics and photonics.

**2:03PM Y33.00015 Influence of structural fluctuations on lifetimes of adsorbate states at hybrid organic-semiconductor interfaces<sup>1</sup>**, M. MÜLLER, CIC nanoGUNE, San-Sebastián, D. SÁNCHEZ-PORTAL, CSIC, San-Sebastián, Spain, H. LIN, Univ. Milano-Bicocca, Italy, G. FRATESI, Univ. Milano, Italy, G.P. BRIVIO, Univ. Milano-Bicocca, Italy, A. SELLONI, Princeton Univ., USA — On the road towards a more realistic description of charge transfer processes at hybrid organic-semiconductor interfaces for photovoltaic applications we extend our first-principles scheme for the extraction of elastic linewidths to include the effects of structural fluctuations. Based on snapshots obtained from Car-Parinello molecular dynamics simulations at room temperature, we set up geometries in which dye molecules at interfaces are attached to a semi-infinite TiO<sub>2</sub> substrate. The elastic linewidths are computed using a Green's function method. This effectively introduces the coupling to a continuum of states in the substrate. In particular we investigate catechol and isonicotinic acid on rutile(110) and anatase(101) at the level of semi-local density functional theory. We perform multiple calculations of linewidths and peak-positions associated with the adsorbate's frontier orbitals for different geometric configurations to obtain a time-averaged analysis of such physical properties. We compare the results from the considered systems to understand the effects of dynamics onto interfacial charge transfer and systematically assess the dependence of the extracted elastic lifetimes on the relative alignment between adsorbate and substrate states.

<sup>1</sup>This project has received funding from the European Union Seventh Framework Programme under grant agreement no. 607323 [THINFACE]

**Friday, March 18, 2016 11:15AM - 1:51PM –**

**Session Y35 GSNP DBIO: Principles of Cell-to-Cell Communication** 338 - Ned Wingreen, Princeton University

**11:15AM Y35.00001 Collective synchronization of divisions in *Drosophila* development.**<sup>1</sup>, MASSIMO VERGASSOLA, Univ of California - San Diego — Mitoses in the early development of most metazoans are rapid and synchronized across the entire embryo. While diffusion is too slow, in vitro experiments have shown that waves of the cell-cycle regulator Cdk1 can transfer information rapidly across hundreds of microns. However, the signaling dynamics and the physical properties of chemical waves during embryonic development remain unclear. We develop FRET biosensors for the activity of Cdk1 and the checkpoint kinase Chk1 in *Drosophila* embryos and exploit them to measure waves in vivo. We demonstrate that Cdk1 chemical waves control mitotic waves and that their speed is regulated by the activity of Cdk1 during the S-phase (and not mitosis). We quantify the progressive slowdown of the waves with developmental cycles and identify its underlying control mechanism by the DNA replication checkpoint through the Chk1/Wee1 pathway. The global dynamics of the mitotic signaling network illustrates a novel control principle: the S-phase activity of Cdk1 regulates the speed of the mitotic wave, while the Cdk1 positive feedback ensures an invariantly rapid onset of mitosis. Mathematical modeling captures the speed of the waves and predicts a fundamental distinction between the S-phase Cdk1 trigger waves and the mitotic phase waves, which is illustrated by embryonic ablation experiments.

<sup>1</sup>In collaboration with Victoria Deneke<sup>1</sup>, Anna Melbinger<sup>2</sup>, and Stefano Di Talia<sup>1</sup> <sup>1</sup> Department of Cell Biology, Duke University Medical Center <sup>2</sup> Department of Physics, University of California San Diego

**11:51AM Y35.00002 Collective Calcium Dynamics in Networks of Communicating Cells**, TOMMY BYRD, Purdue University, GARRETT POTTER, BO SUN, Oregon State University, ANDREW MUGLER, Purdue University — Cells can sense and encode information about their environment with remarkable precision. These properties have been studied extensively for single cells, but intercellular communication is known to be important for both single- and multicellular organisms. Here, we examine calcium dynamics of fibroblast cells exposed to external ATP stimuli, and the effects of communication and stimulus strength on cells' response. Experimental results show that increasing communication strength induces a greater fraction of cells to exhibit oscillatory calcium dynamics, but the frequencies of oscillation do not systematically shift with ATP strength. We developed a model of calcium signaling by adding noise, communication, and cell-to-cell variability to the model of Tang and Othmer<sup>1</sup>. This model reproduces cells' increased tendency to oscillate as a function of communication strength, and frequency encoding is nearly removed at the global level. Our model therefore suggests that the propensity of cells to oscillate, rather than frequency encoding, determines the response to external ATP. These results suggest that the system lies near a critical boundary separating non-oscillatory and oscillatory calcium dynamics.

<sup>1</sup>Tang, Y. and Othmer, H. G., *Proc. Natl. Acad. Sci.* 92, 1995.

**12:03PM Y35.00003 Precision of multicellular gradient sensing with cell-cell communication**, ANDREW MUGLER, Department of Physics and Astronomy, Purdue University, ANDRE LEVCHENKO, Department of Biomedical Engineering and Yale Systems Biology Institute, Yale University, ILYA NEMENMAN, Departments of Physics and Biology, Emory University — Gradient sensing underlies diverse biological processes. In principle, bigger “detectors (cells or groups of cells) make better sensors, since then concentrations measured at the front and back of a detector are more different, and the gradient can be determined with higher precision. Indeed, experiments have shown that populations of cells detect gradients more precisely than single cells. However, this argument neglects the fact that information must be communicated between different parts of the detector, and the communication process introduces its own noise. Here we derive the fundamental limits to the precision of gradient sensing with cell-cell communication and temporal integration. We find that communication imposes its own sensory length scale, beyond which the precision cannot increase no matter how large the cell population grows. We also find that temporal integration couples the internal communication with the external signal diffusion, imposing an additional limit on the precision. We discuss how these limits can be improved by a strategy with two communicated molecular species, which we term “regional excitation/global inhibition. We compare our findings to experiments with communicating epithelial cells, and infer a sensor length scale of about 4 cells.

**12:15PM Y35.00004 Collective synchronization of self/non-self discrimination in T cell activation, across multiple spatio-temporal scales**, GREGOIRE ALTAN-BONNET, National Cancer Institute, Bethesda MD — The immune system is a collection of cells whose function is to eradicate pathogenic infections and malignant tumors while protecting healthy tissues. Recent work has delineated key molecular and cellular mechanisms associated with the ability to discriminate self from non-self agents. For example, structural studies have quantified the biophysical characteristics of antigenic molecules (those prone to trigger lymphocyte activation and a subsequent immune response). However, such molecular mechanisms were found to be highly unreliable at the individual cellular level. We will present recent efforts to build experimentally validated computational models of the immune responses at the collective cell level. Such models have become critical to delineate how higher-level integration through nonlinear amplification in signal transduction, dynamic feedback in lymphocyte differentiation and cell-to-cell communication allows the immune system to enforce reliable self/non-self discrimination at the organism level. In particular, we will present recent results demonstrating how T cells tune their antigen discrimination according to cytokine cues, and how competition for cytokine within polyclonal populations of cells shape the repertoire of responding clones. Additionally, we will present recent theoretical and experimental results demonstrating how competition between diffusion and consumption of cytokines determine the range of cell-cell communications within lymphoid organs. Finally, we will discuss how biochemically explicit models, combined with quantitative experimental validation, unravel the relevance of new feedbacks for immune regulations across multiple spatial and temporal scales.

**12:51PM Y35.00005 A generic spatial-stochastic framework for quantifying noisy information flow in multicellular systems**, THOMAS SOKOLOWSKI<sup>1</sup>, GAŠPER TKAČIK<sup>2</sup>, IST Austria — Spatio-temporal protein signals play a crucial role in communicating information within and between cells. However, their ability to convey signals robustly is hampered by noise in gene regulation and biochemical transport, occurring at low copy numbers. While we increasingly understand distinct strategies of biochemical noise control, it remains unclear how nature orchestrates them to maximize information flow. Our recent work extends our information-theoretic framework for gene regulation to an explicitly spatial setting. We constructed a stochastic model enabling fast calculation of local means and variances in a spatially coupled gene regulatory system, which we use for rigorous quantification of information flow in an ensemble of units sensing a spatially distributed input and exchanging information via diffusion. By applying our framework to the paradigmatic Bcd-Hbk system in early fly development, we demonstrate that diffusive coupling can be of substantial benefit in encoding positional information, and uncover a novel optimal regulatory strategy relying on spatial coupling. Thanks to the generic methodology employed, our framework is universally applicable for realistic predictive modeling and data-driven inference of multicellular systems engaging in noisy communication.

<sup>1</sup>Institute of Science and Technology Austria, Am Campus 1, A-3400 Klosterneuburg, Austria

<sup>2</sup>Institute of Science and Technology Austria, Am Campus 1, A-3400 Klosterneuburg, Austria

**1:03PM Y35.00006 Increased dimensionality of cell-cell communication can decrease the precision of gradient sensing<sup>1</sup>**, TYLER SMITH, Department of Physics, Emory University, ANDRE LEVCHENKO, Department of Biomedical Engineering and Yale Systems Biology Institute, Yale University, ILYA NEMENMAN, Department of Physics, Emory University, ANDREW MUGLER, Department of Physics and Astronomy, Purdue University — Gradient sensing is a biological computation that involves comparison of concentrations measured in at least two different locations. As such, the precision of gradient sensing is limited by the intrinsic stochasticity in the communication that brings such distributed information to the same location. We have recently analyzed such limitations experimentally and theoretically in multicellular gradient sensing in mammary epithelial cell organoids. For 1d chains of collectively sensing cells, the communication noise puts a severe constraint on how the accuracy of gradient sensing increases with the number of cells in the sensor. A question remains as to whether the effect of the noise can be mitigated by the extra spatial averaging allowed in sensing by 2d and 3d cellular organoids. Here we show using computer simulations that, counterintuitively, such spatial averaging decreases gradient sensitivity (while it increases concentration sensitivity). We explain the findings analytically and propose that a recently introduced Regional Excitation - Global Inhibition model of gradient sensing can overcome this limitation and use 2d or 3d spatial averaging to improve the sensing accuracy.

<sup>1</sup>Supported by NSF Grant PHY/1410978 and James S. McDonnell Foundation Grant 220020321

**1:15PM Y35.00007 ABSTRACT WITHDRAWN —**

**1:27PM Y35.00008 Synthetic Quorum Sensing and Induced Aggregation in Model Microcapsule Colonies with Repressilator Feedback**, HENRY SHUM, VICTOR YASHIN, ANNA BALAZS, University of Pittsburgh — We model a system of synthetic microcapsules that communicate chemically by releasing nanoparticles or signaling molecules. These signaling species bind to receptors on the shells of capsules and modulate the target shells permeability, thereby controlling nanoparticle release from the target capsule. Using the repressilator regulatory network motif, whereby three species suppress the production of the next in a cyclic fashion, we show that large amplitude oscillations in nanoparticle release can emerge when many capsules are close together. This exemplifies quorum sensing, which is the ability of cells to gauge their population density and collectively initiate a new behavior once a critical density is reached. We present a physically realizable model in which the oscillations exhibited in crowded populations induce aggregation of the microcapsules, mimicking complex biological behavior of the slime mold *Dictyostelium discoideum* with only simple, synthetic components. We also show that the clusters can be dispersed and reformed repeatedly and controllably by addition of chemical stimuli, demonstrating possible applications in creating reconfigurable or programmable materials.

**1:39PM Y35.00009 Limits to collaborative concentration sensing in cell populations<sup>1</sup>**, SEAN FANCHER, ANDREW MUGLER, Department of Physics and Astronomy, Purdue University — Cells sense chemical concentrations with a precision that approaches the physical limit set by molecular diffusion. Recent experiments have vividly shown that cells can beat this limit when they communicate. We derive the physical limits to concentration sensing for cells that communicate over short distances by directly exchanging small molecules across their membranes (juxtacrine signaling), and over long distances by secreting and absorbing a diffusive messenger molecule (paracrine signaling). In the latter case, we find that the cell spacing that optimizes precision can be large, due to a tradeoff between maintaining communication strength and reducing signal cross-correlations. This leads to the surprising result that paracrine signaling allows more precise sensing than juxtacrine signaling for sufficiently large populations, even though this means that the cells are spaced far apart. We compare our results to recent experiments.

<sup>1</sup>This work is supported by a grant from the Simons Foundation (376198 to A.M.)

**Friday, March 18, 2016 11:15AM - 1:51PM —**  
**Session Y36 GSOF DBIO: Soft Mechanics in Biological Systems** 339 - Moumita Das, Rochester Institute of Technology

**11:15AM Y36.00001 Intermediate response of complex fluids with biophysical implications**, HAIM DIAMANT, Tel Aviv University — Over sufficiently large distances any complex fluid responds as a continuous medium, characterized by bulk viscoelastic moduli. But how large is “sufficiently large”? Close examination of the competing sub-asymptotic term reveals a distinctive spatio-temporal regime, intermediate between the small-scale and large-scale responses. In materials such as semiflexible polymer networks this regime governs the dynamics over a broad range of distances, pushing the crossover to the bulk behavior to a distance much larger than the structural correlation length. The validity of these findings has been confirmed by two-point microrheology of entangled F-actin networks, where the crossover distance was found to be of micron scale—i.e., relevant to biological cells.<sup>1</sup> We discuss consequences of the intermediate response for the fluctuations of small objects and membranes inside actin networks.

<sup>1</sup>A. Sonn-Segev, A. Bernheim-Groswasser, H. Diamant, Y. Roichman, Phys. Rev. Lett. **112**, 088301 (2014).

**11:27AM Y36.00002 Mechanical response of biopolymer double networks<sup>1</sup>**, JOSHUA CARROLL, MOUMITA DAS, Rochester Institute of Technology — We investigate a double network model of articular cartilage (AC) and characterize its equilibrium mechanical response. AC has very few cells and the extracellular matrix mainly determines its mechanical response. This matrix can be thought of as a double polymer network made of collagen and aggrecan. The collagen fibers are stiff and resist tension and compression forces, while aggrecans are flexible and control swelling and hydration. We construct a microscopic model made of two interconnected disordered polymer networks, with fiber elasticity chosen to qualitatively mimic the experimental system. We study the collective mechanical response of this double network as a function of the concentration and stiffness of the individual components as well as the strength of the connection between them using rigidity percolation theory. Our results may provide a better understanding of mechanisms underlying the mechanical resilience of AC, and more broadly may also lead to new perspectives on the mechanical response of multicomponent soft materials.

<sup>1</sup>This work was partially supported by a Cottrell College Science Award

**11:39AM Y36.00003 The mechanics of endothelial gap formation**, JOYJIT CHATTORAJ, EMANUELA DEL GADO, Georgetown Univ, C. COREY HARDIN, Division of Pulmonary and Critical Care Medicine, Massachusetts General Hospital, Boston, MA, RAMASWAMY KRISHNAN, Center for Vascular Biology Research, Beth Israel Deaconess Medical Center, Boston, MA — The vascular endothelium is a layer of specialized cells, referred to as endothelial cells (EC) that line the internal surfaces of blood vessels and are largely responsible for regulating the transit of fluids, solutes and immune system cells from the circulation, across the vessel wall, and into the tissues. We investigate the physics of the mechanical events that may proceed and eventually lead to dramatic increase of its permeability, leading to serious illness. In combination with experiments measuring local stresses and gap formation in EC in different conditions, we devise a minimal model based on an amorphous assembly of adhesive particles, subjected to an imposed tension. Numerical simulations of the model show that, as a function of the rate at which the tension is imposed, the system goes from an elastic regime in which small gaps increase in number to a plastic one, where pre-existing gaps increase in size, and internal stresses display large heterogeneities and long range correlations. This second regime bears intriguing similarities with the experimental finding in EC monolayers.

**11:51AM Y36.00004 A simple polymeric model describes cell nuclear mechanical response**, EDWARD BANIGAN, Department of Physics & Astronomy, Northwestern University, ANDREW STEPHENS, Department of Molecular Biosciences, Northwestern University, JOHN MARKO, Departments of Physics & Astronomy and Molecular Biosciences, Northwestern University — The cell nucleus must continually resist inter- and intracellular mechanical forces, and proper mechanical response is essential to basic cell biological functions as diverse as migration, differentiation, and gene regulation. Experiments probing nuclear mechanics reveal that the nucleus stiffens under strain, leading to two characteristic regimes of force response. This behavior depends sensitively on the intermediate filament protein lamin A, which comprises the outer layer of the nucleus, and the properties of the chromatin interior. To understand these mechanics, we study a simulation model of a polymeric shell encapsulating a semiflexible polymer. This minimalistic model qualitatively captures the typical experimental nuclear force-extension relation and observed nuclear morphologies. Using a Flory-like theory, we explain the simulation results and mathematically estimate the force-extension relation. The model and experiments suggest that chromatin organization is a dominant contributor to nuclear mechanics, while the lamina protects cell nuclei from large deformations.

**12:03PM Y36.00005 The Effect of Predators on Cholera Biofilms: If it Lyses, We Can Smash It**, ARBEN KALZIQI, ERYN BERNARDY, JACOB THOMAS, WILL RATCLIFF, BRIAN HAMMER, PETER YUNKER, Georgia Institute of Technology — Many microbes form biofilms dense clumps of cells and protein on surfaces. Biofilms are complex communities that facilitate the study of biological competition (e.g., two types of microbes may compete to form a biofilm in the same location) and interesting physics (e.g., the source of a biofilm's rigidity). *Vibrio cholerae* can produce biofilms which have a network-like structure; however, cholera can be genetically engineered to kill other cholera with different genotypes, which leaves behind a structureless slime rather than such a biofilm. Through mechanical creep testing of both predator-prey and non-predator populations, we found that the predator-prey population responds viscously and decreases in height with repeated compression, whereas the non-predator population responds elastically and maintains its original height. The current work suggests that cell lysis after killing disrupts biofilm formation, preventing microbial colonies from forming rigid networks.

**12:15PM Y36.00006 Mechanical Properties of a Primary Cilium Measured by Resonant Oscillation**, ANDREW RESNICK, Cleveland State University — Primary cilia are ubiquitous mammalian cellular substructures implicated in an ever-increasing number of regulatory pathways. The well-established 'ciliary hypothesis' states that physical bending of the cilium (for example, due to fluid flow) initiates signaling cascades, yet the mechanical properties of the cilium remain incompletely measured, resulting in confusion regarding the biological significance of flow-induced ciliary mechanotransduction. In this work we measure the mechanical properties of a primary cilium by using an optical trap to induce resonant oscillation of the structure. Our data indicate 1), the primary cilium is not a simple cantilevered beam, 2), the base of the cilium may be modeled as a nonlinear rotatory spring, the linear spring constant 'k' of the cilium base calculated to be  $(4.6 \pm 0.62) \times 10^{-12}$  N/rad and nonlinear spring constant ' $\alpha$ ' to be  $(-1 \pm 0.34) \times 10^{-10}$  N/rad<sup>2</sup>, and 3) the ciliary base may be an essential regulator of mechanotransduction signalling. Our method is also particularly suited to measure mechanical properties of nodal cilia, stereocilia, and motile cilia, anatomically similar structures with very different physiological functions.

**12:27PM Y36.00007 Composition and Humidity Response of the Black Widow Spider's Gumfoot Silk and its Implications on Adhesion**, DHARAMDEEP JAIN, CI ZHANG, LYDIA ROSE COOL, TODD A. BLACKLEDGE, CHRYS WEDEMIOTIS, TOSHIKAZU MIYOSHI, ALI DHINOJWALA, University of Akron — Humidity plays an important part in the performance of biomaterials such as pollen, gecko toe, wheat awns, bird feathers and dragline silk. Capture silk produced by web building spiders form an interesting class of humidity responsive biological glues. The adhesive properties of the widely studied 'viscid silk' produced by orbweb-weaving spiders is highly humidity sensitive. On the other hand, relatively less is known about the dependence of composition and humidity response towards adhesion for 'gumfoot' silk produced by cobweb-weaving spiders. In the present study, we investigate the gumfoot silk produced by Black Widow using adhesion mechanics, microscopy and spectroscopic methods. The results show the presence of hygroscopic salts, glycoproteins and previously known spider coating peptides in silk and their importance in the humidity response and adhesion. The current study elucidates the role of constituents of capture silk in its adhesion mechanism and offers insights to novel ways for fabricating bio-inspired adhesives.

**12:39PM Y36.00008 Flexibility of bacterial type IV pili determined using atomic force microscopy**, JOSH MOGYOROS, SHUN LU, University of Guelph, HANJEONG HARVEY, LORI BURROWS, McMaster University, ROBERT WICKHAM, JOHN DUTCHER, University of Guelph — Type IV pili (T4P) are very thin protein filaments extended and retracted from the surface of certain Gram-negative bacteria. Pili play a major role in processes such as adhesion, twitching motility and biofilm formation. We used atomic force microscopy (AFM) to perform force spectroscopy measurements on T4P of *P. aeruginosa*. Bacteria were adhered to the end of an AFM cantilever that was brought into contact with a substrate, allowing the pili to adhere. Force-separation curves were collected by retracting the cantilever, corresponding to the stretching of the T4P that was well described by the worm-like chain (WLC) model. Distinct peaks were observed in the distributions of the best-fit values of the persistence length  $L_p$  on two different surfaces, providing strong evidence for close-packed bundling of very flexible T4P [1]. Surprisingly, the most prominent value of  $L_p \sim 1$  nm is significantly less than the  $\sim 8$  nm length of the PilA subunit. We have investigated this intriguing result by refining our protocol to combine AFM with fluorescence microscopy to isolate a single bacterium on a colloidal probe, as well as critically examining the applicability of the WLC model. [1] S. Lu et al., Biophys. J. 108, 2865 (2015).

**12:51PM Y36.00009 Passage times of confined cancer cells and deformable particles flowing through a microfluidic channel**, ZEINA KHAN, NABIOLLAH KAMYABI, FAZLE HUSSAIN, SIVA VANAPALLI, Texas Tech University — Circulating tumor cells, the primary cause of cancer metastasis, have to navigate through tight extracellular matrix and capillaries. Unfortunately, understanding of the hydrodynamic interactions between cells and narrow vessel walls is lacking. Using a microfluidic channel of rectangular cross-section, we investigate cell hydrodynamic behavior by measuring cell confinement, passage time through the microchannel, and excess pressure drop. Testing with highly and lowly aggressive cancer cells shows that passage time may not always be indicative of cancer cell aggressiveness as the relationship among passage time, friction and rheology is complex. Transport of deformable particles including droplets of varying viscosity and interfacial tension, as well as elastic particles of different elastic moduli, reveals that passage times depend on particle size and, contrary to prior claims, on viscosity but not on elastic modulus. We also find that particle viscosity and not modulus controls the friction force and lubrication film thickness, suggesting that cancer cell viscosity rather than elasticity controls cell transport on short time-scales.

**1:03PM Y36.00010 Mechanics governs single-cell signaling and multi-cell robustness in biofilm infections.**<sup>1</sup> , VERNITA GORDON, The University of Texas at Austin — In biofilms, bacteria and other microbes are embedded in extracellular polymers (EPS). Multiple types of EPS can be produced by a single bacterial strain - the reasons for this redundancy are not well-understood. Our work suggests that different polymers may confer distinct mechanical benefits. Our model organism is *Pseudomonas aeruginosa*, an opportunistic human pathogen that forms chronic biofilm infections associated with increased antibiotic resistance and evasion of the immune defense. Biofilms initiate when bacteria attach to a surface, sense the surface, and change their gene expression. Changes in gene expression are regulated by a chemical signal, cyclic-di-GMP. We find that one EPS material, called "PEL," enhances surface sensing by increasing mechanical coupling of single bacteria to the surface. Measurements of bacterial motility suggest that PEL may increase frictional interactions between the surface and the bacteria. Consistent with this, we show that bacteria increase cyclic-di-GMP signaling in response to mechanical shear stress. Mechanosensing has long been known to be important to the function of cells in higher eukaryotes, but this is one of only a handful of studies showing that bacteria can sense and respond to mechanical forces. For the mature biofilm, the embedding polymer matrix can protect bacteria both chemically and mechanically. *P. aeruginosa* infections in the cystic fibrosis (CF) lung often last for decades, ample time for the infecting strain(s) to evolve. Production of another EPS material, alginate, is well-known to tend to increase over time in CF infections. Alginate chemically protects biofilms, but also makes them softer and weaker. Recently, it is being increasingly recognized that bacteria in chronic CF infections also evolve to increase PSL production. We use oscillatory bulk rheology to determine the unique contributions of EPS materials to biofilm mechanics. Unlike alginate, increased PSL stiffens biofilms. Increasing both PSL and alginate expression increases the energy cost to break the biofilm. We compare the elastic moduli of biofilms to estimated stresses exerted by phagocytotic immune cells, and infer that increased PSL could confer a mechanical fitness benefit.

<sup>1</sup>This work was supported by start-up funds from The University of Texas at Austin and a gift from ExxonMobile to VDG, and by grants from the Human Frontiers Science Program (HFSP RGY0081/2012-GORDON) and the National Science Foundation (NSF 1337670).

**1:39PM Y36.00011 Suspended Solid-state Membranes on Glass Chips with Sub 1-pF Capacitance for Biomolecule Sensing Applications** , CHEN-CHI CHIEN, ADRIAN BALAN, REBECCA ENGELKE, MARIJA DRNDIC, University of Pennsylvania — Solid-state membranes are finding use in many applications in nanoelectronics and nanomedicine, from single molecule sensors to water filtration, and yet many of their electronics applications are limited by the current noise and low bandwidth stemming from the relatively high capacitance (more than 10 pF) of the membrane chips. To address this problem, we devised an integrated fabrication process to grow and define circular silicon nitride membranes on glass chips that successfully lower the chip capacitance to below 1 pF. We use these devices to demonstrate low-noise, high-bandwidth DNA translocation measurements. We also make use of this versatile, low-capacitance platform to suspend other thin, two-dimensional membranes such as graphene.

**Friday, March 18, 2016 11:15AM - 2:15PM –**  
**Session Y37 GSOF GSNP: Fracture, Friction, and Deformation** 340 - Mark Robbins, John Hopkins University

**11:15AM Y37.00001 Tearing Fracture of Polymer Foam Sheet**<sup>1</sup> , ATSUSHI TAKEI, KO OKUMURA, Ochanomizu Univ. — We study crack propagation in a sheet of polymer foam. The sheet was stretched, and an initial crack was introduced to induce the crack propagation. When the sheet width is shorter than the crack length, the energy release rate (ERR)  $G$  of the system is independent of the crack length and constant during the propagation. Under the constant ERR condition, we find that the crack propagates at a constant speed. We observed the crack propagation for various values of ERR by changing the width of the sheet and the applied strain. Depending on values  $G$  of ERR, the measured velocity of the crack propagation was in the range from 0.01 mm/s to 10000 mm/s. We also found power laws between the velocity of the crack  $V$  and  $G$ . While in the literature the power law with the exponent close to three ( $V \sim G^3$ ) has been reported, we found that polymer foam sheets have different exponents depending on physical characteristics of polymer foam. In this presentation, we report the experimental result and its analysis.

<sup>1</sup>This research was partly supported by ImPACT program of council for science, Technology and Innovation (Cabinet office government of Japan)

**11:27AM Y37.00002 Effect of system compliance on crack nucleation in soft materials** , SHRUTI RATTAN, ALFRED CROSBY, UMass Amherst — Puncture mechanics in soft materials is critical for the development of new surgical instruments, robot assisted-surgery as well as new materials used in personal protective equipment. However, analytical techniques to study this important deformation process are limited. We have previously described a simple experimental method to study the resistive forces and failure of a soft gel being indented with a small tip needle. We showed that puncture stresses can reach two orders of magnitude greater than the material modulus and that the force response is insensitive to the geometry of the indenter at large indentation depths. Currently, we are examining the influence of system compliance on crack nucleation (e.g. puncture) in soft gels. It is well known that system compliance influences the peak force in adhesion and traditional fracture experiments; however, its influence on crack nucleation is unresolved. We find that as the system becomes more compliant, lower peak forces required to puncture a gel of certain stiffness with the same indenter were measured. We are developing scaling relationships to relate the peak puncture force and system compliance. Our findings introduce new questions with regard to the possibility of intrinsic materials properties related to the critical stress and energy for crack nucleation in soft materials.

**11:39AM Y37.00003 Crack propagation in attractive colloidal systems** , LAURA ROSSI, TRIET DANG, University of Amsterdam, MAXIME LEFRANC, PAUL LE FLOCH, ELISABETH BOUCHAUD, ESPCI ParisTech, PETER SCHALL, University of Amsterdam — Despite its importance, the fracture of materials, especially the regime of slow, plastic fracture, remains poorly understood. This is especially true in amorphous materials, where local inhomogeneities and structural disorder are crucial to determine the mode of failure, yet they cannot be modeled with classical homogenization methods. We use new attractive colloidal systems to study fracture at time and length scales much longer than in molecular systems. In this specific project, we focus on gels made of fluorescent pNipam microgel particles aggregated via critical Casimir interactions, to analyze, at the microscopic level, nonlinear and dissipative processes in the material ahead of the propagating crack tip.

**11:51AM Y37.00004 Localized Plastic Deformation in Colloidal Micropillars** , DANIEL STRICKLAND, JYO LYN HOR, CARLOS ORTIZ, DAEYEON LEE, DANIEL GIANOLA, University of Pennsylvania — When driven beyond yield, many amorphous solids exhibit concentrated regions of large plastic strain referred to as shear bands. Shear bands are the result of localized, cooperative rearrangements of particles known as shear transformations (STs). STs are dilatatory: their operation results in an increase of free volume and local softening that leads to spatially concentrated plasticity. However, the evolution of STs into a macroscopic shear band remains poorly understood. To study the process, we perform compression experiments on amorphous colloidal micropillars. The micropillars, which are composed of fluorescent 3  $\mu\text{m}$  PMMA particles, are made freestanding so that shear banding instabilities are not suppressed by confining boundaries. During compression, we observe strong localization of strain in a band of the pillar. As deformation proceeds, the sheared region continues to dilate until it reaches the colloidal glass transition, at which point dilation terminates. We quantify a length scale by measuring the extent of spatial correlations in strain. This length scale decreases gradually with increasing dilation and becomes static beyond the glass transition. Our results reinforce the idea of yield as a stress-induced glass transition in amorphous solids.

**12:03PM Y37.00005 Theory of rate dependent fracture size effects**, ALESSANDRO TALONI, ALESSANDRO SELLERIO, STEFANO ZAPPERI, Center for Complexity and Biosystems - Physics Department, University of Milan La Statale" — The idea that the solid failure can be described by means of the Kramer theory, where the intrinsic energy barrier is reduced proportionally to the applied field, first appeared in material science to treat the kinetic fracture of solids under applied stresses and dates back to '40s. Most previous works focused on the thermal dependence of the average strength or the failure time in creep experiments and did not address the survival distribution and its size dependence. To this end, we start from recent theories developed for single-molecule pulling, where the molecule rate coefficient for rupture (or unbinding) is modified by the presence of an external time-dependent force, and we adjust it to a macroscopic elastic object. We generalize the extreme value theory to account for failures of materials with an explicit dependence on temperature, strain rate and size of the object. We show that in the limit of macroscopic objects, large strain rate and low temperature, thermal fluctuations are negligible and the usual extreme value theory is recovered. We provide the critical interpretation of several experiments in terms of our theory, furnishing a clearcut criterion for thermal effects to become relevant. [Phys. Rev. Applied, 024011]

**12:15PM Y37.00006 Major and minor slip-events in frictional stick-slip**<sup>1</sup>, GEORGIOS TSEKENIS, DEMET TATAR, SHMUEL RUBINSTEIN, DAVID WEITZ, MICHAEL AZIZ, FRANS SPAEPEN, Harvard Univ — Several universal phenomena characterize friction that are independent of the materials involved such as the logarithmic aging of the static friction coefficient and the logarithmic velocity weakening of the dynamic friction coefficient. We study dry friction between rough surfaces with programmed statistical profiles. By measuring the displacement field at the frictional interface we observe stick-slip behavior which reveals two kinds of slip: major events that tend to grow large and unbounded and minor events that usually stay small and bounded.

<sup>1</sup>Research supported by Harvard MRSEC Program under NSF contracts DMR-0820484, DMR-1420570

**12:27PM Y37.00007 Tribological Properties of Nanodiamonds in Aqueous Suspensions: Effect of the Surface Charge.**<sup>1</sup>, J. KRIM, ZIJIAN LIU, D.A. LEININGER, A. KOVILAND, A.I. SMIRNOV, North Carolina State University, O. SHENDAROVA, International Technology Center, Raleigh, NC, D.W. BRENNER, North Carolina State University — The presence of granular nanoparticulates, be they wear particles created naturally by frictional rubbing at a geological fault line or products introduced as lubricant additives, can dramatically alter friction at solid-liquid interfaces. Given the complexity of such systems, understanding system properties at a fundamental level is particularly challenging. The Quartz Crystal Microbalance (QCM) is an ideal tool for studies of material-liquid-nanoparticulate interfaces. We have employed it here to study the uptake and nanotribological properties of positively and negatively charged 5-15 nm diameter nanodiamonds dispersed in water[1] in the both the presence and absence of a macroscopic contact with the QCM electrode. The nanodiamonds were found to impact tribological performance at both nanometer and macroscopic scales. The tribological effects were highly sensitive to the sign of the charge: negatively (positively) charged particles were more weakly (strongly) bound and reduced (increased) frictional drag at the solid-liquid interface. For the macroscopic contacts, negatively charged nanodiamonds appeared to be displaced from the contact, while the positively charged ones were not. Overall, the negatively charged nanodiamonds were more stable in an aqueous dispersion for extended time periods.

<sup>1</sup>Work supported by NSF and DOE

**12:39PM Y37.00008 Transition from superlubrically sliding islands to pinned monolayer, demonstrated in Xe/Cu(111) (\*)**<sup>1</sup>, ROBERTO GUERRA, International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy., ANDREA VANOSSI, CNR-IOM Democritos National Simulation Center, Via Bonomea 265, 34136 Trieste, Italy., ERIO TOSATTI, International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy., TRIESTE NANOFRICTION TEAM — A molecular dynamics simulation case study of Xe on Cu(111) reveals unexpected information on the exceptionally smooth sliding state associated with incommensurate superlubricity which is argued to emerge in the large size limit of naturally incommensurate Xe islands. As coverage approaches a full monolayer, theory predicts an abrupt adhesion-driven two-dimensional density compression on the order of several per cent, implying a hysteretic jump from superlubric free islands to a pressurized  $\sqrt{2} \times \sqrt{2}$  commensurate (and pinned, and therefore immobile) monolayer. These results match with recent quartz crystal microbalance data which show remarkably large slip times with increasing submonolayer coverage, signalling superlubricity, followed by a dramatic drop to zero for the dense commensurate monolayer [1]. Careful analysis of this variety of island sliding phenomena should be essential in future applications of friction at crystal/adsorbate interfaces. (\*) Matching experimental work by M. Pierro, L. Bruschi, G. Mistura, G. Paolicelli, A. di Bona, S. Valeri. [1] M. Pierro, L. Bruschi, G. Mistura, G. Paolicelli, A. di Bona, S. Valeri, R. Guerra, A. Vannessi, E. Tosatti, Nature Nanotechnology 10, 714 (2015).

<sup>1</sup>Supported by ERC Advanced Grant N. 320796 - MODPHYSFRICT

**12:51PM Y37.00009 Elastic deformations disrupt structural superlubricity in large contacts**<sup>1</sup>, TRISTAN A. SHARP, Johns Hopkins University, LARS PASTEWKA, Karlsruher Institut für Technologie, MARK O. ROBBINS, Johns Hopkins University — Force microscopy experiments observe ultra-low friction between solids with incommensurate lattice structures. This phenomenon is referred to as superlubricity and is due to a cancellation of lateral forces because surfaces sample all relative local configurations with equal probability. We use simulations to show that elasticity disrupts superlubricity in sufficiently large circular contacts. The simulations include atomic-scale geometry and reach micron-scales. For rigid solids, cancellation is complete except at the contact boundary. The static friction force per contact area,  $\tau$ , falls as a power of contact radius,  $\tau \sim a^{-3/2}$ . Elastic deformations limit this cancellation when the contact radius  $a$  is larger than a characteristic length scale set by the core width of interfacial dislocations,  $b_{core}$ . For  $a > b_{core}$  sliding of moderately incommensurate contacts is dominated by dislocation motion and, at large  $a$ ,  $\tau$  approaches a constant value near the Peierls stress needed to move edge dislocations. Surprisingly, the stress in commensurate contacts drops to nearly the same value at large  $a$ . We conclude that true structural lubricity does not occur in large contacts, although the constant shear stress drops rapidly with  $b_{core}$ .

<sup>1</sup>NSF IGERT, DAAD

**1:03PM Y37.00010 Subharmonic Shapiro steps in sliding colloidal monolayers**<sup>1</sup>, ANDREA VANOSSI, CNR-IOM Democritos & SISSA, Trieste, Italy, STELLA PARONUZZI, SISSA, Trieste, Italy, GABRIELE FORNASIER, NICOLA MANINI, Dipartimento di Fisica, Università di Milano, Italy, GIUSEPPE E. SANTORO, SISSA, Trieste, Italy, ERIO TOSATTI, SISSA & ICTP, Trieste, Italy — We examine the possibility to observe dynamical mode locking, in the form of Shapiro steps, when a time-periodic potential modulation is applied to two mutually sliding incommensurate 2D lattices. Specifically we present realistic MD simulations of a monolayer of charged colloids that are dragged by an external force over an optically generated periodic potential, where the colloid sliding is enacted through the motion of soliton or antisoliton lines between locally commensurate domains. Clear integer Shapiro steps, with the synchronous rigid advancement of the whole monolayer, known from previous studies [1], are found. The jump between one step and the next during each AC cycle corresponding to particles jumping from one patch to the next, across the soliton boundary. We find additional smaller "subharmonic" steps. Here, the overall colloid advancement takes several AC cycles. At each cycle, different subsets of particles negotiate the soliton line between commensurate domains [2]. The wide parameter tunability of colloid monolayers makes these predictions potentially easy to access in an experimentally rich 2D geometry. [1] A. Libal et al., Phys. Rev. Lett. 96, 188301 (2006). [2] S. Paronuzzi et al., J. Phys. Cond. Matt., in press (2015)

<sup>1</sup>Supported by ERC Advanced Grant N. 320796 MODPHYSFRICT

**1:15PM Y37.00011 Superlubric-pinned Aubry transition of two dimensional monolayers in optical lattices.**<sup>1</sup> , DAVIDE MANDELLI, SISSA, Trieste, ANDREA VANOSI, CNR-IOM Democritos and SISSA, Trieste, NICOLA MANINI, University of Milano, ERIO TOSATTI, SISSA and ICTP, Trieste — Two-dimensional (2D) crystalline colloidal monolayers sliding over a laser-induced optical lattice “corrugation” potential emulate friction between ideal crystal surfaces. Static friction is always present when the monolayer and the optical lattices are commensurate, but when they are incommensurate the presence or absence of static friction depends upon the system parameters. In 1D, at the Aubry dynamical phase transition the static friction goes continuously from zero (superlubricity) to finite as the periodic corrugation strength is increased. We look for the Aubry-like transition in the more realistic 2D case of a monolayer in an incommensurate periodic potential using molecular dynamics simulations. Results confirm a clear and sharp 2D superlubric-pinned transition upon increasing corrugation strength. Unlike the 1D Aubry transition which is continuous, the 2D transition is first-order, with a jump of static friction. At the 2D Aubry transition there is no change of symmetry, a sudden rise of the colloid-colloid interaction energy, and a compensating drop of the colloid-corrugation energy. The observability of the superlubric-pinned colloid transition is proposed and discussed [1]. [1] D. Mandelli, et al., Phys. Rev. B, to be published (2015).

<sup>1</sup>This work has been supported by ERC Advanced Grant N. 320796 MODPHYSFRICT.

**1:27PM Y37.00012 Superlubricity in a nutshell.**<sup>1</sup> , ERIO TOSATTI, SISSA and ICTP, Trieste, DAVIDE MANDELLI, SISSA, Trieste, ANDREA VANOSI, CNR-IOM Democritos and SISSA, Trieste — Cold ion chains in optical lattices emulate the Frenkel-Kontorova model, whose frictional behavior depends on commensurability or incommensurability between the two lattices. In the latter and more interesting case, there are two different regimes: one with pinning and static friction, and one without pinning, called superlubric. Only in an infinite chain the two regimes exist, separated by a dynamical Aubry transition. A cold ion chain is necessarily finite and short, we nevertheless proposed that a clear remnant of that transition should persist in trapped ion chains[1]. Recent experiments showed how in fact a small number of ions suffices to demonstrate incommensuration effects, with a change of friction by orders of magnitude from matched to mismatched geometries[2]. Here we present simulation results suggesting for increasing optical lattice amplitude a clear vestigial Aubry transition for very few ions, with a weak dependence upon the ion number and a stronger one upon the relative mismatch. A properly chosen amplitude should therefore show the vestigial transition from pinning at small mismatch to superlubricity at large mismatch. Alternatively, a chain which at  $T=0$  is pinned at all mismatches could develop an Aubry transition at finite temperature to a state of “thermally induced superlubricity”, due to the thermal smearing of the optical lattice amplitude. [1] A. Benassi et al., Nat. Comm. 2, 236 (2011). [2] A. Bylinskii et al, Science 348, 1115-1118 (2015).

<sup>1</sup>Supported by ERC Advanced Grant N. 320796 MODPHYSFRICT.

**1:39PM Y37.00013 An Artificial Ising System with Phononic Excitations** , HAMED GHAFARI, W.ASHLEY GRIFFITH, University of Texas, PHILIP BENSON , School of Earth & Environmental Sciences, Burnaby Building, Burnaby Road, Portsmouth, M.H.B NASSERI, R.PAUL YOUNG, University of Toronto — Many intractable systems and problems can be reduced to a system of interacting spins. Here, we report mapping collective phononic excitations from different sources of crystal vibrations to spin systems. The phononic excitations in our experiments are due to micro and nano cracking (yielding crackling noises due to lattice distortion). We develop real time mapping of the multi-array sensors to a network-space and then mapping the excitation- networks to spin-like systems. We show that new mapped system satisfies the quench (impulsive) characteristics of the Ising model in 2D classical spin systems. In particular, we show that our artificial Ising system transits between two ground states and approaching the critical point accompanies with a very short time frozen regime, inducing formation of domains separated by kinks. For a cubic-test under a true triaxial test (3D case), we map the system to a 6-spin ring under a transversal-driving field where using functional multiplex networks, the vector components of the spin are inferred (i.e., XY model). By visualization of spin patterns of the ring per each event, we demonstrate that “kinks” (as defects) proliferate when system approach from above to its critical point. We support our observations with employing recorded acoustic excitations during distortion of crystal lattices in nano-indentation tests on different crystals (silicon and graphite), triaxial loading test on rock (poly-crystal) samples and a true 3D triaxial test.

**1:51PM Y37.00014 Fingering Instability of Debonding Soft Elastic Adhesives** , ELIE RAPHAEL, UMR GULLIVER CNRS ESPCI Paris, FALKO ZIEBERT, Albert-Ludwigs-Universitt Freiburg, THOMAS VILMIN, UMR GULLIVER CNRS ESPCI Paris — We study the crack-front fingering instability of an elastic adhesive tape that is peeled off a solid substrate. Our analysis is based on an energy approach using fracture mechanics and scaling laws and provides simple physical explanations for (i) the fact that the wavelength depends only on the thickness of the adhesive film and (ii) the threshold of the instability, and (iii) additionally estimates the characteristic size of the fingers.

**2:03PM Y37.00015 Gluing Soft Interfaces by Nanoparticles**<sup>1</sup> , ZHEN CAO, ANDREY DOBRYNIN, Univ of Akron — Using a combination of the molecular dynamics simulations and scaling analysis we studied reinforcement of interface between two soft gel-like materials by spherical nanoparticles. Analysis of the simulations shows that the depth of penetration of a nanoparticle into a gel is determined by a balance of the elastic energy of the gel and nanoparticle deformations and the surface energy of nanoparticle/gel interface. In order to evaluate work of adhesion of the reinforced interface, the potential of mean force for separation of two gels was calculated. These simulations showed that the gel separation proceeds through formation of necks connecting nanoparticles with two gels. The shapes of the necks are controlled by a fine interplay between nanoparticle/gel surface energies and elastic energy of the neck deformation. Our simulations showed that by introducing nanoparticles at soft interfaces, the work required for separation of two gels could be 10-100 times larger than the work of adhesion between two gels without nanoparticle reinforcement. These results provide insight in understanding the mechanism of gluing soft gels and biological tissues by nano- and micro-sized particles.

<sup>1</sup>NSF DMR-1409710

**Friday, March 18, 2016 11:15AM - 2:03PM –**

**Session Y38 DPOLY: Polymeric Elastomers and Gels** 341 - Jan Genzer, North Carolina State University

**11:15AM Y38.00001 Covalent Fusion of layered Incompatible Gels in Immiscible Solvents** , SANTIDAN BISWAS, AWANEESH SINGH, Univ of Pittsburgh, KRZYSZTOF MATYJASZEWSKI, Carnegie Mellon University, ANNA C. BALAZS, Univ of Pittsburgh — We carry out dissipative particle dynamics (DPD) simulations to model a two layered stackable gel where the gels are incompatible and are present in immiscible solvent. The bottom layer of the gel is created first and then a solution of new initiators, monomers and cross-linkers is introduced on top of it. These components then undergo polymerization and form the second gel layer. We study all possible combinations of free radical polymerization (FRP) and atom transfer radical polymerization (ATRP) mechanisms with the two layers of the gel. For example, the bottom layer gel is created via ATRP, whereas the top layer gel follows FRP. Our focus is to do a systematic study of all these combinations and find out the factors responsible for combining two incompatible gels in immiscible solvents.

**11:27AM Y38.00002 Cyclic topology in polymer networks**, RUI WANG, ALFREDO ALEXANDER-KATZ, JEREMIAH JOHNSON, BRADLEY OLSEN, Massachusetts Institute of Technology — Despite the ubiquity of applications, much of our fundamental knowledge about polymer networks is based on an assumption of ideal end-linked structure. However, polymer networks invariably possess topological defects: loops of different orders which have profound effects on network properties. Here, we demonstrate that all different orders of cyclic topologies are a universal function of a single dimensionless parameter characterizing the conditions for network formation. The theory is in excellent agreement with both experimental measurements of hydrogel loop fractions and Monte Carlo simulations without any fitting parameters. We demonstrate the superposition of the dilution effect and chain-length effect on loop formation. The one-to-one correspondence between the network topology and primary loop fraction demonstrates that the entire network topology is characterized by measurement of just primary loops, a single chain topological feature. Different cyclic defects cannot vary independently, in contrast to the intuition that the densities of all topological species are freely adjustable.

**11:39AM Y38.00003 Capturing dissipation and adhesion using transient network theory**, MICHELLE SING, GARETH MCKINLEY, BRADLEY OLSEN, Massachusetts Institute of Technology — Associative networks are prevalent in many fields and are of interest for applications where it is important that these materials are capable of adhering to their surroundings and/or provide a mechanism for dissipating energy in high-impact systems. However, little is known about the particular molecular behavior that differentiates these materials from their non-dissipative and non-adhesive associative counterparts. Here, we modify our previous work using the Smoluchowski equation to model the full network chain end-to-end distance distribution while tracking the population of individual chain conformations for chains that undergo multiple reaction intermediate steps. Thus, instead of the binary associated/dissociated states traditionally studied, we incorporate the ability for chains to partially dissociate and associate. This partial association/dissociation results in stress relaxation due to chain extension. In steady shear and start-up of steady shear, dissipation within the network becomes a function of both the elastically stored energy and the bond energy released during dissociation events.

**11:51AM Y38.00004 Dynamics of Bottlebrush Networks: A Computational Study<sup>1</sup>**, ANDREY DOBRYNIN, ZHEN CAO, Univ of Akron, SERGEI SHEIKO, Univ of NC - Chapel Hill — We study dynamics of deformation of bottlebrush networks using molecular dynamics simulations and theoretical calculations. Analysis of our simulation results show that the dynamics of bottlebrush network deformation can be described by a Rouse model for polydisperse networks with effective Rouse time of the bottlebrush network strand,  $\tau_R = \tau_0 N_s^2 (N_{sc} + 1)$  where,  $N_s$  is the number-average degree of polymerization of the bottlebrush backbone strands between crosslinks,  $N_{sc}$  is the degree of polymerization of the side chains and  $\tau_0$  is a characteristic monomeric relaxation time. At time scales  $t$  smaller than the Rouse time,  $t < \tau_R$ , the time dependent network shear modulus decays with time as  $G(t) \propto \rho k_B T (\tau_0/t)^{1/2}$ , where  $\rho$  is the monomer number density. However, at the time scale  $t$  larger than the Rouse time of the bottlebrush strands between crosslinks, the network response is pure elastic with shear modulus  $G(t) = G_0$ , where  $G_0$  is the equilibrium shear modulus at small deformation. The stress evolution in the bottlebrush networks can be described by a universal function of  $t/\tau_R$ .

<sup>1</sup>NSF DMR-1409710

replacing MAR16-2015-006437.

**12:03PM Y38.00005 Bottlebrush and comb-like elastomers as ultra-soft electrical and acoustically active materials<sup>1</sup>**, WILLIAM DANIEL, MOHAMMAD VATANKHAH-VARNOSFADERANI, ASHISH PANDYA, Univ of NC - Chapel Hill, JOANNA BURDYNKA, Carnegie Mellon University - CMU, BENJAMIN MORGAN, MATTHEW EVERHART, Univ of NC - Chapel Hill, KRZYSZTOF MATYJASZEWSKI, Carnegie Mellon University - CMU, ANDREY DOBRYNIN, University of Akron- Akron, MICHAEL RUBINSTEIN, SERGEI SHEIKO, Univ of NC - Chapel Hill, UNC MIRT TEAM — Without swelling in a solvent, it is challenging to obtain materials with a modulus below  $10^5$  Pa, which is dictated by chain entanglements. We show that macromolecules can be disentangled by dense grafting of side chains to long polymer chains. The bottlebrush and comb-like architectures demonstrate a unique combination of flexibility and network dilution, leading to significant decrease of the entanglement modulus ( $G_e$ ) and increase of extensibility. Following theoretical predictions, it has been shown that the  $G_e$  is controlled by the polymerization degrees of sidechains ( $n_{sc}$ ) and grafting spacer ( $n_g$ ) as  $G_e \approx (n_g/n_{sc})^{1.5}$ . Using the reduced entanglement density, we developed solvent-free elastomers with moduli on the order of 100 Pa and excellent extensibility. Using bottlebrush architectures we have developed PDMS dielectric actuators with high deformation at low electric field strength. Additionally strong acoustic adsorption leads to materials showing shape and volume control in light opaque environments.

<sup>1</sup>NSF (DMR 1409710, DMR 1122483, DMR 1407645, and DMR 1436201)

**12:15PM Y38.00006 Controlling Phase Separation of Tough Interpenetrating Polymer Networks via Addition of Amphiphilic Block Copolymers.**, BRIAN ROHDE, RAMANAN KRISHNAMOORTI, MEGAN ROBERTSON, Univ of Houston — Interpenetrating polymer networks (IPNs) offer a unique way to combine the mechanical properties of two thermoset systems. Often used to create a material that possesses both high toughness and tensile properties, here we use polydicyclopentadiene, cured via ring opening metathesis polymerization, to contribute high toughness and diglycidyl ether of bisphenol A cured via anhydride chemistry to contribute high tensile strength and modulus. As the uncompatibilized system reacts in the presence of one another, mesoscopic phase separation occurs and dictates the overall efficacy of combining mechanical properties. To control phase separation and drive the system towards more mechanically robust nanostructured IPNs, amphiphilic block copolymers of polybutadiene-*b*-polyethylene oxide, where one block possesses strong affinity to polyDCPD and the other the DGEBA, were added to the system. Here we present a systematic study of the influence of block copolymer composition in the overall blend on degree of phase separation and morphology using a combination of small-angle x-ray scattering (SAXS) and scanning electron microscopy (SEM) techniques. The resultant mechanical properties are then explored in an effort to link mechanical properties to blend morphology.

**12:27PM Y38.00007 Weak hydrogen bonding yields rigid, tough, and elastic hydrogels<sup>1</sup>**, SERGEI SHEIKO, XIAOBO HU, MOHAMMAD VATANKHAH-VARNOSFADERANI, JING ZHOU, QIAOXI LI, University of North Carolina at Chapel Hill, ANDREY DOBRYNIN, University of Akron — Unlike living tissues, synthetic hydrogels are inherently soft and brittle, particularly when built of hydrogen bonds. It remains challenging to design hydrogels that combine high rigidity, strength at break, extensibility, high elasticity. Through free-radical copolymerization of *N*,*N*-dimethylacrylamide and methacrylic acid, we have designed a network system based on tunable composition of covalent bonds (permanent cross-links) and hydrogen bonds (sacrificial and recoverable crosslinks) with the following rationale: 1) Maintain a high total number of cross-links to ensure high modulus; 2) Introduce a high fraction of H-bonding to ensure high energy dissipation; and 3) Incorporate a small fraction of permanent cross-links to ensure shape control. By tuning the chemical composition and microstructure we have obtained materials with superb mechanical properties. The hydrogels contain 70 wt% water (similar to living cartilage, skin, and ligaments), while display modulus of 28 MPa, strength of 2 MPa, fracture energy of  $9300 \text{ J}\cdot\text{m}^{-2}$ , extensibility of 800%, excellent fatigue-resistance, and great elasticity allowing for complete and fast strain recovery. The results agreed with theoretical predictions for modulus relaxation of dual networks with dynamic and permanent crosslinks.

<sup>1</sup>We gratefully acknowledge funding from the National Science Foundation (DMR 1122483, DMR 1407645, and DMR 1436201).

**12:39PM Y38.00008 Cavitation of a Physically Associating Gel**, SATISH MISHRA, SANTANU KUNDU, Mississippi State University — Self-assembly of block copolymers in selective solvents form ordered structures such as micelles, vesicles, and physically crosslinked gels due to difference in their interaction with solvents. These gels have wide range of applications in tissue engineering, food science and biomedical field due to their tunable properties and responsiveness with changing environmental conditions. Pressurization of a defect inside a physically associating gel can lead to elastic instability (cavitation) leading to failure of the gel. The failure behavior involves dissociation of physical networks. A thermoreversible, physically associating gel with different volume fractions of a triblock copolymer, poly (methyl methacrylate)-poly (n-butyl acrylate)-poly (methyl methacrylate) [PMMA-PnBA-PMMA] in 2-ethyl 1-hexanol, a midblock selective solvent, is considered here. Mechanical properties were investigated using shear rheology and cavitation experiments. The experimental data is fitted with a constitutive model that captures the stiffening behavior followed by softening behavior of a physical gel. Finite element analysis has been performed on cavitation rheology geometry to capture the failure behavior and to calculate energy release rate during cavitation experiments.

**12:51PM Y38.00009 Tough Stretchable Physically-Crosslinked Hydrogel Fiber Mats from Electrospun Statistical Copolymers.**, YIMING YANG, R.A. WEISS, BRYAN VOGT, University of Akron — Nature uses supramolecular interactions combined with hierarchical structures to produce water-laden materials with combination of properties that are challenging to obtain in synthetic systems. Here we describe a simple method based on electrospinning of a self-associating amphiphilic copolymer. Immersion of the copolymer mats in water generates supramolecular hydrogels that are crosslinked by association of the fluorinated hydrophobic moieties in the copolymer. These robust hydrogel fiber mats exhibit extensibility greater than 225 % and the elastic modulus can be comparable to the bulk hydrogel despite the porous structure of the as-spun mat. Moreover, the stress dissipation by re-arrangement of the physically associated network leads to coalescence of the fibers that propagates from the surfaces to the interior of the mat. Both the mechanical properties and this fiber coalescence behavior can be tuned by selection of the copolymer composition and the initial fiber dimensions. These tough, stretchable hydrogel fiber mats could find utility in a variety of biomedical applications due to their unique properties.

**1:03PM Y38.00010 Amphiphile-modified supramolecular hydrogels: optimized network structure and enhanced stiffness at "Goldilocks" amphiphile content**, CHAO WANG, BRYAN VOGT, R.A. WEISS, University of Akron — Hydrogels formed by hydrophobic physical crosslinks have high mechanical strength (larger than 100kPa). 1 Surfactants, such as sodium dodecyl sulfate (SDS), can be used to control the mechanical strength and modulus of these hydrogels. Here we describe the change in the viscoelastic behavior of physically crosslinked copolymer hydrogels synthesized from N,N-dimethylacrylamide (DMA) and 2-(N-ethylperfluoro-octane sulfonamido) ethyl methacrylate (FOSM) by the addition of a SDS solution. Without confinement, SDS dissociates the FOSM micelle-like microstructure and facilitates swelling, which decreases the crosslink density of the hydrogel and reduces the modulus and strength of the hydrogel. With 1-dimensional macroscopic confinement, similar behavior was observed, but only for soaking times in the salt solution smaller than 15 h. For longer times (larger than 15 h), SDS improved the mechanical strength and modulus of the hydrogel presumably by reducing the imperfections in the hydrogel network and forming complexes with FOSM. 1. Hao, J.; Weiss, R. a. Mechanical Behavior of Hybrid Hydrogels Composed of a Physical and a Chemical Network. Polymer 2013, 54, 21742182.

**1:15PM Y38.00011 Advancing Reversible Shape Memory by Tuning Network Architecture**, QIAOXI LI, JING ZHOU, MOHAMMAD VATANKHAH VARNOSFADERANI, University of North Carolina at Chapel Hill, DMYTRO NYKYPANCHUK, OLEG GANG, Brookhaven National Lab-CFN, SERGEI SHEIKO, University of North Carolina at Chapel Hill, UNIVERSITY OF NORTH CAROLINA AT CHAPEL HILL COLLABORATION, BROOKHAVEN NATIONAL LAB-CFN COLLABORATION — Recently, reversible shape memory (RSM) has been realized in conventional semi-crystalline elastomers without applying any external force and synthetic programming. The mechanism is ascribed to counteraction between thermodynamically driven relaxation of a strained polymer network and kinetically preferred self-seeding recrystallization of constrained network strands. In order to maximize RSM's performance in terms of (i) range of reversible strain, (ii) rate of strain recovery, and (iii) relaxation time of reversibility, we have designed a systematic series of networks with different topologies and crosslinking densities, including purposely introduced dangling chains and irregular meshes. Within a broad range of crosslink density ca. 50-1000 mol/m<sup>3</sup>, we have demonstrated that the RSM's properties improve significantly with increasing crosslink density, regardless of network topology. Actually, one of the most irregular networks with densest crosslinking allowed achieving up to 80% of the programmed strain being fully reversible, fast recovery rate up to 0.05 K<sup>-1</sup>, and less than 15% decrease of reversibility after hours of annealing at partial melt state. With this understanding and optimization of RSM, we pursue an idea of shape control through self-assembly of shape-memory particles. For this purpose, 3D printing has been employed to prepare large assemblies of particles possessing specific shapes and morphologies.

**1:27PM Y38.00012 Increasing the Mechanical Strength of Block Polymer Ion Gels Through the Stepwise Self-Assembly of a Thermoresponsive ABC Triblock Terpolymer**, CECILIA HALL, CAN ZHOU, SCOTT DANIELSEN, TIMOTHY LODGE, Univ of Minnesota - Twin Cities — Blends of network-forming block polymers and ionic liquids have remarkable potential for solid electrolytes, as they allow the combination of desirable mechanical and electrical properties. While ABA triblock copolymers have successfully been implemented as the network component of ion gels, these networks contain looped defects, where the endblocks of the polymer loop back into the same spherical core instead of forming a bridge between two cores. We demonstrate that the ABC triblock terpolymer poly(ethylene-*alt*-propylene)-*block*-poly(ethylene oxide)-*block*-poly(*N*-isopropylacrylamide) (PEP-*b*-PEO-*b*-PNIPAm) in the ionic liquid 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonate)imide forms a thermoreversible gel network with negligible looping defects. PEP-core micelles exist at all temperatures, while cooling causes association of the PNIPAm micelle corona to form a bridging network. Small-angle x-ray scattering and dynamic light scattering were used to characterize the high-temperature micelles. These gels show enhanced mechanical properties and the ability to form gels at lower concentrations than the corresponding thermoresponsive ABA triblock copolymers.

**1:39PM Y38.00013 Rheology and Relaxation Timescales of ABA Triblock Polymer Gels**, ANDREW PETERS, TIMOTHY LODGE, Univ of Minn - Minneapolis — When dissolved in a midblock selective solvent, ABA polymers form gels composed of aggregated end block micelles bridged by the midblocks. While much effort has been devoted to the study of the structure of these systems, the dynamics of these systems has received less attention. We examine the underlying mechanism of shear relaxation of ABA triblock polymer gels, especially as a function of chain length, composition, and concentration. Recent work using time-resolved small-angle neutron scattering of polystyrene (PS)-*block*-poly(ethylene-*alt*-propylene) (PEP) in squalane has elucidated many aspects of the dynamics of diblock chain exchange. By using rheology to study bulk relaxation phenomena of the triblock equivalent, PS-PEP-PS, we apply the knowledge gained from the chain exchange studies to bridge the gap between the molecular and macroscopic relaxation phenomena in PS-PEP-PS triblock gels.

**1:51PM Y38.00014 Non-continuum, anisotropic nanomechanics of random and aligned electrospun nanofiber matrices**, DAPHNEY CHERY, BIAO HAN, Drexel University, ROBERT MAUCK, VIVEK SHENOY, University of Pennsylvania, LIN HAN, Drexel University — Polymer nanofiber assemblies are widely used in cell culture and tissue engineering, while their nanomechanical characteristics have received little attention. In this study, to understand their nanoscale structure-mechanics relations, nanofibers of polycaprolactone (PCL) and poly(vinyl alcohol) (PVA) were fabricated via electrospinning, and tested via AFM-nanoindentation with a microspherical tip ( $R \approx 10 \mu\text{m}$ ) in PBS. For the hydrophobic, less-swollen PCL, a novel, non-continuum linear F-D dependence was observed, instead of the typical Hertzian  $F-D^{3/2}$  behavior, which is usually expected for continuum materials. This linear trend is likely resulted from the tensile stretch of a few individual nanofibers as they were indented in the normal plane. In contrast, for the hydrophilic, highly swollen PVA, the observed typical Hertzian response indicates the dominance of localized deformation within each nanofiber, which had swollen to become hydrogels. Furthermore, for both matrices, aligned fibers showed significantly higher stiffness than random fibers. These results provide a fundamental basis on the nanomechanics of biomaterials for specialized applications in cell phenotype and tissue repair.

**Friday, March 18, 2016 11:15AM - 2:15PM –**

**Session Y39 DBIO: Methods in Biological Physics** 342 - Tatsiana Mironava, State University of New York, Stonybrook

**11:15AM Y39.00001 “Calibration-on-the-spot”: How to calibrate an EMCCD camera from its images<sup>1</sup>**, KIM I. MORTENSEN, HENRIK FLYVBJERG, Department of Micro- and Nanotechnology, Technical University of Denmark — In localization-based microscopy, super-resolution is obtained by analyzing isolated diffraction-limited spots imaged, typically, with EMCCD cameras. To compare experiments and calculate localization precision, the photon-to-signal amplification factor is needed but unknown without a calibration of the camera. Here we show how this can be done *post festum* from just a recorded image. We demonstrate this (i) theoretically, mathematically, (ii) by analyzing images recorded with an EMCCD camera, and (iii) by analyzing simulated EMCCD images for which we know the true values of parameters. In summary, our method of *calibration-on-the-spot* allows calibration of a camera with unknown settings from old images on file, with no other info needed. Consequently, *calibration-on-the-spot* also makes future camera calibrations before and after measurements unnecessary, because the calibration is encoded in recorded images during the measurement itself, and can at any later time be decoded with *calibration-on-the-spot*.

<sup>1</sup>This work was supported by the Lundbeck Foundation and the Danish Council for Strategic Research Grant No. 10-092322 (PolyNano).

**11:27AM Y39.00002 Live-cell thermometry with nitrogen vacancy centers in nanodiamonds**, HARISHANKAR JAYAKUMAR, Department of Physics, CUNY-City College of New York, HELMUT FEDDER, Department of Physics, University of Stuttgart, ANDREW CHEN, LIUDI YANG, CHENGHAO LI, Department of Biomedical Engineering, CUNY-City College of New York, JOERG WRACHTRUP, Department of Physics, University of Stuttgart, SIHONG WANG, Department of Biomedical Engineering, CUNY-City College of New York, CARLOS MERILES, Department of Physics, CUNY-City College of New York — The ability to measure temperature is typically affected by a tradeoff between sensitivity and spatial resolution. Good thermometers tend to be bulky systems and hence are ill-suited for thermal sensing with high spatial localization. Conversely, the signal resulting from nanoscale temperature probes is often impacted by noise to a level where the measurement precision becomes poor. Adding to the microscopist toolbox, the nitrogen vacancy (NV) center in diamond has recently emerged as a promising platform for high-sensitivity nanoscale thermometry [1,2]. Of particular interest are applications in living cells because diamond nanocrystals are biocompatible and can be chemically functionalized to target specific organelles. Here we report progress on the ability to probe and compare temperature within and between living cells using nanodiamond-hosted NV thermometry. We focus our study on cancerous cells, where atypical metabolic pathways arguably lead to changes in the way a cell generates heat, and thus on its temperature profile. 1. V. Acosta et al., *Phys. Rev. Lett.* **104**, 070801 (2010). 2. G. Kucsko et al., *Nature* **500**, 54 (2013).

**11:39AM Y39.00003 Production and NMR signal optimization of hyperpolarized <sup>13</sup>C-labeled amino acids**, CHRISTOPHER PARISH, PETER NIEDBALSKI, SARAH FERGUSON, ANDHIKA KISWANDHI, LLOYD LUMATA, University of Texas at Dallas — Amino acids are targeted nutrients for consumption by cancers to sustain their rapid growth and proliferation. <sup>13</sup>C-enriched amino acids are important metabolic tracers for cancer diagnostics using nuclear magnetic resonance (NMR) spectroscopy. Despite this diagnostic potential, <sup>13</sup>C NMR of amino acids however is hampered by the inherently low NMR sensitivity of the <sup>13</sup>C nuclei. In this work, we have employed a physics technique known as dynamic nuclear polarization (DNP) to enhance the NMR signals of <sup>13</sup>C-enriched amino acids. DNP works by transferring the high polarization of electrons to the nuclear spins via microwave irradiation at low temperature and high magnetic field. Using a fast dissolution method in which the frozen polarized samples are dissolved rapidly with superheated water, injectable solutions of <sup>13</sup>C-amino acids with highly enhanced NMR signals (by at least 5,000-fold) were produced at room temperature. Factors that affect the NMR signal enhancement levels such as the choice of free radical polarizing agents and sample preparation will be discussed along with the thermal mixing physics model of DNP. The authors would like to acknowledge the support by US Dept of Defense award no. W81XWH-14-1-0048 and Robert A. Welch Foundation grant no. AT-1877.

**11:51AM Y39.00004 Real-time tracking of dissociation of hyperpolarized <sup>89</sup>Y-DTPA: a model for degradation of open-chain Gd<sup>3+</sup> MRI contrast agents<sup>1</sup>**, SARAH FERGUSON, PETER NIEDBALSKI, CHRISTOPHER PARISH, ANDHIKA KISWANDHI, University of Texas at Dallas, ZOLTAN KOVACS, University of Texas Southwestern Medical Center, LLOYD LUMATA, University of Texas at Dallas — Gadolinium (Gd) complexes are widely used relaxation-based clinical contrast agents in magnetic resonance imaging (MRI). Gd-based MRI contrast agents with open-chain ligand such as Gd-DTPA, commercially known as magnevist, are less stable compared to Gd complexes with macrocyclic ligands such as GdDOTA (Dotarem). The dissociation of Gd-DTPA into Gd ion and DTPA ligand under certain biological conditions such as high zinc levels can potentially cause kidney damage. Since Gd is paramagnetic, direct NMR detection of the Gd-DTPA dissociation is quite challenging due to ultra-short relaxation times. In this work, we have investigated Y-DTPA as a model for Gd-DTPA dissociation under high zinc content solutions. Using dissolution dynamic nuclear polarization (DNP), the <sup>89</sup>Y NMR signal is amplified by several thousand-fold. Due to the relatively long T<sub>1</sub> relaxation time of <sup>89</sup>Y which translates to hyperpolarization lifetime of several minutes, the dissociation of Y-DTPA can be tracked in real-time by hyperpolarized <sup>89</sup>Y NMR spectroscopy. Dissociation kinetic rates and implications on the degradation of open-chain Gd<sup>3+</sup> MRI contrast agents will be discussed.

<sup>1</sup>This work was supported by the U.S. Department of Defense award number W81XWH-14-1-0048 and by the Robert A. Welch Foundation research grant number AT-1877.

**12:03PM Y39.00005 Optimization of <sup>13</sup>C dynamic nuclear polarization: isotopic labeling of free radicals<sup>1</sup>**, PETER NIEDBALSKI, CHRISTOPHER PARISH, ANDHIKA KISWANDHI, LLOYD LUMATA, University of Texas at Dallas — Dynamic nuclear polarization (DNP) is a physics technique that amplifies the nuclear magnetic resonance (NMR) signals by transferring the high polarization of the electrons to the nuclear spins. Thus, the choice of free radical is crucial in DNP as it can directly affect the NMR signal enhancement levels, typically on the order of several thousand-fold in the liquid-state. In this study, we have investigated the efficiency of four variants of the well-known 4-oxo-TEMPO radical (normal 4-oxo-TEMPO plus its <sup>15</sup>N-enriched and/or perdeuterated variants) for use in DNP of an important metabolic tracer [1-<sup>13</sup>C]acetate. Though the variants have significant differences in electron paramagnetic resonance (EPR) spectra, we have found that changing the composition of the TEMPO radical through deuteration or <sup>15</sup>N doping yields no significant difference in <sup>13</sup>C DNP efficiency at 3.35 T and 1.2 K. On the other hand, deuteration of the solvent causes a significant increase of <sup>13</sup>C polarization that is consistent over all the 4-oxo-TEMPO variants. These findings are consistent with the thermal mixing model of DNP.

<sup>1</sup>This work is supported by US Dept of Defense award no. W81XWH-14-1-0048 and the Robert A. Welch Foundation grant no. AT-1877.

**12:15PM Y39.00006 ABSTRACT WITHDRAWN –**

**12:27PM Y39.00007 Simulated biophysical experimental techniques for chlorhexidine in dmPC/cholesterol systems**, BRAD VAN OOSTEN, THAD HARROUN, Brock University — We have investigated the use of molecular dynamic simulations and the MARTINI force field to simulate isothermal titration calorimetry and differential scanning calorimetry techniques. The goal of these simulations was to observe how well they can reproduce the concentration effects of the addition of the small molecule chlorhexidine (CHX) into a model DMPC membrane containing varying concentrations of cholesterol. We constructed a coarse grained model for CHX compatible with the MARTINI force field. We were able to mimic an isothermal titration calorimetry experiment by repeatedly adding CHX into a DMPC membrane. With the increased concentration, we observed a decreasing affinity between CHX and the membrane as well as a resulting increase in the reaction time before the system was equilibrated. We then performed a controlled cooling of the membrane with various CHX concentrations to mimic a differential scanning calorimetry experiment. A change in membrane structure accompanied by a spike in the specific heat was measured at specific temperature  $T_m$  signaling a phase transition. We then varied the concentration of CHX as well as the addition of varying concentrations of cholesterol to observe trends in the change to  $T_m$  due to the addition of CHX and cholesterol.

Department of Electrical Engineering

Department of Physics

Biophotonics Laboratory

**12:39PM Y39.00008 Detection of carotenoids present in blood o Raman spectroscopy**, MARYAM LIAQAT, Federal University of Pernambuco, Recife, Brazil, Faisalabad, Pakistan, MUHAMMAD SALEEM, National Institute of Lasers and Optronics (NILOP) Islamabad, SAHER JABEEN<sup>2</sup>, University of Agriculture, Faisalabad, Pakistan — Raman spectroscopy is simple stable po other biomolecules. Human blood possesses different kind of carotenoids that play a key role for protecting bacterial diseases. Carotenoids are antioxidative components which are capable to overcome the attack of di Carotenoids are not prepared by human body, therefore it is recommended to eat carotenoids enrich vegeta concentration of useful carotenoids component in non-vegetable consumed items. In present research work, blood components like plasma, serum, carotenoids present in blood of different animal species like goat, sheep, beta carotene is investigated. The Raman shift ranges from 600-1700  $\text{cm}^{-1}$  for samples. Different characte which are not characterized before in animal samples.

<sup>1</sup>Lecturer: department of clinical medicine and surgery

<sup>2</sup>Student of Philosophy of Statistics

Department of Electrical Engineering

**12:51PM Y39.00009 Direct simulation of amphiphilic nanoparticle mediated membrane inter-actions**, MUKARRAM TAHIR, ALFREDO ALEXANDER-KATZ, Massachusetts Inst of Tech-MIT — Membrane fusion is a critical step in the transport of biological cargo through membrane-bound compartments like vesicles. Membrane proteins that alleviate energy barriers for initial stalk formation and eventual rupture of the hemifusion intermediate during fusion generally assist this process. Gold nanoparticles functionalized with a combination of hydrophobic and hydrophilic alkanethiol ligands have recently been shown to induce membrane re-arrangements that are similar to those associated with these fusion proteins. In this work, we utilize molecular dynamics simulation to systematically design nanoparticles that exhibit targeted interactions with membranes. We introduce a method for rapidly parameterizing nanoparticle topology for the MARTINI biomolecular force field to permit long timescale simulation of their interactions with lipid bilayers. We leverage this model to investigate how ligand chemistry governs the nanoparticle's insertion efficacy and the perturbations it generates in the membrane environment. We further demonstrate through unbiased simulations that these nanoparticles can direct the fusion of lipid assemblies such as micelles and vesicles in a manner that mimics the function of biological fusion peptides and SNARE proteins.

**1:03PM Y39.00010 Exposure to TiO<sub>2</sub> nanoparticles increases Staphylococcus aureus infection of HeLa cells**, YAN XU, State Univ of NY- Stony Brook, MING-TZO WEI, Lehigh University, STEPHEN.G WALKER, HONG ZHAN WANG, CHRIS GONDON, PETER BRINK, State Univ of NY- Stony Brook, SHOSHANA GUTERMAN, Yeshiva University High School for Girls, EMMA ZAWACKI, University of California at Los Angeles, ELIANA APPLEBAUM, Stern College for Women, MIRIAM RAFAILOVICH, State Univ of NY- Stony Brook, H. DANIEL OUYANG, Lehigh University, TATSIANA MIRONAVA, State Univ of NY- Stony Brook — TiO<sub>2</sub> is one of the most common nanoparticles in industry from food additives to energy generation. Even though TiO<sub>2</sub> is also used as an anti-bacterial agent in combination with UV, we found that, in the absence of UV, exposure of HeLa cells to TiO<sub>2</sub> nanoparticles largely increased their risk of bacterial invasion. HeLa cells cultured with low dosage rutile and anatase TiO<sub>2</sub> nanoparticles (0.1 mg/ml) for 24 hrs prior to exposure to bacteria had 350% and 250% respectively more bacteria infected per cell. The increase was attributed to increased LDH leakage, and changes in the mechanical response of the cell membrane. On the other hand, macrophages exposed to TiO<sub>2</sub> particles ingested 40% fewer bacteria, further increasing the risk of infection. In combination, these two factors raise serious concerns regarding the impact of exposure to TiO<sub>2</sub> nanoparticles on the ability of organisms to resist bacterial infection.

**1:15PM Y39.00011 Effect of TiO<sub>2</sub> nanoparticles on adipose derived stromal cell differentiation, morphology, ECM deposition and its susceptibility to bacterial infections.**, TATSIANA MIRONAVA, YAN XU, MIRIAM RAFAILOVICH, Stony Brook University — The growing annual production of Titanium dioxide (TiO<sub>2</sub>) nanoparticles is proportional to an increase in the chances of occupational and consumer exposure. Considering, that these nanoparticles are currently being used in multiple personal care products many concerns have arisen about their health impact. Human skin is in constant contact with the external environment and is one of the most important routes of exposure to TiO<sub>2</sub>. In this study we have investigated the effect of two forms of TiO<sub>2</sub>, rutile and anatase, on human adipose derived stromal cells (ADSCs). Here, we focus on the effects of TiO<sub>2</sub> exposure on intracellular lipid accumulation and expression of adipogenic markers; on whether different forms of TiO<sub>2</sub> have similar effects on cell function; and whether nanoparticle localization inside cells correlates with loss of cell function. In addition presence of bacteria on the skin is taken into account in its complex interaction with ADSCs and TiO<sub>2</sub> nanoparticles. Altogether, the present study indicates that nanosized TiO<sub>2</sub> particles adversely effects the differentiation of ADSCs, have profound effects on cell function and increase the rate of bacterial infection.

**1:27PM Y39.00012 Effect of cell donor age on the cellular response to nanoparticle exposure.**, FAN YANG, MIRIAM RAFAILOVICH, TATSIANA MIRONAVA, Stony Brook University — As human age there are many significant changes that occur in the skin. Here we investigate how the age-dependent changes in dermal fibroblast mechanics affect cell response to the AuNPs nanoparticles. To analyze these processes we exposed cells from donors of different age groups to AuNPs of two different sizes. Our results indicate that there are significant changes in cell rigidity with age, which in turn lead to different penetration rates of AuNPs through cell membrane and overall nanoparticle toxicity. Cell proliferation results revealed that all cell groups exposed to the same concentration of AuNPs had a very similar decrease in cell proliferation and similar impact on cell morphology. However, recovery data demonstrated that the rate of recovery from the damage is much faster for neonatal cells as compared to 30- and 80-years old cell group. Therefore, we conclude that nanoparticle uptake depends on cell membrane mechanics that in turn is a function of cell donor age.

**1:39PM Y39.00013 Mechanics of Cellulose Synthase Complexes in Living Plant Cells<sup>1</sup>**, NINA ZEHFROOSH, Department of Physics, University of Massachusetts, Amherst, DERUI LIU, Biology Department, University of Massachusetts, Amherst, KIERAN P. RAMOS, Department of Physics, University of Massachusetts, Amherst, XIAOLI YANG, Biology Department, University of Massachusetts, Amherst, LORI S. GOLDNER, Department of Physics, University of Massachusetts, Amherst, TOBIAS I. BASKIN, Biology Department, University of Massachusetts, Amherst — The polymer cellulose is one of the major components of the world's biomass with unique and fascinating characteristics such as its high tensile strength, renewability, biodegradability, and biocompatibility. Because of these distinctive aspects, cellulose has been the subject of enormous scientific and industrial interest, yet there are still fundamental open questions about cellulose biosynthesis. Cellulose is synthesized by a complex of transmembrane proteins called "Cellulose Synthase A" (CESA) in the plasma membrane. Studying the dynamics and kinematics of the CESA complex will help reveal the mechanism of cellulose synthesis and permit the development and validation of models of CESA motility. To understand what drives these complexes through the cell membrane, we used total internal reflection fluorescence microscopy (TIRFM) and variable angle epi-fluorescence microscopy to track individual, fluorescently-labeled CESA complexes as they move in the hypocotyl and root of living plants. A mean square displacement analysis will be applied to distinguish ballistic, diffusional, and other forms of motion. We report on the results of these tracking experiments.

<sup>1</sup>This work was funded by NSF/PHY-1205989.

**1:51PM Y39.00014 Electronic measurements in an alternating magnetic field (AMF) for studying magnetic nanoparticle hyperthermia**, Z. BOEKLHEIDE, Z. A. HUSSEIN, S. HARTZELL, Lafayette College — Magnetic nanoparticle hyperthermia is a promising cancer treatment in which magnetic nanoparticles are injected into a tumor and then exposed to an alternating magnetic field (AMF). This process releases heat and damages tumor cells, but the exact mechanisms behind the effectiveness of this therapy are still unclear. Accurate sensors are required to monitor the temperature and, potentially, other parameters such as magnetic field or mechanical stress during clinical therapy or lab research. Often, optical rather than electronic temperature sensors are used to avoid eddy current self-heating in conducting parts in the AMF. However, eddy current heating is strongly dependent on the size and geometry of the conducting part, thus micro- and nano-scale electronics are a promising possibility for further exploration into magnetic nanoparticle hyperthermia. This presentation quantitatively discusses the eddy current self-heating of thin wires (thermocouples) and will also present a proof of concept thin film resistive thermometer and magnetic field sensor along with measurements of their eddy current self-heating. The results show that electronic measurements are feasible in an AMF with both thin wires and patterned thin film sensors under certain conditions.

**2:03PM Y39.00015 Non-invasive measurement of the blood pressure pulse using multiple PPGs<sup>1</sup>**, JOHN SEYMOUR, GARY PENNINGTON, Towson University — Heart disease, the leading cause of death in the US, may be spotted early on by looking at photoplethysmogram (PPG) data. This experiment explores a new method of continuously monitoring the blood pressure pulse with PPG data. In contrast to the traditional sphygmomanometer (cuff) method, which yields only the systolic and diastolic pressure during measurement, this method tracks the blood pressure pulse wave in a non-invasive continuous manner. This procedure allows for fast, inexpensive, and detailed analysis of the patient's blood pressure implementable on a large scale. We also explore the second derivative of the PPG data. In combination with the above method, the patient's heart risk can be effectively detected.

<sup>1</sup>We acknowledge Fisher Endowment Grant support from the Jess and Mildred Fisher College of Science and Mathematics, Towson University.

## Friday, March 18, 2016 11:15AM - 2:27PM –

**Session Y40 GSNP GSOFD DBIO: Robophysics: Physics Meets Robotics II** 343 - Daniel Goldman, Georgia Tech

**11:15AM Y40.00001 Managing and capturing the physics of robotic systems**, JUSTIN WERFEL, Harvard University — Algorithmic and other theoretical analyses of robotic systems often use a discretized or otherwise idealized framework, while the real world is continuous-valued and noisy. This disconnect can make theoretical work sometimes problematic to apply successfully to real-world systems. One approach to bridging the separation can be to design hardware to take advantage of simple physical effects mechanically, in order to guide elements into a desired set of discrete attracting states. As a result, the system behavior can effectively approximate a discretized formalism, so that proofs based on an idealization remain directly relevant, while control can be made simpler. It is important to note, conversely, that such an approach does not make a physical instantiation unnecessary nor a purely theoretical treatment sufficient. Experiments with hardware in practice always reveal physical effects not originally accounted for in simulation or analytic modeling, which lead to unanticipated results and require nontrivial modifications to control algorithms in order to achieve desired outcomes. I will discuss these points in the context of swarm robotic systems recently developed at the Self-Organizing Systems Research Group at Harvard.

**11:27AM Y40.00002 Robot flow, clogging and jamming in confined spaces**, DARIA MONAENKOVA, VADIM LINEVICH, MICHAEL A.D. GOODISMAN, DANIEL I. GOLDMAN, Georgia Institute of Technology — We hypothesized that when a collection of robots operate in confined space, maximization of individual effort could negatively affect the collective performance by impeding the mobility of the individuals. To test our hypothesis, we built and programmed groups of 1-4 autonomous robotic diggers to construct a tunnel in a model cohesive soil. The robots' mobility, defined in terms of the residence time (T) required for a robot to move one body-length within the tunnel, was compared between groups of maximally active robots (mode 1), groups with different levels of activity between individuals (mode 2), and maximally active robots with a "giving up" behavior (mode 3), in which the robot ceased the attempt to excavate in a crowded tunnel. In small groups of two robots, T was ~3 sec and did not depend on the mode of operation. However, an increase in the number of robots caused an increase in T which depended upon mode. The residence time in groups of four robots in mode 1 (~9 sec) significantly exceeded the residence time in mode 2 and 3 (~4 sec), indicating that crowding was causing slower movement of individuals, particularly under maximum effort (mode 1). We will use our robophysical studies to discover principles of collective construction in subterranean social animals.

**11:39AM Y40.00003 Legged-locomotion on inclined granular media**, JENNIFER RIESER, FEIFEI QIAN, DANIEL GOLDMAN, Georgia Institute of Technology — Animals traverse a wide variety of complex environments, including situations in which the ground beneath them can yield (e.g. dry granular media in desert dunes). Locomotion strategies that are effective on level granular media can fail when traversing a granular slope. Taking inspiration from successful legged-locomotors in sandy, uneven settings, we explore the ability of a small (15 cm long, 100 g), six-c-shaped legged robot to run uphill in a bed of 1-mm-diameter poppy seeds, using an alternating tripod gait. Our fully automated experiments reveal that locomotor performance can depend sensitively on both environmental parameters such as the inclination angle and volume fraction of the substrate, and robot morphology and control parameters like leg shape, step frequency, and the friction between the feet of the robot and the substrate. We assess performance by measuring the average speed of the robot, and we find that the robot tends to perform better at higher step frequency and lower inclination angles, and that average speed decreases more rapidly with increasing angle for higher step frequency.

**11:51AM Y40.00004 Robotic and mathematical modeling reveal general principles of appendage control and coordination in terrestrial locomotion<sup>1</sup>** , BENJAMIN MCINROE, UC Berkeley, HENRY ASTLEY, Georgia Tech, CHAOHUI GONG, CMU Robotics Institute, SANDY KAWANO, NIMBioS, PERRIN SCHIEBEL, Georgia Tech, HOWIE CHOSET, CMU Robotics Institute, DANIEL I GOLDMAN, Georgia Tech — The transition from aquatic to terrestrial life presented new challenges to early walkers, necessitating robust locomotion on complex, flowable substrates (e.g. sand, mud). Locomotion on such substrates is sensitive to limb morphology and kinematics. Although early walker morphologies are known, principles of appendage control remain elusive. To reveal limb control strategies that facilitated the invasion of land, we study both robotic and mathematical models. Robot experiments show that an active tail is critical for robust locomotion on granular media, enabling locomotion even with poor foot placement and limited ability to lift the body. Using a granular resistive force theory model, we construct connection vector fields that reveal how appendage coordination and terrain inclination impact locomotor performance. This model replicates experimental results, showing that moving limbs/tail in phase is most effective (suggesting a locomotor template). Varying limb trajectories and contacts, we find gaits for which tail use can be neutral or harmful, suggesting limb-tail coordination to be a nontrivial aspect of locomotion. Our findings show that robot experiments coupled with geometric mechanics provide a general framework to reveal principles of robust terrestrial locomotion.

<sup>1</sup>This work was supported by NSF PoLS

**12:03PM Y40.00005 Compliant Synergies in Locomotion** , MATTHEW TRAVERS, HOWIE CHOSET, Carnegie Mellon University, GOLDMAN @ GEORGIA TECH. PHYSICS DEPARTMENT COLLABORATION — Biological systems appear to have natural mechanisms that allow them to readily compensate for unexpected environmental variations when compared to their mechanical (i.e., robotic) counterparts. We hypothesize that the basis for this discrepancy is almost innate: what biology appears to be born with, built-in mechanisms for coordinating their many degrees of freedom, we struggle to “program.” We therefore look toward biology for inspiration. In particular, we are interested in kinematic synergies, low-dimensional representations that explicitly encode the underlying structure of how systems coordinate their internal degrees of freedom to achieve high-level tasks. In this work, we derive parametric representations of kinematic synergies and present a new compliant locomotion control framework that enables the parameters to be directly controlled in response to external disturbances. We present results of this framework implemented on two separate platforms, a snake-like and hexapod robot. Our results show that, using synergies, the locomotion control of these very different systems can be reduced to simple, extremely capable, and common forms, thus offering new insights into both robotic as well as biological locomotion in complex terrains.

**12:15PM Y40.00006 Instability and maneuverability of a multi-legged robot<sup>1</sup>** , SHINYA AOI, Kyoto University — Our previous study showed that a centipede like multi-legged robot composed of many modules, each of which has one pair of legs, produces body undulations through a supercritical Hopf bifurcation of walking in a straight line with parallel bodies when the gait speed increases over a critical value or when the body segment joint stiffness decreases below a critical value (Aoi et al., PRE 2013, featured by Nat Phys 2013). So far, it is unclear if centipedes actively produce or resist body undulations during their locomotion and the previous study discussed the underlying mechanism responsible for the body undulations in centipede locomotion based on the robot experimental results and dynamic analysis using a simplified physical model. Furthermore, centipedes produce agile locomotion despite many legs being in contact with the ground during their locomotion, which may impede their agile motions. The present study investigated the relationship between the instability of walking in a straight line and maneuverability of the robot using a quick turn task and some evaluation criteria for maneuverability.

<sup>1</sup>KAKENHI 26630097

**12:27PM Y40.00007 Are snakes particles or waves? Scattering of a limbless locomotor through a single slit** , FEIFEI QIAN, Georgia Institute of Technology, JIN DAI, CHAOHUI GONG, HOWIE CHOSET, Carnegie Mellon University, DANIEL GOLDMAN, Georgia Institute of Technology — Droplets on vertically vibrated fluid surfaces can walk and diffract through a single slit by a pilot wave hydrodynamic interaction [Couder, 2006; Bush, 2015]. Inspired by the correspondence between emergent macroscale dynamics and phenomena in quantum systems, we tested if robotic snakes, which resemble wave packets, behave emergently like particles or waves when interacting with an obstacle. In lab experiments and numerical simulations we measured how a multi-module snake-like robot swam through a single slit. We controlled the snake undulation gait as a fixed serpenoid traveling wave pattern with varying amplitude and initial phase, and we examined the snake trajectory as it swam through a slit with width  $d$ . Robot trajectories were straight before interaction with the slit, then exited at different scattering angle  $\theta$  after the interaction due to a complex interaction of the body wave with the slit. For fixed amplitude and large  $d$ , the snake passed through the slit with minimal interaction and  $\theta$  was  $\approx 0$ . For sufficiently small  $d$ ,  $\theta$  was finite and bimodally distributed, depending on the initial phase. For intermediate  $d$ ,  $\theta$  was sensitive to initial phase, and the width of the distribution of  $\theta$  increased with decreasing  $d$ .

**12:39PM Y40.00008 Multi-terrain locomotor interactions in flying snakes<sup>1</sup>** , ISAAC YEATON, GRANT BAUMGARDNER, SHANE ROSS, JOHN SOCHA, Virginia Tech — Arboreal snakes of the genus *Chrysopelea* are the only known snakes to glide. To execute aerial locomotion, a snake uses one of several stereotyped jumps from a tree into the air, while simultaneously flattening its body into an aerodynamically favorable shape. Large amplitude traveling waves are propagated posteriorly during the stable glide, while landing involves body wrapping, passive body compression, and energy absorption through compliance in the landing substrate to dissipate the accumulated kinetic energy from the glide. In all of these locomotor events, from interacting with cylindrical branches, falling through the air, grasping compliant tree branches and leaves, to landing on solid ground, snakes appropriate the same body morphology and perhaps the same basic neural mechanisms. Here we discuss our use of computational models and animal experiments to understand how flying snakes interact with and locomote on and through multiple media, potentially providing principles for legless locomotor designs.

<sup>1</sup>Supported by NSF 1351322

**12:51PM Y40.00009 Aerodynamic control with passively pitching wings** , NICK GRAVISH, ROBERT WOOD, Harvard University — Flapping wings may pitch passively under aerodynamic and inertial loads. Such passive pitching is observed in flapping wing insect and robot flight. The effect of passive wing pitch on the control dynamics of flapping wing flight are unexplored. Here we demonstrate in simulation and experiment the critical role wing pitching plays in yaw control of a flapping wing robot. We study yaw torque generation by a flapping wing allowed to passively rotate in the pitch axis through a rotational spring. Yaw torque is generated through alternating fast and slow upstroke and downstroke. Yaw torque sensitively depends on both the rotational spring force law and spring stiffness, and at a critical spring stiffness a bifurcation in the yaw torque control relationship occurs. Simulation and experiment reveal the dynamics of this bifurcation and demonstrate that anomalous yaw torque from passively pitching wings is the result of aerodynamic and inertial coupling between the pitching and stroke-plane dynamics.

**1:03PM Y40.00010 Crucial advantages of tail use in the evolution of vertebrate terrestrial locomotion.** , HENRY ASTLEY, Georgia Inst of Tech, BENJAMIN MCINROE, U C Berkeley, SANDY KAWANO, National Institute for Mathematical and Biological Synthesis, RICK BLOB, Clemson University, DANIEL GOLDMAN, Georgia Inst of Tech — In the invasion of terrestrial environment, the first tetrapods faced the challenge of locomotion on flowable substrates (e.g. sand and mud), sometimes oriented at inclines. Although the morphology of many early tetrapods is known, robotic studies have revealed that effective locomotion on these substrates also depends strongly upon kinematics; slight differences in movements of the same appendage can lead to success or failure. Using a model organism (the mudskipper) and a robotic physical model, we demonstrate how muscular tails provided critical locomotor advantages on granular substrates that the first invaders of land likely encountered. Mudskippers use their tails for additional propulsion with increasing frequency as the slope of the granular material increases, and the decline in locomotor performance with slope is shallower when the tail is used. Experiments with a robotic model of the mudskipper showed that, while the tail did not always provide a benefit to locomotion, use of the tail made the robot's performance more robust, achieving effective locomotion on a wider range of slopes, limb postures and foot placements. These results suggest that, rather than simply being an inert appendage, the tails of early tetrapods were vital to their first forays into terrestrial habitats.

**1:15PM Y40.00011 Mutually opposing forces during locomotion can eliminate the tradeoff between maneuverability and stability** , NOAH COWAN, SHAHIN SEFATI, Johns Hopkins University, IZAAK NEVELN, Northwestern University, EATAI ROTH, TERENCE MITCHELL, Johns Hopkins University, JAMES SNYDER, MALCOLM MACIVER, Northwestern University, ERIC FORTUNE, New Jersey Institute of Technology — A surprising feature of animal locomotion is that organisms typically produce substantial forces in directions other than what is necessary to move the animal through its environment, such as perpendicular to, or counter to, the direction of travel. The effect of these forces has been difficult to observe because they are often mutually opposing and therefore cancel out. Using a combination of robotic physical modeling, computational modeling, and biological experiments, we discovered that these forces serve an important role: to simplify and enhance the control of locomotion. Specifically, we examined a well-suited model system, the glass knifefish *Eigenmannia virescens*, which produces mutually opposing forces during a hovering behavior. By systematically varying the locomotor parameters of our biomimetic robot, and measuring the resulting forces and kinematics, we demonstrated that the production and differential control of mutually opposing forces is a strategy that generates passive stabilization while simultaneously enhancing maneuverability. Mutually opposing forces during locomotion are widespread across animal taxa, and these results indicate that such forces can eliminate the tradeoff between stability and maneuverability, thereby simplifying robotic and neural control.

**1:27PM Y40.00012 A robotic platform for studying sea lion thrust production** , MEGAN LEFTWICH, RAHI PATEL, ADITYA KULKARNI, CHEN FRIEDMAN, The George Washington University — California Sea Lions are agile swimmers and, uniquely, use their foreflippers (rather than hind flipper undulation) to generate thrust. Recently, a sea lion flipper from a deceased subject was externally scanned in high detail for fluid dynamics research. The flipper's geometry is used in this work to build an accurate scaled down flipper model (approximately 68% of the full size span). The flipper model is placed in a water flume to obtain lift and drag force measurements. The unique trailing edge features are then examined for their effect on the measured forces by comparing to similar flipper models with a smooth trailing edge, sinusoidal trailing edge, and a saw-tooth trailing edge. Additionally, a robotic flipper is being designed and built, replicating the sea lion foreflipper anatomical structure. The robot is actuated by a set of servo motors and replicates the sea lion flipper clap motion based on previously extracted kinematics. The flipper tip speed is designed to match typical full scale Reynolds numbers for an acceleration from rest maneuver. The model is tested in the water flume as well to obtain the forces and flow structures during the thrust production phase of the flipper motion.

**1:39PM Y40.00013 Controlled locomotion of robots driven by a vibrating surface<sup>1</sup>** , PAUL UMBANHOWAR, KEVIN M. LYNCH, Northwestern University — Robots typically derive their powers of movement from onboard actuators and power sources, but other scenarios are possible where the external environment provides part or all of the necessary forcing and control. I will discuss details of a system where the robots are just planar solid objects and the requisite driving forces originate from frictional sliding-interactions with a periodically oscillated and nominally horizontal surface. For the robots to move, the temporal symmetry of the frictional forces must be broken, which is achieved here by modulating the normal force using vertical acceleration of the surface. Independent of the initial conditions and vibration waveform, a sliding locomotor reaches a unique velocity limit cycle at a given position. Its resulting motion can be described in terms of velocity fields which specify the robots cycle-averaged velocity as a function of position. Velocity fields with non-zero spatial divergence can be generated by combining translational and rotational surface motions; this allows the simultaneous and open-loop collection, dispersal, and transport of multiple robots. Fields and field sequences can simultaneously move multiple robots between arbitrary positions and, potentially, along arbitrary trajectories.

<sup>1</sup>Supported by NSF CMMI 0700537

**1:51PM Y40.00014 Dynamical states in the sensorimotor loop of a rolling robot** , BULCSÚ SÁNDOR, TIM JAHN, LAURA MARTIN, RODRIGO ECHEVESTE, CLAUDIUS GROS, Institute for Theoretical Physics, Goethe University Frankfurt — We investigate the closed sensorimotor loop of a simple rolling robot as a dynamical system. Using the LpzRobots simulation package <sup>1</sup>, we construct robots with cylindrical body, controlled by a single proprioceptive neuron with a time dependent threshold. Despite its simplicity, we obtain a rich set of rolling modes, as a result of the self-organizing processes arising through the feedback within the sensorimotor loop. These rolling modes are robust against environmental noise, since they correspond to stable limit cycle attractors. However, for certain parameters they also allow for explorative behavior via internal noise induced switching. Furthermore, we also find a region of parameters in which the motion is fully embodied, where, in engineering terms, the engine powering the motion of the robot is turned on dynamically through the feedback of its very motion <sup>2</sup>.

<sup>1</sup>R. Der & G. Martius, **The Playful Machine: Theoretical Foundation and Practical Realization of Self-Organizing Robots**, Springer Science & Business Media, Vol. 15, 2012

<sup>2</sup>B. Sándor, T. Jahn, L. Martin & C. Gros, **The sensorimotor loop as a dynamical system: How regular motion primitives may emerge from self-organized limit cycles**, to be published, 2015

**2:03PM Y40.00015 Vibration Propagation in Spider Webs<sup>1</sup>** , ROSS HATTON, ANDREW OTTO, Oregon State Univ, DAMIAN ELIAS, Univ. California, Berkeley — Due to their poor eyesight, spiders rely on web vibrations for situational awareness. Web-borne vibrations are used to determine the location of prey, predators, and potential mates. The influence of web geometry and composition on web vibrations is important for understanding spiders behavior and ecology. Past studies on web vibrations have experimentally measured the frequency response of web geometries by removing threads from existing webs. The full influence of web structure and tension distribution on vibration transmission; however, has not been addressed in prior work. We have constructed physical artificial webs and computer models to better understand the effect of web structure on vibration transmission. These models provide insight into the propagation of vibrations through the webs, the frequency response of the bare web, and the influence of the spider's mass and stiffness on the vibration transmission patterns.

<sup>1</sup>Funded by NSF-1504428.

**2:15PM Y40.00016 Proprioceptive Actuation Design for Dynamic Legged locomotion<sup>1</sup>**, SANGBAE KIM, PATRICK WENSING, MIT, BIOMIMETIC ROBOTICS LAB TEAM — Designing an actuator system for highly-dynamic legged locomotion exhibited by animals has been one of the grand challenges in robotics research. Conventional actuators designed for manufacturing applications have difficulty satisfying challenging requirements for high-speed locomotion, such as the need for high torque density and the ability to manage dynamic physical interactions. It is critical to introduce a new actuator design paradigm and provide guidelines for its incorporation in future mobile robots for research and industry. To this end, we suggest a paradigm called proprioceptive actuation, which enables highly- dynamic operation in legged machines. Proprioceptive actuation uses collocated force control at the joints to effectively control contact interactions at the feet under dynamic conditions. In the realm of legged machines, this paradigm provides a unique combination of high torque density, high-bandwidth force control, and the ability to mitigate impacts through backdrivability. Results show that the proposed design provides an impact mitigation factor that is comparable to other quadruped designs with series springs to handle impact. The paradigm is shown to enable the MIT Cheetah to manage the application of contact forces during dynamic bounding, with results given down to contact times of 85ms and peak forces over 450N. As a result, the MIT Cheetah achieves high-speed 3D running up to 13mph and jumping over an 18-inch high obstacle.

<sup>1</sup>The project is sponsored by DARPA M3 program

## **Friday, March 18, 2016 11:15AM - 1:15PM – Session Y41 DBIO: Multi-cellular Systems 344 - Simon Sponberg, Georgia Institute of Technology**

**11:15AM Y41.00001 Tension, cell shape and triple-junction angle anisotropy in the Drosophila germband<sup>1</sup>**, MONICA LACY, M. SHANE HUTSON, CHRISTIAN MEYER, XENA MCDONALD, Vanderbilt University — In the field of tissue mechanics, the embryonic development of Drosophila melanogaster offers many opportunities for study. One of Drosophila's most crucial morphogenetic stages is the retraction of an epithelial tissue called the germband. During retraction, the segments of the retracting germband, as well as the individual germband cells, elongate in response to forces from a connected tissue, the amnioserosa. Modeling of this elongation, based on tissue responses to laser wounding, has plotted the internal germband tension against the external amnioserosa stress, creating a phase space to determine points and regions corresponding to stable elongation. Although the resulting fits indicate a necessary opposition of internal and external forces, they are inconclusive regarding the exact balance. We will present results testing the model predictions by measuring cell shapes and the correlations between cell-edge directions and triple-junction angles. These measures resolve the ambiguity in pinpointing the internal-external force balance for each germband segment.

<sup>1</sup>Research was supported by NIH Grant Numbers 1R01GM099107 and 1R21AR068933.

**11:27AM Y41.00002 Small angle x-ray diffraction through living muscle links the lattice structure to macroscopic material properties**, TRAVIS TUNE, Georgia Inst of Tech, TOM IRVING, Illinois Institute of Technology, SIMON SPONBERG, Georgia Inst of Tech — Muscle is a unique hierarchical material composed of millions of molecular motors arranged on filaments in a regular lattice structure. The macroscopic, material behavior of muscle can be characterized by its workloop, a periodically activated force-length curve. Muscle is capable of operating as a spring, motor, brake, or strut, defined by its workloop. We are interested in the multiscale physics of muscle that drive its energetic versatility – the ability of muscle to alter its function. Here we introduce a system of two muscles from the cockroach whose workloops are not explained by our current understanding of the determinants of workloop function (the classic force-length, force-velocity, and twitch response). Differences in material behavior may arise from structural differences in the muscles active lattice. Using the BIOCat beam at the Advanced Photon Source at Argonne NL, we tested for differences in the two muscles lattice structure. Small-angle x-ray scattering (SAXS) revealed a difference of 4-8

**11:39AM Y41.00003 Curvature dependent modulation of fish fin stiffness**, KHOI NGUYEN, Okinawa Institute of Science and Technology, NING YU, Brown University, MAHESH BANDI, Okinawa Institute of Science and Technology, MADHUSUDHAN VENKADESAN, Yale University, SHREYAS MANDRE, Brown University — Propulsion and maneuvering ability of fishes depends on the stiffness of their fins. However, increasing stiffness by simply adding material to thicken the fin would incur a substantial energetic cost associated with flapping the fin. We propose that fishes increase stiffness of the fin not by building thicker fins, but by geometrically coupling out-of-plane bending of the fin's rays with in-plane stretching of a stiff membrane that connects the rays. We present a model of fin elasticity for ray-finned fish, where we decompose the fin into a series of elastic beams (rays) with springy interconnections (membrane). In one limit, where the membranes are infinitely extensible, the fin's stiffness is no more than the sum of the stiffness of individual rays. At the other limit of an inextensible membrane, fin stiffness reaches an asymptotic maximum. The asymptote value increases monotonically with curvature. We propose that musculature at the base of the fin controls fin curvature, and thereby modulates stiffness.

**11:51AM Y41.00004 Heterogeneous Force Chains in Cellularized Biopolymer Network**, LONG LIANG, Department of Physics, Arizona State University, CHRISTOPHER ALLEN RUCKSACK JONES, BO SUN, Department of Physics, Oregon State University, YANG JIAO, Materials Science and Engineering, Arizona State University, Tempe, AZ — Biopolymer Networks play an important role in coordinating and regulating collective cellular dynamics via a number of signaling pathways. Here, we investigate the mechanical response of a model biopolymer network due to the active contraction of embedded cells. Specifically, a graph (bond-node) model derived from confocal microscopy data is used to represent the network microstructure, and cell contraction is modeled by applying correlated displacements at specific nodes, representing the focal adhesion sites. A force-based stochastic relaxation method is employed to obtain force-balanced network under cell contraction. We find that the majority of the forces are carried by a small number of heterogeneous force chains emerged from the contracting cells. The force chains consist of fiber segments that either possess a high degree of alignment before cell contraction or are aligned due to the reorientation induced by cell contraction. Large fluctuations of the forces along different force chains are observed. Importantly, the decay of the forces along the force chains is significantly slower than the decay of radially averaged forces in the system, suggesting that the fibrous nature of biopolymer network structure could support long-range mechanical signaling between cells.

**12:03PM Y41.00005 Three-Dimensional Cell Behavior in Microgels<sup>1</sup>**, TAPOMOY BHATTACHARJEE, GLYN PALMER, STEVEN GHIVIZZANI, BENJAMIN KESELOWSKY, W GREGORY SAWYER, THOMAS ANGELINI, University of Florida — The number of dimensions in which particles can freely move strongly influences the collective behavior that emerges from their individual fluctuations. Thus, in 2D systems of cells in petri-dishes, our growing understanding of collective migration may be insufficient to explain cell behavior in 3D tissues. To study cell behavior in 3D, polymer scaffolds are used. Contemporary designs of 3D cell growth scaffolds enable cell migration and proliferative expansion by incorporating of degradable motifs. Matrix degradation creates space for cells to move and proliferate. However, different cell types and experimental conditions require the design of different scaffolds to optimize degradation with specific cell behaviors. By contrast, liquid like solids made from packed microgels can yield under cell generated stresses, allowing for cell motion without the need for scaffold degradation. Moreover, the use of microgels as 3D culture media allows arranging cells in arbitrary structures, harvesting cells, and delivering drugs and nutrients. Preliminary data describing cell behavior in 3D microgel culture will be presented.

<sup>1</sup>: This material is based on work supported by the National Science Foundation under grant no. DMR-1352043.

**12:15PM Y41.00006 Frequency-dependent micromechanics of cellularized biopolymer networks**, CHRIS JONES, JIHAN KIM, DAVID MCINTYRE, BO SUN, Oregon State University — Mechanical interactions between cells and the extracellular matrix (ECM) influence many cellular behaviors such as growth, differentiation, and migration. These are dynamic processes in which the cells actively remodel the ECM. Reconstituted collagen gel is a common model ECM for studying cell-ECM interactions *in vitro* because collagen is the most abundant component of mammalian ECM and gives the ECM its material stiffness. We embed micron-sized particles in collagen and use holographic optical tweezers to apply forces to the particles in multiple directions and over a range of frequencies up to 10 Hz. We calculate the local compliance and show that it is dependent on both the direction and frequency of the applied force. Performing the same measurement on many particles allows us to characterize the spatial inhomogeneity of the mechanical properties and shows that the compliance decreases at higher frequencies. Performing these measurements on cell-populated collagen gels shows that cellular remodeling of the ECM changes the mechanical properties of the collagen and we investigate whether this change is dependent on the local strain and distance from nearby cells.

**12:27PM Y41.00007 Asymmetries arising from the space-filling nature of vascular networks**, DAVID HUNT, VAN SAVAGE, University of California - Los Angeles — Cardiovascular networks span the body by branching across many generations of vessels. The structural features of the network that accomplish this density and ubiquity of capillaries are often called space-filling. Some strategies do not lead to biologically adaptive structures, requiring too much construction material or space, delivering resources too slowly, or using too much power to move blood through the system. We empirically measure the structure of real networks to compare with predictions of model networks that are space-filling and constrained by a few guiding biological principles. We devise a numerical method that enables the investigation of space-filling strategies and determination of which biological principles influence network structure. Optimization for only a single principle creates unrealistic networks that represent an extreme limit of the possible structures that could be observed in nature. We first study these extreme limits for two competing principles, minimal total material and minimal path lengths. We combine these two principles and enforce various thresholds for balance in the network hierarchy, which provides a novel approach that highlights the trade-offs faced by biological networks and yields predictions that better match empirical data.

**12:39PM Y41.00008 Spatio-temporal Model of Xenobiotic Distribution and Metabolism in an in Silico Mouse Liver Lobule<sup>1</sup>**, XIAO FU, JAMES SLUKA, SHERRY CLENDENON, JAMES GLAZIER, Indiana Univ - Bloomington, JENNIFER RYAN, KENNETH DUNN, Indiana Univ - Indianapolis, ZEMIN WANG, JAMES KLAUNIG, Indiana Univ - Bloomington — Our study aims to construct a structurally plausible in silico model of a mouse liver lobule to simulate the transport of xenobiotics and the production of their metabolites. We use a physiologically-based model to calculate blood-flow rates in a network of mouse liver sinusoids and simulate transport, uptake and biotransformation of xenobiotics within the in silico lobule. Using our base model, we then explore the effects of variations of compound-specific (diffusion, transport and metabolism) and compound-independent (temporal alteration of blood flow pattern) parameters, and examine their influence on the distribution of xenobiotics and metabolites. Our simulations show that the transport mechanism (diffusive and transporter-mediated) of xenobiotics and blood flow both impact the regional distribution of xenobiotics in a mouse hepatic lobule. Furthermore, differential expression of metabolic enzymes along each sinusoids portal to central axis, together with differential cellular availability of xenobiotics, induce non-uniform production of metabolites. Thus, the heterogeneity of the biochemical and biophysical properties of xenobiotics, along with the complexity of blood flow, result in different exposures to xenobiotics for hepatocytes at different lobular locations.

<sup>1</sup>We acknowledge support from National Institute of Health GM 077138 and GM 111243

**12:51PM Y41.00009 Modeling oxygen transport in the placenta**, FILOCHE, Physique de la Matière Condensée, Université de Lorraine, S.M. 207, Boulevard S. P. 23, 54506 Vandœuvre-lès-Nancy Cedex, France — Efficient functioning of the placenta is essential for the health of the fetus. The placenta is a complex organ, the structure of which is based on its histological cross-section. The efficiency of oxygen transport from the mother to the fetus is determined by the estimate oxygen uptake of a placental unit. We have developed a model to estimate the incoming oxygen flow and the absorbing villous surface area. The villi density and the effective villi radius - are determined by the oxygen uptake. The oxygen uptake is also identified: maximal oxygen uptake is 22 healthy placental cross-sections demonstrate that the oxygen transport efficiency is rather low (around 30-40%). In this paper, we present a preliminary assessment in the human placenta.

Department of Chemistry and Biochemistry, UCLA, Los Angeles, CA 90095, USA

**1:03PM Y41.00010 ABSTRACT WITHDRAWN —**

**Friday, March 18, 2016 11:15AM - 1:15PM —**

**Session Y42 DPOLY: Renewable and Sustainable Polymers** 345 - Megan Robertson, University of Houston

**11:15AM Y42.00001 Sustainable epoxy and oxetane thermosets from photo-initiated cationic polymerization.**, CHANG RYU, Rensselaer Polytechnic Institute — A group of sustainable materials are proposed and produced from multifunctional epoxides and oxetanes obtained from renewable sources. Monomers are photopolymerized using diaryliodonium salts designed and synthesized by our group as initiator. A detailed investigation of the network formation of epoxidized linseed oil revealed that crosslinks is markedly dependent to the thickness and viscosity of substrate. Copolymerization studies of difunctional oxetane showed that limonene dioxide was effective in increasing the reaction rates and shorten the inherent induction period, also known as kick-starting effect. Such oxetane thermoset can achieve desirable curing rates and Tg compared to petroleum based epoxy used in applications such as large scale surface coatings.

**11:51AM Y42.00002 Structure and Dynamics of Cellulose Molecular Solutions**, HOWARD WANG, XIN ZHANG, University of Maryland, College Park, MADHUSUDAN TYAGI, YIMIN MAO, NIST Center for Neutron Research, ROBERT BRIBER, University of Maryland, College Park — Molecular dissolution of microcrystalline cellulose has been achieved through mixing with ionic liquid 1-Ethyl-3-methylimidazolium acetate (EMIMAc), and organic solvent dimethylformamide (DMF). The mechanism of cellulose dissolution in tertiary mixtures has been investigated by combining quasielastic and small angle neutron scattering (QENS and SANS). As SANS data show that cellulose chains take Gaussian-like conformations in homogenous solutions, which exhibit characteristics of having an upper critical solution temperature, the dynamic signals predominantly from EMIMAc molecules indicate strong association with cellulose in the dissolution state. The mean square displacement quantities support the observation of the stoichiometric 3:1 EMIMAc to cellulose unit molar ratio, which is a necessary criterion for the molecular dissolution of cellulose. Analyses of dynamics structure factors reveal the temperature dependence of a slow and a fast process for EMIMAc bound to cellulose and in DMF, respectively, as well as a very fast process due possibly to the rotational motion of methyl groups, which persisted to near the absolute zero.

**12:03PM Y42.00003 Thermodynamics of coil-hyperbranched poly(styrene-*b*-acrylated epoxidized soybean oil) block copolymers.** , FANG-YI LIN, AUSTIN HOHMANN, NACÚ HERNÁNDEZ, ERIC COCHRAN, Iowa State University — Here we present the phase behavior of a new type of coil-hyperbranched diblock copolymer: poly(styrene-*b*-acrylated epoxidized soybean oil), or PS-PAESO. PS-PAESO is an example of a biorenewable thermoplastic elastomer (bio-TPE). To date, we have shown that bio-TPEs can be economical commercial substitutes for their petrochemically derived analogues—such as poly(styrene-*b*-butadiene-*b*-styrene) (SBS)—in a range of applications including pressure sensitive adhesives and bitumen modification. From a polymer physics perspective, PS-PAESO is an interesting material in that it couples a linear coil-like block with a highly branched block. Thus in contrast to the past five decades of studies on linear AB diblock copolymers, coil-hyperbranched block copolymers are relatively unknown to the community and can be expected to deviate substantially from the standard “universal” phase behavior in the AB systems. To explore these new materials, we have constructed a library of PS-PAESO materials spanning a range of molecular weight and composition values. The phase transition behavior and the morphology information will be interpreted by isochronal temperature scanning in dynamic shear rheology, small angle X-ray scattering and the corresponding transmission electron microscopy.

**12:15PM Y42.00004 Mechanochemical modification of lignin and application of the modified lignin for thermoplastics and thermosets** , XIAOJIE GUO, JINWEN ZHANG, JUNNA XIN, Washington State University — In this work, mechanochemical modification of lignin and use of the modified lignin in thermoplastics and thermosets were studied. Oleated lignin was successfully prepared by transesterification between lignin and methyl, and the oleation reaction was performed in a solvent-free and room temperature ball milling process with a relatively short time. PLA/lignin blends were prepared through melt extrusion. Compared with the PLA/lignin blends, the PLA/oleated lignin blends exhibited finer dispersion of lignin in the blends, increased glass transition temperature and higher tensile properties, suggesting improved compatibility between lignin and PLA. Carboxylic and anhydride groups were also introduced into the structure of lignin via mechanochemical modification, and the resulting lignin derivatives were used as curing agents for epoxies. The dynamic mechanical properties and thermal stability of the cured epoxy resins were studied using dynamic mechanical analysis (DMA) and thermogravimetric analysis (TGA).

**12:27PM Y42.00005 Alignment of Fatty Acid-Derived Triblock Copolymers under Large Amplitude Oscillatory Shear** , WENYUE DING, SHU WANG, University of Houston, SAMEER KESAVA, ENRIQUE GOMEZ, The Pennsylvania State University, MEGAN ROBERTSON, University of Houston — Linear ABA triblock copolymers find widespread utilization as thermoplastic elastomers (TPEs): materials which exhibit elastomeric behavior at room temperature and can be readily processed at elevated temperatures. Traditional TPEs are derived from fossil fuels; however, the finite availability of petroleum and the environmental impact of petroleum processing has led to an increased interest in developing alternative sources for polymers. Vegetable oils and their fatty acids are promising replacements for petroleum sources due to their abundance, low cost, lack of toxicity, biodegradability and ease of functionalization that provides convenient routes to polymerization. In this study, triblock copolymer TPEs were synthesized containing lauryl and stearyl acrylate, derived from fatty acids found in vegetable oils. Small-angle X-ray scattering experiments revealed highly aligned triblock copolymer morphologies after the application of large amplitude oscillatory shear. The temperature and frequency dependence of the degree of alignment was investigated. In contrast to prior studies on shear-aligned morphologies in bulk and thin film block copolymers, hexagonal close packed and face centered cubic spherical structures were observed.

**12:39PM Y42.00006 PLA branching with anhydrides and tri-functional aziridine<sup>1</sup>** , LIANGLIANG GU, YUEWEN XU, RAJASEKHAR NAREDLA, THOMAS HOYE, CHRISTOPHER MACOSKO, Univ of Minn - Minneapolis — Branched PLA was prepared by melt blending with tri-functional aziridine (T-Az) and pyromellitic dianhydride (PMDA). <sup>1</sup>HNMR, gel permeation chromatography (GPC) and rheology were used to characterize the topological structures of branched PLA. Fast reaction between PLA carboxyl end group and T-Az resulted in 3-arm stars and increased the molecular weight. However, the 3-arm stars did not show strain hardening behavior under extensional flow. After modifying PLA hydroxyl end group with PMDA, PLA can react with T-Az on both chain ends and form long chain branched structure, which showed strain hardening in extension. It was found that that only 10% of the PLA hydroxyl end groups reacted with PMDA.

<sup>1</sup>This work is supported by Center for Sustainable Polymers.

**12:51PM Y42.00007 Wear Characteristics of Oleophobic Coatings in Aerospace Applications** , HAMZA SHAMS, BILAL A. SIDDIQUI, DHA Suffa University (DSU), SAJID SALEEM, National University of Sciences and Technology (NUST) — This paper investigates the wear characteristics of oleophobic coatings when applied over Inconel 718, which has widespread applications in the aerospace industry. Coatings once applied were selectively exposed to controlled uni- and then multi-directional sand storm conditions. Size and speed of sand particles colliding with the work surface were carefully moderated to simulate sand storm conditions. Study of friction was performed using Lateral Force Microscopy (LFM) coupled with standard optical microscopy. The analysis has been used to devise a coefficient of friction value and in turn suggest wear behavior of the coated surface including the time associated with exposure of the base substrate. The analysis after validation aims to suggest methods for safe usage of these coatings for aerospace applications.

**1:03PM Y42.00008 The influence of starch oxidization and aluminate coupling agent on interfacial interaction, rheological behavior, mechanical and thermal properties of poly(propylene carbonate)/starch blends<sup>1</sup>** , GUO JIANG, SHUI-DONG ZHANG, HAN-XIONG HUANG, School of Mechanical & Automotive Engineering, South China University of Technology, THE KEY LABORATORY OF POLYMER PROCESSING ENGINEERING OF THE MINISTRY OF EDUCATION TEAM — Poly(propylene carbonate) (PPC) is a kind of new biodegradable polymer that is synthesized by copolymerization of propylene oxide and carbon dioxide. In this work, PPC end-capped with maleic anhydride (PPCMA)/thermoplastic starch (TPS), PPCMA/thermoplastic oxidized starch (TPOS) and PPCMA/AL-TPOS (TPOS modified by aluminate coupling agent) blends were prepared by melt blending to improve its thermal and mechanical properties. FTIR results showed that there existed hydrogen-bonding interaction between PPCMA and starch. SEM observation revealed that the compatibility between PPCMA and TPOS was improved by the oxidation of starch. The enhanced interfacial interactions between PPCMA and TPOS led to a better performance of PPC blends such as storage modulus ( $G'$ ), loss modulus ( $G''$ ), complex viscosity ( $\eta^*$ ), tensile strength and thermal properties. Furthermore, the modification of TPOS by aluminate coupling agent (AL) facilitated the dispersion of oxidized starch in PPC matrix, and resulted in increasing the tensile strength and thermal stability.

<sup>1</sup>National Natural Science Foundation of China, National Science Fund of Guangdong Province

**Friday, March 18, 2016 11:15AM - 1:27PM –**  
**Session Y43 GSNP: Statistical Mechanics of Frustrated Systems, Including Constraint Satisfaction, Satisfiability and NP-Complete Problems** 346 - Jonathsan Machta, University of Massachusetts, Amherst

**11:15AM Y43.00001 Order-to-chaos transition in the hardness of random Boolean satisfiability problems**, MELINDA VARGA, Department of Physics, University of Notre Dame, ROBERT SUMI, MARIA ERCSEY-RAVASZ, Faculty of Physics, Babes-Bolyai University, Romania, ZOLTAN TOROCZKAI, Department of Physics, University of Notre Dame — Transient chaos is a phenomenon characterizing the dynamics of phase space trajectories evolving towards an attractor in physical systems. We show that transient chaos also appears in the dynamics of certain algorithms searching for solutions of constraint satisfaction problems (e.g., Sudoku). We present a study of the emergence of hardness in Boolean satisfiability ( $k$ -SAT) using an analog deterministic algorithm. Problem hardness is defined through the escape rate  $\kappa$ , an invariant measure of transient chaos, and it expresses the rate at which the trajectory approaches a solution. We show that the hardness in random  $k$ -SAT ensembles has a wide variation approximable by a lognormal distribution. We also show that when increasing the density of constraints  $\alpha$ , hardness appears through a second-order phase transition at  $\alpha_c$  in the random 3-SAT ensemble where dynamical trajectories become transiently chaotic, however, such transition does not occur for 2-SAT. This behavior also implies a novel type of transient chaos in which the escape rate has an exponential-algebraic dependence on the critical parameter. We demonstrate that the transition is generated by the appearance of non-solution basins in the solution space as the density of constraints is increased.

**11:27AM Y43.00002 Population Annealing: Theory and Application in Spin Glasses**<sup>1</sup>, JONATHAN MACHTA, Univ of Mass - Amherst, WENLONG WANG, HELMUT G. KATZGRABER, Texas A&M University — Population annealing is an efficient sequential Monte Carlo algorithm for simulating equilibrium states of systems with rough free energy landscapes. The theory of population annealing is presented, and systematic and statistical errors are discussed. The behavior of the algorithm is studied in the context of large-scale simulations of the three-dimensional Ising spin glass and the performance of the algorithm is compared to parallel tempering. It is found that the two algorithms are similar in efficiency though with different strengths and weaknesses.

<sup>1</sup>Supported by NSF DMR-1151387, DMR-1208046 and DMR-1507506

**11:39AM Y43.00003 Bond and temperature chaos in spin glasses revealed through thermal boundary conditions**<sup>1</sup>, WENLONG WANG, Texas AM Univ, JONATHAN MACHTA COLLABORATION<sup>2</sup>, HELMUT G. KATZGRABER COLLABORATION<sup>3</sup> — Spin glasses are complex systems with rugged energy landscapes that exhibit chaotic behavior. Unfortunately, despite decades of study, there is still no clear understanding of the chaotic behavior found in these systems. The use of thermal boundary conditions has become a useful approach to study such phenomena. Here we discuss how to efficiently simulate bond and temperature chaos using thermal boundary conditions and population annealing Monte Carlo. We provide a simple scaling argument for bond and temperature chaos, and present numerical results of the scaling exponents. Similarities and differences of bond chaos and temperature chaos are also discussed.

<sup>1</sup>NSF DMR-120804

<sup>2</sup>UMass Amherst

<sup>3</sup>Texas AM Univ

**11:51AM Y43.00004 Can we predict the difficulty of optimization problems without solving them?**, HELMUT G. KATZGRABER, CHAO FANG, RICHARD LAWRENCE, OLIVER MELCHERT, HUMBERTO MUNOZ-BAUZA, ANDREW J. OCHOA, WENLONG WANG, ZHENG ZHU, Texas A&M University — Surprisingly often. Based on previous results of a large-scale numerical study of the equilibrium three-dimensional Edwards-Anderson Ising spin glass where it was demonstrated that autocorrelation times are directly correlated with the roughness of the free-energy landscape [Phys. Rev. E 87, 012104 (2013)], we show that a generalized spin-glass order parameter can be used as a proxy to the computational difficulty of various paradigmatic optimization problems. Our results are illustrated with different optimization algorithms, as well as optimization problems. Furthermore, we show numerical evidence that the order-parameter distribution does mirror salient features in the free-energy landscape of complex systems for moderate system sizes.

**12:03PM Y43.00005 TemperSAT: A new efficient fair-sampling random  $k$ -SAT solver**, CHAO FANG, ZHENG ZHU, HELMUT G. KATZGRABER, Department of Physics and Astronomy, Texas A&M University — The set membership problem is of great importance to many applications and, in particular, database searches for target groups. Recently, an approach to speed up set membership searches based on the NP-hard constraint-satisfaction problem (random  $k$ -SAT) has been developed [S. Weaver *et al.* JSAT 8, 129 (2014)]. However, the bottleneck of the approach lies in finding the solution to a large SAT formula efficiently and, in particular, a large number of independent solutions is needed to reduce the probability of false positives. Unfortunately, traditional random  $k$ -SAT solvers such as WalkSAT are biased when seeking solutions to the Boolean formulas. By porting parallel tempering Monte Carlo to the sampling of binary optimization problems, we introduce a new algorithm (TemperSAT) whose performance is comparable to current state-of-the-art SAT solvers for large  $k$  with the added benefit that theoretically it can find many independent solutions quickly. We illustrate our results by comparing to the currently fastest implementation of WalkSAT, WalkSAT/ $lm$ .

**12:15PM Y43.00006 ICANP2: Isoenergetic cluster algorithm for NP-complete Problems**, ZHENG ZHU, CHAO FANG, HELMUT G. KATZGRABER, Texas AM University — NP-complete optimization problems with Boolean variables are of fundamental importance in computer science, mathematics and physics. Most notably, the minimization of general spin-glass-like Hamiltonians remains a difficult numerical task. There has been a great interest in designing efficient heuristics to solve these computationally difficult problems. Inspired by the rejection-free isoenergetic cluster algorithm developed for Ising spin glasses [Phys. Rev. Lett. 115, 077201 (2015)], we present a generalized cluster update that can be applied to different NP-complete optimization problems with Boolean variables. The cluster updates allow for a wide-spread sampling of phase space, thus speeding up optimization. By carefully tuning the pseudo-temperature (needed to randomize the configurations) of the problem, we show that the method can efficiently tackle problems on topologies with a large site-percolation threshold. We illustrate the ICANP2 heuristic on paradigmatic optimization problems, such as the satisfiability problem and the vertex cover problem.

**12:27PM Y43.00007 ABSTRACT WITHDRAWN —**

**12:39PM Y43.00008 Lower-Critical Spin-Glass Dimension from 23 Sequenced Hierarchical Models**, MEHMET DEMIRTAS, Sabanci University and Cornell University, ASLI TUNCER, Istanbul Technical University, A. NIHAT BERKER, Sabanci University and MIT — The lower-critical dimension for the existence of the Ising spin-glass phase is calculated, numerically exactly, as  $d_L = 2.520$  for a sequence of hierarchical lattices, from an essentially exact (correlation coefficient  $R^2 = 0.999999$ ) near-linear fit to 23 different diminishing fractional dimensions. To obtain this result, the phase transition temperature between the disordered and spin-glass phases, the corresponding critical exponent  $y_T$ , and the runaway exponent  $y_R$  of the spin-glass phase are calculated for consecutive hierarchical lattices as dimension is lowered.[1]

[1] M. Demirtas, A. Tuncer, and A.N. Berker, Phys. Rev. E 92, 022136 (2015).

**12:51PM Y43.00009 Odd  $q$ -State Clock Spin-Glass Models in Three Dimensions, Asymmetric Phase Diagrams, and Multiple Algebraically Ordered Phases**, EFE ILKER, Sabanci University and Case Western Reserve University, A. NIHAT BERKER, Sabanci University and MIT — Distinctive orderings and phase diagram structures are found, from renormalization-group theory, for odd  $q$ -state clock spin-glass models in  $d = 3$  dimensions [1]. These models exhibit asymmetric phase diagrams, as is also the case for quantum Heisenberg spin-glass models. No finite-temperature spin-glass phase occurs. For all odd  $q \geq 5$ , algebraically ordered antiferromagnetic phases [2,3] occur. One such phase is dominant and occurs for all  $q \geq 5$ . Other such phases occupy small low-temperature portions of the phase diagrams and occur for  $5 \leq q \leq 15$ . All algebraically ordered phases have the same structure, determined by an attractive finite-temperature sink fixed point where a dominant and a subdominant pair states have the only non-zero Boltzmann weights. The phase transition critical exponents quickly saturate to the high  $q$  value as previously observed for even  $q$ -state clock models [4].

- [1] E. Ilker and A. N. Berker, Phys. Rev. E **90**, 062112 (2014)
- [2] A. N. Berker and L. P. Kadanoff, J. Phys. A **13**, L259 (1980)
- [3] A. N. Berker and L. P. Kadanoff, J. Phys. A **13**, 3786 (1980)
- [4] E. Ilker and A. N. Berker, Phys. Rev. E **87**, 032124 (2013)

**1:03PM Y43.00010 Spinodals of the Ising model on the order-4 pentagonal tiling of the hyperbolic plane**<sup>1</sup>, HOWARD L. RICHARDS, Physics, Marshall University — In the Euclidean plane, the Ising model on a regular lattice does not have a true spinodal – that is, there is no local minimum of the free energy that persists forever (in the limit of infinitely large systems) except for the global minimum, which characterizes the stable state. However, a local minimum can persist for a very long time, so the minimum can be referred to as a “metastable” state. The manner in which the metastable state decays depends on the strength of the magnetic field and the system size; the “thermodynamic spinodal” is the transition between systems large enough to contain a single critical droplet and systems that are too small to do so, and the “dynamic spinodal” marks the transition between decay as a Poisson process to decay that is “deterministic”, meaning the standard deviation of the lifetime of the metastable state is small compared with its mean value. However, in the hyperbolic plane, true metastability exists, and evidence shows that the thermodynamic spinodal and dynamic spinodal are numerically close to the true spinodal, the field below which the metastable state cannot decay through the nucleation and growth of droplets.

<sup>1</sup>This research was supported by NSF grant OCI-1005117.

**1:15PM Y43.00011 Weak confinement in the three-state Potts Field Theory**, SERGEI RUTKEVICH, Univ Duisburg-Essen — Kink topological excitations are quite common in one-dimensional quantum ferromagnetic systems with the spontaneously broken discrete symmetry. Application of the external magnetic field  $h$  induces the long-range attractive force between kinks leading to their confinement. While in the Ising Field Theory the particle sector in the confinement regime contains only the two-kink bound states (“the mesons”), in the three-state Potts Field Theory (PFT) the three-kink bound states (“the baryons”) can exist as well. In the weak confinement regime, which is realized at small external magnetic fields, the meson masses in the PFT can be determined analytically in the leading order in  $h$  by means of the solution of a quantum-mechanical problem for two non-relativistic particles interacting with a linear attractive potential, and my means of the WKB method. The masses of lightest baryons in the three-state PFT were calculated by the numerical solution of a three-particle quantum-mechanical problem. The obtained mass spectra for the PFT mesons and baryons were confirmed recently by Lencés and Takács in numerical calculations based on the truncated conformal space approach.

## Friday, March 18, 2016 11:15AM - 2:15PM –

Session Y48 GQI: Decoherence in Superconducting Qubits: Noise 349 - Frederick Wellstood, University of Maryland

**11:15AM Y48.00001 Design and Simulation of Microwave Attenuators for Superconducting Quantum Devices**, JAY LEFEBVRE, Department of Physics, University of Maryland, College Park, JEN-HAO YEH, Laboratory for Physical Sciences, College Park, MD and Department of Physics, University of Maryland, College Park, MD, FREDERICK WELLSTOOD, Department of Physics, University of Maryland, College Park, MD and Joint Quantum Institute, University of Maryland, College Park, BENJAMIN PALMER, Laboratory for Physical Sciences, College Park, MD and Department of Physics, University of Maryland, College Park, MD — We have found that dephasing times for quantum superconducting transmons operating nominally at  $T = 20$  mK can be limited by thermal photons in the read-out cavity due to non-equilibrium noise on our input microwave line. In an effort to reduce this noise, we have used finite-element simulations to design attenuators that provide better thermalization of the input microwave signals being delivered to our devices. Our thermal simulations incorporate both electron-phonon decoupling effects due to dissipated power in each element of the attenuator as well as phonon thermal conduction and Kapitza boundary effects. We combine the resulting thermal map with a thermal noise model of each dissipative element of the filter to estimate the effective noise temperature of our filter design.

**11:27AM Y48.00002 Cavity Dephasing in Transmon Qubits from Non-equilibrium Noise**, JEN-HAO YEH, Laboratory for Physical Sciences, College Park, MD and Department of Physics, University of Maryland, College Park, MD, JAY LEFEBVRE, Department of Physics, University of Maryland, College Park, MD, FREDERICK WELLSTOOD, Department of Physics, University of Maryland, College Park, MD and Joint Quantum Institute, University of Maryland, College Park, MD, BENJAMIN PALMER, Laboratory for Physical Sciences, College Park, MD and Department of Physics, University of Maryland, College Park, MD — The dephasing times for transmon qubits in a 3D cavity can be limited by coupling of the cavity input and output lines to non-equilibrium noise from higher temperature stages. In our system, the dominant source of thermal photons in the cavity is the last microwave attenuator in the microwave input line which is mounted on the 20 mK stage. Guided by thermal and microwave simulations, we have fabricated microwave attenuators and tested them in a 3D transmon measurement system. The performance of the attenuators was quantified by measuring the Ramsey decay time of a transmon qubit as a function of the temperature of the mixing chamber and power dissipated in the attenuator. Based on the Ramsey decay times and properties of the transmon-cavity system, we estimate the effective output noise temperature of the attenuator and compare our results to simulations.

**11:39AM Y48.00003 Qubit dephasing due to photon shot noise from coherent and thermal sources<sup>1</sup>**, S. GUSTAVSSON, F. YAN, A. KAMAL, T. P. ORLANDO, W. D. OLIVER, MIT, J. BIRENBAUM, A. SEARS, D. HOVER, T. GUDMUNDSEN, J. YODER, MIT Lincoln Laboratory — We investigate qubit dephasing due to photon shot noise in a superconducting flux qubit transversally coupled to a coplanar microwave resonator. Due to the AC Stark effect, photon fluctuations in the resonator cause frequency shifts of the qubit, which in turn lead to dephasing. While this is universally understood, we have made the first quantitative spectroscopy of this noise for both thermal (i.e., residual photons from higher temperature stages) and coherent photons (residual photons from the readout and control pulses). We find that the bandwidth of the shot noise from thermal and coherent photons differ by approximately a factor of two, which we attribute to differences in the correlation time for the two noise sources. By comparing the results with noise spectra measured without any externally applied photons, we conclude that the qubit coherence times in our setup were limited by photon shot noise from thermal radiation, with an average resonator photon population of 0.006. Equipped with this knowledge, we improved the filtering for thermal noise and thereby improved the qubit coherence times by more than a factor of two, with T2 echo times approaching 100  $\mu$ s. From the measured T2 decay, we determine an upper bound on the residual photon population of 0.0004.

<sup>1</sup>This research was funded by the Office of the Director of National Intelligence (ODNI), Intelligence Advanced Research Projects Activity (IARPA) via MIT LL under Air Force Contract No. FA8721-05-C-0002.

**11:51AM Y48.00004 Suppression of photon shot noise dephasing in a tunable coupling superconducting qubit**, GENG YAN ZHANG, YANBING LIU, JAMES RAFTERY, ANDREW HOUCK, Princeton University — We report on the suppression of photon shot noise dephasing in a tunable coupling qubit (TCQ). This is achieved by eliminating the dispersive coupling rate,  $\chi$ , between the TCQ and the readout cavity. We observe that the coherence time approaches twice the relaxation time and becomes less sensitive to thermal photon noise when  $\chi$  is tuned close to zero. Experimental results of tunable  $\chi$  and its impact on qubit coherence will be presented.

**12:03PM Y48.00005 Dephasing of superconducting asymmetric transmon qubits**, M. HUTCHINGS, MATTHEW WARE, YEBIN LIU, Syracuse university, JARED B. HERTZBERG, JERRY M. CHOW, IBM T.J. Watson Research Center, Yorktown Heights, NY 10598, USA, B. L. T. PLOURDE, Syracuse university — As quantum computing implementations based on superconducting qubits increase in scale and complexity, fabrication tolerances and frequency crowding make it desirable to have layouts with at least some of the qubit frequencies being tunable. Split-junction transmon qubits allow for the tuning of qubit energy levels with a magnetic flux. However, this tunability can lead to excess dephasing due to flux noise. By making the two junctions asymmetric, the modulation range of the qubit energy bands can be reduced along with the sensitivity to flux noise. Such asymmetric transmons have been used previously for demonstrations of flux-modulated first-order sideband transitions between a qubit and cavity. We will report on the sensitivity of qubit dephasing to magnetic flux noise for different junction asymmetry. For large asymmetries, of the order of 10:1, the dephasing due to flux noise is greatly reduced compared to a symmetric junction device, whilst still maintaining a useful level of frequency tunability.

**12:15PM Y48.00006 Paramagnetic Spins on -Al<sub>2</sub>O<sub>3</sub> with Varied Surface Termination<sup>1</sup>**, KEITH RAY, Lawrence Livermore National Laboratory, DONGHWA LEE, Chonnam National University, NICOLE ADELSTEIN, San Francisco State University, JONATHAN DUBOIS, VINCENZO LORDI, Lawrence Livermore National Laboratory — Superconducting qubits (SQs) are promising building blocks for a quantum computer, however, coherence in SQs is reduced by unintended coupling to magnetic noise sources. The microscopic origins of the magnetic noise have not been satisfactorily characterized. Building on previous computational studies [PRL 112, 017001 (2014)] of magnetic spins induced by molecules adsorbed on bare Al terminated Al<sub>2</sub>O<sub>3</sub>, we present a density functional theory investigation of magnetic noise associated with other Al<sub>2</sub>O<sub>3</sub> surfaces likely to be encountered in experiment. We calculate the exchange interaction between native defects and adsorbed molecules, as well as the magnetic states energy splitting and anisotropy, on fully hydroxylated Al<sub>2</sub>O<sub>3</sub>, with and without a water over-layer. We also present simulated x-ray adsorption and x-ray magnetic circular dichroism spectra of these systems with the aim of aiding experimental surface characterization.

<sup>1</sup>This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344.

**12:27PM Y48.00007 Suppression of 1/f Flux Noise in Superconducting Quantum Circuits**, PRADEEP KUMAR, University of Wisconsin, Madison, JOHN FREELAND, Advanced Photon Source, Argonne National Lab, Argonne, IL, CLARE YU, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine, CA, ZHE WANG, State Key Laboratory of Surface Physics and Department of Physics, Fudan University, Shanghai, China, HUI WANG<sup>1</sup>, CHUNTAI SHI<sup>2</sup>, Department of Physics and Astronomy, University of California, Irvine, CA, DAVID PAPPAS, National Institute of Standards and Technology, Boulder, CO, ROBERT MCDERMOTT, University of Wisconsin, Madison — Low frequency 1/f magnetic flux noise is a dominant contributor to dephasing in superconducting quantum circuits. It is believed that the noise is due to a high density of unpaired magnetic defect states at the surface of the superconducting thin films. We have performed X-ray absorption spectroscopy (XAS) and X-ray magnetic circular dichroism (XMCD) experiments that point to adsorbed molecular oxygen as the dominant source of magnetism in these films. By improving the vacuum environment of our superconducting devices, we have achieved a significant reduction in surface magnetic susceptibility and 1/f flux noise power spectral density. These results open the door to realization of superconducting qubits with improved dephasing times.

<sup>1</sup>State Key Laboratory of Surface Physics and Department of Physics, Fudan University, Shanghai, China

<sup>2</sup>University of Wisconsin, Madison

**12:39PM Y48.00008 Measurement of the Magnetic Flux Noise Spectrum in Superconducting Xmon Transmon Quantum Bits**, BEN CHIARO, UC - Santa Barbara, D. SANK, J. KELLY, Google - Santa Barbara, Z. CHEN, B. CAMPBELL, A. DUNSWORTH, P. O'MALLEY, C. NEILL, C. QUINTANA, A. VAINSENCHE, J. WENNER, UC - Santa Barbara, R. BAREND, Y. CHEN, A. FOWLER, E. JEFFREY, A. MIGRANT, J. MUTUS, P. ROUSHAN, T. WHITE, Google - Santa Barbara, J. M. MARTINIS, UC - Santa Barbara and Google - Santa Barbara — Dephasing induced by magnetic flux noise limits the performance of modern superconducting quantum processors. We measure the flux noise power spectrum in planar, frequency-tunable, Xmon transmon quantum bits (qubits), with several SQUID loop geometries. We extend the Ramsey Tomography Oscilloscope (RTO) technique by rapid sampling up to 1 MHz, without state reset, to measure the flux noise power spectrum between 10<sup>-2</sup> and 10<sup>5</sup> Hz. The RTO measurements are combined with idle gate randomized benchmarking and Ramsey decay to give a more complete picture of dephasing in SQUID-based devices.

**12:51PM Y48.00009 1/f noise driven qubit dynamics in presence of a bosonic thermostat**, KOSTYANTYN KECHEDZHI, FEDIR VASKO, ANDRE PETUKHOV, NASA Ames Research Center, Mail Stop 269-3, Moffet Field, CA 94035, VADIM SMELYANSKIY, Google, Venice, CA 90291, US — Motivated by observations of distinct sources of noise in superconducting flux qubits over a wide frequency range, we analyze a qubit, a two level system, coupled to two microscopic sources of noise: 1/f low frequency noise and the Ohmic high frequency noise. The noise sources are treated as independent and characterized by different temperatures. We analyze the steady state regime of the resulting out-of-equilibrium dynamics focusing in particular on the effects of the interplay of the two types of noise on spectroscopic characteristics of the qubit. We calculate both analytically and numerically the steady state population of the qubit energy levels, relaxation and dephasing times and effective renormalization of the qubit's energy level splitting.

**1:03PM Y48.00010 1/f permittivity noise probed uniformly in a film with two level systems: The power law of field saturation and the relationship to loss**, KEVIN OSBORN, Laboratory for Physical Sciences and Joint Quantum Institute, ARUNA RAMANAYAKA, BAHMAN SARABI, Laboratory for Physical Sciences and University of Maryland Physics Dept., U. OF MARYLAND TEAM — Noise from atomic tunneling two-level systems (TSs) limit the performance of various superconducting devices, ranging in application from astronomy to quantum computing. We study superconducting resonators with films containing TS and measure the resulting 1/f frequency noise caused by resonant TS. The resonators are designed such that they apply a uniform ac electric field to the films which allows a direct measurement of permittivity noise in the film as a function the electric field. An intrinsic value of noise is found as well as the power law for ac-field saturation. The temperature dependence of 1/f noise below 200 mK fits to a relationship found previously in high-Q resonators. However, our data lead us to a model different than a previous experimental study; in our work TS phenomena are modeled with frequency diffusion. Our measured noise times the temperature is found to be the same to within error in the different films when normalized to the loss tangent at low temperature, despite dramatically different loss tangents. Following from the general nature of the TS models, we expect the same permittivity noise in many other devices.

**1:15PM Y48.00011 Flux noise due to magnetic impurities in superconducting circuits: Optimal spin texture and role of phase transition<sup>1</sup>**, ROGÉRIO DE SOUSA, Department of Physics and Astronomy, University of Victoria, British Columbia, Canada — Superconducting quantum interference devices (SQUIDs) and other superconducting circuits are limited by intrinsic flux noise with spectral density  $1/f^\alpha$  with  $\alpha < 1$  whose origin is believed to be due to spin impurities. We present a theory of flux noise in the presence of phase transitions and arbitrary spin textures in the impurity spin system [1]. At higher temperatures we find that the spin-spin correlation length scale (describing, e.g., the average size of ferromagnetic spin clusters) greatly impacts the scaling of flux noise with wire geometry. At lower temperatures we find that flux noise is quite sensitive to the particular spin texture realized by the spin system ground state. Remarkably, we show that flux-noise is exactly equal to zero when the spins form a poloidal texture. Flux noise is nonzero for other spin textures, but gets reduced in the presence of correlated ferromagnetic fluctuations between the top and bottom wire surfaces, where the flux vectors are antiparallel. This demonstrates the idea of engineering spin textures and/or intersurface correlation as a method to reduce flux noise in superconducting circuits.  
[1] S. LaForest and R. de Sousa, Phys. Rev. B **92**, 054502 (2015).

<sup>1</sup>This research was supported by the Natural Sciences and Engineering Research Council of Canada (RGPIN/342982- 2010, EGP/429649-2012) through its Discovery and Engage programs.

**1:27PM Y48.00012 Spin noise and magnetic screening of impurities in a BCS superconductor<sup>1</sup>**, MATTHIAS LE DALL, Department of Physics and Astronomy, University of Victoria, British Columbia, Canada, LUIS G. G. V. DIAS DA SILVA, Instituto de Física, Universidade de São Paulo, Brazil, ROGÉRIO DE SOUSA, Department of Physics and Astronomy, University of Victoria, British Columbia, Canada — The coupling of a localized impurity to a BCS superconductor (SC) leads to the formation of impurity Cooper-pairs via the proximity effect, generating two bound states within the SC energy gap, the so-called Yu-Rusinov-Shiba (YSR) states. They are similar to the Andreev Bound States that originate from Andreev reflection, e.g. when the impurity is hosted in a Josephson junction, and are known to produce sharp sub-gap resonances in charge noise [de Sousa et al., PRB 2009], providing a natural explanation for the observation of microresonators in superconducting devices [Simmonds et al., PRL 2004]. Here we present a theory for the spin noise generated by magnetic impurities in a SC, and discuss the impact of the Shiba states on models of flux noise in superconducting qubits. We use a combination of analytical methods and the numerical renormalization group technique to calculate the spin noise of an Anderson impurity in a SC, unveiling the competition between the proximity effect and Kondo correlations. Both mechanisms produce magnetic screening and a corresponding reduction in spin noise, giving rise to new insights on the kinds of impurities that are responsible for the observed  $1/f^\alpha$  flux noise in superconducting circuits.

<sup>1</sup>This research is supported by NSERC CRD/478366-2015.

**1:39PM Y48.00013 Geometrical Effects in Noise Spectra of Superconducting Flux Qubits<sup>1</sup>**, ANDRE PETUKHOV, NASA Ames Research Center, Moffett Field, California, VADIM SMELYANSKIY, Google Inc, Venice, California, JOHN MARTINIS, University of California, Santa Barbara and Google Inc, Santa Barbara, California — We present theoretical study of geometrical effects related to spin diffusion in superconducting flux qubits. We adopt a model of a long superconducting wire surrounded by a thin oxide layer with spins distributed uniformly over cross-sectional area of the oxide layer. Using a continuous transformation from a round cylinder to a flat wire strip, we demonstrate that the noise spectral density tends to a power law  $S(\omega) \propto (\omega/\Gamma)^{-s}$  with  $s \gtrsim 3/4$ , approaching  $s = 3/4$  for very thin wires. The  $\omega^{-s}$  dependence is valid in a broad frequency range above  $\omega \gtrsim \Gamma$  stretching up to four orders of magnitude in units of characteristic diffusion decay rate  $\Gamma \sim 1 - 10^2$  Hz. The effect is highly sensitive to a cross-sectional aspect ratio of a thin wire thus revealing its geometrical origin. We substantiate our findings by detailed comparison with available experimental data and conclude that  $3/4$  power law distinguishes spin diffusion flux noise from generic “ $1/f$ ” family.

<sup>1</sup>Supported by the AFRL Information Directorate under grant F4HBKC4162G001

**1:51PM Y48.00014 Suppression of dephasing by qubit motion in superconducting circuits<sup>1</sup>**, D.V. AVERIN, Dep-t of Physics and Astronomy, Stony Brook University, SUNY, K. HU, Y. P. ZHONG, C. SONG, H. WANG, Dep-t of Physics, Zhejiang University, China, S. HAN, Dep-t of Physics and Astronomy, University of Kansas — We suggest and demonstrate a protocol which suppresses dephasing due to the low-frequency noise by qubit motion, i.e., transfer of the logical qubit of information in a system of  $n \geq 2$  physical qubits. The protocol requires only the nearest-neighbor coupling and is applicable to different qubit structures. Motion of a logical qubit limits the correlation time of the effective noise seen by this qubit and suppresses its decoherence rate. This effect is qualitatively similar to the dynamic decoupling, but relies on the different resource: additional physical qubits, not extra control pulses. In this respect, suggested protocol can serve as the basis for an alternative approach to scalable quantum circuits. We further analyze its effectiveness against noises with arbitrary correlations. Our analysis, together with experiments using up to three superconducting qubits, shows that for the realistic uncorrelated noises, qubit motion increases the dephasing time of the logical qubit as  $\sqrt{n}$ . In general, the protocol provides a diagnostic tool for measurements of the noise correlations.

<sup>1</sup>This work was supported by the National Basic Research Program of China (2014CB921200, 2012CB927404), US NSF grants PHY-1314758 and PHY-1314861, the National Natural Science Foundation of China, and Zhejiang Provincial Natural Science Foundation

**2:03PM Y48.00015 Long range correlations by local dissipation in lattice waveguide QED**, BAPTISTE ROYER, ARNE L. GRIMSMO, Univ of Sherbrooke, ALEXANDRE BLAIS, Univ of Sherbrooke, CIFAR — In waveguide QED, superconducting qubits acting as artificial atoms are coupled to 1D superconducting transmission lines playing the role of common bath for the qubits. By controlling their effective separation and coupling to the transmission line, it is possible to engineer various types of dissipation-induced interactions between the qubits. In this talk, we consider the situation where multiple superconducting qubits are coupled to a lattice of superconducting transmission lines. We show that this can lead to the creation of highly entangled dark states using local dissipation only. Using tensor networks techniques, we study such large-scale highly-correlated systems.

**Friday, March 18, 2016 11:15AM - 1:15PM –**

**Session Y50 DAMOP: Fluctuation-Induced Forces** Hilton Baltimore Holiday Ballroom 1 - Jeremy Munday, University of Maryland

**11:15AM Y50.00001 Nanoscale Radiative Heat Transfer between Graphene Ribbon Arrays<sup>1</sup>**

, ZHUOMIN ZHANG<sup>2</sup>, XIANGLEI LIU<sup>3</sup>, Georgia Institute of Technology — Near-field radiative heat transfer between two graphene sheets can exceed that between blackbodies due to surface plasmons excited by the graphene sheet. This study shows that, by patterning a single layer of graphene sheet into ribbons, a giant enhancement of the near-field radiative heat flux, by more than one order of magnitude higher than that between two graphene sheets, can be achieved. The mechanism lies in that when the graphene sheet is patterned into an array of ribbons, the closed circular dispersion of graphene plasmons is opened to become hyperbolic, leading to broadband singularities of density of states. Extremely high-k evanescent waves can now couple with hyperbolic graphene plasmons. Exact numerical simulations are used by combining the scattering theory and rigorous coupled-wave analysis. Furthermore, effective medium calculations are used to support the arguments and provide clear physical insights. The findings from this study may open promising pathways for highly efficient thermal management, energy harvesting, and subwavelength thermal imaging.

<sup>1</sup>This work was supported by the Department of Energy, Office of Science, Basic Energy Sciences (DE-FG02-06ER46343).

<sup>2</sup>Professor

<sup>3</sup>PhD student

**11:27AM Y50.00002 Failure of local FDT in fluctuation-induced interactions.**

, DIEGO DALVIT, Los Alamos National Laboratory, FRANCESCO INTRAVAIA, Max-Born Institute, Germany, RYAN BEHUNIN, Yale University, CARSTEN HENKEL, University of Potsdam, Germany, KURT BUSCH, Humboldt University, Germany — In the study of non-equilibrium fluctuation-induced interactions (e.g., quantum friction, near-field heat transfer, and non-equilibrium Casimir forces) the local fluctuation-dissipation theorem (FDT) is widely used without much justification. Here, we report the failure of the local FDT in a specific example of quantum friction of an atom moving at constant velocity above a surface. A generalized non-equilibrium FDT is derived, which contains a contribution akin to the local FDT and an additional one corresponding to a velocity-dependent current term. We show that in the low-velocity limit the frictional force arising from the current term is of the same order of magnitude as that predicted by the local FDT, which underestimates the total force by almost 50 percent.

**11:39AM Y50.00003 Fluctuation-Induced Interactions in external magnetic fields: Casimir force and Radiative Heat Transfer**

, RAUL ESQUIVEL-SIRVENT, Univ Nacl Autonoma de Mexico — Thermally induced electromagnetic fields give rise to the Casimir force and the near field heat transfer between two bodies separated by a gap. These phenomena are described by Rytov's theory of fluctuating electromagnetic fields and both the Casimir force and the near field heat transfer depend on the local dielectric function of the bodies. In this work we present a theoretical calculation on the modulation of fluctuation-induced interactions in the presence of an external magnetic field. The system consists of two parallel plates separated by a gap  $d$ . Each plate is isotropic and has a local dielectric function. Applying an external magnetic field parallel to the plates, in the so called Voigt configuration, the plates become anisotropic. In particular, we consider plates of InSb. For the Casimir force the two plates are kept at the same temperature and the external field reduces the magnitude of the force. Similarly if the two plates are kept at different temperature the near field radiative heat transfer is modulated by the magnitude of the external magnetic field. The results are extended to semiconducting quantum wells. In both cases, the excitation of magnetoplasmons provides an explanation for the observed effect.

**11:51AM Y50.00004 Short distance expansion for fluctuation induced interactions**

, THORSTEN EMIG, CNRS and MIT, GIUSEPPE BIMONTE, Universita' di Napoli Federico II — Fluctuation induced interactions become most prominent in close to proximity to surfaces. Examples include van der Waals and Casimir forces, heat transfer, and spectral shifts for atoms and molecules. In many situations, the surfaces are curved or structured which makes the computation of the interaction in general complicated. Here we present a versatile and powerful approach to this problem which is based on a derivative expansion. It applies to distances much smaller than the radii of surface curvature. Explicit results include orientational effects for anisotropic particles, thermal effects, and spectral modifications.

**12:03PM Y50.00005 Unified boundary conditions and Casimir forces for fields with arbitrary spin<sup>1</sup>**

, ROBERT BENNETT, University of Freiburg, ADAM STOKES, University of Leeds — The electromagnetic Casimir effect is well-known and has been extensively studied for the last half-century. This attractive force between parallel plates arises from the imposition of boundary conditions upon the fluctuating spin-1 photon field, so a natural further question is whether fields of different spin can cause similar forces when confined in the same way. However, so far it has not been clear what the appropriate boundary conditions for physically-confined spinor fields may be. Here we present work that generalises the physically well-motivated electromagnetic boundary conditions to fields of arbitrary spin, thus arriving at physically reasonable boundary conditions<sup>2</sup> and Casimir forces<sup>3</sup> for a selection of interesting fields. For example, the so-called 'bag model' boundary conditions from nuclear physics emerge from our generalised boundary condition as a special case, as do the linearised gravity boundary conditions suggested in a remarkable recent proposal<sup>4</sup> concerning possible measurement of gravitonic Casimir forces.

<sup>1</sup>Supported by the UK Engineering and Physical Sciences Research Council (EPSRC)

<sup>2</sup>A. Stokes and R. Bennett, New J. Phys. 17 073012 (2015)

<sup>3</sup>A. Stokes and R. Bennett, Ann. Phys NY 360 246 (2015)

<sup>4</sup>James Q. Quach, Phys. Rev. Lett. 114 081104 (2015)

**12:15PM Y50.00006 Measurement and control of electrostatic patch potentials**

, JOSEPH L GARRETT, JEREMY N MUNDAY, University of Maryland, College Park — Electrostatic patch potentials hinder many precision measurements, particularly measurements of the Casimir force. Despite the improved force sensitivity achieved over the last decade, only recently have attempts been made to measure and quantify the effects of patch potentials. Here we present an analysis of patch potentials measured by Kelvin probe force microscopy (KPFM) and discuss methods to control these potentials (e.g. humidity, material choice, etc).

**12:27PM Y50.00007 An experimental apparatus for Casimir torque measurements** , DAVID A.T. SOMERS<sup>1</sup>, JEREMY N. MUNDAY<sup>2</sup>, Univ of Maryland-College Park — We have developed an experiment to measure the Casimir torque. In our experiment, a solid birefringent crystal causes a nematic liquid crystal director to rotate such that the extraordinary axes are aligned. A transparent and isotropic dielectric spacer layer is used to separate the two birefringent materials and an all-optical technique is used for detection. In this talk, we report on the progress of this experiment.

<sup>1</sup>Department of Physics, Institute for Research in Electronics and Applied Physics

<sup>2</sup>Electrical and Computer Engineering, Institute for Research in Electronics and Applied Physics

**12:39PM Y50.00008 Parameterization of lattice spacings for lipid multilayers in ionic solutions** , HORIA PETRACHE, Indiana University Purdue University Indianapolis, MERRELL JOHNSON, Indiana University Purdue University Fort Wayne, DANIEL HARRIES, The Hebrew University of Jerusalem, SOENKE SEIFERT, Argonne National Laboratory — Lipids, which are molecules found in biological cells, form highly regular layered structures called multilamellar lipid vesicles (MLVs). The repeat lattice spacings of MLVs depend on van der Waals and electrostatic forces between neighboring membranes and are sensitive to the presence of salt. For example, addition of salt ions such as sodium and potassium makes the MLVs swell, primarily due to changes in electrical polarizabilities. However, a more complicated behavior is found in some ionic solutions such as those containing lithium ions. Using x-ray scattering, we show experimentally how the interactions between membranes depend on the type of monovalent ions and construct parameterizations of MLVs swelling curves that can help analyze van der Waals interactions.

**12:51PM Y50.00009 Johnson-Nyquist Noise Coupling Formulation of Near-Field Heat Transfer for 1D Conductors** , MIKA PRUNNILA, SAMPO LAAKSO, DAVID GUNNARSSON, VTT Technical Research Centre of Finland — Near-field heat transfer has been formulated using different levels of theoretical sophistication and complexity ranging from fluctuational electrodynamics to quasi-static Coulomb interaction description. Our goal is to find a simple description for the near-field heat transfer between coupled 1D electron systems (conductors). We will show that by considering distributed Johnson-Nyquist voltage sources, arising from the dissipative part of the electron systems' response, a compact fundamental formula for the near-field heat transfer can be found. We will describe the details of the derivation and discuss the regime of validity of our approach. Several special cases will be considered and experimental configurations will be discussed. The presented analysis is especially suitable for closely spaced graphene ribbons and nanowires. We will also show that by including inductive responses, which are necessary at high frequencies, speed of light emerges in the heat flow formula, thereby showing the link between fundamental physical quantities/constants and near-field heat transfer in coupled 1D systems. Our formulation also provides the possibility to use different boundary conditions for the physical system and this enables design of near-field heat transfer circuits.

**1:03PM Y50.00010 ABSTRACT WITHDRAWN —**

**Friday, March 18, 2016 11:15AM - 2:15PM —**

**Session Y52 DAMOP: Atomic Physics: New Frontiers II** Hilton Baltimore Holiday Ballroom 3 - Seth Aubin, College of William and Mary

**11:15AM Y52.00001 A fully controllable Kondo system: Coupling a flux qubit and an ultracold Fermi gas** , KELLY PATTON, School of Science and Technology, Georgia Gwinnett College — We show that a composite spin-1/2 Kondo system can be formed by coupling a superconducting quantum interference device (SQUID) to the internal hyperfine states of a trapped ultracold atomic Fermi gas. Here, the SQUID, or flux qubit, acts as an effective magnetic impurity that induces spin-flip scattering near the Fermi energies of the trapped gas. Although the ultracold gas and SQUID are at vastly different temperatures, the formation of a strongly correlated Kondo state between the two systems is found when the gas is cooled below the Kondo temperature. We find that the Kondo temperature of this hybrid system is within current experimental limits. Furthermore, the momentum distribution of the trapped fermions is calculated. We find that it clearly contains an experimental signature of this correlated state and the associated Kondo screening length. In addition to probing Kondo physics, the controllability of this system can be used to systematically explore the relaxation and equilibration of a strongly correlated system that has been initially prepared in a selected nonequilibrium state.

**11:27AM Y52.00002 Broken selection rule in the quantum Rabi model** , GUILLERMO ROMERO, University of Santiago of Chile, POL FORN-DÍAZ<sup>1</sup>, University of Waterloo, C. J. P. M. HARMANS, TU Delft, ENRIQUE SOLANO, University of the Basque Country, HANS MOOIJ, TU Delft — We report the spectroscopic observation of a resonant transition that breaks a selection rule in the quantum Rabi model, implemented using an *LC* resonator and a superconducting qubit. The eigenstates of the system consist of a superposition of bare qubit-oscillator states with a relative sign. In the limit of low qubit-oscillator coupling strength, the matrix element between excited eigenstates of different sign is very small in presence of an oscillator drive, establishing a sign-preserving selection rule. Here, our qubit-resonator system operates in the ultrastrong coupling regime, where the coupling strength is 10% of the resonator frequency, allowing sign-changing transitions to be activated and, therefore, detected. This work shows that sign-changing transitions are an unambiguous, distinctive signature of systems operating in the ultrastrong coupling regime of the quantum Rabi model. These results pave the way to further studies of sign-preserving selection rules in multiqubit and multiphoton models.

<sup>1</sup>First author in this collaboration

**11:39AM Y52.00003 "Magnetic" refrigeration in synthetic quantum magnets** , MICHAEL ZALETEL, Station Q, Microsoft Research , NORMAN YAO, Department of Physics, UC Berkeley — The advent of ultracold atomic systems has promised to expand upon our understanding of strongly correlated quantum ground states; by contrast to their material cousins, cold atomic experiments benefit from unique tools such as direct optical imaging and tunable short- and long-range interactions. However, despite advances in coherent quantum control, ultracold atoms remain much too hot. Although sub-nanokelvin temperatures are the norm in experiments, the entropy of the system remains extensively far above the ground state. One strategy to combat this is to shift the entropy elsewhere for example, placing a gapless system near a gapped system can effectively "cool" the latter. In this talk, we will demonstrate that typical atomic systems can act as their own coolant. As an example, we consider a 1D optical lattice geometry where spin-1 atoms interact via a generic AKLT-type Hamiltonian. We will discuss why decreasing the density of atoms in one region is sufficient to cool the complementary portion of the system to the ground state, wherein coherent edge dynamics are observed.

**11:51AM Y52.00004 Dissipative topological insulator with fractional winding number and single edge state** , TONY LEE, Indiana University-Purdue University Indianapolis (IUPUI) — Photonic experiments offer an opportunity to find novel topological states. We consider a one-dimensional tight-binding model in the presence of gain and loss as well as long-range hopping. The system is described by a non-Hermitian Hamiltonian with PT symmetry and exceptional points. The unique feature of the model is that the Hamiltonian encircles an exceptional point in momentum space, leading to novel topological features. The winding number has a fractional value 1/2 because the Brillouin zone has a periodicity of 4 $\pi$  instead of 2 $\pi$ . There is only one edge state due to the coalescence of eigenvectors. The edge state is topologically protected by a chiral symmetry but disappears when the bulk gap closes. We also discuss experimental realization with optical waveguides.

**12:03PM Y52.00005 Simulating the Generalized Gibbs Ensemble (GGE): A Hilbert space Monte Carlo approach**, VINCENZO ALBA, SISSA — By combining classical Monte Carlo and Bethe ansatz techniques we devise a numerical method to construct the Truncated Generalized Gibbs Ensemble (TGGE) for the spin-1/2 isotropic Heisenberg (XXX) chain. The key idea is to sample the Hilbert space of the model with the appropriate GGE probability measure. The method can be extended to other integrable systems, such as the Lieb-Liniger model. We benchmark the approach focusing on GGE expectation values of several local observables. As finite-size effects decay exponentially with system size, moderately large chains are sufficient to extract thermodynamic quantities. The Monte Carlo results are in agreement with both the Thermodynamic Bethe Ansatz (TBA) and the Quantum Transfer Matrix approach (QTM). Remarkably, it is possible to extract in a simple way the steady-state Bethe-Gaudin-Takahashi (BGT) roots distributions, which encode complete information about the GGE expectation values in the thermodynamic limit. Finally, it is straightforward to simulate extensions of the GGE, in which, besides the local integral of motion (local charges), one includes arbitrary functions of the BGT roots. As an example, we include in the GGE the first non-trivial quasi-local integral of motion.

**12:15PM Y52.00006 Minimally entangled typical thermal states versus matrix product purifications for the simulation of equilibrium states and time evolution**, MORITZ BINDER, THOMAS BARTHEL, Duke Univ — We compare matrix product purifications and minimally entangled typical thermal states (METTS) for the simulation of equilibrium states and finite-temperature response functions of strongly correlated quantum many-body systems. For METTS, we highlight the interplay of statistical and DMRG truncation errors, discuss the use of self-averaging effects, and describe schemes for the computation of response functions. We assess the computation costs and accuracies of the two methods for critical and gapped spin chains and the Bose-Hubbard model. For the same computation cost, purifications yield more accurate results than METTS except for temperatures well below the systems energy gap. (Phys. Rev. B 92, 125119 (2015))

**12:27PM Y52.00007 Interacting Bose gas confined in a Kronig-Penney potential<sup>1</sup>**, O. A. RODRÍGUEZ, Posgrado en Ciencias Físicas, UNAM, M. A. SOLÍS, Instituto de Física, UNAM — We analyze the effect of the 1D periodic Kronig-Penney potential, composed of barriers of width  $b$  and separated a distance  $a$ , over an interacting Bose gas. At  $T = 0$ , the Gross-Pitaevskii equation is solved analytically in terms of the Jacobi elliptic functions for repulsive or attractive interaction between bosons. By applying the boundary conditions for periodic solutions as well as the normalization of the wave function, we arrive to a set of nonlinear equations from which we obtain the density profile and the chemical potential of the condensate as a function of the particle momentum. The profiles for attractive and repulsive interactions are compared with that of the non-interacting case. For attractive interaction we are able to observe a pronounced spatial localization in the middle of every two barriers. We reproduce the well known results when the Kronig-Penney potential becomes a Dirac Comb.

<sup>1</sup>We acknowledge partial support from grants PAPIIT IN111613 and CONACyT 221030

**12:39PM Y52.00008 Concept of contact spectrum and its applications in atomic quantum Hall states<sup>1</sup>**, MINGYUAN HE, SHAO-LIANG ZHANG, HON-MING CHAN, QI ZHOU, Department of Physics, The Chinese University of Hong Kong — A unique feature of ultracold atoms is the separation of length scales,  $r_0 \ll k_F^{-1}$ , where  $k_F$  and  $r_0$  are the Fermi momentum characterizing the average particle distance and the range of interaction between atoms respectively. For  $s$ -wave scattering, Shina Tan discovered that such diluteness leads to universal relations, all of which are governed by contact, among a wide range of thermodynamic quantities. In this talk, I will show that the concept of contact can be generalized to an arbitrary partial-wave scattering. Contact of all partial-wave scatterings form a contact spectrum, which establishes universal thermodynamic relations with notable differences from those in the presence of  $s$ -wave scattering alone. Moreover, such a contact spectrum has an interesting connection with a special bipartite entanglement spectrum of atomic quantum Hall states, and enables an intrinsic probe of these highly correlated states using two-body short-ranged correlations.

<sup>1</sup>Funding acknowledgement: GRF/14306714

**12:51PM Y52.00009 Energy transfer in mesoscopic vibrational systems enabled by eigenfrequency fluctuations**, JUAN ATALAYA<sup>1</sup>, Michigan State University — Energy transfer between low-frequency vibrational modes can be achieved by means of nonlinear coupling if their eigenfrequencies fulfill certain nonlinear resonance conditions. Because of the discreteness of the vibrational spectrum at low frequencies, such conditions may be difficult to satisfy for most low-frequency modes in typical mesoscopic vibrational systems. Fluctuations of the vibrational eigenfrequencies can also be relatively strong in such systems. We show that energy transfer between modes can occur in the absence of nonlinear resonance if frequency fluctuations are allowed. The case of three modes with cubic nonlinear coupling and no damping is particularly interesting. It is found that the system has a non-thermal equilibrium state which depends only on the initial conditions. The rate at which the system approaches to such state is determined by the parameters such as the noise strength and correlation time, the nonlinearity strength and the detuning from exact nonlinear resonance. We also discuss the case of many weakly coupled modes. Our results shed light on the problem of energy relaxation of low-frequency vibrational modes into the continuum of high-frequency vibrational modes. The results have been obtained with Mark Dykman.

<sup>1</sup>Alternative email: jatalaya2012@gmail.com

**1:03PM Y52.00010 Quantum memory and phase gate in Optical cavities based on EIT<sup>1</sup>**, HALYNE BORGES, CELSO VILLAS-BÔAS, Federal University of São Carlos — In this work we investigate theoretically the implementation of an optical quantum memory in a system composed by a single atom, trapped in a high finesse optical cavity. In order to analyse the feasibility of implementing a quantum memory in the atom-cavity system based on the EIT phenomenon, we investigated in detail which parameter configuration the memory efficiency is optimized considering the two different setups. Our results shows that for a asymmetric one-sided cavity, which is the experimental setup commonly used to observe the EIT effect, the memory efficiency value saturates at about 8.5%. Meanwhile, for an one-sided cavity, we observe for a sufficiently high value of the coupling constant  $g$ , the efficiency has its maximum value increased considerably, close to 100%. However, this experimental setup is not suitable to observe cavity-EIT in the transmission spectrum, being necessary another kind of experiment, such as measurements phase difference field that leaves the cavity induced by the control field. Considering this configuration we also showed the implementation of a quantum phase gate based on the same nonlinear effect, where the pulse probe can experience a phase shift on the order of  $\pi$ , due to the presence or absence of a control pulse.

<sup>1</sup> Supported by FAPESP (Proc. 2014/12740-1) and INCT-IQ

**1:15PM Y52.00011 Beyond quantum-classical analogies: high time for agreement?** , MICHELE MARROCCO, ENEA — Lately, many quantum-classical analogies have been investigated and published in many acknowledged journals. Such a surge of research on conceptual connections between quantum and classical physics forces us to ask whether the correspondence between the quantum and classical interpretation of the reality is deeper than the correspondence principle stated by Bohr. Here, after a short introduction to quantum-classical analogies from the recent literature, we try to examine the question from the perspective of a possible agreement between quantum and classical laws. A paradigmatic example is given in the striking equivalence between the classical Mie theory of electromagnetic scattering from spherical scatterers and the corresponding quantum-mechanical wave scattering analyzed in terms of partial waves. The key features that make the correspondence possible are examined and finally employed to deal with the fundamental blackbody problem that marks the initial separation between classical and quantum physics. The procedure allows us to recover the blackbody spectrum in classical terms and the proof is rich in consequences. Among them, the strong analogy between the quantum vacuum and its classical counterpart.

**1:27PM Y52.00012 Application of axiomatic formal theory to the Abraham–Minkowski controversy** , MICHAEL CRENSHAW, USArmy AMRDEC — Continuum electrodynamics is an axiomatic formal theory whose axioms are the macroscopic Maxwell equations. We demonstrate that valid theorems of the formal theory are inconsistent with conservation laws and with special relativity because continuum electrodynamics allows transformations of the Maxwell equations that constitute an improper tensor transformation that changes the conservation properties, the relativity properties, and the space-time embedding of the coupled equations of motion. The inconsistencies are resolved by a reformulation of physical principles in a flat non-Minkowski material spacetime in which the timelike coordinate corresponds to  $ct/n$ . Applying Lagrangian field theory, we derive equations of motion for the macroscopic electric and magnetic fields in a simple dielectric medium. We construct a new formal theory of continuum electrodynamics and we derive a tensor energy-momentum continuity theorem that trivially resolves the century-old Abraham–Minkowski momentum controversy. We derive the theory of special relativity in a dielectric, including the material Lorentz factor and the material Lorentz transformation. We derive the momentum of a polariton in the context of material special relativity to confirm the resolution of the Abraham-Minkowski debate.

**1:39PM Y52.00013 Particle beams carrying orbital angular momentum, charge, mass and spin** , TEUNTJE TIJSSEN, H H Wills Physics Laboratory, University of Bristol, ARMEN HAYRAPETYAN, JOERG GOETTE, Max Planck Institute for the Physics of Complex Systems, Dresden, MARK DENNIS, H H Wills Physics Laboratory, University of Bristol — Electron beams carrying vortices and angular momentum have been of much experimental and theoretical interest in recent years. In addition, optical vortex beams are a well-established field in optics and photonics. In both cases, the orbital angular momentum associated with the beams axial vortex has effects on the overall spin of the beam, due to spin-orbit interactions. A simple model of these systems are Bessel beam solutions (of either the Dirac equation or Maxwell equations) with a nonzero azimuthal quantum number, which are found by separation in cylindrical coordinates. Here, we generalize this approach, considering the classical field theory of Bessel beams for particles which are either massive or massless, uncharged or charged and of a variety of different spins ( $0, \frac{1}{2}, 1, \dots$ ). We regard the spin and helicity states and different forms of spin-orbit terms that arise. Moreover, we analyse the induced electromagnetic field when the particles carry charge. Most importantly, this unified field theory approach leads to the prediction of effects for vortex beams of neutrons, mesons and neutrinos.

**1:51PM Y52.00014 Harmonic Fractions and an Integer Power Law to Demonstrate a Relationship of the Neutron to the Properties of Hydrogen and Cosmic Observables** , D. W. CHAKERES, Department of Radiology, The Ohio State University, Columbus, OH, 43210, R. VENTO, Retired, Columbus State Community College, Columbus, OH, 43215, D. I. PANCHENKO, J. A. TOBAR, S. S. MOSES, V. M. ANDRIANARIJAONA, Department of Physics, Pacific Union College, Angwin, CA, 94508 — Power laws and harmonic oscillator systems represent a ubiquitous relationship among many physical phenomena. This study demonstrates a close power law relationship of the annihilation frequency of the neutron, approximately  $2.27 \cdot 10^{23}$  Hz, when used as a dimensionless base, to fundamental quantum properties of hydrogen and present-day cosmic observables. The following set of the three smallest integers:  $\{-1, 0, 1\}$ , and the set of partial harmonic fractions:  $\{3/2, 1/2, 2/3, -3/4, 4/5\}$ , are associated with each physical entity investigated as a frequency equivalent. They are listed as follows: twice the maximum energy of a cosmic ray,  $3/2$ ; the base identity of the neutron,  $1$ ; the Bohr radius,  $4/5$ ; Rydberg's constant,  $2/3$ ; twice the peak spectral radiance of cosmic microwave background radiation,  $1/2$ ; Planck's constant,  $0$ ; the Sun's galactic radius,  $-1/2$ ; the Sun's galactic period,  $-2/3$ ; Hubble's constant,  $-3/4$ ; the dimension of the observable universe,  $-4/5$ ; and twice the gravitational binding energy of the electron in hydrogen,  $-1$ . When viewed in the physically equivalent frequency domain, the neutron partitions an abundance of physical constants from the very small to the very large.

**2:03PM Y52.00015 Branching ratio, transition frequency and lifetime measurements in  $^{88}\text{Sr}^+$  with trapped ions<sup>1</sup>** , HELENA ZHANG, MICHAEL GUTIERREZ, GUANG HAO LOW, ISAAC CHUANG, Massachusetts Inst of Tech-MIT — Precise measurements of atomic properties, such as branching ratios and transition frequencies and lifetimes, are important in the study of astrophysical objects as well as verification of relativistic many-body theories. We report on a new measurement of the branching ratio of the  $5P_{1/2}$  and  $5P_{3/2}$  states in  $^{88}\text{Sr}^+$  to  $10^{-4}$  fractional uncertainty, a  $10^3$  times improvement over current results, using ions confined in a Paul trap. Using a fiber frequency comb and pulsed spectroscopy, we measure the absolute frequencies of the  $5S_{1/2} - 5P_{1/2}$  and  $5S_{1/2} - 5P_{3/2}$  transitions to within 200 kHz, previously only known to tens of MHz. By fitting the fluorescence curve of the ion with optical Bloch equations, we obtain a new measurement for the lifetime of the  $5P_{1/2}$  and  $5P_{3/2}$  states without using a pulsed laser source.

<sup>1</sup>Supported by the IARPA MQCO program and the ARO Quantum Algorithms program

**Friday, March 18, 2016 11:15AM - 2:03PM –**

**Session Y53 DCMF: Superconductivity: Proximity Effects and SN Junctions III** Hilton Baltimore Holiday Ballroom 4 -

**11:15AM Y53.00001 Scanning Tunneling Microscopy Study of Graphene/Cuprate Heterostructures.** , MINGHAO CHENG, ALEXANDER KERELSKY, XINJUE ZHONG, DA WANG, YUFENG HAO, JAMES HONE, XIAOYANG ZHU, AHBAY PASUPATHY, Columbia University in the City of New York — We study the properties of single-layer graphene co-laminated to BSCCO-2212 single crystals using UHV-Low Temperature-STM. Samples were prepared by transferring large-area single layer graphene grown on copper substrate using the chemical vapor deposition to the freshly-cleaved surface of a BSCCO single crystal in an inert atmosphere. Under optimal conditions, the graphene acts as a protective film for the freshly-cleaved surface of BSCCO allowing for high-quality spectroscopic measurements to be performed subsequently. We will show evidence of this protection from topographic imaging of the BSCCO through the graphene monolayer. More interestingly, the d-wave superconductivity of BSCCO couples to the Dirac Fermions of graphene via the proximity effect. We will describe the signatures of this coupling as probed by point spectroscopy and spectroscopic imaging in the STM.

**11:27AM Y53.00002 Experimental study of electrical conduction across high-Tc superconductor-graphene interfaces<sup>1</sup>**, DAVID PERCONTE, FABIAN CUELLAR, MARIE-BLANDINE MARTIN, BRUNO DLUBAK, MAELIS PIQUEMAL-BANCI, ROZENN BERNARD, JUAN TRASTOY, CONSTANCE MOREAU-LUCHAIRE, PIERRE SENEOR, JAVIER VILLEGAS, Unite Mixte de Physique CNRS/Thales, PIRAN KIDAMBI, JOHN ROBERTSON, STEPHAN HOFMANN, Cambridge University, Eng. Dept. — Proximity-induced superconductivity presents unusual features in graphene (i.e. specular Andreev reflection [1]) due to its particular electronic structure. It has been theoretically discussed that, if a d-wave superconductor is put contact with graphene, the latter will sustain d-wave superconductivity, and further unusual features (such as oscillatory behavior) should be observed in the superconductor-graphene junction conductance [2]. Motivated by these prospects, we experimentally investigate YBCO-graphene junctions. We will show differential conductance measurements as a function of temperature, magnetic field, and graphene doping. The observed behavior will be discussed in the frame of the theory developed in [1,2,3]. [1] C.W.J. Beenakker, Phys. Rev. Lett. 97, 067007 (2006); [2] J. Linder et al., Phys. Rev. Lett. 99, 147001 (2007); [3] S. Kashiwaya et al., Phys. Rev. B 53, 2667 (1996).

<sup>1</sup>work supported by Labex Nanosaclay

**11:39AM Y53.00003 Proximity superconductivity in graphene Landau levels**, GAURAV CHAUDHARY, Univ of Texas, Austin, XIAO LI, Univ of Maryland, College Park, ALLAN MACDONALD, Univ of Texas, Austin — We study monolayer graphene sheets in the quantum Hall regime that are proximity coupled to an s-wave superconducting thin film. At magnetic fields near  $H_{c2}$  triangular vortex lattice states form in the superconductor and induce similar vortex lattice states in the graphene sheets. We use the Bogoliubov-de Gennes theory to study the properties of quasiparticle excitations in the graphene sheets, and find that the quantized Hall conductance survives even in such a vortex lattice state. We further explore the possibility of realizing topological superconductivity in such a system. In addition, we propose that under some circumstances the vortex cores may host zero-energy bound states which are Majorana fermions.

**11:51AM Y53.00004 ABSTRACT WITHDRAWN —**

**12:03PM Y53.00005 Proximity Effect at Graphene - High Tc Superconductor Junctions**, DA WANG, EN-MIN SHIH, GHIDEWON AREFE, YOUNGDUCK KIM, DREW EDELBERG, ERICK ANDRADE, DENNIS WANG, JAMES HONE, CORY DEAN, ABHAY PASUPATHY, Columbia university, DEPARTMENT OF PHYSICS, COLUMBIA UNIVERSITY, NEW YORK, NY 10027, USA COLLABORATION — The proximity effect is a well-known mesoscopic phenomenon where Cooper pairs from a superconductor (S) enter into a normal metal (N) that is well coupled to it. Since graphene was discovered a decade ago, the proximity effect at superconductor-graphene junctions has been extensively studied and interesting phenomena such as specular Andreev reflection and ballistic transport at graphene Josephson junctions have been observed. However, superconductors used in these experiments to date are of conventional low Tc, such as aluminum (Tc=1.2K), NbSe2 (Tc=7K), and MoRe (Tc=8K). Understanding how the proximity effect works between high-Tc superconductors (pnictides and cuprates) and the Dirac Fermions of graphene remains largely unexplored. The chief technical challenge here is to create high-quality junctions between high-Tc superconductors and graphene. In this work, we will introduce a home-made setup that allows us to exfoliate, transfer and encapsulate superconductor-graphene junctions in a well controlled inert atmosphere. Transport measurements of the proximity effect at graphene-iron pnictide (FeSe, FeTeSe) and graphene-cuprate (BSCCO) junctions will be described.

**12:15PM Y53.00006 Proximity superconductivity in ballistic graphene at high magnetic fields**, J. R. PRANCE, Department of Physics, University of Lancaster, Lancaster, UK, M. BEN SHALOM, M. J. ZHU, V. I. FALKO, A. MISHCHENKO, A. V. KRETININ, K. S. NOVOSELOV, C. R. WOODS, School of Physics and Astronomy, University of Manchester, Oxford Road, M13 9PL Manchester, UK, K. WATANABE, T. TANIGUCHI, National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044 Japan, A. K. GEIM, School of Physics and Astronomy, University of Manchester, Oxford Road, M13 9PL Manchester, UK — We present measurements of the superconducting proximity effect in graphene-based Josephson junctions with a mean free path of several microns, which exceeds the junctions' length [1]. The junctions exhibit low contact resistance and large supercurrents. We observe Fabry-Pérot oscillations in the normal-state resistance and the critical current of the junctions. The proximity effect is mostly suppressed in magnetic fields of <10 mT showing the conventional Fraunhofer interference pattern; however, unexpectedly, a weak proximity effect survives in magnetic fields as high as 1 T. Superconducting states randomly appear and disappear as a function of field and carrier concentration, and each exhibits a supercurrent carrying capacity close to the universal limit of  $e\Delta/h$  where  $\Delta$  is the superconducting gap of the contacts. We attribute the high-field supercurrent to mesoscopic Andreev states that persist near graphene edges. Our work reveals new proximity regimes that can be controlled by quantum confinement and cyclotron motion. [1] Ben Shalom et al., arXiv:1504.03286 (2015)

**12:27PM Y53.00007 Proximity induced Superconductivity in Epitaxial Graphene<sup>1</sup>**, FABIAN D. NATTERER, NIST/CNST, JEONGHOON HA, NIST/CNST - UMD, HONGWOO BAEK, NIST/CNST - Seoul National University, DUMING ZHANG, WILLIAM CULLEN, NIST/CNST - UMD, NIKOLAI B. ZHITENEV, NIST/CNST, YOUNG KUK, Seoul National University, JOSEPH A. STROSCIO, NIST/CNST — The intimate electrical contact of a superconductor with a normal metal leads to an exchange of carriers through their boundary. Cooper pairs leak into the normal metal via Andreev reflection and enable the normal metal to acquire superconducting-like properties. The electron-hole conversion process in graphene is prominent due to relativistic quantum mechanics governing low energy chiral carriers in a multi-valley system. In the present experiment, we reveal spatial measurements of the proximity effect in graphene from a graphene-superconductor interface. Superconducting aluminum films were grown on epitaxial graphene on SiC. The aluminum films were discontinuous with networks of trenches in the film morphology reaching down to the substrate to exposed graphene terraces. Scanning tunneling spectra measured on the graphene terraces show a clear decay of the superconducting gap width with increasing separation from the graphene-aluminum edges. The decay length for the superconducting energy gap extends beyond 400 nm. Subtle deviations in the exponentially decaying energy gap were also observed on a much smaller length scale of tens of nanometers.

<sup>1</sup>Funding from SNSF (project 158468), NIST/CNST grant 70NANB10H193, and KRF-2010-00349

**12:39PM Y53.00008 Contact spectroscopy on S/TI/N devices: Induced pairing on the surface of a topological insulator<sup>1</sup>**, MARTIN P. STEHNO, PROSPER NGABONZIZA, MARIEKE SNELDER, University of Twente, HIROAKI MYOREN, Saitama University, YU PAN, ANNE DE VISSER, Y. HUANG, MARK S. GOLDEN, University of Amsterdam, ALEXANDER BRINKMAN, University of Twente — Translating concepts of topological quantum computation into applications requires fine-tuning of parameters in the model Hamiltonians of candidate systems. Such level of control has proven difficult to achieve in devices where superconductors are used to induce pairing in topological insulator (TI) materials. While local probe experiments have indicated features of p-wave superconducting correlations in TIs (as suggested by theory), results on extended devices often remain ambiguous. We present contact spectroscopy data on superconductor/topological insulator/normal metal devices with bulk-insulating TI material and compare these with bulk conducting samples. We discuss the magnitude of the induced gap and unusual features in the conductance traces of the bulk-insulating samples that may suggest the presence of p-wave type correlations in the TI.

<sup>1</sup>This work is financially supported by the Dutch Foundation for Fundamental Research on Matter (FOM), the Netherlands Organization for Scientific Research (NWO), and by the European Research Council (ERC).

**12:51PM Y53.00009 Signatures of Induced Superconductivity in NbTi Contacted InAs Quantum Wells<sup>1</sup>**, ANTHONY MCFADDEN, ECE Department, University of California - Santa Barbara, JAVAD SHABANI, Physics Department, City College of New York, BORZOYEH SHOJAEI, Materials Department, University of California - Santa Barbara, JOON SUE LEE, California NanoSystems Institute, University of California - Santa Barbara, CHRIS PALMSTRM, ECE and Materials Department, University of California - Santa Barbara — We have studied electrical transport through InAs quantum wells grown by MBE with unannealed superconducting NbTi contacts deposited *ex-situ* and patterned by optical photolithography. Characterization of the InAs 2DEG's without superconducting contacts yields typical mobilities greater than 100,000 cm<sup>2</sup>/Vs at a density of 4e11 cm<sup>-2</sup>. NbTi-InAs-NbTi (SNS) and NbTi-InAs (SN) devices with dimensions greater than 1 μm are fabricated using optical lithography. Although the dimensions of the fabricated SNS devices are too large to observe a supercurrent, signatures of superconductivity induced in the InAs are present. We observe two superconducting critical temperatures: one of the NbTi leads ( $T_c \sim 8K$ ), and a second ( $T_c < 4.5K$ ) attributed to superconductivity induced in the InAs channel.  $dI/dV$  vs  $V$  spectroscopy on SNS junctions below the second critical temperature shows a conductance maximum at zero applied voltage while conductance minima appear at finite bias voltage which is attributed to the presence of an induced superconducting gap in the InAs quantum well.

<sup>1</sup>This work has been supported by Microsoft research

**1:03PM Y53.00010 Large superconducting double-gap, a pronounced pseudogap and evidence for proximity-induced topological superconductivity in the Bi<sub>2</sub>Te<sub>3</sub>/Fe<sub>1+y</sub>Te interfacial superconductor<sup>1</sup>**, J. Y. SHEN, M. Q. HE, Q. L. HE, K. T. LAW, I. K. SOU, R. LORTZ, Department of Physics, Hong Kong University of Science and Technology, A. P. PETROVIC, School of Physical and Mathematical Sciences, Nanyang Technological University — We investigate directional point-contact spectroscopy on a Bi<sub>2</sub>Te<sub>3</sub>/Fe<sub>1+y</sub>Te heterostructure, fabricated via van der Waals epitaxy, which is interfacial superconducting with an onset  $T_C$  at 12K and zero resistance below 8K. A large superconducting twin-gap structure is seen down to 0.27K, together with a zero bias conductance peak. The anisotropic smaller gap ( $\Delta_1$ ) is around 5 meV at 0.27K and closes at 8K, while the other one ( $\Delta_2$ ), as large as 12 meV, is isotropic and eventually evolves into a pseudogap closing at 40K. Both, the two-gap BTK and Dynes models can well reproduce our data, demonstrating  $\Delta_1$  should be associated with the proximity-induced superconductivity in the topological Bi<sub>2</sub>Te<sub>3</sub> layer, while  $\Delta_2$  may be attributed to an intrinsically-doped FeTe thin film at the interface.

<sup>1</sup>This work was supported by grants from the Research Grants Council of the Hong Kong Special Administrative Region, China (603010, SEG HKUST03).

**1:15PM Y53.00011 Proximity-induced superconducting gap in low-dimensional materials**, CHRISTOPHER REEG, DMITRII MASLOV, Univ of Florida - Gainesville — The ability to induce a sizable gap in the excitation spectrum of a metal placed in contact with a conventional superconductor has become increasingly important in recent years in the context of engineering a topological superconductor. Conventional studies of the proximity effect involving sufficiently bulky metals have shown that Andreev reflection processes at the superconductor/metal interface induce a nonzero pairing amplitude in the metal but do not endow it with a gap. Conversely, when the metal is an atomically thin layer, the tunneling of Cooper pairs can induce an excitation gap equal to the bulk gap of the superconductor (provided that the superconductor/metal interface is sufficiently transparent). We study how these two seemingly different views of the proximity effect evolve into one another as the thickness of the metal is changed. More specifically, we show that there is a thickness scale associated with the decrease of the induced gap, and that this scale is much larger than the Fermi wavelength. As a result, by proximity to most conventional superconductors, a sizable excitation gap can be induced in metals that are tens of atomic layers thick.

**1:27PM Y53.00012 General conditions for proximity induced odd-frequency superconductivity in two-dimensional electronic systems<sup>1</sup>**, ENRICO ROSSI, Department of Physics, College of William and Mary, CHRISTOPHER TRIOLA, Nordita and Center for Quantum Materials (CQM), DRISS BADIANE, Department of Physics, College of William and Mary, ALEXANDER V. BALATSKY, Institute for Materials Science, Los Alamos National Laboratory; Nordita and Center for Quantum Materials (CQM) — We obtain the general conditions for the emergence of odd-frequency superconducting pairing in a two-dimensional (2D) electronic system proximity-coupled to a superconductor, making minimal assumptions about both the 2D system and the superconductor. Using our general results we show that a simple heterostructure formed by a monolayer of a group VI transition metal dichalcogenide, such as molybdenum disulfide, and an s-wave superconductor with Rashba spin-orbit coupling will exhibit odd-frequency superconducting pairing.

<sup>1</sup>Work supported by US DOE BES E304, KAW, ACS-PRF-53581-DNI5, and NSF-DMR-1455233.

**1:39PM Y53.00013 Growth and fabrication of proximity-coupled topological quantum wire circuits from thin InAs films**, CAROLYN KAN, CHI XUE, YANG BAI, JAMES ECKSTEIN, Univ of Illinois - Urbana — The realization of topological states in strongly spin orbit coupled semiconductors proximity-coupled to conventional superconductors requires delicate materials engineering. Key areas for improvement include the crystalline quality of the semiconductor itself, but a high-quality interface between the semiconductor and superconductor is essential. Recent results have demonstrated the necessity of forming an in situ interface to eliminate the soft gap observed in earlier experiments. While much work has focused on vertically grown nanowires, we take a lithographic approach to fabricating quantum wires out of MBE-grown thin films, which allow for increased flexibility and scalability of device structures. Notably, our films are grown entirely in situ in linked MBE systems, vastly improving interface transmission and cleanliness. Aspects of growth architecture aimed toward increasing the InAs mobility, such as substrate choice and layer structure, are also discussed.

**1:51PM Y53.00014 Superfluid density through 2D superconductor junctions.**, HYOUNGDO NAM, CHIH-KANG SHIH, Department of Physics, The University of Texas at Austin, Austin, TX 78712, USA. — As S. Qin et al. [1] reported, two monolayer (2 ML) lead film on a silicon (111) substrate has one of two different atomic structures on the silicon substrate: the unstrained 1x1 and the pseudomorphically strained  $\sqrt{3} \times \sqrt{3}$  (i.e. the same lattice constant as the Si  $\sqrt{3} \times \sqrt{3}$  lattice). Most interestingly, although these two different regions show the same quantum well state features, they have different  $T_c$ 's (5 K and 4 K). These two different regions of 2 ML film naturally form superconductor-superconductor (SS or SS') junctions along silicon step edges. Physical connection of the junction is only 1 ML thickness because of the step height difference of substrate. We will present this study of SS (or SS') junction system using scanning tunneling microscopy/spectroscopy and *in-situ* double-coil mutual inductance measurement. The transition of superconducting gaps across either SS or SS' junctions should show how to locally affect each other. Double coil measurement show a global  $T_c$  close to the lower  $T_c$  region with sizable superfluid density. We will discuss the phase rigidity and its relationship to the superfluid density in this ultra-thin Pb film that is only 2 ML thick. [1] 'Superconductivity at the two-dimensional limit' S. Qin, J. Kim, Q. Niu, and C. K. Shih, *Science* **324**, 1314 (2009).

**Friday, March 18, 2016 11:15AM - 2:15PM –**

Session Y55 DBIO DCOMP DPOLY: Physics of Proteins: Pushing the Envelope on Understanding and Designing Function Hilton Baltimore Holiday Ballroom 6 - Wouter Hoff, Oklahoma State University

**11:15AM Y55.00001 Enhancing MD simulations of proteins using vague and combinatorics information** , KEN DILL, Stony Brook University — We have developed MELD, a method that 'melds' together replica-exchange molecular dynamics simulations with external information. Traditionally, accelerating MD simulations has only been possible by using information that is precise and correct. In contrast, MELD allows us to leverage information that is vague or corrupted. For example, we give generic instructives, such as 'make a hydrophobic core', 'make good secondary structures', or 'search only compact structures'. Normally, such information implies a loss of ability to compute free energies and populations. But, MELD satisfies detailed balance. We show that it can fold small proteins much faster than brute-force MD can, that it gives reasonable populations, and that it can succeed in CASP, the blind protein-structure prediction event.

**11:51AM Y55.00002 Molecular and cellular constraints on proteins** , TANJA KORTEEMME, UCSF — Engineering proteins with new sequences, structures and functions has many exciting practical applications, and provides new ways to dissect design principles for function. Recent successes in computational protein design provide a cause for optimism. Yet many functions are currently too complex to engineer predictively, and successful design of new biological activities also requires an understanding of the functional pressures acting on proteins in the context of cells and organisms. I will present two vignettes describing our progress with dissecting both molecular and cellular constraints on protein function. In the first, we characterized the cost and benefit of protein production upon sequence perturbations in a classic system for gene regulation, the *lac* operon. Our results were unexpected in light of the common assumption that the dominant fitness costs are due to protein *expression*. Instead, we discovered a direct linear relationship between cost and *lac* permease *activity*, not protein or mRNA production. The magnitude of the cost of permease activity, relative to protein production, has consequences for regulation. Our model predicts an advantage of direct regulation of protein *activity* (not just expression), providing a new explanation for the long-known mechanism of "inducer exclusion" that inhibits transport through the permease. Similar pressures and cost/benefit tradeoffs may be key to engineering synthetic systems with improved fitness. In the second vignette, I will describe our recent efforts to develop computational approaches that predict protein sequences consistent with multiple functional conformations. We expect such "multi-constraint" models to improve predictions of functional sequences determined by deep mutational scanning in bacteria, to provide insights into how the balance between functional conformations shapes sequence space, and to highlight molecular and cellular constraints that cannot be captured by the model.

**12:27PM Y55.00003 Response of proteins to mechanical force** , DAVE THIRUMALAI, Univ of Maryland-College Park — No abstract available.

**1:03PM Y55.00004 Kinetic Cooperativity, Loop Dynamics, and Allostery from NMR and MD simulations** , RAFAEL BRUSCHWEILER, The Ohio State University — The hallmark of glucokinase (GCK), which catalyzes the phosphorylation of glucose during glycolysis, is its kinetic cooperativity whose understanding at atomic detail has remained open since its discovery over 40 years ago. I will discuss how the origin of kinetic cooperativity is rooted in intramolecular protein dynamics using NMR relaxation data of 17 isoleucines distributed over all parts of GCK. Residues of glucose-free GCK located in the small domain display a distinct exchange behavior involving multiple conformers that are substantially populated, whereas in the glucose-bound form these dynamic processes are quenched. The conformational exchange process directly competes with the enzymatic turnover at physiological glucose concentrations, thereby generating the sigmoidal rate dependence that defines kinetic cooperativity. The flexible nature of protein loops and the timescales of their dynamics are critical for many biologically important events at the molecular level, such as protein interaction and recognition processes. Based on a library of proteins, rules about loop dynamics in terms of amplitude and timescales can be derived using molecular dynamics (MD) simulations and NMR data. These rules have been implemented in the new web server ToeLoop (for Timescales Of Every Loop) that permits the prediction of loop dynamics based on an average 3D protein structure (<http://spin.ccic.ohio-state.edu/index.php/loop/index>).

**1:39PM Y55.00005 Unraveling protein catalysis through neutron diffraction.** , DEAN MYLES, Neutron Science Directorate, Oak Ridge National Laboratory, Oak Ridge, TN. 37831 — Neutron scattering and diffraction are exquisitely sensitive to the location, concentration and dynamics of hydrogen atoms in materials and provide a powerful tool for the characterization of structure-function and interfacial relationships in biological systems. Modern neutron scattering facilities offer access to a sophisticated, non-destructive suite of instruments for biophysical characterization that provide spatial and dynamic information spanning from Angstroms to microns and from picoseconds to microseconds, respectively. Applications range from atomic-resolution analysis of individual hydrogen atoms in enzymes, through to multi-scale analysis of hierarchical structures and assemblies in biological complexes, membranes and in living cells. Here we describe how the precise location of protein and water hydrogen atoms using neutron diffraction provides a more complete description of the atomic and electronic structures of proteins, enabling key questions concerning enzyme reaction mechanisms, molecular recognition and binding and protein-water interactions to be addressed. Current work is focused on understanding how molecular structure and dynamics control function in photosynthetic, cell signaling and DNA repair proteins. We will highlight recent studies that provide detailed understanding of the physiochemical mechanisms through which proteins recognize ligands and catalyze reactions, and help to define and understand the key principles involved.